NBS CIRCULAR 539

VOLUME I

Standard X-ray Diffraction Powder Patterns

UNITED STATES DEPARTMENT OF COMMERCE

NATIONAL BUREAU OF STANDARDS

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Standard X-ray Diffraction Powder Patterns

Howard E. Swanson and Eleanor Tatge



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STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Vol. I—Data for 54 Inorganic Substances

Howard E. Swanson and Eleanor Tatge

In continuation of the National Bureau of Standards project for improving the file of X-ray diffraction patterns published by the American Society for Testing Materials, sets of patterns in the file, each representing a different chemical, have been reviewed with the object of supplanting them with single standard patterns. Reports are made on substances for each of which a pattern prepared at the Bureau is offered to replace a set now in the file. Four additional reports are included, one for high cristobalite, for which no pattern was prepared at the NBS, and three, which are not represented in the ASTM file, on selenium dioxide, zinc borate, and magnesium tungstate.

The substances reported upon are Mg, Al, Ni, Cu, Zn, Ge, Mo, Pd, Ag, Sn, Te, W, Ta, Pt, Au, Pb, BeO, MgO, SiO_2 (low cristobalite), SiO_2 (high cristobalite), CaO, TiO_2 (rutile), TiO_2 (anatase), NiO, CuO, GeO_2, As_2O_3, SeO_2, SnO_2, CeO_2, ThO_2, $Ca(OH)_2$, NH_4Cl, LiF, LiCl, NaF, KF, KCl, KBr, KI, CaF_2, BaF_2, Hg_2Cl_2, $HgCl_2$, HgI_2, PbFCl, KCN, NaCN (cubic), NaCN (orthorhombic), $Sr(NO_3)_2$, $Ba(NO_3)_2$, ZnB_2O_4, Mg_2SiO_4, and $MgWO_4$.

The ASTM patterns are tabulated for comparison with additional patterns from the literature and one prepared at the NBS. Miller indices are derived from the calculation of spacings by desk calculator or the electronic computer SEAC. Interplanar spacings in angstroms (except where otherwise noted) and relative intensities from 1 to 100 are tabulated. For the NBS pattern the three strongest lines are given, as well as the lattice constants and the computed density. The index of refraction of the sample is noted if it could be determined. Crystal-structure data from the literature are noted.

1. Introduction

Three hundred or more substances are represented in the X-ray Diffraction Pattern card file [1][1] of the American Society for Testing Materials by more than one pattern each, many of the patterns differing materially from each other. Upon the recommendation of the Joint Committee on Chemical Analysis by X-ray Diffraction Methods,[2] a critical examination of repeated patterns in the card file is being undertaken as part of a program for the general improvement of the file. Patterns made recently for 53 substances at the National Bureau of Standards are presented, compared with those in the file and in the literature, and recommended for adoption as standard patterns, 50 of them to replace 170 patterns now in the file, and three of them (SeO_2, ZnB_2O_4, and $MgWO_4$) offered as additions to the file. Also, the patterns for β-cristobalite (SiO_2), for which no NBS pattern was prepared, are discussed, and one in the ASTM file is recommended as a standard. The eight patterns given in an earlier paper [218], in which the technique used in the NBS laboratory was outlined, are included in this paper with some slight revisions. A complete list of the patterns reported is given on page 3.

Briefly, for preparing the NBS pattern, a Geiger-counter spectrometer with a 160-degree arc was used, which permits recording the patterns into the back reflection region. Copper Kα x-radiation with a wavelength of 1.5405 A was considered most satisfactory for general use. Separate charts were made for interplanar spacing and for intensity measurements so that the flat sample surface desirable for the former did not preclude the disorientation of particles necessary for the latter. Actual peak height from background was used for intensity measurements. Samples

[1] Figures in brackets indicate the literature references at the end of this volume. They are in alphabetical order.

[2] The Joint Committee represents the American Crystallographic Society, American Society for Testing Materials, and the Institute of Physics (England).

used were sufficiently fine-grained, usually less than 25 microns, to give reproducible results. The spacings for all NBS standard patterns were corrected by an internal standard of tungsten, except that for the tungsten pattern, silver was used. The unit cell used for tungsten calibration was 3.1648 A and for silver calibration, 4.0861 A, both at 25°C [119]. Lines occasionally hidden by tungsten lines were obtained from the intensity diagrams. All spacing errors inherent in sample mountings, sample density variations, spectrometer alinement, and recorder lag were easily compensated by the use of the internal standard. The samples used were of high chemical purity, and chemical or spectrographic analyses are given (rarely both). Phase purity was checked microscopically where possible. The temperature was allowed to vary not more than ±1°C from that recorded in the respective tables.

The diffraction lines were indexed and the lattice constants determined. For the cubic substances the indexing was done by comparing theoretical spacings calculated on a desk calculator. The electronic computer SEAC (National Bureau of Standards Eastern Automatic Computer), used under the direction of Dr. Fred Ordway, proved a time-saving device for computing the spacings for many of the substances.

So far as possible the interplanar spacing data reproduced in the tables were reduced to angstrom units as internationally agreed upon in 1946 [264]. In some cases the data are known to be, or assumed to be, in kX units, which are less than angstroms by a factor of 1.00202 [264], and thus easily converted. In others, Bragg angle data are computed to obtain spacings directly in angstroms; or the wavelength of the radiation used in preparing the pattern is compared with the actual wavelength in angstroms to obtain a conversion factor. The dates heading the column are those of the first publication of the basic data.

With regard to other units, the values of the coefficient of linear thermal expansion given are those which could be readily located in the literature and which cover a satisfactory temperature range. The density is given in grams per cubic centimeter. Indices of refraction for the NBS materials were obtained in white light with oils standardized by sodium light; indices quoted from the literature are accompanied by subscript *D* for the sodium *D* line, or *Li* for lithium.

Lattice constants from the literature are presented in order of date in unnumbered tables in the text for comparison with those obtained from the NBS data. They are tabulated in angstrom units and are given at 25°C, the most commonly stated temperature, if a coefficient of expansion is available from the literature for use in recalculating. This results in an occasional difference between the NBS lattice constant given in the text (at 25°C) and that appearing with the tabulated pattern (at the experimental temperature, usually 26°C, noted at the head of the column).

The cumulative maximum error of interplanar spacing and lattice constant measurements on NBS patterns varies not more than ±5 in the last significant figure recorded. In most cases the last significant figure for the density depends rather on the precision to which atomic weights are known than on that of the lattice constant, which is usually greater.

The original sources are noted of all patterns, tabulated lattice constants, and, where practicable, structure data. For some of the simpler structures it was not always easy to ascertain who was first responsible for the determination of the structure of the compound in question and a reference could not be given with certainty.

2. Patterns

The duplicate patterns considered here are listed in table 1. In the table the file card numbers are given for both the old (1940-41) and new (1950) files of the ASTM, followed by the index numbers (interplanar spacings for the three strongest lines).

Tables 2 to 55 list Miller indices, interplanar spacings, and relative-intensity measurements for the substances considered. Also, in the case of cubic materials, the lattice constants calculated from each spacing are given and averaged at the bottom of the table. The text preceding each table furnishes the following information: Origin of the patterns (such as ASTM cards, or literature); source of the NBS material, its chemistry, and its treatment preliminary to preparing the pattern; basis for converting the spacings of each pattern to angstrom units; the three strongest lines of the NBS pattern—the lines used for indexing the ASTM cards; crystal structure data, such as the type of lattice, space group, and the number of molecules in the unit cell; the lattice constant determined from the NBS pattern, compared with constants obtained from the literature; the density, calculated from the NBS lattice constant; and the index of refraction, if it could be determined on the NBS material, or was easily available for other pure material from the literature.

A complete list of the patterns given is magnesium (hexagonal); aluminum (cubic); nickel (cubic); copper (cubic); zinc (hexagonal); germanium (cubic); molybdenum (cubic); palladium (cubic); silver (cubic); tin—white or β (tetragonal); tellurium (hexagonal); tungsten (cubic); tantalum (cubic); platinum (cubic); gold (cubic); lead (cubic); BeO—bromellite (hexagonal); MgO—periclase (cubic); SiO_2—low or α cristobalite (tetragonal); SiO_2—high or β cristobalite (cubic); CaO—lime (cubic); TiO_2—rutile (tetragonal); TiO_2—anatase (tetragonal); NiO—bunsenite (cubic); CuO—tenorite (monoclinic); GeO_2 (hexagonal); As_2O_3—arsenolite (cubic); SeO_2—selenolite (tetragonal); SnO_2—cassiterite (tetragonal); CeO_2 (cubic); ThO_2—thorianite (cubic); $Ca(OH)_2$—portlandite (hexagonal); NH_4Cl—salammoniac (cubic); LiF (cubic); LiCl (cubic); NaF—villiaumite (cubic); KF (cubic); KCl—sylvite (cubic); KBr (cubic); KI (cubic); CaF_2—fluorite (cubic); BaF_2 (cubic); Hg_2Cl_2—calomel (tetragonal); $HgCl_2$ (orthorhombic); HgI_2 (tetragonal); PbFCl—matlockite (tetragonal); KCN (cubic); NaCN (cubic); NaCN (orthorhombic); $Sr(NO_3)_2$ (cubic); $Ba(NO_3)_2$—nitrobarite (cubic); ZnB_2O_4 (cubic); Mg_2SiO_4—forsterite (orthorhombic); and $MgWO_4$ (monoclinic).

TABLE 1. *ASTM card to be superseded*

Card number		Index lines		Source
Old	1950	Old	1950	
1. Magnesium				
2942	3124	2.44	2.44	[100]
	1-1151	2.75	2.75	
	1-1148	1.61	1.61	
2924	3080	2.45	2.45	[85]
	1-1135	2.77	2.77	
	1-1141	2.60	2.60	
2. Aluminum				
3060	3224	2.33	2.33	[102]
	1-1180	2.025	2.03	
	1-1179	1.21	1.21	
3049	3242	2.34	2.34	[59]
	1-1186	1.221	1.22	
	1-1176	2.02	2.02	
-------	3223	-----	2.32	[170]
	3-0938	-----	2.03	
	3-0932	-----	1.43	
3061	3225	2.33	2.33	[85]
	1-1181	2.02	2.02	
	1-1180	1.430	1.43	
H-2503	3243	2.33	2.33	Crystallographic Laboratory, Cambridge.
	2-1117	1.22	1.22	
	2-1109	2.02	2.02	
3. Nickel				
3462	3645	1.95	1.95	[103]
	1-1272	1.13	1.13	
	1-1272	0.74	0.74	
3362	3595	2.038	2.04	[104]
	1-1270	1.067	1.07	
	1-1258	1.766	1.77	

TABLE 1. *ASTM cards to be superseded—Con.*

Card number		Index lines		Source
Old	1950	Old	1950	
3. Nickel—Con.				
3379	3577	2.03	2.03	[85]
	1-1263	1.76	1.76	
	1-1260	1.244	1.24	
3397	3578	2.01	2.01	[59]
	1-1264	1.741	1.74	
	1-1266	1.053	1.05	
---------	3575	-----	2.03	[123]
	3-1051	-----	1.78	
	3-1043	-----	1.25	
---------	3597	-----	2.02	[144]
	3-1057	-----	1.06	
	3-1051	-----	1.75	
4. Copper				
3312	3504	2.08	2.08	[59]
	1-1244	1.798	1.80	
	1-1242	1.083	1.08	
---------	3498	-----	2.09	[124]
	3-1027	-----	1.81	
	3-1005	-----	1.28	
II-2828	3499	2.08	2.08	[242]
	2-1231	1.81	1.81	
	2-1225	1.28	1.28	
3311	3500	2.08	2.08	[85]
	1-1243	1.81	1.81	
	1-1241	1.277	1.28	
---------	3501	-----	2.08	[88]
	3-1026	-----	1.81	
	3-1015	-----	1.28	
---------	3526	-----	2.08	Allis-Chalmers Manufacturing Co.
	3-1035	-----	1.27	
	3-1018	-----	1.09	
5. Zinc				
3315	3524	2.077	2.08	[104]
	1-1247	1.339	1.34	
	1-1244	1.332	1.33	
3308	3470	2.08	2.08	[85]
	1-1237	2.46	2.46	
	1-1238	2.30	2.30	
6. Germanium				
---------	1761	-----	3.24	Schatzlein
	3-0502	-----	1.99	
	3-0486	-----	1.70	
---------	1676	-----	3.26	Fuller, and [85].
	3-0480	-----	1.99	
	3-0478	-----	1.70	

TABLE 1. *ASTM cards to be superseded—Con.*

Card number		Index lines		Source
Old	1950	Old	1950	
7. Molybdenum				
3170	3331	2.215	2.22	[104]
	1-1213	1.283	1.28	
	1-1208	0.839	0.84	
3155	3330	2.23	2.23	[59]
	1-1212	1.283	1.28	
	1-1205	0.994	0.99	
3169	3328	2.22	2.22	[85]
	1-1211	1.281	1.28	
	1-1207	1.57	1.57	
8. Palladium				
3883	3938	1.192	1.19	[104]
	1-1310	2.274	2.27	
	1-1310	1.398	1.40	
3895	3940	1.163	1.16	[59]
	1-1312	2.21	2.21	
	1-1312	1.925	1.93	
II-4108	3941	1.16	1.16	[60]
	2-1438	2.21	2.21	
	2-1439	1.92	1.92	
3151	3300	2.23	2.23	[85]
	1-1202	1.94	1.94	
	1-1201	1.371	1.37	
9. Silver				
---------	4095	-----	-----	[231; 249]
	3-1316	-----	-----	
	3-1316	-----	-----	
3010	3193	2.37	2.37	[59]
	1-1173	1.23	1.23	
	1-1164	2.05	2.05	
---------	3178	-----	2.36	[124]
	3-0916	-----	2.03	
	3-0921	-----	1.44	
---------	3221	-----	2.32	[124]
	3-0936	-----	2.05	
	3-0931	-----	1.44	
3022	3176	2.36	2.36	[85]
	1-1168	2.04	2.04	
	1-1167	1.232	1.23	
10. Tin				
2269	2314	2.91	2.91	[85]
	1-0919	2.79	2.79	
	1-0926	2.01	2.01	
II-1471	2186	2.95	2.95	British Museum.
	2-0678	2.81	2.81	
	2-0709	2.02	2.02	

TABLE 1. *ASTM cards to be superseded—Con.*

Card number		Index lines		Source
Old	1950	Old	1950	
11. Tellurium				
3910	3974	1.075	1.08	[25]
	1-1313	1.092	1.09	
	1-1313	3.845	3.85	
1765	1751	3.22	3.22	[208]
	1-0738	2.34	2.34	
	1-0727	2.22	2.22	
---------	1705	-----	3.23	[170]
	3-0493	-----	3.58	
	3-0488	-----	2.35	
II-1111	1753	3.22	3.22	[88]
	2-0515	2.33	2.33	
	2-0511	2.22	2.22	
1737	1752	3.24	3.24	[85]
	1-0739	2.34	2.34	
	1-0714	2.22	2.22	
---------	1830	-----	3.19	Institute of Physics, Cardiff.
	3-0518	-----	2.33	
	3-0506	-----	2.21	
12. Tungsten				
3154	3324	2.23	2.23	[59]
	1-1208	1.289	1.29	
	1-1203	0.997	1.00	
313	3325	2.23	2.23	[85]
	1-1209	1.290	1.29	
	1-1204	0.846	0.85	
13. Tantalum				
3847	3905	1.335	1.34	[104]
	1-1309	2.315	2.32	
	1-1309	0.872	0.87	
II-2491	3236	2.34	2.34	[189]
	2-1114	1.35	1.35	
	2-1104	1.04	1.04	
3063	3235	2.33	2.33	[85]
	1-1184	1.346	1.35	
	1-1182	1.65	1.65	
14. Platinum				
3884	3939	1.183	1.18	[104]
	1-1311	2.265	2.27	
	1-1311	1.387	1.39	
3118	3285	2.27	2.27	[59]
	1-1195	1.179	1.18	
	1-1190	1.956	1.96	
3132	3265	2.25	2.25	[85]
	1-1191	1.95	1.95	
	1-1194	1.382	1.38	

TABLE 1. *ASTM cards to be superseded—Con.*

Card number		Index lines		Source
Old	1950	Old	1950	
15. Gold				
3038	3194	2.35	2.35	[59]
	1-1174	1.225	1.23	
	1-1174	2.03	2.03	
II-2471	3175	2.36	2.36	[88; 60; 124]
	2-1093	2.04	2.04	
	2-1095	1.23	1.23	
3036	3179	2.35	2.35	[85]
	1-1170	2.03	2.03	
	1-1172	1.227	1.23	
16. Lead				
2426	2580	2.81	2.81	[59]
	1-1004	1.480	1.48	
	1-0995	2.44	2.44	
---------	3861	-----	1.48	[137]
	3-1159	-----	0.84	
	3-1156	-----	2.79	
II-1698	2581	2.82	2.82	[60]
	2-0830	1.48	1.48	
	2-0811	2.44	2.44	
2367	2440	2.85	2.85	[85]
	1-0966	2.47	2.47	
	1-0972	1.74	1.74	
II-1663	2579	2.84	2.84	Harcourt.
	2-0829	1.48	1.49	
	2-0799	1.74	1.74	
---------	3842	-----	1.49	[88]
	3-1154	-----	2.84	
	3-1153	-----	1.71	
17. Beryllium oxide				
3336	3474	2.06	2.06	[85]
	1-1240	2.34	2.34	
	1-1248	2.19	2.19	
---------	3475	-----	2.05	[147]
	3-1014	-----	2.33	
	3-1035	-----	1.34	
---------	3222	-----	2.33	[2]
	3-0937	-----	2.05	
	3-0928	-----	1.35	
---------	3220	-----	2.34	United Steel Companies, England.
	3-0935	-----	2.06	
	3-0926	-----	2.19	
18. Magnesium oxide				
II-3816	3850	1.48	1.48	[87]
	2-1400	1.27	1.27	
	2-1395	1.21	1.21	

TABLE 1. *ASTM cards to be superseded—Con.*

Card number		Index lines		Source
Old	1950	Old	1950	
18. Magnesium oxide—Con.				
II-2798	3418	2.10	2.10	United Steel Companies, England, and [256].
	2-1195	1.48	1.49	
	2-1207	2.42	2.43	
3286	3424	2.10	2.10	[85]
	1-1234	1.485	1.49	
	1-1235	1.213	1.21	
---------	3426	-----	2.10	[48]
	3-0995	-----	1.48	
	3-0998	-----	0.940	
19. Silicon dioxide (α-cristobalite)				
II-612	1005	4.03	4.03	United Steel Companies, England, and [149, 6].
	2-0288	2.48	2.48	
	2-0285	2.83	2.83	
---------	1006	-----	-----	Continuation of preceding card.
	2-0289	-----	-----	
	2-0286	-----	-----	
1010	1004	4.04	4.04	[85]
	1-0445	2.48	2.48	
	1-0438	2.85	2.85	
-- ------	1007	-----	4.04	Allis-Chalmers Manufacturing Co.
	3-0273	-----	2.47	
	3-0271	-----	3.14	
---------	1002	-----	4.07	[220]
	3-0271	-----	2.50	
	3-0267	-----	1.54	
---------	1003	-----	4.04	[11]
	3-0272	-----	4.48	
	3-0270	-----	2.85	
---------	1008	-----	4.03	[48]
	3-0274	-----	2.47	
	3-0272	-----	2.84	
20. Silicon dioxide (β-cristobalite)				
956	0964	4.14	4.14	[254]
	1-0430	2.53	2.53	
	1-0424	1.639	1.64	
---------	0965	-----	4.14	[8]
	3-0259	-----	2.52	
	3-0257	-----	1.64	
II-588	0963	4.14	4.14	[255, 8]
	2-0276	2.53	2.53	
	2-0278	1.64	1.64	
21. Calcium oxide				
II-2441	3140	2.40	2.40	United Steel Companies, England, and [89; 40].
	2-1079	1.70	1.70	
	2-1088	1.45	1.45	

TABLE 1. *ASTM cards to be superseded—Con.*

Card number		Index lines		Source
Old	1950	Old	1950	
21. Calcium oxide—Con.				
2989	3183	2.39	2.39	[85]
	1-1172	1.69	1.69	
	1-1160	2.76	2.76	
---------	3784	-----	1.69	[48]
	3-1127	-----	2.39	
	3-1123	-----	0.98	
22. Titanium dioxide (rutile)				
3653	3774	1.69	1.69	[85]
	1-1292	3.24	3.24	
	1-1292	2.49	2.49	
II-1089	1774	3.24	3.24	British Museum, Crystallographic Lab., Cambridge, and [19, 125, 246].
	2-0526	1.68	1.68	
	2-0494	1.36	1.36	
---------	3773	1.69	1.69	United Steel Companies, England.
	3-1124	3.25	3.25	
	3-1122	1.36	1.36	
23. Titanium dioxide (anatase)				
---------	4111	-----	-----	[233]
	3-1332	-----	-----	
	3-1332	-----	-----	
II-911	1390	3.47	3.47	British Museum, Crystallographic Lab., Cambridge, and [246].
	2-0411	1.88	1.88	
	2-0406	1.69	1.69	
1406	1324	3.52	3.52	[85]
	1-0572	1.88	1.88	
	1-0562	1.70	1.70	
II-676	1323	3.51	3.51	United Steel Companies, England.
	2-0391	1.89	1.89	
	2-0387	1.70	1.70	
24. Nickelous oxide				
II-2809	3516	2.09	2.09	United Steel Companies, England, and [139; 93; 134]
	2-1238	1.48	1.48	
	2-1216	2.41	2.41	
---------	4066	-----	-----	[46]
	3-1287	-----	-----	
	3-1287	-----	-----	
3309	3471	2.08	2.08	[85]
	1-1238	2.40	2.40	
	1-1238	1.474	1.47	
25. Cupric oxide				
---------	3014	-----	2.52	[165]
	3-0867	-----	2.31	
	3-0867	-----	1.04	

TABLE 1. *ASTM cards to be superseded—Con.*

Card number		Index lines		Source
Old	1950	Old	1950	
25. Cupric oxide—Con.				
II-2252	3012	2.52	2.52	[186]
	2-1036	2.32	2.32	
	2-1040	1.86	1.87	
---------	4042	-----	-----	[225]
	3-1263	-----	-----	
	3-1263	-----	-----	
II-2253	3017	2.52	2.52	Harcourt; Waldo; British Museum; and [226].
	2-1037	2.30	2.30	
	2-1041	1.41	1.41	
2851	3013	2.51	2.51	[85]
	1-1111	2.31	2.31	
	1-1117	1.85	1.85	
---------	3086	-----	2.48	[88]
	3-0886	-----	2.32	
	3-9884	-----	1.87	
26. Germanium dioxide				
1528	1446	3.41	3.41	[85]
	1-0625	2.35	2.35	
	1-0617	1.87	1.87	
II-938	1458	3.43	3.43	[260]
	2-0430	1.56	1.56	
	2-0419	1.42	1.42	
27a. Arsenic trioxide (arsenolite)				
---------	4022	-----	-----	[24]
	3-1234	-----	-----	
	3-1234	-----	-----	
II-4177	3975	1.068	1.07	[181]
	2-1451	0.965	0.965	
	2-1451	3.20	3.20	
1820	1778	3.18	3.18	[85]
	1-0747	6.3	6.3	
	1-0754	2.53	2.53	
II-1154	1853	3.19	3.19	[153]
	2-0549	1.55	1.55	
	2-0530	1.95	1.96	
27b. Arsenic trioxide (claudetite)				
II-1155	1855	3.19	3.19	[153]
	2-0550	1.068	1.07	
	2-0531	3.53	3.53	
28. Selenium oxide. No ASTM patterns.				
29. Stannic oxide				
1556	1432	3.40	3.40	[245]
	1-0617	2.67	2.67	
	1-0625	1.77	1.77	

TABLE 1. *ASTM cards to be superseded—Con.*

Card number		Index lines		Source
Old	1950	Old	1950	
29. Stannic oxide—Con.				
1626	1574	3.34	3.34	[85]
	1-0667	2.64	2.64	
	1-0657	1.75	1.75	
II-3351	3735	1.76	1.76	[19]
	2-1341	1.50	1.50	
	2-1337	1.21	1.21	
II-3357	3734	1.75	1.75	Harcourt; and Institute of Mines, Leningrad, USSR.
	2-1336	3.33	3.33	
	2-1340	2.63	2.63	
---------	1576	-----	3.32	[88]
	3-0444	-----	2.62	
	3-0439	-----	1.75	
---------	3736	-----	1.75	British Museum.
	3-1111	-----	3.30	
	3-1116	-----	2.62	
---------	3732	-----	1.76	United Steel Companies, England.
	3-1110	-----	3.35	
	3-1114	-----	2.64	
30. Ceric oxide				
II-3085	3675	1.92	1.92	[183]
	2-1306	1.64	1.64	
	2-1306	1.11	1.11	
1927	1936	3.11	3.11	[85]
	1-0802	1.90	1.90	
	1-0800	1.62	1.62	
31. Thorium oxide				
II-2995	3634	1.98	1.98	[183]
	2-1288	1.69	1.69	
	2-1278	1.14	1.14	
1769	1773	3.22	3.22	[85]
	1-0745	1.68	1.68	
	1-0731	1.97	1.97	
32. Calcium hydroxide				
II-2043	2911	2.63	2.63	[89]
	2-0983	1.80	1.80	
	2-0967	1.93	1.93	
2687	--------	2.63	2.63	[85]
	--------	4.93	4.93	
	--------	1.93	1.93	
II-2049	2856	2.62	2.62	No reference—United Steel?
	2-0953	4.91	4.91	
	2-0968	1.92	1.72	
II-2050	2857	2.62	2.62	United Steel Companies, England.
	2-0954	4.89	4.89	
	2-0969	1.92	1.92	

TABLE 1. *ASTM cards to be superseded—Con.*

Card number		Index lines		Source
Old	1950	Old	1950	
33. Ammonium chloride				
2570	2762	2.718	2.72	[9]
	1-1051	1.568	1.57	
	1-1044	1.924	1.92	
2539	2754	2.734	2.73	[92]
	1-1049	1.577	1.58	
	1-1037	3.874	3.87	
II-1850	2758	2.73	2.73	[256, 82]
	2-0904	1.58	1.58	
	2-0887	1.93	1.93	
2569	2761	2.72	2.72	[85]
	1-1050	1.57	1.57	
	1-1043	3.85	3.85	
---------	2773	-----	2.74	United Steel Companies, England.
	3-0810	-----	0.91	
	3-0785	-----	1.03	
34. Lithium fluoride				
3408	3559	2.00	2.00	[57]
	1-1258	2.31	2.31	
	1-1270	1.422	1.42	
3407	3558	2.00	2.00	[85]
	1-1257	2.32	2.32	
	1-1269	1.419	1.42	
II-2511	3226	2.32	2.32	Crystallographic Laboratory, Cambridge.
	2-1107	2.01	2.01	
	2-1111	1.42	1.42	
35. Lithium chloride				
2194	2214	2.96	2.96	[57]
	1-0895	2.55	2.55	
	1-0900	1.814	1.81	
2193	2212	2.96	2.96	[85]
	1-0894	2.56	2.56	
	1-0899	1.81	1.81	
II-1364	2096	3.01	3.01	Crystallographic Laboratory, Cambridge.
	2-0638	2.59	2.59	
	2-0640	1.83	1.83	
36. Sodium fluoride				
3062	3231	2.33	2.33	[57]
	1-1182	1.636	1.64	
	1-1181	1.335	1.34	
3075	3232	2.32	2.32	[85]
	1-1183	1.64	1.64	
	1-1184	1.336	1.34	
II-2522	3233	2.31	2.31	Crystallographic Laboratory, Cambridge, and [256].
	2-1112	1.63	1.63	
	2-1115	1.34	1.34	

TABLE 1. *ASTM cards to be superseded—Con.*

Card number		Index lines		Source
Old	1950	Old	1950	
37. Potassium fluoride				
2614	2829	2.69	2.69	[57]
	1-1069	1.887	1.89	
	1-1056	1.192	1.19	
2656	2830	2.66	2.66	[85]
	1-1070	1.88	1.88	
	1-1069	3.08	3.08	
II-2042	2901	2.63	2.63	Crystallographic Laboratory, Cambridge.
	2-0976	1.87	1.87	
	2-0966	1.19	1.19	
38. Potassium chloride				
1911	1913	3.12	3.12	[57]
	1-0795	2.21	2.21	
	1-0796	1.812	1.81	
1904	1914	3.13	3.13	[85]
	1-0796	2.21	2.21	
	1-0786	1.81	1.81	
39. Potassium bromide				
1705	1664	3.27	3.27	[57]
	1-0708	2.32	2.32	
	1-0695	1.465	1.47	
1676	1661	3.29	3.29	[85]
	1-0701	2.33	2.33	
	1-0680	1.468	1.47	
40. Potassium iodide				
1393	1302	3.53	3.53	[57]
	1-0559	2.49	2.49	
	1-0555	1.578	1.58	
---------	1306	-----	3.50	[170]
	3-0360	-----	2.48	
	3-0365	-----	1.57	
1392	1299	3.53	3.53	[85]
	1-0558	2.50	2.50	
	1-0554	4.08	4.08	
41. Calcium fluoride				
3475	3650	1.93	1.93	[85]
	1-1273	3.16	3.16	
	1-1274	1.65	1.65	
II-3061	3651	1.93	1.93	William Jessop & Sons, Ltd., England; and United Steel Companies, England.
	2-1301	3.15	3.15	
	2-1302	1.64	1.64	
II-3071	3684	1.93	1.93	United Steel Companies, England.
	2-1312	1.11	1.11	
	2-1305	3.15	3.15	
---------	3654	-----	1.90	British Museum.
	3-1079	-----	3.10	
	3-1088	-----	1.63	

TABLE 1. *ASTM cards to be superseded—Con.*

Card number		Index lines		Source
Old	1950	Old	1950	
42. Barium fluoride				
II-2633	3305	2.20	2.20	[221]
	2-1147	1.87	1.87	
	2-1157	1.43	1.43	
1346	1311	3.58	3.58	[85]
	1-0563	2.19	2.19	
	1-0533	1.86	1.86	
43. Mercurous chloride				
1869	1792	3.155	3.16	[90]
	1-0757	4.143	4.14	
	1-0768	1.962	1.96	
---------	1842	-----	3.17	[112]
	3-0522	-----	1.96	
	3-0516	-----	1.04	
II-1222	1921	3.13	3.13	[196]
	2-0574	1.94	1.94	
	2-0560	4.05	4.05	
945	0959	4.16	4.16	[85]
	1-0426	3.17	3.17	
	1-0420	1.97	1.97	
44. Mercuric chloride				
812	0852	4.35	4.35	[85]
	1-0377	3.00	3.00	
	1-0365	2.70	2.70	
II-524	0826	4.34	4.34	[26]
	2-0249	4.08	4.08	
	2-0255	3.36	3.36	
45. Mercuric iodide				
3204	3336	2.183	2.18	[91]
	1-1216	3.563	3.56	
	1-1217	6.192	6.19	
---------	4060	-----	-----	[99]
	3-1281	-----	-----	
	3-1281	-----	-----	
1362	1312	3.56	3.56	[85]
	1-0564	2.18	2.18	
	1-0542	4.11	4.11	
46. Lead fluochloride				
II-856	1310	3.54	3.54	British Museum.
	2-0388	2.25	2.25	
	2-0377	1.77	1.77	
---------	3928	-----	1.22	[164]
	3-1184	-----	1.29	
	3-1182	-----	1.79	

TABLE 1. *ASTM cards to be superseded—Con.*

Card number		Index lines		Source
Old	1950	Old	1950	
47. Potassium cyanide				
---------	4078	-----	-----	[22]
	3-1299	-----	-----	
	3-1299	-----	-----	
II-1064	1666	3.26	3.26	[159]
	2-0485	2.30	2.30	
	2-0482	1.97	1.97	
1711	1667	3.26	3.26	[85]
	1-0705	2.30	2.30	
	1-0700	1.96	1.96	
48. Sodium cyanide (cubic)				
II-1530	2348	2.92	2.92	[159]
	1-0742	2.06	2.06	
	1-0739	3.37	3.37	
2234	2346	2.94	2.94	[85]
	1-0932	2.07	2.07	
	1-0913	1.69	1.69	
49. Sodium cyanide (orthorhombic)				
---------	2234	-----	2.96	[240]
	3-0638	-----	2.03	
	3-0638	-----	2.82	
50. Strontium nitrate				
732	0733	4.50	4.50	[85]
	1-0336	2.35	2.35	
	1-0336	2.24	2.24	
51. Barium nitrate				
2933	3111	2.44	2.44	[85]
	1-1144	4.69	4.69	
	1-1144	2.34	2.34	
52. Zinc borate. No ASTM patterns.				
53. Magnesium silicate				
3627	3752	1.74	1.74	[85]
	1-1290	3.89	3.89	
	1-1290	2.77	2.77	
---------	3760	-----	1.74	[48]
	3-1119	-----	2.44	
	3-1117	-----	2.49	
54. Magnesium tungstate. No ASTM patterns.				

2.1. Magnesium (Hexagonal)

In addition to the two patterns recorded in the ASTM file (see table 1) four were found in the literature: 1920, Bohlin [18]; 1923, Owen and Preston [176]; 1929, Grime and Morris-Jones [84]; and 1933, Finch and Quarrell [69]. These are compared in table 2 with a pattern prepared at the NBS.

The magnesium sample used for the NBS pattern was obtained from the Dow Chemical Co. Spectrographic analysis at the NBS indicates the presence of calcium <0.01 percent, and traces of Al, Cu, Fe, and Si.

In table 2 the data of Hull and Bohlin were derived directly in angstrom units from the published Bragg angle data. The electron diffraction measurements of Finch and Quarrell

TABLE 2. *Magnesium (hexagonal)*

hkl	1917 Hull Mo, 0.7093 A		1920 Bohlin Cu, 1.5405 A		1923 Owen and Preston Mo, 0.7093 A	1929 Grime and Morris-Jones Cu, 1.5405 A		1933 Finch and Quarrell Electron diffraction	1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A		1953 Swanson and Tatge Cu, 1.5405 A, 26°C	
	d	*I*	*d*	*I*	*d*	*d*	*I*	*d*	*d*	*I*	*d*	*I*
	A		*A*		*A*	*A*		*A*	*A*		*A*	
-------	-------	-----	3.06	m	----------	--------	------	----------	--------	------	---------	------
100	2.75	47	2.81	m	2.75	2.791	m	2.85	2.78	30	2.780	35
002	-------	-----	2.63	s	----------	2.613	m	2.53	2.61	25	2.606	41
-------	-------	-----	2.49	s	----------	--------	------	----------	--------	------	---------	------
101	2.45	100	2.48	vs	2.41	2.459	s	2.19	2.45	100	2.453	100
102	1.90	33	1.93	s-m	1.89	1.903	m	1.96	1.90	20	1.901	20
003	-------	-----	1.76	vw	----------	--------	------	----------	--------	------	---------	------
110	1.61	47	1.62	m-w	----------	1.606	m	1.62	1.60	20	1.605	18
111	-------	-----	1.55	vw	1.58	--------	------	1.52	--------	------	---------	------
103	1.48	40	1.49	m	1.46	1.474	m	1.43	1.474	20	1.473	18
200	-------	-----	1.41	vw	----------	--------	------	----------	--------	------	1.389	2
112	1.37	40	1.38	m	} 1.34	{ 1.367	m	1.37	1.381	18	1.366	16
201	1.34	13	1.35	m	}	{ 1.344	m	----------	1.344	13	1.343	9
004	-------	-----	1.31	w	1.29	--------	------	----------	1.306	3	1.303	2
202	1.227	7	1.24	w	1.21	--------	------	----------	1.227	3	1.227	2
104	} 1.186	1	1.19	w	1.16	--------	------	1.19	1.182	3	1.1795	2
113	}											
203	1.089	10	1.093	w	1.076	1.083	w	1.11	1.084	4	1.0851	2
210	-------	-----	-------	-----	----------	--------	------	1.06	--------	------	1.0506	1
211	1.032	20	1.035	w	1.017	1.030	w	1.03	1.032	7	1.0296	7
114	1.012	1	1.016	vw	----------	1.012	w	----------	1.012	3	1.0112	3
105	0.976	13	0.980	w	----------	0.9761	w	0.98	0.976	4	0.9757	2
204	-------	-----	-------	-----	0.961	--------	------	.95	--------	------	.9505	1
300	0.931	1	-------	-----	.935	--------	------	.93	0.927	1	.9265	1
213	.904	10	-------	-----	.902	0.8998	w	.90	.900	3	.8988	4
302	.872	7	-------	-----	.865	.8745	vw	----------	.872	1	.8729	2
205	.836	1	-------	-----	} .830	--------	------	{ 0.84	--------	------	.8337	2
106	-------	-----	-------	-----	}			{ .83	--------	------	.8288	1
214	-------	-----	-------	-----	----------	--------	------	----------	--------	------	.8177	1
303	-------	-----	-------	-----	0.812	--------	------	----------	--------	------	---------	------
-------	0.763	7	-------	-----	.758	--------	------	----------	{ 0.765 .741 }	1	---------	------

are presented as published. Measurements by the remaining workers were converted to angstroms from kX units. The two patterns published by Hull gave the same interplanar spacings; only the one reproduced on the ASTM card is given in the table. The Bohlin pattern shows two lines for approximately the spacing required for 101, one of which is extraneous to the structure. Bohlin also found lines at 001 and 003 not found in any other pattern, and at 111, occurring only in the electron diffraction pattern of Finch and Quarrell. It is surprising that neither Hull, nor Owen and Preston reported the strong 002 line.

Two patterns were published by Hull [100]; they are much alike, and only one appears in the ASTM file and in table 2. The three lines 104, 300, and 205 recorded in table 2 as <1, were miscalculated in converting them for the ASTM card as 3 rather than as 0.3. The intensities of Hanawalt, Rinn, and Frevel and of the NBS compare closely except that the 002 line is almost twice as strong for the pattern of the latter. The NBS sample, in minute spheres formed upon atomizing the material, was particularly satisfactory for this determination as particle orientation was not possible.

The structure of magnesium, which is hexagonal close-packed, was worked out by Hull [103] in 1917. The space group is D_{6h}^4 (C6/mmc); there are two atoms in the unit cell.

Some recent unit cell determinations, after the addition of corrections for temperature and conversion to angstrom units, are tabulated:

Unit cell at 25°C, angstroms

		a	c
1932	Stenzel and Weertz [212]	3.2091	5.2104
1935	Jette and Foote [119]	3.2095	5.2107
1935	Owen, Pickup, and Roberts [175]	3.2091	5.2115
1938	Ievinš, Straumanis, and Karlsons [114]	3.20927	5.21033
1939	Raynor and Hume-Rothery [191]	3.20948	5.2113
1940	Foote and Jette [71, 72]	3.2095	5.2107
1942	Raynor [190]	3.20949	5.21096
1953	Swanson and Tatge	3.2094	5.2103

The 1939 determinations of Raynor and Hume-Rothery [191] of the coefficients of expansion were used in correcting for temperature: 27.9×10^{-6} parallel to c, and 27×10^{-6} parallel to a. The density based on the NBS unit-cell determination is 1.737.

2.2. Aluminum (Cubic)

Five patterns of aluminum recorded on ASTM cards (see table 1) are compared in table 3 with a pattern prepared at the NBS and one by Scherrer [202] obtained from the literature. The material used for the NBS sample was a melting-point Standard Sample of aluminum prepared in the chemistry laboratories of the Bureau. The chemical analysis (in percent) is Si, 0.011; Cu, .006; Fe, .007; Ti, .0001; Zr, .003; Ga, .004; Mo, .00002; S, .0001; Al, 99.9+ (by difference).

The intensity measurements on the ASTM card accompanying the spacings ascribed to the Crystallographic Laboratory correspond to those of the 1925 Davey pattern except for one line, and were probably supplied from that source; the 400, a very weak line, has the intensity given as 80, surely a misprint for the 40 of the Davey pattern. This set of intensity measurements is the only one showing the 311 line stronger than the 200. All patterns show the 111 line as the strongest. The order shown by the NBS pattern is 111, 200, and 311 as first, second, and third strongest lines.

Aluminum has a face-centered cubic lattice [102], four atoms to the unit cell, and the space group O_h^5 (Fm3m). Unit cell values from the literature are compared below with the NBS determination.

Unit cell, angstroms at 25°C

		a
1933	Owen and Yates [178]	4.0495
1935	Jette and Foote [119]	4.0496
1936	Jevins and Straumanis [121]	4.04961
1936	Straumanis and Ievinš [216]	4.0489
1940	Foote and Jette [71]	4.0496
1941	Lu and Chang [141]	4.0498
1941	Van Bergen [230]	4.04955
1948	Axon and Hume-Rothery [4]	4.0495
1953	Swanson and Tatge	4.0494

These were accompanied by temperature data, and by means of a coefficient of expansion of 23.84×10^{-6} [4, 67, 127, 230] were converted to angstroms at 25°C. Using the

NBS lattice constant, the density was calculated as 2.697 at 25°C.

For table 3, the spacings of three of the five ASTM patterns were converted to angstroms from the kX units in which they were given. The Olshausen interplanar spacings were calculated for the table directly from the measurements given of the Bragg angle. Hull used 0.712 as the wavelength for molybdenum radiation; his spacings were converted to angstroms to correspond with a wavelength of 0.709 A. The pattern by Scherrer, a slight improvement on that of Hull made the year before, was calculated for table 3 directly in angstroms from Bragg angle data. Agreement among the patterns on spacings is excellent, as demonstrated by the uniform unit-cell values shown at the bottom of the table.

TABLE 3. *Aluminum (cubic)*

hkl	1917 Hull Mo, 0.7093 A			1918 Scherrer Cu, 1.5405 A			1925 Davey Mo, 0.7093 A			1925 Olshausen Cu, 1.5405 A		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		A	A		A	A		A	A		A
111	2.32	100	4.02	2.33	s	4.036	2.34	100	4.05	2.32	vs	4.02
200	2.02	60	4.04	2.021	m-s	4.042	2.02	90	4.04	2.02	s	4.04
220	1.42	50	4.02	1.426	m	4.033	1.434	80	4.056	1.428	s	4.039
311	1.20	60	3.98	1.220	s	4.043	1.223	100	4.056	1.219	s	4.043
222	1.17	20	4.05	1.168	w-m	4.046	1.172	50	4.060	1.168	m	4.046
400	1.01	5	4.04	1.010	w-m	4.040	1.015	40	4.060	1.010	m	4.040
331	0.93	25	4.05	0.928	m	4.045	0.930	70	4.054	0.931	s	4.058
420	.90	25	4.02	.905	m	4.047	.907	70	4.056	.907	s	4.056
422	.82	10	4.02	.827	m-s	4.051	.827	50	4.051	.830	s	4.066
511	.78	15	4.05	.780	s	4.053	.779	60	4.048	---	---	---
440	.71	2	4.02	---	---	---	.716	20	4.050	---	---	---
531	.68	4	4.02	---	---	---	---	---	---	---	---	---
Average unit cell from last five lines			4.03	---	---	4.047	---	---	4.052	---	---	4.053

hkl	1938 Banawalt, Binn, and Frevel Mo, 0.7093 A			---- Crystallographic Laboratory Mo, 0.7093 A, 25°C			1953 Swanson and Tatge Cu, 1.5405 A, 23°C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		A	A		A	A		A
111	2.33	100	4.04	2.337	100	4.048	2.338	100	4.050
200	2.02	40	4.04	2.025	90	4.050	2.024	47	4.048
220	1.433	30	4.053	1.432	80	4.050	1.431	22	4.047
311	1.221	30	4.050	1.220	100	4.046	1.221	24	4.0489
222	1.170	7	4.053	1.169	50	4.050	1.1690	7	4.0495
400	1.013	2	4.052	1.012	80	4.048	1.0124	2	4.0496
331	0.930	4	4.054	0.929	70	4.049	0.9289	8	4.0490
420	.907	4	4.056	.906	70	4.052	.9055	8	4.0495
422	.828	1	4.056	.827	50	4.051	.8266	8	4.0495
511	.779	1	4.048	.779	60	4.048	---	---	---
440	---	---	---	---	---	---	---	---	---
531	---	---	---	---	---	---	---	---	---
Average unit cell from last five lines			4.053	---	---	4.050	---	---	4.0494

2.3. Nickel (Cubic)

An unusually large number of patterns has been published for nickel. Table 4 is based on 15 patterns, 6 of which are in the ASTM card index file of X-ray diffraction patterns (see table 1), nine additional patterns found in the literature, and the proposed standard pattern made at the NBS. The literature sources are 1917, Hull [103]; 1920, Bohlin [18]; 1922, Wever [247]; 1925, Levi and Tacchini [139]; 1925, Clark, Asbury, and Wick [49]; 1926, Holgersson [95]; 1928, Roux and Cournot [195]; 1929, Greenwood [83]; 1939, Boochs [20].

With regard to the ASTM cards, the earliest pattern recorded, the 1917 pattern of Hull [103], was retracted in 1921 [106], and is replaced in table 4 by a second pattern from the same 1917 publication, not in the ASTM file. Hull's 1921 pattern was published twice in successive articles in the same journal [104, 106]. The ASTM card ascribes it to the second of these. Jung's published pattern [123] comprises four lines, of which the fourth is omitted from the ASTM card, probably due to its lack of precision.

The sample of nickel used for the NBS pattern was prepared by the Johnson, Matthey & Co., Ltd., laboratories of London, England; it is numbered 3236. Their spectrographic analysis (in percent) showed as impurities Mg, <0.01; Si, <0.01; Ca, <0.01.

Table 4 compares the interplanar spacings, intensity measurements and unit cell dimensions of the 15 patterns. Nine of the investigators published θ or sin θ values rather than interplanar spacings. The spacings were calculated for the table directly in angstrom units. The spacings of the Davey, the Hanawalt, Rinn, and Frevel, and the Boochs patterns were converted to angstrom from kX units. The two Hull patterns, one made with tungsten radiation with a wavelength given as 0.212, the other with molybdenum (wavelength 0.712), and the spacings of the Roux and Cournot pattern giving the wavelength of the molybdenum radiation used as 0.712, were converted to angstrom units on the basis of the wavelengths used. Wever tabulated the θ values for several samples of nickel; these are closely parallel and one, of a sample of high purity, was selected for table 4. Only one of two similar patterns published by Davey was chosen for the table. Mazza and Nasini likewise published several patterns, of which one was selected for the ASTM card and is reproduced here. Comparison of the lattice constants for the lines of each pattern shows that none of the interplanar spacings of the published patterns is accurate to more than two decimal places.

Five of the patterns record intensity measurements numerically. The older ones show the effects of uncorrected absorption and focusing errors. Those of Hanawalt, Rinn, and Frevel and of the NBS, although utilizing different radiations in their preparation, agree in designating the three strongest or index lines as the 111, 200, and 320.

The common form of nickel discussed here has a face-centered cubic lattice [103], four atoms to the unit cell, and the space group O_h^5 ($Fm3m$). About 40 lattice constants were found in the literature, many of these of high precision. Six, accompanied by the necessary data for conversion to angstroms at 25°C, are tabulated below with the NBS determination. For the conversion the coefficient of expansion of 13.4×10^{-6} was used, an average of two recent values [122, 179].

Unit cell in angstroms, 25°C

1931	Phragmén [185]	3.5255
1932	Owen and Iball [173]	3.5254
1934	Jesse [118]	3.525
1935	Jette and Foote [71, 119, 120]	3.5239
1936	Owen and Yates [179]	3.5247
1941	Lu and Chang [141]	3.5247
1941	Fricke [76]	3.5239
1953	Swanson and Tatge	3.5238

The density, based on the NBS lattice constant, is 8.907 at 25°C.

TABLE 4. *Nickel (cubic)*

hkl	1917 Hull W, 0.2086 A		1920 Bohlin Cu, 1.5405 A			1921 Hull Mo, 0.7093 A			1922 Wever Cu, 1.5405 A			1925 Levi and Tacchini Cu, 1.5405 A		
	d	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A	*A*	*A*		*A*	*A*		*A*	*A*		*A*	*A*		*A*
111	1.98	3.43	2.05	vs	3.55	2.03	100	3.51	2.04	vs	3.53	2.05	vs	3.55
200	1.74	3.48	1.77	s	3.54	1.76	50	3.52	1.76	s	3.52	1.73	s	3.46
220	1.23	3.49	1.25	s-m	3.54	1.25	40	3.54	1.25	m	3.53	1.23	ms	3.48
311	1.05	3.48	1.065	s	3.532	1.062	60	3.522	1.063	s	3.526	1.057	s	3.506
222	------	------	1.020	w	3.533	1.018	10	3.526	1.019	w	3.530	1.011	mw	3.502
400	------	------	------	---	------	0.880	2	3.520	0.879	vw	3.515	0.880	mw	3.520
331	------	------	------	---	------	.809	20	3.526	.807	s	3.519	.810	s	3.531
420	------	------	------	---	------	.788	16	3.524	.787	s	3.520	.790	vs	3.533
422	------	------	------	---	------	.720	10	3.527	------	----	------	------	----	------
511	------	------	------	---	------	.678	10	3.523	------	----	------	------	----	------
440	------	------	------	---	------	.622	1	3.518	------	----	------	------	----	------
531	------	------	------	---	------	.595	8	3.520	------	----	------	------	----	------
600	------	------	------	---	------	.587	4	3.522	------	----	------	------	----	------
Average unit cell for last five lines---		[a]3.48	------	---	[b]3.533	------	-----	3.522	------	----	3.522	------	----	3.518

hkl	1925 Davey Mo, 0.7093 A			1925 Clark, Asbury and Wick Mo, 0.7093 A		1926 Holgersson Fe, 1.9360 A			1927 Jung Fe, 1.9360 A			1929 Roux and Cournot Mo, 0.7093 A		
	d	*I*	*a*	*d*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*	*A*	*A*		*A*	*A*		*A*	*A*		*A*
111	2.01	100	3.48	1.96	3.39	1.96	80	3.409	2.037	vs	3.528	2.063	vs	3.573
200	1.745	88	3.490	1.76	3.52	1.715	80	3.430	1.780	vs	3.560	1.786	s	3.572
220	1.235	75	3.493	1.249	3.533	1.227	30	3.470	1.253	vs	3.544	1.238	w	3.502
311	1.055	88	3.499	1.069	3.545	1.053	100	3.492	1.127	w	3.738	1.081	m	3.585
222	1.011	63	3.502	1.025	3.551	1.011	60	3.502	------	----	------	------	--	------
400	0.877	50	3.508	------	------	------	-----	------	------	----	------	------	--	------
331	.806	63	3.513	0.822	3.539	------	-----	------	------	----	------	------	--	------
420	.784	63	3.506	.794	3.551	------	-----	------	------	----	------	------	--	------
422	.717	63	3.513	------	------	------	-----	------	------	----	------	------	--	------
511	------	-----	------	------	------	------	-----	------	------	----	------	------	--	------
440	------	-----	------	------	------	------	-----	------	------	----	------	------	--	------
531	------	-----	------	------	------	------	-----	------	------	----	------	------	--	------
600	------	-----	------	------	------	------	-----	------	------	----	------	------	--	------
Average unit cell for last five lines---			3.508	------	3.544	------	-----	3.461	------	----	[c]3.544	------	--	[d]3.558

[a] Average of last three lines.
[b] Average of last two lines.
[c] Average of three lines preceding last line.
[d] Average of four lines.

(Continued)

TABLE 4. *Nickel (cubic)*—Con.

hkl	1929 Greenwood Cu, 1.5405 A		1929 Mazza and Nasini Cu, 1.5405 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A			1939 Boochs Electron diffraction		1953 Swanson and Tatge Cu, 1.5405 A, 26°C		
	d	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*a*	*d*	*I*	*a*
	A	A	A		A	A		A	A	A	A		A
111	1.836	3.180	2.02	100	3.50	2.03	100	3.52	2.0351	3.5249	2.034	100	3.523
200	1.767	3.534	1.75	54	3.50	1.76	50	3.52	----------	--------	1.762	42	3.524
220	-------	-------	1.24	47	3.51	1.247	32	3.527	1.2511	3.5386	1.246	21	3.524
311	1.071	3.552	1.06	65	3.52	1.063	32	3.526	1.0736	3.5607	1.0624	20	3.5236
222	1.023	3.550	1.01	19	3.50	1.019	4	3.530	----------	--------	1.0172	7	3.5237
400	0.887	3.548	0.88	10	3.52	-------	-----	-------	----------	--------	0.8810	4	3.5240
331	.812	3.540	.80	33	3.49	0.810	8	3.531	----------	--------	.8084	14	3.5237
420	.791	3.547	.78	32	3.49	.790	8	3.533			.7880	15	3.5240
422	-------	-------	------	-----	------	.720	8	3.527	----------	--------	--------	-----	--------
511	-------	-------	------	-----	------	.679	8	3.528	----------	--------	--------	-----	--------
440	-------	-------	------	-----	------	-------	-----	-------	----------	--------	--------	-----	--------
531	-------	-------	------	-----	------	-------	-----	-------	----------	--------	--------	-----	--------
600	-------	-------	------	-----	------	-------	-----	-------	----------	--------	--------	-----	--------
Average unit cell for last five lines—	3.547		------	-----	3.50	-------	-----	3.530	----------	[a] 3.5414	--------	-----	3.5238

[a] Average of last three lines.

2.4. Copper (Cubic)

The six patterns for copper in the ASTM file (see table 1) are supplemented in table 5 by two from the literature, by Sidhu [207] and by Terrey and Wright [219]. The NBS pattern was made with a sample of copper from the metallurgical laboratory of the Bureau. It had been heated in a hydrogen atmosphere at 300°C. Spectrographic examination at the NBS showed the following impurities from 0.001 to 0.01 percent: Ag, Al, Bi, Fe, Si, and Zn.

The spacings for the Jung patterns were calculated for table 5 directly in angstroms from the published Bragg angle data. For the other patterns the spacings were converted from kλ to angstrom units, except that of Allis-Chalmers (presumably a personal communication), which was left as it appears on the ASTM card, the unit employed not being known. The second of the two Jung patterns appearing on one ASTM card was published with additional Cu_2O lines which are omitted in the table. For the Jung and the Waldo patterns two columns of intensity measurements are given, the first as originally published, the second as converted to numerical values on the ASTM card. For most of the patterns the three strongest lines are 111, 200, and 220.

The lattice was first determined by Bragg [31] in 1914 as face-centered cubic. The space group is O_h^5 ($Fm3m$) [107], and there are four atoms in the unit cell. Nine unit cell determinations are compared below with that of the NBS. All were converted to angstroms at 25°C; the coefficient of expansion 16.99×10^{-6} [67] was used.

Unit cell in angstroms at 25°C

1933	Owen and Yates [178]	3.6155
1933	Obinata and Wasserman [168]	3.6155
1936	Hume-Rothery, Lewin, and Reynolds [109]	3.6148
1939	Owen and Roberts [177]	3.6151
1940	Foote and Jette [71]	3.6151
1941	Lu and Chang [141]	3.6149
1941	Fricke [76]	3.615
1942	Hume-Rothery and Andrews [108]	3.6151
1945	Hume-Rothery [107]	3.616
1953	Swanson and Tatge	3.6150

From the NBS unit-cell determination the density was calculated as 8.932 at 25°C.

TABLE 5. *Copper (cubic)*

hkl	1925 Davey Mo, 0.7093 A			1926 Jung Cu, 1.5405 A				1926 Jung Cu, 1.5405 A				1928 Terrey and Wright Cu, 1.5405 A		1935 Waldo Mo, 0.7093 A			
	d	*I*	*a*	*d*	*I*[a]	*I*[b]	*a*	*d*	*I*[a]	*I*[b]	*a*	*d*	*a*	*d*	*I*[a]	*I*[b]	*a*
	A		*A*	*A*			*A*	*A*			*A*	*A*	*A*	*A*			*A*
111	2.08	100	3.60	2.08	s	100	3.60	2.08	vs	100	3.62	2.085	3.610	2.08	s	100	3.60
200	1.802	86	3.604	1.806	s	100	3.612	1.806	w	40	3.612	1.804	3.609	1.814	m	80	3.628
220	1.274	71	3.603	1.283	s	100	3.629	1.281	s	80	3.623	1.276	3.609	1.276	m	80	3.609
311	1.085	86	3.599	1.094	s	100	3.641	1.091	ms	70	3.618	1.089	3.611	1.089	m	80	3.612
222	1.040	56	3.603	1.051	ms	80	3.641	1.049	w	40	3.634	1.043	3.612	1.042	w	50	3.610
400	0.902	29	3.608	0.907	w	40	3.628	-------	---	---	------	-------	-------	0.903	vw	20	3.612
331	.828	56	3.609	-------	--	---	-----	-------	---	---	------	-------	-------	.830	w	40	3.618
420	.808	42	3.613	-------	--	---	-----	-------	---	---	------	-------	-------	.809	w	40	3.618
422	.736	42	3.606	-------	--	---	-----	-------	---	---	------	-------	-------	.736	vw	20	3.606
Average unit cell for last five lines			3.608	-------	--	---	3.630	-------	---	---	[d] 3.622	-- ----	3.610	-------	---	---	3.613

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A			1942 Harcourt Cu, 1.5405 A			---- Allis-Chalmers Fe, 1.9360 A			1948 Sidhu Cu, 1.5405 A			1953 Swanson and Tatge Cu, 1.5405 A, 26° C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	(c)		(c)	*A*		*A*	*A*		*A*
111	2.08	100	3.60	2.08	100	3.60	2.08	100	3.60	2.08	vs	3.60	2.088	100	3.617
200	1.81	53	3.62	1.81	50	3.62	1.80	70	3.60	1.81	s	3.62	1.808	46	3.6154
220	1.280	33	3.620	1.278	40	3.615	1.27	90	3.59	1.28	m	3.62	1.278	20	3.6150
311	1.091	33	3.618	1.090	40	3.615	1.09	90	3.62	1.09	m	3.62	1.0900	17	3.6151
222	1.045	9	3.620	1.045	10	3.620	1.04	70	3.60	1.04	w	3.60	1.0436	5	3.6151
400	0.907	3	3.628	0.905	5	3.620	------	---	-------	0.905	vw	3.620	0.9038	3	3.6152
331	-------	---	--------	.830	5	3.618	------	---	-------	.830	m	3.618	.8293	9	3.6148
420	-------	---	--------	.810	5	3.622	------	---	-------	.809	s	3.618	.8083	8	3.6148
422	-------	---	--------	-------	---	-------	------	---	-------	------	---	-------	--------	---	--------
Average unit cell for last five lines			[d] 3.622	-------	---	3.619	------	---	3.60	------	---	[e] 3.619	--------	---	3.6150

[a] As first published. [b] On ASTM card. [c] Unit not known. [d] Average of four lines only. [e] Average of three lines only.

2.5. Zinc (Hexagonal)

Two patterns for zinc recorded in the ASTM file (see table 1) are compared in table 6 with a pattern made at the NBS and with 12 found in the literature. The literature sources are 1925, Peirce, Anderson, and van Dyck [184]; 1926, Freeman, Sillers, and Brandt [73]; 1928, Roux and Cournot [195]; 1929, Osawa and Ogawa [171]; 1929, McLennan and Monkman [148]; 1933, Finch and Quarrell [69]; 1935, Kotin and Losada [132]; 1936, Brindley [37]; 1937, Wollan and Harvey [251]; 1937, Miller [154]; 1938, Wroński [252]; 1943, Köhler [128].

The sample of zinc used to obtain the NBS pattern presented here was supplied by the New Jersey Zinc Co., and was numbered 11837. Spectrographic analysis at the Bureau showed a trace of lead and faint traces of copper,

magnesium, and silicon. A lump of zinc sublimed in an evacuated tube yielded a fine powder.

The interplanar spacings of all patterns listed in table 6 are in angstroms, some of them changed from kX units, some computed directly in angstroms from Bragg angle data, and others converted from angstrom units based on old wavelength values. Only experimental data are listed; published spacings computed by some investigators in the course of work on intensity measurements do not appear in the table. Freeman, Sillers, and Brandt in 1926 published a pattern showing the presence of every possible line. The Köhler pattern of 1943 misses the 006 line, and shows an extraneous line between 114 and 210.

There is general agreement that 101 is the strongest line. The patterns since 1936 give 002 and 100 as second and third strongest, respectively, except for that of Wroński, 1938, which places these in reverse order.

The structure of zinc [106] is based on a hexagonal lattice, space group D^4_{6h} (C6/mmc). There are two atoms to the unit cell. Values, presumed all in kX units, found in the literature were converted to angstrom units for the following table and corrected for temperature by means of the coefficients of expansion

TABLE 6. *Zinc (hexagonal)*

hkl	1921 Hull Mo, 0.7093 A		1925 Peirce, Anderson and van Dyck Mo, 0.7093 A		1926 Freeman, Sillers and Brandt Mo, 0.7093 A		1928 Roux and Cournot Cu, 1.5405 A		1929 Osawa and Ogawa Fe, 1.9360 A	1929 McLennan and Monkman Cu, 1.5405 A	1933 Finch and Quarrell Electron diffraction
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*d*	*d*
	A		A		A		A		A	A	A
002	2.462	30	2.479	25	2.461	30	2.489	vs	2.477	----------	2.56
100	2.284	10	2.306	13	2.293	20	2.356	w	----------	----------	2.32
101	2.069	100	2.094	100	2.078	100	2.130	vs	2.099	2.078	2.12
102	1.678	20	1.690	25	1.677	15	1.742	m	1.687	1.684	1.74
103	1.334	100	1.340	44	1.335	30	1.402	s	1.343	1.339	1.39
110	1.327	100	----------	------	1.324	30	1.304	w	----------	1.329	1.35
004	1.230	5	1.236	2	1.231	3	1.232	w	----------	----------	1.30
112	1.167	70	1.173	25	1.166	35	1.201	w	1.174	1.169	1.19
200	1.148	5	1.150	------	1.146	3	------	------	----------	----------	1.17
201	1.117	40	1.124	19	1.117	35	------	------	1.123	1.119	1.13
104	1.084	5	1.090	3	1.085	1	------	------	1.090	1.085	
202	1.040	10	1.046	2	1.039	1	------	------	1.046	1.043	1.06
203	0.943	20	0.944	------	0.940	3	------	------	----------	0.943	0.96
105	-------	-------	----------	------	.905	5	------	------	----------	----------	.93
114	0.906	20	0.908	6	.901	5	------	------	----------	----------	----------
---	-------	-------	----------	------	----------	-------	------	------	----------	----------	----------
210	-------	-------	----------	------	0.866	-------	------	------	----------	0.870	0.87
211	0.856	30	0.859	6	.853	8	------	------	----------	.856	.86
204	-------	-------	.847	2	.839	1	------	------	----------	----------	----------
006	0.824	10	----------	------	.821	1	------	------	----------	0.825	----------
212			----------	------	.817	1	------	------	----------	.821	0.84
106	-------	-------	----------	------	.773	-------	------	------	----------	----------	.80
213	0.770	20	0.772	3	.766	3	------	------	----------	----------	.79
300			----------	------	.764	3	------	------	----------	----------	
205	.753	10	----------	------	.748	-------	------	------	----------	----------	.78
302	.734	20	----------	------	.729	1	------	------	----------	----------	.74
214	.714	5	----------	------	----------	-------	------	------	----------	----------	.72
116	.700	5	----------	------	----------	-------	------	------	----------	----------	----------

TABLE 6. *Zinc (hexagonal)*—Con.

hkl	1935 Kotin and Losada Cu, 1.5405 A		1936 Brindley Cu, 1.5405 A	1937 Wollan and Harvey Cu, 1.5405 A	1937 Miller Mo, 0.7093 A	1938 Wroński Cu, 1.5405 A	1938 Hanawalt, Rinn and Frevel Mo, 0.7093 A		1943 Köhler Cu, 1.5405 A		1953 Swanson and Tatge Cu, 1.5405 A, 26° C	
	d	*I*	*I*	*I*	*I*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A						A		A		A	
002	2.475	100	35	33	32	41	2.46	25	2.48	81	2.473	53
100	2.310	100	28	30	26	44	2.30	20	2.31	68	2.308	40
101	2.092	80	100	100	100	100	2.08	100	2.09	100	2.091	100
102	1.687	60	15	15	16	26	1.68	14	1.69	50	1.687	28
103	1.337	36	28	15	34	56	1.333	18	1.34	53	1.342	25
110				14					1.33	36	1.332	21
004	1.237	31	----------	----------	2	----------	-------	-----	1.23	8	1.237	2
112	1.176	23	13	14	16	32	1.171	12	1.171	33	1.1729	23
200	1.155	25	----------	----------	----------	----------	-------	-----	1.153	6	1.1538	5
201	1.124	21	9	11	11	26	1.122	8	1.123	22	1.1236	17
104	1.090	25	----------	----------	----------	----------	-------	-----	1.089	8	1.0901	3
202	1.046	21	----------	----------	----------	----------	1.042	2	1.045	6	1.0456	5
203	0.9458	11	4	4	4	12	0.943	2	0.945	17	0.9454	8
105	.9086	7	8	7	5	15	.907	2	.909	17	.9093	6
114							------	-----	.906	25	.9064	11
----	-------	------	----------	----------	----------	----------	-------	-----	.905	14	------	------
210	0.8726	10	----------	----------	----------	----------	-------	-----	.872	8	0.8722	5
211	.8593	11	10	11	6	26	-------	-----	.859	31	.8589	9
204	.8438	5	----------	----------	----------	----------	-------	-----	.857	19	.8437	2
006	------	-----	4	4	1	----------	-------	-----	------	----	.8245	1
212	------	-----							0.822	14	.8225	9
106	-------	-----	----------	----------	----------	----------	-------	-----	-------	-----	-------	------
213	-------	-----	----------	----------	----------	----------	-------	-----	-------	-----	-------	------
300	-------	-----	----------	----------	----------	----------	-------	-----	-------	-----	-------	------
205	-------	-----	----------	----------	----------	----------	-------	-----	-------	-----	-------	------
302	-------	-----	----------	----------	----------	----------	-------	-----	-------	-----	-------	------
214	-------	-----	----------	----------	----------	----------	-------	-----	-------	-----	-------	------
116	-------	-----	----------	----------	----------	----------	-------	-----	-------	-----	-------	------

60.8×10^{-6} parallel to the *c*-axis and 14.3×10^{-6} perpendicular to it [175].

Unit cell at 25°C in angstrom units

		a	*c*
1929	McLennan and Monkman [148]	2.662	4.960
1932	Stenzel and Weertz [212]	2.6643	4.9472
1932	Boas [17]	2.6640	4.9468
1933	Hansen and Stenzel [86]	2.6646	4.9466
1933	Owen and Iball [174]	2.6646	4.947
1935	Jette and Foote [119]	2.6649	4.9468
1935	Owen, Pickup, and Roberts [175]	2.6648	4.9474
1953	Swanson and Tatge	2.665	4.947

The density, based on the NBS unit cell, is 7.134 at 25°C.

2.6. Germanium (Cubic)

The two patterns for germanium in the ASTM file (see table 1) were not published elsewhere; information regarding the first is limited to the author's name and date, and the second is a combined pattern from two sources. The two patterns are compared in table 7 with one prepared at the NBS and three from the literature, by Kolkmeijer [130], Nitka [166], and König [129].

The germanium used for the NBS pattern was obtained from Johnson, Matthey & Co., Ltd., numbered 4065. Their spectrographic examination showed faint traces of silver, copper, sodium, and iron present as impurities.

The Kolkmeijer and Nitka patterns were published as Bragg angle data and the values of the spacings were calculated for table 7 directly in angstroms. The spacings of the other patterns were converted from kX units to angstroms. In Nitka's pattern the reflection from the 400 plane was omitted; it is shown by the other patterns to be very weak. In the patterns of Nitka, König, and Fuller no reflections were recorded with indices higher than 511. König noted and indexed as 222 a reflection in his electron diffraction pattern which is not consistent with the assumed diamond structure of germanium as found in X-ray patterns.

The intensity measurements of the patterns of Kolkmeijer and Nitka are estimated values represented by letters. No intensity values accompany the electron diffraction pattern by König. Schatzlein's pattern shows the customary high values associated with the absorption and focusing errors of much film work. A comparison between the Fuller pattern and the NBS pattern, after a rough conversion of the Fuller-Hanawalt intensity measurements from molybdenum to copper radiation by means of the ASTM conversion chart ([1] page 108 of index covering original set of cards, or card No. vii of the introduction to the 1950 file), indicates good agreement of values. The NBS pattern is in close agreement with those of other investigators using copper radiation.

Germanium, cubic, has the structure of diamond and the space group O_h^7 (Fd3m) [105] with eight atoms in the unit cell. The lattice constant determined at the NBS is compared in the following table with determinations found in the literature, after their conversion to angstrom units at 25°C. The coefficient of expansion of 5.92×10^{-6} was used for the temperature conversions.

Unit cell, angstroms at 25°C

1937	Nitka [166]	5.659
1952	Straumanis and Aka [215a]	5.657640
1953	Swanson and Tatge	5.6576

The density, based on the NBS lattice constant, is 5.325 at 25°C.

TABLE 7. *Germanium (cubic)*

hkl	1922 Kolkmeijer Cu, 1.5405 A			1937 Nitka Fe, 1.9360 A			1938 Schatzlein Cu, 1.5405 A			1944 König Electron diffraction		---- Fuller Hanawalt Mo, 0.7093 A			1953 Swanson and Tatge Cu, 1.5405 A, 26°C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*		*A*	*A*		*A*	*A*		*A*
111	3.18	vs	5.51	3.270	s	5.664	3.25	100	5.62	3.28	5.61	3.26	100	5.66	3.266	100	5.657
220	1.97	s-vs	5.57	2.000	vs	5.657	1.99	100	5.63	1.99	5.63	1.99	66	5.64	2.000	57	5.657
311	1.69	s-vs	5.61	1.708	s	5.665	1.70	100	5.64	1.69	5.61	1.70	53	5.65	1.706	39	5.658
(222)	-----	----	-----	-----	----	-----	-----	---	------	1.62	5.61	-----	---	-----	------	---	------
400	1.42	w	5.68	-----	----	-----	1.41	40	5.64	1.41	5.64	1.41	8	5.65	1.414	7	5.657
331	1.28	m-s	5.58	1.298	m	5.657	1.30	50	5.67	1.29	5.62	1.29	16	5.63	1.298	10	5.658
422	1.14	s-vs	5.58	1.155	vs	5.658	1.12	60	5.49	1.15	5.63	1.15	27	5.64	1.1547	17	5.6569
511	1.08	w	5.61	1.090	s	5.664	1.09	40	5.66	1.08	5.61	1.09	13	5.67	1.0888	7	5.6576
440	0.995	w	5.629	-----	----	-----	1.00	30	5.66	------	------	0.998	7	5.646	1.0000	3	5.6569
531	.954	s-m	5.644	-----	----	-----	0.958	100	5.67	------	------	-----	---	-----	0.9562	11	5.6571
620	.893	m	5.647	-----	----	-----	.898	90	5.68	------	------	-----	---	-----	.8946	6	5.6579
533	.861	w	5.646	-----	----	-----	.865	30	5.67	------	------	-----	---	-----	.8628	4	5.6574
444	.814	w	5.640	-----	----	-----	.818	30	5.66	------	------	-----	---	-----	.8166	2	5.6575
711	.792	s-m	5.656	-----	----	-----	.793	90	5.66	------	------	-----	---	-----	.7923	8	5.6579
Average unit cell for last five lines			5.647	-----	----	5.660	-----	---	5.67	------	5.62	-----	---	5.65	------	---	5.6576

2.7. Molybdenum (Cubic)

Molybdenum is represented in table 8 by three patterns from the ASTM file (see table 1); no additional patterns were found in the literature. A pattern was made at the NBS from a sample prepared by fused salt electrolysis by Seymour Senderoff of the Bureau. Spectrographic analysis showed very weak lines of Al, Fe, Mg, and Si, and traces of Ca, Cu, Mn, and Pb. The unit-cell size remained unchanged after heating the finely divided powder in a vacuum furnace at 1,430°C for 1 hour.

The spacings of the three ASTM card patterns were converted to angstrom units for table 8. For the Davey and the Hanawalt, Rinn, and Frevel patterns the conversion was from kX units to angstroms; for the Hull pattern the radiation wavelength cited as 0.712 unit for molybdenum was used as the basis for the conversion. Only the first of four series of interplanar spacings published by Davey is given on an ASTM card, and only this is represented in table 8. Two patterns closely resembling these were published a year later by Davey in a German article [60]. Copper radiation used for the recording of the NBS pattern permitted the determination of only seven lines.

The first and second strongest lines are generally agreed upon as the 110 and 211, respectively. Hull and Davey list the 321 and 310 as third strongest, but their intensity values show the effect of sample absorption when compared with those of Hanawalt, Rinn, and Frevel and of the NBS, which agree upon the 200 as third strongest.

The molybdenum lattice is body centered cubic [106]. Molybdenum has the space group O_h^9 (Im3m), and two atoms in the unit cell. Correcting temperatures to 25°C with the

TABLE 8. *Molybdenum*

hkl	1921 Hull Mo, 0.7093 A			1925 Davey Mo, 0.7093 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A			1953 Swanson and Tatge Cu, 1.5405 A, 26°C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*	*A*		*A*
110	2.215	100	3.132	2.23	100	3.16	2.22	100	3.14	2.225	100	3.147
200	1.569	50	3.138	1.576	80	3.152	1.57	36	3.14	1.574	21	3.147
211	1.283	100	3.143	1.286	100	3.149	1.284	57	3.145	1.285	39	3.147
220	1.109	35	3.137	1.114	70	3.151	1.116	17	3.157	1.1127	11	3.1472
310	0.993	60	3.140	0.996	90	3.149	0.997	23	3.153	0.9952	17	3.1472
222	.907	10	3.142	.910	40	3.151	.910	7	3.152	.9085	7	3.1472
321	.839	70	3.139	.842	80	3.149	.843	23	3.154	.8411	26	3.1472
400	.784	5	3.136	----------	-----	----------	.789	3	3.156	----------	-----	----------
411	.739	30	3.135	0.743	60	3.154	.743	14	3.152	----------	-----	----------
420	.702	20	3.139	.704	50	3.150	.705	11	3.152	----------	-----	----------
332	.669	20	3.138	----------	-----	----------	.673	9	3.157	----------	-----	----------
422	.641	20	3.140	----------	-----	----------	.644	6	3.155	----------	-----	----------
510	.616	35	3.141	----------	-----	----------	.618	14	3.151	----------	-----	----------
521	.574	25	3.144	----------	-----	----------	----------	-----	----------	----------	-----	----------
440	.554	5	3.134	----------	-----	----------	----------	-----	----------	----------	-----	----------
530	.538	25	3.137	----------	-----	----------	----------	-----	----------	----------	-----	----------
600	.523	20	3.138	----------	-----	----------	----------	-----	----------	----------	-----	----------
Average unit cell for last five lines			3.139	----------	-----	3.145	----------	-----	3.151	----------	-----	3.1472

coefficient of expansion Michel [152] gives as 5×10^{-6}, and converting to angstrom units, the following lattice constants compare thus with the NBS determinations:

Unit cell at 25°C in angstrom units

1935	Jette and Foote [119]_____	3.1474
1941	Lu and Chang [141]_____	3.1467
1953	Swanson and Tatge_____	3.1472

The density, using the NBS unit-cell value, is 10.220 at 25°C.

2.8. Palladium (Cubic)

Four patterns recorded on ASTM cards (see table 1) and two patterns by Barth and Lund [7] and Jaeger and Zanstra [116] are represented in table 9. The sample of sponge palladium used for the NBS pattern was obtained from Johnson, Matthey & Co., Ltd. Spectrographic analysis (in percent) at the Bureau showed Ag, 0.1 to 0.01; Ca, 0.01 to 0.001; Cu, 0.01 to 0.001; Mg, 0.01 to 0.001; Pb, <0.0001; Pt, 0.01 to 0.001; Si, 0.1 to 0.01. The sample was heated at 700°C for 15 minutes in vacuum and rechecked for a change in unit-cell size. No appreciable change took place.

There is good agreement among various workers on the interplanar spacings of palladium. The spacings of the Hull pattern were converted to angstrom units on the basis of 0.712 as the wavelength used by Hull for molybdenum radiation. Those of the other patterns were converted from kX units. The two Davey patterns are essentially the same. The two most recent patterns, the Hanawalt, Rinn, and Frevel, and that of the NBS agree closely.

In contrast to the agreement of spacings among various workers, the intensity values are not in complete accord. The 311 is recorded on all but two patterns as either first or second strongest. The two most recent patterns, that of Hanawalt, Rinn, and Frevel, and that of the NBS, show the 111, 200, and 220 as first, second, and third strongest lines, putting the 311 in fourth place.

On the Hull card of the 1950 file the lattice constant is given as 3.950 and the density as 11.40. Although these data are referred to Wyckoff and to "C.C.," respectively, they are in fact from Hull's own published work. The two Davey cards of the new file both have lattice constants and densities ascribed to Wyckoff and to "C.C.," respectively; on the 1925 card these data are from Davey's own work, while on the 1926 card the lattice constant is from Wyckoff as represented, and the source of the density was not determined.

Palladium crystallizes in the cubic system [178] and has a space group O_h^5 (Fm3m). Two unit cell determinations made at specified temperatures were found in the literature. Converted to angstrom from kX units and corrected to 25°C temperature, these are compared below with the NBS determination. For the correction, a coefficient of expansion of 11.8×10^{-6} published by Owen and Yates [178] was used.

Unit cell, angstroms at 25°C

1931	Stenzel and Weerts [213]__	3.889
1933	Owen and Yates [178]_____	3.8905
1953	Swanson and Tatge_____	3.8898

The density calculated from the NBS lattice constant is 12.04 at 25°C.

TABLE 9. *Palladium (cubic)*

hkl	1921 Hull Mo, 0.7093 A			1925 Barth and Lunde Fe, 1.9360 A			1925 Davey Mo, 0.7093 A			1926 Davey Mo, 0.7093 A		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*	*A*		*A*
111	2.264	67	3.921	2.249	100	3.895	2.21	89	3.83	2.21	90	3.83
200	1.958	27	3.916	1.938	67	3.876	1.929	89	3.858	1.927	90	3.854
220	1.392	67	3.937	1.370	67	3.875	1.366	78	3.864	1.365	80	3.861
311	1.187	100	3.938	1.169	90	3.877	1.165	100	3.864	1.164	100	3.861
222	-------	-------	-------	1.119	30	3.869	1.116	33	3.866	1.116	30	3.866
400	-------	-------	-------	-------	-------	-------	0.967	33	3.868	0.967	30	3.868
331	0.905	20	3.945	-------	-------	-------	.887	78	3.866	.887	80	3.866
420	.882	7	3.944	-------	-------	-------	.865	78	3.868	.865	80	3.868
422	.804	7	3.939	-------	-------	-------	.790	56	3.870	.790	60	3.870
511	.756	2	3.928	-------	-------	-------	.745	67	3.871	.745	70	3.871
440	-------	-------	-------	-------	-------	-------	.684	22	3.869	.684	20	3.869
531	0.665	3	3.934	-------	-------	-------	.655	56	3.875	.655	60	3.875
600	.653	1	3.918	-------	-------	-------	.646	56	3.876	.646	60	3.876
620	-------	-------	-------	-------	-------	-------	.613	33	3.877	.613	30	3.877
Average unit cell for last five lines			3.933	-------	-------	3.878	-------	-------	3.874	-------	-------	3.874

hkl	1931 Jaeger and Zanstra Fe, 1.9360 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A			1953 Swanson and Tatge Cu, 1.5405 A, 26°C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*
111	2.221	60	3.847	2.23	100	3.86	2.246	100	3.891
200	1.926	50	3.852	1.94	50	3.88	1.945	42	3.889
220	1.367	90	3.866	1.374	27	3.886	1.376	25	3.891
311	1.166	100	3.867	1.172	27	3.887	1.1730	24	3.8904
222	1.117	40	3.876	1.122	5	3.887	1.1232	8	3.8909
400	----------	-------	----------	0.972	1	3.888	0.9723	3	3.8890
331	----------	-------	----------	.893	5	3.892	.8924	13	3.8896
420	----------	-------	----------	.871	5	3.895	.8697	11	3.8893
422	----------	-------	----------	.795	2	3.895	----------	-------	----------
511	----------	-------	----------	.750	2	3.897	----------	-------	----------
440	----------	-------	----------	----------	-------	----------	----------	-------	----------
531	----------	-------	----------	----------	-------	----------	----------	-------	----------
600	----------	-------	----------	----------	-------	----------	----------	-------	----------
620	----------	-------	----------	----------	-------	----------	----------	-------	----------
Average unit cell for last five lines			3.862	----------	-------	3.893	----------	-------	3.8898

2.9. Silver (Cubic)

There are six cards for silver in the ASTM file of diffraction patterns (see table 1). One of these (number 2-1098), for a "bismuth rich" silver, is not listed in either table 1 or 10. Three lines in this pattern are not silver lines and are probably due to a compound of silver and bismuth. When this card was duplicated for the 1950 reprinting, a unit cell measurement of pure silver was included that does not depend on any of the interplanar spacings on the card and misleadingly indicates that the pattern is for pure silver. Another card (3-1316), which is

TABLE 10. *Silver (cubic)*

hkl	1925 Davey Mo, 0.7093 A			1926 Jung Cu, 1.5405 A				1926 Jung Cu, 1.5405 A			
	d	*I*	*a*	*d*	*I*[a]	*I*[b]	*a*	*d*	*I*[a]	*I*[b]	*a*
	A		*A*	*A*			*A*	*A*			*A*
111	2.37	100	4.11	2.35	s	100	4.07	2.33	s	100	4.03
200	2.05	80	4.10	2.03	m	80	4.06	2.05	ms	90	4.10
220	1.445	80	4.087	1.442	m	80	4.079	1.435	m	80	4.059
311	1.232	90	4.086	1.230	m	80	4.079	1.223	m	80	4.056
222	1.180	50	4.088	1.179	w	60	4.084	1.182	w	60	4.095
400	1.021	20	4.084								
331	0.937	60	4.084	0.935	m	80	4.077				
420	.914	60	4.088	.912	m	80	4.080				
422	.835	40	4.091								
511	.786	40	4.084								
440	.722	10	4.084								
531											
Average unit cell for last five lines			4.086				4.080				4.070

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A			1942 Harcourt Cu, 1.5405 A			1953 Swanson and Tatge Cu, 1.5405 A, 27° C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*
111	2.36	100	4.09	2.35	100	4.07	2.359	100	4.086
200	2.04	53	4.08	2.04	55	4.08	2.044	38	4.088
220	1.448	27	4.096	1.44	45	4.07	1.445	25	4.087
311	1.234	53	4.093	1.230	65	4.079	1.231	26	4.083
222	1.181	5	4.091	1.178	20	4.081	1.1796	13	4.0863
400	1.024	1	4.096	1.020	10	4.080	1.0215	4	4.0860
331	0.940	8	4.097	0.938	55	4.089	0.9375	15	4.0864
420	.917	5	4.101	.914	55	4.088	.9137	10	4.0862
422	.836	3	4.096	.8351	55	4.0911	.8341	13	4.0862
511	.787	4	4.089						
440									
531	0.692	5	4.094						
Average unit cell for last five lines			4.095			4.086			4.0862

[a] As first published. [b] On ASTM card.

listed in table 1, gives no pattern, but only a unit cell measurement—a measurement actually appearing in only one [231] of the two papers to which it is ascribed. Of the remaining four patterns, the two by Jung [124] were published in the same paper. All four are compared in table 10 with a more recently published pattern by Harcourt [88], and one prepared at the NBS.

The NBS pattern was made from a sample furnished by Johnson, Matthey & Co., Ltd., London, with a purity of more than 99.999 percent. Their spectrographic analysis indicated faint traces of calcium, iron, and copper.

The interplanar spacings of the Jung patterns were calculated directly in angstroms from the Bragg angle data given; the spacings of the other patterns were converted from kX units. All patterns show 111 as the strongest line, but there is considerable difference as to the second and third strongest—Hanawalt, Rinn, and Frevel agree with the NBS on 200 and 311, respectively.

The atoms in silver are arranged in a face-centered lattice [231]. Silver has the space group O_h^5 (Fm3m), and four atoms in the unit cell. Published unit cell values are compared in the following table with that derived from the NBS pattern. Conversion to 25°C was made by means of a coefficient of expansion of 19.59×10^{-6} [67], and all were corrected from kX to angstrom units.

Unit cell in angstroms at 25°C

1930	Sachs and Weerts [200]	4.0863
1932	Owen and Iball [173]	4.0862
1933	Owen and Yates [178]	4.0860
1933	Saini [201]	4.0862
1935	Jette and Foote [119]	4.0861
1936	Hume-Rothery, Lewin, and Reynolds [109]	4.0862
1939	Owen and Roberts [177]	4.0860
1940	Foote and Jette [71]	4.0861
1953	Swanson and Tatge	4.0862

The density of silver based on the NBS unit cell is 10.500 at 25°C.

2.10. Tin (White or β) (Tetragonal)

The two patterns in the ASTM X-ray diffraction pattern file for tin are both for the tetragonal modification, referred to as white or β-tin (see table 1). Three patterns for tin not included in the ASTM file were found in the literature; these are by Bijl and Kolkmeijer [14], Van Arkel [228], and Willot and Evans [248].

The sample of tin used for the NBS pattern was furnished by Johnson, Matthey & Co., Ltd., London, with the notation that the metal had been specially purified by Capper, Pass, & Sons, Limited, who furnished the following analysis (in percent): lead, 0.0012; antimony, 0.001; iron, 0.00027; copper, 0.0002; arsenic, 0.0002; bismuth, 0.00012; sulfur, 0.00003; tin, 99.997 (by difference). Spectrographic analysis by Johnson, Matthey & Co., Ltd., showed the following impurities: lead, faint; bismuth, faint; iron, very faint; sodium, faint; cadmium, very faint; calcium, very faint; magnesium, very faint; aluminum, barely visible; copper, barely visible; indium, barely visible in one spectrum only. The sample was annealed for 12 hours at 160°C before it was mounted in the spectrometer.

Interplanar spacings and intensity measurements of the six patterns are compared in table 11. The interplanar spacings of Bijl and Kolkmeijer and of Van Arkel were calculated directly in angstrom units from their published Bragg angle data; for the remaining patterns they were converted from kX units to angstroms. Intensity values are given numerically by only three of the patterns. These are in agreement with those of the NBS in designating the 200, 101, and 211 as the first, second, and third strongest lines, respectively.

White or β-tin belongs to the tetragonal system; Mark and Polanyi [142] in 1923 assigned it to space group D_{4h}^{19} (I4/amd), a body-centered lattice with two atoms in the unit cell. Recent unit cell measurements have

TABLE 11. *Tin (white or β)*

hkl	1919 Bijl and Kolkmeijer Cu, 1.541 A		1923 Van Arkel Cu, 1.541 A		1934 Willot and Evans Cu, 1.541 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A		---- British Museum Cu, 1.5405 A		1953 Swanson and Tatge Cu, 1.5405 A, 26° C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*		*A*		*A*	
200	----	----	----	----	2.914	s	2.92	100	2.96	100	2.915	100
101	2.74	m	2.83	m	2.792	s	2.80	80	2.82	80	2.793	90
220	----	----	----	----	2.062	w	2.05	32	2.08	60	2.062	34
211	1.987	vs	2.03	vs	2.015	s	2.01	80	2.02	70	2.017	74
----	----	----	----	----	----	----	----	----	1.98	40	----	----
301	----	----	1.65	w	1.659	m	1.65	24	1.60	20	1.659	17
112	1.465	s	1.50	s	1.483	m	1.483	24	1.495	60	1.484	23
400	----	----	1.44	w	1.457	w	1.453	20	1.446	60	1.458	13
321					1.442	m					1.442	20
----	----	----	----	----	----	----	----	----	1.343	20	----	----
420	1.315	vw	1.29	m	1.304	w	1.301	16	1.312	40	1.304	15
411					1.292	w			1.296	20	1.292	15
312	1.192	vs	1.20	vs	1.205	m	1.202	20	1.214	60	1.205	20
501	1.081	m	1.09	m	1.096	w	1.094	11	1.102	40	1.0950	13
103	----	----	1.041	----	1.041	w	1.042	8	1.046	40	1.0434	3
332											1.0401	5
440	1.033	s	1.030	s	1.027	w	1.024	6	1.031	20	1.0309	2
521											1.0252	5
213	0.975	s	0.982	----	0.982	w	0.982	3	----	----	0.9824	5
600			.968	----							.9718	2
303	----	----	----	----	----	----	----	----	----	----	.9310	3
512	0.926	vs	0.928	----	0.930	m	0.929	6	----	----	.9286	13
620	----	----	----	----	----	----	----	----	----	----	.9219	5
611	----	----	0.919	----	----	----	----	----	----	----	.9178	5
323	0.881	s	.886	----	0.887	w	0.887	2	----	----	.8868	4
541	----	----	.874	----	.875	w	----	----	----	----	.8755	2
413	----	----	.847	----	.848	w	0.849	3	----	----	.8485	4
532											.8466	10
631	----	----	.841	----	.839	w	----	----	----	----	.8386	4
640	0.807	m	.805	----	----	----	0.807	2	----	----	.8086	6
701											.8058	3
004	----	----	.796	----	----	----	----	----	----	----	----	----
104	----	----	.789	----	----	----	----	----	----	----	----	----
503	0.783	m	----	----	----	----	----	----	----	----	----	----
433												
114												

been made by several workers, whose results are compared in the following table after conversion to angstroms at 26°C. In making the temperature corrections coefficients of expansion obtained from Kosolapov and Trapeznikov [131] of 46.4×10^{-6} perpendicular to the c axis and of 22.4×10^{-6} parallel with it were used.

Unit cell in angstroms at 26°C

		a	c
1932	Stenzel and Weertz [212]	5.8326	3.1821
1935	Jette and Foote [119]	5.83126	3.1814
1936	Kosolapov and Trapeznikov [131]	5.8311	3.1810
1938	Ievinš, Straumanis, and Karlsons [114]	5.83146	3.18129
1953	Swanson and Tatge	5.831	3.182

The density of tin based on the NBS lattice constant is 7.286 at 26°C.

2.11. Tellurium (Hexagonal)

Of the eight patterns in table 12, six are recorded on ASTM cards (see table 1), one, by Bose and Ray [21], was found in the literature, and one was prepared at the NBS. The sample used for the NBS pattern was prepared in the laboratories of Johnson, Matthey and Co., Ltd., London, and was numbered 3824. Their spectrographic analysis showed Si, Fe, Mg, and Al present as faint traces. After being finely ground the sample was annealed in a vacuum furnace at approximately 400°C for 15 minutes.

For purposes of comparison, the spacings of the patterns in table 12 were converted to angstrom units except for those by Olshausen and by Bose and Ray, whose Bragg angle data enabled the derivation of interplanar spacings directly in angstrom units, and those of Bradley and Slattery for which a correction factor could not be determined. The patterns by Harcourt, by Hanawalt, Rinn, and Frevel, and by the Institute of Physics at Cardiff, Wales, were presumed to be in kX units, and were converted accordingly. The Olshausen pattern includes a spacing of 3.58 A, incompatible with the tellurium structure and parameters, and another such spacing, of 5.8 A, is included in the Hanawalt, Rinn, and Frevel pattern.

With the exception of the Slattery pattern of 1924, all patterns accompanied by numerical relative intensity values are in agreement with the NBS pattern as to the three strongest lines: 101, 102, and 110, in decreasing order.

The tellurium lattice is hexagonal close-packed. The space group was determined in 1924 [25] as enantiomorphic D_3^4 or D_3^6 ($C3_12$ or $C3_22$). There are three atoms in the unit cell. The only precision determination of the lattice constants found in the literature is by Straumanis [215], whose measurements, corrected for temperature and converted from kX to angstrom units are compared with the NBS values in the table below. For the temperature correction the coefficient of expansion given in the same paper was used; 27.51×10^{-6} perpendicular to the c axis, and -1.70×10^{-6} parallel to it.

Unit cell in angstroms at 25°C

		a	c
1940	Straumanis [215]	4.45653	5.92682
1953	Swanson and Tatge	4.4570	5.9290

The density calculated from the NBS lattice constants is 6.2311 at 25°C.

TABLE 12. *Tellurium (hexagonal)*

hkl	1924 Bradley Mo, 0.7093 A		1925 Slattery Mo, 0.7093 A		1925 Olshausen Cu, 1.5405 A		1927 Harcourt Cu, 1.5405 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A		1941 Bose and Ray Cu, 1.5405 A		---- Institute Physics, Wales Cu, 1.5405 A		1953 Swanson and Tatge Cu, 1.5405 A, 26°C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	(a)		(a)		A		A		A		A		A		A	
---	------	----	-------	---	------	----	-------	---	5.8	19	------	-----	--------	----	------	----
100	3.845	84	3.83	20	3.81	w	3.86	50	3.87	14	3.67	w	3.80	40	3.86	20
---	------	----	-------	---	3.58	m	-------	---	--------	-----	------	-----	--------	---	------	----
101	3.220	5	3.22	100	3.224	s	3.23	100	3.25	100	3.05	vs	3.20	100	3.230	100
102	2.344	11	2.34	50	2.350	m	2.33	80	2.34	48	2.86	vvw	2.33	80	2.351	37
110	2.219	16	2.22	40	2.215	m	2.22	70	2.22	32	2.12	s	2.21	80	2.228	31
111	2.078	63	2.08	20	2.019	vw	2.07	50	2.08	14	------	-----	2.06	60	2.087	11
003	1.968	63	1.969	20	1.965	w	1.97	50	1.96	14	1.99	w	1.96	60	1.980	8
200	------	----	-------	---	------	----	-------	---	--------	-----	------	-----	--------	----	1.930	4
201	1.830	27	1.834	40	1.836	m	1.82	60	1.83	28	1.87	vvw	1.82	80	1.835	20
112	1.765	79	1.777	20	------	----	1.77	30	1.77	10	1.78	vvw	1.77	20	1.781	7
103	------	----	-------	---	------	----	-------	---	--------	-----	------	-----	--------	----	1.758	2
202	1.614	52	1.614	25	1.619	m	1.61	60	1.61	20	1.55	vvw	1.61	60	1.616	12
113	1.464	32	1.469	30	1.471	m	1.47	50	1.473	28	------	-----	1.47	60	1.479	13
210					1.448	w	1.448	30					1.45	40	1.459	8
211	1.410	50	1.412	20	1.409	w	1.413	50	1.421	13	1.41	vvw	1.41	60	1.417	8
104	1.375	50	1.377	20	1.377	w	1.378	50	1.383	16	------	-----	1.38	60	1.383	7
203																
212	1.308	68	1.307	10	1.305	m	1.303	30	1.312	8	------	-----	1.30	40	1.309	6
300	1.287	68	-------	---	------	----	-------	---	--------	-----	------	-----	--------	----	1.287	1
301	1.255	74	1.267	3	------	----	1.254	20	1.260	5	------	-----	1.25	20	1.257	4
114	------	----	-------	---	------	----	1.232	20	--------	-----	------	-----	--------	----	1.234	1
302	------	----	-------	---	------	----	-------	---	--------	-----	------	-----	--------	----	1.1802	3
204	1.172	21	1.171	30	1.171	m	1.172	70	1.177	14	------	-----	1.17	60	1.1740	8
213																
105	1.131	84	1.130	8	1.129	vw	1.127	20	1.121	5	------	-----	--------	----	1.1334	3
221	1.092	95	-------	---	1.096	vw	-------	---	--------	-----	------	-----	1.09	10	1.0951	2
303	------	----	-------	---	------	----	-------	---	--------	-----	------	-----	--------	----	1.0784	1
310	1.075	100	-------	---	------	----	-------	---	--------	-----	------	-----	--------	----	1.0705	1
311	------	----	-------	---	1.049	w	1.050	20	1.047	5	------	-----	1.05	20	1.0535	3
115	------	----	-------	---	------	----	-------	---	--------	-----	------	-----	--------	----	1.0432	2
222	1.038	42	-------	---	1.038	w	1.039	10	--------	-----	------	-----	1.04	20	1.0399	3
214	------	----	-------	---	------	----	-------	---	--------	-----	------	-----	--------	----	1.0104	2
205	------	----	-------	---	1.009	w	1.007	10	1.007	5	------	-----	1.00	20	1.0071	3
312																
006	------	----	-------	---	------	----	-------	---	--------	-----	------	-----	--------	----	0.9889	1
304	------	----	-------	---	------	----	-------	---	--------	-----	------	-----	--------	----	.9714	2
223	------	----	-------	---	0.966	vd	-------	---	0.970	2	------	-----	--------	----	.9650	1
313	------	----	-------	---	.944	w	-------	---	--------	-----	------	-----	--------	----	.9413	1
215	------	----	-------	---	.921	w	-------	---	--------	-----	------	-----	--------	----	.9201	2
116	------	----	-------	---	.905	w	0.900	10	--------	-----	------	-----	--------	----	.9032	2
224	------	----	-------	---	.889	w	-------	---	--------	-----	------	-----	--------	----	.8909	1
320															.8858	1
206	------	----	-------	---	------	----	-------	---	--------	-----	------	-----	--------	----	.8760	1
321	------	----	-------	---	------	----	-------	---	--------	-----	------	-----	--------	----	.8719	1
305	------	----	-------	---	0.870	m	0.866	10	0.868	2	------	-----	0.868	10	.8675	4
314																
403																
322	------	----	-------	---	.851	----	-------	---	--------	-----	------	-----	--------	----	.8485	1
411	------	----	-------	---	.838	----	-------	---	--------	-----	------	-----	--------	----	.8339	2
107	------	----	-------	---	------	----	-------	---	--------	-----	------	-----	--------	----	.8270	1
216	------	----	-------	---	------	----	-------	---	--------	-----	------	-----	--------	----	.8180	2
225	------	----	-------	---	------	----	-------	---	--------	-----	------	-----	--------	----	.8119	1
412	------	----	-------	---	------	----	-------	---	--------	-----	------	-----	--------	----	.8102	2
404	------	----	-------	---	------	----	-------	---	--------	-----	------	-----	--------	----	.8082	3
323																
315	------	----	-------	---	------	----	-------	---	--------	-----	------	-----	--------	----	.7945	2
117	------	----	-------	---	------	----	-------	---	--------	-----	------	-----	--------	----	.7917	1

[a] Unit not known.

2.12. Tungsten (Cubic)

Two tungsten patterns from the ASTM file (see table 1) and five additional patterns from the literature, of which three comprise interplanar spacings only, are compared in table 13 with a pattern prepared at the NBS. The patterns from the literature are by Becker [12], Debye [62], Neuburger [160], Sidhu [207], and Zeidenfeld [261]. The NBS pattern was made from a sample prepared and contributed by the Westinghouse Electric Corporation, who provided the following chemical analysis (in

TABLE 13. *Tungsten (cubic)*

hkl	1917 Debye Pt L, 1.3103 A			1925 Davey Mo, 0.7093 A			1926 Becker Cu, 1.5405 A		1931 Zeidenfeld Cu, 1.5405 A	
	d	*I*	*a*	*d*	*I*	*a*	*d*	*a*	*d*	*a*
	A		*A*	[a]		[a]	*A*	*A*	[a]	[a]
110	2.16	s	3.06	2.23	100	3.15	2.227	3.15	2.22	3.14
200	1.55	m	3.11	1.579	63	3.158	1.575	3.15	1.58	3.16
211	1.27	s	3.13	1.289	75	3.157	1.284	3.15	1.29	3.16
220	1.10	m	3.14	1.116	63	3.157	1.115	3.154	1.12	3.17
310	0.992	s	3.138	0.997	75	3.153	1.000	3.163	1.008	3.188
222	.907	m-w	3.141	.912	33	3.159	0.910	3.152	0.918	3.180
321	.840	s	3.142	.842	63	3.150	.842	3.149	----------	----------
400	.789	w	3.157	.788	25	3.152	.788	3.150	----------	----------
411	.745	s	3.158	.744	50	3.157	----------	----------	----------	----------
420	.708	s	3.165	.706	50	3.157	----------	----------	----------	----------
332	.673	s	3.156	----------	-------	----------	----------	----------	----------	----------
431	----------	-------	----------	----------	-------	----------	----------	----------	----------	----------
Average unit cell for last five lines			3.156	----------	-------	3.155	----------	3.154	----------	[b] 3.184

hkl	1934 Neuburger Fe K, 1.9340 1.9321 20°C		1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A			1948 Sidhu Cu, 1.5405 A			1953 Swanson and Tatge Cu, 1.5405 A, 26°C		
	d	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A	*A*	*A*		*A*	*A*		*A*	*A*		*A*
110	2.24	3.16	2.23	100	3.16	2.23	vs	3.16	2.238	100	3.165
200	1.58	3.16	1.58	29	3.17	1.58	w	3.16	1.582	15	3.164
211	1.291	3.162	1.292	71	3.165	1.29	m	3.16	1.292	23	3.165
220	1.119	3.166	1.119	17	3.165	1.12	w	3.17	1.1188	8	3.1644
310	1.001	3.165	1.002	29	3.168	1.00	w	3.17	1.0009	11	3.1648
222	----------	----------	0.915	6	3.169	0.914	vw	3.166	0.9137	4	3.1651
321	----------	----------	.848	34	3.171	.849	s	3.176	.8459	18	3.1651
400	----------	----------	-------	-------	-------	.829	vw	3.316	.7912	2	3.1648
411	----------	----------	.746	11	3.167	-------	------	-------	----------	-----	----------
420	----------	----------	.708	6	3.168	-------	------	-------	----------	-----	----------
332	----------	----------	.675	6	3.167	-------	------	-------	----------	-----	----------
431	----------	----------	.623	6	3.178	-------	------	-------	----------	-----	----------
Average unit cell for last five lines		[c] 3.164	-------	-------	3.170	-------	------	[d] 3.171	----------	-----	3.1648

[a] Unit not known. [b] Average for last two lines. [c] Average for last three lines. [d] Average for two lines preceding last line.

percent) by A. Pettel, Jr.: SiO_2, 0.04; K, 0.05; Mo, 0.01; Al_2O_3, 0.01; Fe, 0.01. This was verified by spectrographic analysis at the Bureau.

For table 13, data given in Bragg angles were used directly to derive interplanar spacings in angstroms for the patterns of Debye, Becker, Neuburger, and Sidhu. Davey's pattern was left in its original form, since the radiation wavelength was not given. Zeidenfeld gave a radiation wavelength of too few significant figures to show whether his data are in kX units or angstroms. The spacings of Hanawalt, Rinn, and Frevel were converted from kX units to angstroms.

Only three sets of intensity measurements are given with numerical values. Those of Hanawalt, Rinn, and Frevel, and of Swanson and Tatge show the same three strongest or index lines: 110, 211, and 321. Sidhu's estimated intensities agree with them.

The tungsten lattice is body-centered cubic with two atoms in the unit cell. Tungsten has the space group O_h^9 (Im3m) [160]. The lattice parameters derived by several investigators are compared in the table following. They were converted to angstrom units at 25°C. The coefficient of expansion of 4.3×10^{-6} of Michel [152] was used.

Unit cell at 25°C in angstroms

1932	Owen and Iball [173]	3.1657
1934	Neuburger [160]	3.1654
1935	Jette and Foote [119]	3.1648
1936	Cohen [51]	3.16473
1936	Straumanis and Ievinš [216]	3.1651
1941	Lu and Chang [141]	3.1650
1953	Swanson and Tatge	3.1648

The density determined from the NBS lattice constant is 19.265 at 25°C.

A less common form of tungsten, likewise stable at room temperature but with a simple cubic lattice, is represented by a third tungsten card in the ASTM file (old file number II-2579, new file number 2-1138, index lines 2.25, 2.06, 1.34). This form, of different structure, is not to be confused with the form discussed here.

2.13. Tantalum (Cubic)

The three patterns given in the ASTM file (see table 1) are supplemented by three additional patterns found in the literature, by Becker and Ebert [13], McLennon and Monkman [148], and Horn and Ziegler [96]. One of the ASTM patterns (Quill [189]) is recorded as made with molybdenum radiation although copper radiation was actually employed. These patterns are compared with an NBS pattern in table 14.

The sample of tantalum used for the NBS pattern was procured from Johnson, Matthey & Co., Ltd, London. The material contained dissolved gases which caused broadening of diffraction peaks, and TaH, which contributed extra lines. After annealing at 1,500°C in vacuum for 30 minutes in a tantalum boat the sample gave very sharp lines including only traces of the hydride. The spectrographic analysis furnished with the sample indicated faint traces of Nb, Al, Si, Fe, and Mn.

The interplanar spacings of table 14 are all given in angstrom units. The Becker, and the Ebert and Quill patterns were originally recorded as a series of Bragg angles, from which the interplanar spacings in angstroms were derived directly for the table. Hull's pattern was calculated by him with the use of a wavelength of 0.712, on the basis of which his spacings were converted to angstrom units. The McLennon and Monkman, and the Hanawalt, Rinn, and Frevel interplanar spacings were converted from kX units to angstroms. The Horn and Ziegler data are published presumably in angstroms.

The Horn and Ziegler measurements as well as those of Hull and Quill suffer from focusing and absorption effects. The Hanawalt, Rinn, and Frevel data agree with those of the NBS in designating the three strongest lines as the 110, 211, and 200, in decreasing strength.

The tantalum lattice is body-centered cubic; the space group is O_h^9 (Im3m) [104]. There are two atoms in the unit cell. Two measurements of the lattice constant are compared in the table below with that of the NBS.

TABLE 14. *Tantalum (cubic)*

hkl	1921 Hull Mo, 0.7093 A			1925 Becker and Ebert Cu, 1.5405 A		1929 McLennon and Monkman Cu, 1.5405 A		1932 Quill Cu, 1.5405 A		
	d	*I*	*a*	*d*	*a*	*d*	*a*	*d*	*I*	*a*
	A		*A*	*A*	*A*	*A*	*A*	*A*		*A*
110	2.306	67	3.274	2.30	3.25	2.330	3.296	2.340	vs	3.309
200	1.630	20	3.270	1.64	3.28	1.648	3.297	1.650	s	3.300
211	1.330	100	3.269	1.33	3.26	1.346	3.297	1.348	vvs	3.302
220	1.153	27	3.290	1.154	3.264	1.165	3.296	1.168	s	3.304
310	1.029	20	3.266	1.032	3.263	1.041	3.293	1.044	vs	3.301
222	0.942	13	3.278	0.941	3.260	0.952	3.298	0.9537	s	3.3037
321	.869	53	3.260	.871	3.259	.881	3.296	.8821	vvs	3.3005
400	.815	3	3.270	.814	3.256	----------	----------	.8257	s	3.3028
411	.770	20	3.278	----------	----------	----------	----------	----------	----------	----------
420	.729	3	3.273	----------	----------	----------	----------	----------	----------	----------
332	.694	3	3.269	----------	----------	----------	----------	----------	----------	----------
422	.664	3	3.268	----------	----------	----------	----------	----------	----------	----------
510	.641	7	3.275	----------	----------	----------	----------	----------	----------	----------
Average unit cell for last five lines			3.273	----------	3.260	----------	3.296	----------	----------	[a] 3.3023

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A			1947 Horn and Ziegler Cu, 1.5405 A			1953 Swanson and Tatge Cu, 1.5405 A, 26°C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*
110	2.33	100	3.30	2.328	100	3.292	2.338	100	3.306
200	1.65	20	3.30	1.653	30	3.306	1.653	21	3.306
211	1.349	30	3.304	1.348	90	3.302	1.350	38	3.306
220	1.169	5	3.302	1.168	40	3.304	1.1687	13	3.3056
310	1.044	5	3.302	1.046	60	3.308	1.0453	19	3.3055
222	----------	----------	----------	0.9554	30	3.3096	0.9543	7	3.3058
321	0.883	5	3.303	.8846	90	3.3099	.8835	29	3.3058
400	----------	----------	----------	.8271	20	3.3084	.8265	8	3.3060
411	----------	----------	----------	----------	----------	----------	----------	----------	----------
420	----------	----------	----------	----------	----------	----------	----------	----------	----------
332	----------	----------	----------	----------	----------	----------	----------	----------	----------
422	----------	----------	----------	----------	----------	----------	----------	----------	----------
510	----------	----------	----------	----------	----------	----------	----------	----------	----------
Average unit cell for last five lines			[b] 3.3028	----------	----------	[a] 3.3093	----------	----------	3.3057

[a] Average for three lines only.
[b] Average for four lines only.

The data were converted to angstroms at 25°C; the coefficient of expansion of 6.6×10^{-6} [94] was used.

Unit cell in angstroms at 25°C

1932	Owen and Iball [173]	3.3183
1936	Neuburger [161]	3.3027
1953	Swanson and Tatge	3.3058

The density as calculated from the NBS lattice constant is 16.626 at 25°C.

2.14. Platinum (Cubic)

Three patterns for platinum are given in the X-ray diffraction pattern files of the ASTM (see table 1). Four additional patterns were obtained from the literature; these were made by Barth and Lunde [7], Jaeger and Zanstra [116], Rusterholz [199], and by Uspenski and Konobejewski [227]. The sample used to obtain a pattern at the NBS was prepared by R. Gilchrist of the Chemistry Division of the Bureau. The NBS Spectroscopic Laboratory estimated the purity at >99.99 percent.

All the interplanar spacings of the eight patterns of table 15 are given in angstrom units except those of Davey, for which a conversion constant could not be determined. The spacings of Hull were converted to angstroms on the basis of the wavelength $\lambda = 0.712$ given for molybdenum $K\alpha$ radiation; the remainder were calculated directly in angstroms from the Bragg angle data given.

It may be observed from table 15 that several of the patterns omit the weak 400 line. The three earliest patterns, by Hull, by Uspenski and Konobejewski, and by Davey, made with molybdenum radiation, include 511, 531, and 600 lines beyond the range of patterns made with copper radiation. The pattern of Hanawalt, Rinn, and Frevel agrees with that of the NBS upon 111 and 200 as the two strongest lines, but shows 220 and 311 as equal in strength whereas the NBS pattern shows 311 as plainly stronger. This is evidently due to the difference in the radiation used, for upon recalculation of the Hanawalt, Rinn, and Frevel intensity values derived with molybdenum radiation to a copper radiation base ([1] page 108 of index covering original set of cards, or card number vii of introduction to 1950 file), the 311 is plainly the stronger in this pattern also. The earlier intensity measurements vary widely, suffering from the defects common to uncorrected film values.

The platinum lattice is face-centered cubic [106], O_h^5 (Fm3m), with four atoms in the unit cell. Of the many unit cell determinations found in the literature, two are accompanied by the temperature at which they were measured. These values were converted to 25°C by means of the coefficient of expansion 8.3×10^{-6}, an average of two published values [66, 178]. After conversion from kX to angstrom units, comparison with the NBS data gives:

Unit cell at 25°C, angstroms

1933	Owen and Yates [178]	3.9240
1937	Moellier [155]	3.9226
1953	Swanson and Tatge	3.9231

The density based on the NBS lattice constant is 21.472 at 25°C.

TABLE 15. *Platinum (cubic)*

hkl	1921 Hull Mo, 0.7093 A			1923 Uspenski and Konobejewski Rh, 0.6133 A		1925 Davey Mo, 0.7093 A			1925 Barth and Lunde Cu, 1.5405 A		
	d	*I*	*a*	*d*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*	*A*	(a)		(a)	*A*		*A*
111	2.256	67	3.908	2.29	3.97	2.27	100	3.93	2.252	100	3.901
200	1.950	27	3.900	1.96	3.92	1.956	86	3.912	1.951	63	3.902
220	1.382	67	3.909	1.37	3.87	1.385	86	3.917	1.379	63	3.900
311	1.178	100	3.907	1.17	3.88	1.179	100	3.910	1.175	100	3.897
222	1.133	13	3.925	1.11	3.85	1.130	57	3.914	1.126	25	3.901
400	0.979	7	3.916	----	----	0.978	29	3.912	----	----	----
331	.899	34	3.919	0.883	3.849	.897	71	3.910	0.896	13	3.906
420	.875	34	3.913	----	----	.875	71	3.913	----	----	----
422	.797	27	3.904	----	----	.798	57	3.909	----	----	----
511	.755	13	3.923	0.739	3.840	.753	43	3.913	----	----	----
440	----	----	----	----	----	----	----	----	----	----	----
531	0.660	13	3.905	----	----	----	----	----	----	----	----
600	.655	7	3.930	----	----	----	----	----	----	----	----
Average unit cell for last five lines			3.915	----	[b] 3.845	----	----	3.911	----	----	3.901

hkl	1931 Jaeger and Zanstra Fe, 1.9360 A			1931 Rusterholz Cu, 1.5405 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A			1953 Swanson and Tatge Cu, 1.5405 A, 26°C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*	*A*		*A*
111	2.228	60	3.859	2.274	47	3.939	2.25	100	3.90	2.265	100	3.9229
200	1.931	63	3.862	1.969	27	3.938	1.95	30	3.90	1.9616	53	3.9232
220	1.368	90	3.869	1.393	26	3.940	1.385	16	3.917	1.3873	31	3.9239
311	1.170	100	3.880	1.188	63	3.940	1.180	16	3.914	1.1826	33	3.9222
222	1.122	70	3.887	1.137	21	3.939	1.130	3	3.914	1.1325	12	3.9230
400	----	----	----	----	----	----	----	----	----	0.9808	6	3.9232
331	----	----	----	0.904	91	3.939	0.899	3	3.919	.9000	22	3.9229
420	----	----	----	.881	100	3.939	.876	2	3.918	.8773	20	3.9230
422	----	----	----	----	----	----	----	----	----	.8008	29	3.9232
511	----	----	----	----	----	----	----	----	----	----	----	----
440	----	----	----	----	----	----	----	----	----	----	----	----
531	----	----	----	----	----	----	----	----	----	----	----	----
600	----	----	----	----	----	----	----	----	----	----	----	----
Average unit cell for last five lines			3.871	----	----	3.939	----	----	3.916	----	----	3.9231

[a] Unit not known.

[b] Average for two lines only.

2.15. Gold (Cubic)

Three patterns for gold are included in the X-ray diffraction pattern file of the ASTM (see table 1). These are compared in table 16 with a pattern prepared at the NBS. The sample used for the NBS pattern was purified by R. Gilchrist of the Chemistry Division of the Bureau. Spectrographic analysis showed faint traces of silicon and calcium (about 0.001 percent each), and possibly a faint trace of silver; thus the sample is about 99.997 percent gold.

In table 16 all interplanar spacings are given in angstrom units. The spacings of the Davey, the Hanawalt, Rinn, and Frevel, and the Harcourt patterns were converted from kX units. Jung presented his data in Bragg angle values from which interplanar spacings were computed directly in angstroms for the table. The intensity measurements of Hanawalt, Rinn, and Frevel, of Harcourt, and of Swanson and Tatge agree as to the three strongest or index lines: 111, 200, and 311.

The gold lattice is face-centered cubic [232]; the space group is O_h^5 ($Fm3m$). There are four atoms per unit cell. Four measurements of the unit cell edge at specified temperatures were found in the literature. These values were corrected to 25°C by the use of the coefficient of expansion of 15.2×10^{-6} [66], and converted from kX to angstrom units. They compare with the NBS determination, after all are corrected for units and temperature, as follows:

Unit cell at 25°C, angstroms

1930	Sachs and Weerts [200]	4.0785
1933	Owen and Yates [178]	4.0786
1935	Jette and Foote [119]	4.0786
1938	Esser, Eilander, and Bungardt [66]	4.078
1953	Swanson and Tatge	4.0786

The density determined from the NBS lattice constant is 19.302 at 25°C.

TABLE 16. *Gold (cubic)*

hkl	1925 Davey Mo, 0.7093 A			1926 Davey Mo, 0.7093 A			1926 Jung Cu, 1.5405 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A			1942 Harcourt Cu, 1.5405 A			1953 Swanson and Tatge Cu, 1.5405 A, 26°C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*	*A*		*A*	*A*		*A*	*A*		*A*
111	2.35	100	4.07	2.35	100	4.08	2.349	s	4.069	2.35	100	4.07	2.36	100	4.09	2.355	100	4.079
200	2.03	75	4.06	2.03	75	4.07	2.038	ms	4.076	2.03	53	4.06	2.04	67	4.08	2.039	52	4.078
220	1.439	75	4.070	1.440	75	4.072	1.436	s	4.062	1.442	33	4.078	1.44	44	4.07	1.442	32	4.078
311	1.227	88	4.071	1.228	88	4.074	1.229	s	4.076	1.229	40	4.077	1.23	56	4.08	1.230	36	4.079
222	1.175	62	4.071	1.175	62	4.071	1.179	w	4.084	1.175	9	4.071	1.177	12	4.078	1.1774	12	4.0786
400	1.018	38	4.072	1.018	38	4.072	-----	--	-----	1.021	3	4.084	1.019	3	4.076	1.0196	6	4.0784
331	0.935	75	4.075	0.935	75	4.075	0.935	s	4.073	0.937	9	4.084	0.935	22	4.075	0.9358	23	4.0790
420	.911	75	4.073	.911	50	4.073	.913	s	4.083	.912	7	4.078	.912	22	4.078	.9120	22	4.0786
422	.832	50	4.074	.832	50	4.074	-----	--	-----	.834	4	4.084	.832	33	4.074	.8325	23	4.0784
511	-----	---	-----	.784	---	4.077	-----	--	-----	.786	4	4.082	.786	33	4.082	------	---	------
Average unit cell for last five lines			4.073	-----	---	4.074	-----	--	4.076	-----	---	4.082	-----	---	4.077	------	---	4.0786

2.16. Lead (Cubic)

Lead is represented by six patterns in the ASTM X-ray diffraction pattern file (see table 1). An additional pattern to those of the ASTM cards, by Solomon and Jones [16], 1931, was found in the literature. They are compared in table 17 with a pattern prepared at the NBS.

The sample of lead used for the NBS diffraction pattern was obtained from the American Smelting and Refining Company. Spectrographic analysis at the NBS showed faint traces of bismuth and magnesium; the purity of the sample is believed greater than 99.999 percent. It was annealed for one hour at 180°C in petrolatum.

The interplanar spacings of the Levi and the Solomon and Jones patterns were calculated for table 17 directly in angstrom units from the published Bragg angle data. The remaining published patterns were converted from kX units to angstroms. The interplanar spacings for the 1925 pattern of Davey were selected for the ASTM card from two sets of values published in adjacent columns. These two sets were averaged to obtain the pattern published by Davey in German in 1926. Two cards in the ASTM file have patterns credited to Harcourt; the interplanar spacings of these are identical and are given only once in table 17.

The intensity measurements of the Levi pattern were published as visual estimates, which were given numerical designations for the ASTM cards. The intensity measurements of the two Davey patterns are identical, as published; the strongest line has a value of 6, the others proportionately lower. These were converted to a base 100 for the strongest line in transferring the data to the ASTM cards. However, the converted figures were given to two places for the 1925 pattern, and rounded off to one place for the 1926 pattern, with the result shown in table 17. The intensity values for the Solomon and Jones pattern, which is not included in the ASTM file, are given in the table as they were published. The intensity measurements of both Harcourt patterns are given; column I_1 refers to the set published in 1942, I_2 to the set found only in the ASTM file.

Lead has a face-centered cubic lattice [232]. It belongs to the space group O_h^5 ($Fm3m$), and has four atoms to the unit cell. The length of the unit cell edge has been determined, with great accuracy, by many investigators. The following lattice constants, of fairly recent date, are converted to angstroms for comparison at a standard temperature. As published they are supposedly all in kX units. The temperature correction was made by means of Owen and Yates' [178] value of 29.1×10^{-6} for the coefficient of expansion at 20°C.

Unit cell in angstroms at 25°C

1932	Owen and Iball [173]	4.9505
1933	Owen and Yates [178]	4.9506
1933	Obinata and Schmid [167]	4.9496
1934	Ölander [169]	4.9492
1941	Stokes and Wilson [214]	4.9503
1941	Fricke [76]	4.950
1941	Lu and Chang [141]	4.9500
1946	Klug [126]	4.9508
1953	Swanson and Tatge	4.9505

The density of lead based on the NBS determination of the unit cell is 11.341 at 25°C.

TABLE 17. *Lead (cubic)*

hkl	1925 Davey Mo, 0.7093 A			1925 Levi Cu, 1.5405 A				1926 Davey Mo, 0.7093 A			1931 Solomon and Jones Cu, 1.5405 A		
	d	*I*	*a*	*d*	*I*[a]	*I*[b]	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*			*A*	*A*		*A*	*A*		*A*
111	2.82	100	4.88	2.80	s	80	4.84	2.83	100	4.90	2.840	m	4.919
200	2.44	83	4.88	2.43	s	80	4.86	2.44	80	4.88	2.461	m	4.922
220	1.735	83	4.907	1.731	ms	70	4.896	1.739	80	1.919	1.742	s	4.927
311	1.483	100	4.919	1.481	vs	100	4.912	1.483	100	4.919	1.486	s	4.929
222	1.418	33	4.912	1.421	ms	70	4.922	1.418	30	4.912	1.423	m	4.929
400	1.232	67	4.928	1.234	mw	50	4.936	1.232	70	4.928	1.229	w	4.916
331	1.130	67	4.926	1.133	s	80	4.939	1.130	70	4.926	1.130	m	4.926
420	1.101	50	4.924	1.105	s	80	4.942	1.102	50	4.928	1.102	m	4.928
422	1.007	50	4.933	1.008	ms	70	4.938	1.007	50	4.933	1.005	m	4.923
511	0.949	33	4.931	0.951	ms	70	4.942	0.950	30	4.936	0.948	m	4.926
440	.873	33	4.938	.875	m	60	4.950	.873	30	4.938	.870	w	4.921
531	.835	17	4.940	.837	vs	100	4.952	.835	20	4.940	-------	-------	-------
620	.823	17	4.938	.825	s	80	4.950	.823	20	4.938	-------	-------	-------
533	-------	-------	-------	.783	s	80	4.952	.781	20	4.939	-------	-------	-------
622	-------	-------	-------	-------	----	-----	-------	-------	-------	-------	-------	-------	-------
444	-------	-------	-------	-------	----	-----	-------	-------	-------	-------	-------	-------	-------
Average unit cell for last five lines			4.936	-------	----	-----	4.949	-------	-------	4.938	-------	-------	4.925

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A			1942 Harcourt Cu, 1.5405 A				1953 Swanson and Tatge Cu, 1.5405 A, 26°C		
	d	*I*	*a*	*d*	*I*[a]	*I*[b]	*a*	*d*	*I*	*a*
	A		*A*	*A*			*A*	*A*		*A*
111	2.86	100	4.95	2.85	90	100	4.94	2.855	100	4.945
200	2.47	50	4.94	2.450	70	90	4.900	2.475	50	4.950
220	1.74	50	4.92	1.744	80	90	4.933	1.750	31	4.950
311	1.493	50	4.952	1.488	100	100	4.935	1.493	32	4.950
222	1.431	17	4.957	1.426	40	80	4.940	1.429	9	4.950
400	---------	-------	---------	1.235	10	50	4.940	1.238	2	4.950
331	1.136	17	4.952	1.135	70	90	4.947	1.1359	10	4.9513
420	1.107	17	4.951	1.107	70	90	4.951	1.1069	7	4.9502
422	---------	-------	---------	1.011	70	90	4.953	1.0105	6	4.9504
511	---------	-------	---------	0.9534	70	90	4.9540	0.9526	5	4.9500
440	---------	-------	---------	.877	10	50	4.961	.8752	1	4.9508
531	---------	-------	---------	.8382	70	90	4.9589	.8369	9	4.9510
620	---------	-------	---------	.8267	60	90	4.9602	.8251	4	4.9507
533	---------	-------	---------	----------	---------	---------	----------	---------	--------	----------
622	---------	-------	---------	----------	---------	---------	----------	---------	--------	----------
444	---------	-------	---------	----------	---------	---------	----------	---------	--------	----------
Average unit cell for last five lines			4.953	----------	---------	---------	[c]4.9577	---------	--------	4.9506

[a] As first published.
[b] On ASTM card.
[c] Average for 511, 531, and 620 lines.

2.17. Beryllium Oxide, BeO (Hexagonal)

In addition to four patterns for beryllium oxide (bromellite) included in the ASTM file (see table 1), patterns by Zachariasen [258, 259] and by Claassen [47], found in the literature, are compared with an NBS pattern in table 18. Since the two Zachariasen patterns are very similar, only the first is reproduced in the table.

The sample of BeO used for the Bureau pattern was prepared by the Brush Beryllium Company. The material, No. 1743-1747, is of fluorescent grade, and was prepared at a furnace temperature of 1,150°C. Spectrographic analysis at the Bureau laboratory indicated about 0.03 percent Al, <0.01 percent each of Ca, Fe, Mg, and Si, and traces of Cu, Pb, and Sn.

For the McKeehan pattern the ASTM card carries spacings derived from the author's Bragg angle data, while for table 18, d was obtained directly from the author's log d values, and converted from kX to angstrom units. The Claassen interplanar spacings were calculated directly in angstrom units for table 18, from the Bragg angle data published. Since it is not clear from the ASTM card whether the pattern of the United Steel Companies, England, is in kX or angstroms, it was not altered. All others were converted to angstroms upon the assumption that they are published in kX units. Two lines, 114 and 212, not previously observed, show up in the NBS pattern. The 004 and 104 appearing in the two Zachariasen patterns and in the United Steel Companies pattern were observed only with difficulty in the NBS pattern. In the United Steel Companies pattern the line of interplanar spacing 0.993 is indexed as a compound reflection from 104 and 113 planes. As the presence of a 113 reflection is not

TABLE 18. *Beryllium oxide*, BeO *(hexagonal)*

hkl	1922 McKeehan Mo, 0.7093 A		1925 Zachariasen Cu, 1.5405 A		1925 Aminoff Fe, 1.9360 A		1926 Claassen Cu, 1.5405 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A		---- United Steel Co, 1.7902 A		1953 Swanson and Tatge Cu, 1.5405 A, 26°C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		A		A		A		A		(a)		A	
100	2.34	80	2.34	100	2.33	100	2.40	81	2.34	80	2.34	100	2.337	91
002	2.18	60	2.20	60	2.18	50	2.20	58	2.19	50	2.19	80	2.189	61
101	2.06	100	2.07	100	2.05	100	2.14	100	2.06	100	2.06	100	2.061	100
102	1.601	30	1.60	50	1.59	50	1.60	24	1.59	24	1.60	60	1.598	22
110	1.349	80	1.35	80	1.34	75	1.35	39	1.353	32	1.35	70	1.349	29
103	1.239	80	1.24	80	1.20	75	1.24	31	1.242	32	1.24	70	1.238	24
200	-------	-----	1.167	20	1.165	25	1.169	4	1.172	4	1.17	40	1.1682	4
112	1.148	60	1.149	70	1.144	75	1.151	31	1.152	20	1.15	60	1.1482	16
201	-------	-----	1.129	20-30	1.123	25	1.101	4	1.132	4	1.13	40	1.1287	5
004	-------	-----	1.119	0-10	-------	-----	-------	-----	-------	------	1.09	20	1.0958	<1
202	-------	-----	1.031	10-20	1.025	25	1.026	-----	1.034	3	1.03	40	1.0308	3
104	-------	-----	0.995	0-10	-------	-----	0.988	4	-------	------	0.993	20	0.9920	<1
203	0.910	20	.911	70	-------	-----	.918	-----	0.917	8	.914	70	.9118	10
210	.885	10	.881	40	-------	-----	.886	13	.882	2	-------	-----	.8832	4
211	.866	10	.864	50	-------	-----	.866	7	.872	2	-------	-----	.8657	5
114	-------	-----	-------	-----	-------	-----	-------	-----	-------	------	-------	-----	.8498	2
105	0.820	20	-------	-----	-------	-----	-------	-----	0.824	8	-------	-----	.8199	14
212	-------	-----	-------	-----	-------	-----	-------	-----	-------	------	-------	-----	.8179	8
---	0.780	10	-------	-----	-------	-----	-------	-----	0.782	3	-------	-----	----------	-------
---	-------	-----	-------	-----	-------	-----	-------	-----	.760	8	-------	-----	----------	-------
---	0.755	20	-------	-----	-------	-----	-------	-----	-------	------	-------	-----	----------	-------

[a] Unit not known.

compatible with the structure worked out by Zachariasen, the line is indexed only 104 in table 18.

The intensity values of the Claassen, the Hanawalt, Rinn, and Frevel, and the NBS patterns are closely comparable, with the 101, 100, and 002 lines appearing as the first, second, and third strongest, respectively.

Zachariasen [259] in 1926 recorded the space group determination of C_{6v}^4 (C6mc) for hexagonal beryllium oxide. There are two molecules in the hexagonal unit cell. Two lattice constants found in the literature compare with that determined from the NBS data as follows:

Unit cell, in angstroms

		a	c
1925	Aminoff [2]	2.69	4.37
1926	Zachariasen [259]	2.699	4.401
1953	Swanson and Tatge (26°C)	2.698	4.380

The density, based on the NBS lattice constant, is 3.008 at 26°C. The material used was too finely divided for determination of the refractive index.

2.18. Magnesium Oxide, MgO (Cubic)

Four patterns for magnesium oxide (periclase) listed in table 19 appear in the ASTM file (see table 1). The pattern of Hansen and Brownmiller, card number 2-1395, is erroneously labelled $Mg(OH)_2$ in the 1950 file, although correctly ascribed to MgO in the old file. However, it appeared in the old index as $Mg(OH)_2$ and was repeated thus in the new. Two of the patterns of table 19 are combined on one ASTM card; the United Steel Companies, England, interplanar spacings parallel the intensity measurements of Wyckoff and Armstrong. Five patterns were obtained from the literature; they are by Büssem, Schusterius, and Ungewiss [43], Frevel [74], Gerlach [79], Menzer [151], and Passerini [182].

The NBS pattern was made from a sample contributed by the Radio Corporation of America as a pure compound prepared for use in phosphor research [135]. The MgO was crystallized in a graphite crucible which was maintained at 1,800°C for three hours. An NBS spectrographic analysis shows calcium and silicon between 0.01 and 0.1 percent; aluminum, boron, chromium, iron, and nickel, between 0.001 and 0.01 percent.

Some of the patterns of table 19 were corrected to angstroms from kX units. Those of Gerlach, of Passerini, of Wyckoff and Armstrong, of Büssem, Schusterius, and Ungewiss, and of Menzer were calculated directly in angstroms from the published Bragg angle data. Two errors occur in the Hansen and Brownmiller pattern; the spacing for $hkl = 200$ is published as 2.01, doubtless in error for 2.10, as the ASTM card notes; and the spacing 1.243 is superfluous to the pattern. The Hanawalt, Rinn, and Frevel, and the Frevel patterns show two $K\alpha_2$ lines which are not listed in table 19, where only $K\alpha_1$ lines are tabulated. In the table the complete pattern of Wyckoff and Armstrong is given, of which only the intensity values for the first eight of 16 lines appear on the ASTM card. The two strongest lines are given in almost every case as 200 and 220, but the third strongest is not universally agreed upon. Three patterns (including the two of most recent date) and the NBS pattern agree that 420 is third strongest.

TABLE 19. *Magnesium oxide, MgO (cubic)*

hkl	1921 Gerlach and Pauli Cu, 1.5405 A			1928 Hansen and Brownmiller Mo, 0.7093 A				1929 Passerini Co, 1.7889 A			1929 Wyckoff and Armstrong Mo, 0.7093 A			1937 Büssem, Schusterius, and Ungewiss Cu, 1.5405 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A		
	d	*I*	*a*	*d*	I^a	I^b	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*			*A*	*A*		*A*	*A*		*A*	*A*		*A*	*A*		*A*
111	-----	--	-----	2.44	w	40	4.23	-----	--	------	2.43	20	4.21	2.44	9	4.23	2.44	6	4.23
200	2.11	s	4.22	2.01	m	60	4.02	2.07	vs	4.14	2.10	100	4.20	2.102	100	4.204	2.10	100	4.20
220	1.492	s	4.220	1.486	vs	100	4.203	1.476	vs	4.175	1.484	58	4.197	1.489	48	4.211	1.488	75	4.209
311	1.278	mw	4.239	1.269	vs	100	4.209	-----	--	------	1.267	6	4.202	1.270	8	4.212	1.269	6	4.209
---	-----	--	-----	1.246	m	60	-----	-----	--	------	-----	---	-----	------	---	-----	-----	---	-----
222	1.219	s	4.223	1.214	s	80	4.205	1.212	s	4.198	1.210	15	4.192	1.215	16	4.209	1.215	15	4.209
400	1.047	s	4.188	1.051	m	60	4.204	1.056	ms	4.224	1.049	6	4.196	1.052	9	4.208	1.052	4	4.208
331	-----	--	-----	0.965	w	40	4.206	-----	--	------	0.964	4	4.202	0.9657	5	4.209	0.965	1	4.206
420	0.948	s	4.240	.941	s	80	4.208	0.944	vs	4.222	.938	14	4.195	.9409	25	4.208	.942	10	4.213
422	.861	s	4.218	.858	s	80	4.203	-----	--	------	.857	8	4.198	.8603	23	4.215	.862	4	4.223
511	.813	ms	4.224	.808	w	40	4.198	-----	--	------	.808	1	4.198	.8113	7	4.216	-----	---	-----
440	-----	--	-----	.742	m	60	4.197	-----	--	------	.742	2	4.197	------	---	-----	-----	---	-----
531	-----	--	-----	-----	--	---	-----	-----	--	------	.709	1	4.194	------	---	-----	-----	---	-----
600	-----	--	-----	0.699	m	60	4.194	-----	--	------	.699	3	4.194	------	---	-----	-----	---	-----
620	-----	--	-----	.663	m	60	4.193	-----	--	------	.663	2	4.193	------	---	-----	-----	---	-----
533	-----	--	-----	-----	--	---	-----	-----	--	------	.640	< 1	4.196	------	---	-----	-----	---	-----
622	-----	--	-----	0.632	m	60	4.192	-----	--	------	.632	1	4.192	------	---	-----	-----	---	-----
640	-----	--	-----	.581	m	60	4.189	-----	--	------	-----	---	-----	------	---	-----	-----	---	-----
642	-----	--	-----	.560	m	60	4.191	-----	--	------	-----	---	-----	------	---	-----	-----	---	-----
Average unit cell for last five lines---			4.219	-----	--	---	4.192	-----	--	[c]4.205	-----	---	4.194	------	---	4.211	-----	---	4.212

hkl	---- United Steel ----------			1944 Frevel Mo, 0.7093 A			1946 Clark Co, 1.7889 A				1947 Menzer Cu, 1.5405 A			1953 Swanson and Tatge Cu, 1.5405 A, 26°C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	I^a	I^b	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*			*A*	*A*		*A*	*A*		*A*
111	2.430	20	4.209	2.430	8	4.209	2.42	vvw	10	4.19	2.430	8	4.209	2.431	10	4.210
200	2.104	100	4.208	2.107	100	4.214	2.10	vs	100	4.20	2.104	100	4.208	2.106	100	4.212
220	1.488	60	4.209	1.490	50	4.214	1.484	s	80	4.197	1.485	51	4.200	1.489	52	4.211
311	1.269	10	4.209	1.271	4	4.215	1.265	vw	20	4.195	1.265	7	4.195	1.270	4	4.212
---	------	-----	-------	------	-----	-----	------	-----	-----	-----	------	-----	-----	------	----	-----
222	1.214	10	4.205	1.218	12	4.219	1.210	m	60	4.192	1.211	14	4.195	1.216	12	4.212
400	1.0521	10	4.2084	1.055	4	4.220	1.050	vw	20	4.200	1.051	6	4.204	1.0533	5	4.213
331	0.9654	5	4.2081	0.9681	1	4.220	0.9641	vvw	10	4.202	0.9647	3	4.205	0.9665	2	4.213
420	.9410	10	4.2083	.9424	-----	4.215	.9394	ms	70	4.201	.9403	23	4.205	.9419	17	4.212
422	------	-----	-------	.8600	-----	4.213	------	-----	-----	-----	.8588	18	4.207	.8600	15	4.213
511	------	-----	-------	------	-----	-----	------	-----	-----	-----	.8101	5	4.209	.8109	3	4.214
440	------	-----	-------	------	-----	-----	------	-----	-----	-----	------	-----	-----	------	----	-----
531	------	-----	-------	------	-----	-----	------	-----	-----	-----	------	-----	-----	------	----	-----
600	------	-----	-------	------	-----	-----	------	-----	-----	-----	------	-----	-----	------	----	-----
620	------	-----	-------	------	-----	-----	------	-----	-----	-----	------	-----	-----	------	----	-----
533																
622	------	-----	-------	------	-----	-----	------	-----	-----	-----	------	-----	-----	------	----	-----
640	------	-----	-------	------	-----	-----	------	-----	-----	-----	------	-----	-----	------	----	-----
642	------	-----	-------	------	-----	-----	------	-----	-----	-----	------	-----	-----	------	----	-----
Average unit cell for last five lines-------			[d]4.2083	------	-----	4.217	------	-----	-----	4.198	------	-----	4.206	------	----	4.213

[a] Published intensity values. [b] Intensity values as they appear on ASTM card. [c] Average of four lines only. [d] Average of three lines only.

Magnesium oxide has a face-centered cubic lattice [101], space group O_h^5 ($Fm3m$), and four molecules in the unit cell. Unit cell values are tabulated below for comparison. They are all given in angstrom units, the three published ones converted from kX units, at 25°C. The coefficient of expansion 14.45×10^{-6} [42] was used.

Unit cell in angstroms at 25°C

1935	Büssem, Bluth, and Grochtmann [42]	4.211
1936	Straumanis and Ievinš [216]	4.2115
1944	Frevel [74]	4.214
1953	Swanson and Tatge	4.213

The density calculated from the NBS lattice constant is 3.581 at 25°C. The NBS sample shows an index of refraction of $n = 1.732$.

2.19. Silicon Dioxide (low or α-cristobalite), SiO_2 (Tetragonal)

Seven ASTM patterns (see table 1) for α-cristobalite are represented by nine original patterns (some are combined on the cards) in table 20. These are compared with an additional pattern from the literature, by Jay [117], and one produced at the NBS. An eighth card (number 956 of the original set) is mistakenly referred to in the original ASTM index [1] as the α form. This card, which is not itself designated α or β, is represented in the new edition by a pattern labelled correctly "β-Cristobalite" (card number 1-0430).

The NBS sample was obtained from the Radio Corporation of America Laboratories, Princeton, N. J. It was purified in connection with the RCA Phosphor project [135], and had been heated for two hours at 1,420°C; a trace of tridymite showed up in the X-ray diagram.

All the patterns of the table were changed from kX to angstrom units except that of Thilo, which was calculated directly in angstroms from Bragg angle data given. With regard to intensity measurements, the three strongest lines are the same as those of the NBS pattern—101, 200, 102—although some of the patterns show 111 equal in intensity to 102, except for the British Museum pattern, in which 102 appears stronger than 200. The intensity values of most of the patterns were published as visual estimates, but are given in the table in the numerical conversion shown on the ASTM cards; the measured intensities of Barth and of Hanawalt, Rinn, and Frevel are converted to a base of 100 for the strongest line as on the ASTM cards.

Early workers considered alpha cristobalite cubic or nearly so. Nieuwenkamp [163] established the tetragonal structure of the mineral, showing that it has the space group D_4^4 ($P4_12_1$), and the enantiomorphous form D_4^8 ($P4_32_1$). There are four molecules in the unit cell. The following table compares lattice constants from his data with those later determined by Jay [117] and those based on the NBS pattern, all in angstrom units.

Unit cell, in angstroms

		a	c
1935	Nieuwenkamp [163]	4.97	6.93
1944	Jay [117] (22°C)	4.9715	6.9193
1953	Swanson and Tatge (27°C)	4.973	6.95

The density was calculated from the NBS unit cell as 2.32 at 27°C. The indices of refraction were determined as $\epsilon = 1.484$ and $\omega = 1.486$.

TABLE 20. *Silicon dioxide (low or α-cristobalite), SiO_2 (tetragonal)*

hkl	1928 McVey and Thompson Mo, 0.7093 A		1932 Barth Mo, 0.7093 A		---- United Steel ----		1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A		---- Allis-Chalmers Fe, 1.9360 A		1939 Thilo Fe, 1.9360 A	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*		*A*		*A*	
----------	-------	------	-------	-------	-------	-------	-------	-------	6.23	10	-------	-------
----------	-------	------	-------	-------	-------	-------	-------	-------	5.34	10	-------	-------
----------	-------	------	5.0	10	-------	-------	-------	-------	-------	-------	4.70	40
----------	-------	------	-------	-------	-------	-------	-------	-------	-------	-------	4.52	80
----------	-------	------	-------	-------	-------	-------	-------	-------	4.30	10	4.23	40
101	4.04	vs	4.06	100	4.04	100	4.05	100	4.05	100	4.07	100
----------	-------	------	-------	-------	-------	-------	-------	-------	-------	-------	3.59	20
----------	-------	------	-------	-------	-------	-------	-------	-------	-------	-------	3.51	20
----------	-------	------	-------	-------	-------	-------	-------	-------	-------	-------	3.237	10
111	3.13	m	3.15	40	3.14	60	3.14	16	3.15	60	3.149	80
----------	-------	------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------
102	2.84	m	2.86	50	2.840	70	2.86	20	2.85	60	2.858	80
----------	-------	------	-------	-------	-------	-------	-------	-------	-------	-------	2.745	40
200	2.47	s	2.49	90	2.486	80	2.49	32	2.47	80	2.493	100
112	-------	------	-------	-------	2.466	40	-------	-------	-------	-------	-------	-------
201	-------	------	2.35	5	-------	-------	-------	-------	-------	-------	2.348	20
210	-------	------	2.20	5	-------	-------	-------	-------	2.21	10	2.228	10
211	2.11	f	2.12	10	2.116	50	2.11	5	2.12	40	2.121	40
----------	-------	------	-------	-------	-------	-------	-------	-------	-------	-------	2.065	20
202	2.01	f	2.029	20	2.039	50	2.02	5	2.02	40	2.019	40
113	1.93	m	1.937	30	1.928	60	1.93	12	1.92	60	1.933	80
212	1.87	m	1.877	30	1.871	60	1.87	12	1.86	60	1.871	80
----------	-------	------	-------	-------	-------	-------	-------	-------	-------	-------	1.785	20
220	-------	------	1.751	5	1.758	20	-------	-------	-------	-------	1.740	10
004	-------	------	-------	-------	1.729	40	-------	-------	1.72	10	1.729	20
203	1.69	f	1.698	20	1.690	60	1.69	5	1.68	40	1.692	80
104	-------	------	-------	-------	1.633	20	-------	-------	1.64	10	1.647	20
301	1.60	f	1.615	40	1.611	60	1.61	12	1.60	30	1.612	80
213	-------	------	-------	-------	1.600	40	-------	-------	-------	-------	-------	-------
330	} -------	------	1.577	5	1.570	40	1.57	1	1.57	10	1.569	20
222												
311	1.53	m	1.530	20	1.533	60	1.53	4	1.53	20	1.535	100
302	1.49	f	1.452	20	1.4946	60	1.500	6	1.49	20	1.504	80
----------	-------	------	-------	-------	-------	-------	-------	-------	1.46	10	1.468	10
312	1.43	m	1.433	30	1.4313	50	1.436	5	1.43	20	1.431	80
204	-------	------	-------	-------	1.4197	40	-------	-------	1.42	20	1.397	40
223	1.40	f	1.400	10	1.3979	40	1.403	2	1.39	10	1.364	80
214	-------	------	1.368	10	1.3655	50	1.373	3	1.36	20	1.350	20
321	-------	------	-------	-------	1.3521	20	-------	-------	1.35	20	1.332	80
303	1.34	f	-------	-------	1.3458	20	-------	-------	-------	-------	-------	-------
105	-------	------	1.341	10	1.3332	50	1.342	3	1.33	20	1.297	80
313	-------	------	1.304	10	1.2989	50	1.303	3	1.29	20	1.280	80
322	1.28	f	1.281	10	1.2810	50	1.282	3	1.28	20	-------	-------
----------	-------	------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------
224	-------	------	1.231	10	1.2329	20	1.237	1	1.23	10	-------	-------
401	-------	------	-------	-------	1.2234	40	-------	-------	1.22	10	-------	-------
410	-------	------	1.207	10	1.2058	20	1.205	1	1.20	40	-------	-------
323	-------	------	1.182	20	1.1836	40	1.183	2	1.18	20	-------	-------
215	1.17	f	-------	-------	1.1749	40	-------	-------	1.17	10	-------	-------
314	-------	------	-------	-------	1.1633	20	-------	-------	1.16	10	-------	-------
331	-------	------	-------	-------	1.1552	20	-------	-------	1.15	10	-------	-------
420	1.10	f	1.117	30	1.1098	40	-------	-------	1.11	10	-------	-------
421	-------	------	-------	-------	1.0976	50	1.097	3	1.09	50	-------	-------
116	-------	------	-------	-------	1.0957	50	-------	-------	-------	-------	-------	-------
225	-------	------	-------	-------	1.0874	10	-------	-------	-------	-------	-------	-------
324	-------	------	-------	-------	1.0782	20	-------	-------	1.08	10	-------	-------
413	-------	------	-------	-------	1.0686	10	-------	-------	1.07	10	-------	-------
422	-------	------	1.061	5	-------	-------	-------	-------	-------	-------	-------	-------
333	-------	------	1.044	5	-------	-------	-------	-------	1.05	10	-------	-------
315	-------	------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------
423	-------	------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------
500	-------	------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------
414	0.989	f	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------
----------	-------	------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------
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(Continued)

TABLE 20. *Silicon dioxide (low or α-cristobalite), SiO_2 (tetragonal)*—Con.

hkl	1941 Baumann Cu, 1.5405 A		1944 Jay Co, 1.7889 A, 22° C		---- British Museum Cu, 1.5405 A		1946 Clark Mo, 0.7093 A		1953 Swanson and Tatge Cu, 1.5405 A, 27°C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*		*A*	
101	4.05	100	4.04	vs	4.00	100	4.03	100	4.04	100
111	3.14	60	3.19	m	3.20	80	3.13	60	3.138	12
					2.95	40				
102	2.86	80	2.841	ms	2.83	40	2.84	70	2.845	14
200	2.48	100	2.486	s	2.51	60	2.47	80	2.489	18
112			2.466	w			2.45	10	2.468	6
201									2.342	<1
210										
211			2.116	wm	2.11	40	2.10	20	2.121	4
202			2.019	wm	2.02	40	2.01	20	2.024	3
113	1.93	40	1.928	m	1.93	40	1.915	40	1.932	4
212	1.87	40	1.8703	m	1.86	40	1.859	40	1.874	4
220			1.7580	vw	1.78	20	1.749	10	1.756	1
004			1.7300	w			1.724	10	1.736	1
203			1.6909	wm	1.69	40	1.684	20	1.692	3
104			1.6338	vw			1.626	10	1.642	1
301	1.61	40	1.6117	m			1.603	40	1.612	5
213			1.6007	w	1.60	60	1.593	10	1.604	2
310			1.572	w	1.54	40	1.564	10	1.574	1
222			1.567							
311	1.53	20	1.533	m			1.423	20	1.535	2
302			1.4945	m	1.49	60	1.486	20	1.495	3
312			1.4314	wm	1.43	40	1.425	20	1.432	2
204			1.4197	w			1.413	10	1.423	1
223			1.3979	w			1.392	10	1.401	1
214	1.37	20	1.3655	wm	1.37	40	1.359	10	1.368	1
321			1.3521	vw			1.345	10	1.353	1
303			1.3458	vw	1.34	40	1.338	10	1.345	1
105			1.3332	wm			1.328	20	1.336	1
313			1.2989	wm	1.31	40	1.294	20	1.301	2
322			1.2810	wm	1.28	40	1.275	20	1.282	2
					1.27	40				
224			1.2329	vw	1.24	40	1.226	10	1.235	<1
401			1.2234	w			1.217	10	1.224	<1
410	1.203	20	1.2058	wm			1.199	10	1.207	1
323			1.1836	w	1.18	40	1.177	10	1.1842	2
215			1.1749	w			1.169	10	1.1762	1
314			1.1633	vw			1.158	10	1.1659	1
331			1.1552	vw					1.1556	<1
420			1.1098	w			1.103	10	1.1112	1
421	1.095	40	1.0976	m	1.10	60	1.091	20	1.0989	3
116			1.0957							
225			1.0892	vvw						
324			1.0782	wm						
413			1.0686	vw						
422			1.0611	w						
333			1.0448	wm						
315			1.0388	w						
423			1.0013	wm						
500			0.9942	wm						
414			.9892	m						
	0.969	40								
	.836	40								

2.20. Silicon Dioxide (High or β-Cristobalite), SiO_2 (Cubic)

Although an NBS pattern was not made for high or β-cristobalite, the published patterns were reviewed in order to select the most suitable one for retention in the ASTM file. Three cards in the latest edition of the ASTM file of X-ray diffraction patterns record two patterns for high or β-cristobalite; the two patterns are combined on the third card (see table 1). Two references are given to Wyckoff [254, 255]—one on the simple card, one on the combined card; they were published the same year, the one in German a translation of the one in English, and the patterns are identical. Two literature references to Barth and Posnjak [8], one on a simple, one on a combined card, are identical, although the combined card erroneously lists the junior author first. The older edition of the ASTM file labelled the Wyckoff pattern simply "cristobalite" and listed it in the accompanying index as "α-cristobalite." In the 1950 edition the card is correctly labelled and indexed. The combined pattern apparently represents an average of the two published patterns, with the addition of lines given by one or the other.

TABLE 21. *Silicon dioxide (high or β-cristobalite), SiO_2 (cubic)*

hkl	1925 Wyckoff Mo, 0.7093 A, 290 °C			1932 Barth and Posnjak Mo, 0.7093 A, 500°C			---- Combined[a] Mo, 0.7093 A		
	d	I	a	d	I	a	d	I	a
	A		A	A		A	A		A
111	4.137	100	7.165	4.15	100	7.19	4.14	100	7.17
211	-----	--	-----	2.92	5	7.15	2.92	5	7.15
220	2.524	45	7.139	2.53	80	7.16	2.53	90	7.16
311	-----	--	-----	2.17	10	7.20	2.17	10	7.20
222	2.070	13	7.171	2.07	30	7.17	2.07	30	7.17
320	-----	--	-----	1.99	5	7.18	1.99	5	7.18
400	1.779	tr.	7.116	1.793	5	7.172	1.79	10	7.16
411	-----	--	-----	1.688	5	7.162	1.69	5	7.17
331	1.637	35	7.136	1.639	60	7.144	1.639	70	7.144
422	1.455	30	7.128	1.469	50	7.148	1.457	60	7.138
511	1.372	10	7.129	1.379	20	7.165	1.376	20	7.150
440	1.261	15	7.133	1.265	30	7.156	1.263	30	7.145
531	1.203	28	7.117	1.209	30	7.153	1.206	50	7.135
620	1.125	10	7.115	1.130	20	7.147	1.127	20	7.128
533	1.085	tr.	7.115	1.089	5	7.141	1.087	10	7.128
444	1.031	tr.	7.143	1.029	5	7.129	1.030	10	7.136
711	0.993	5	7.091	1.000	10	7.141	0.997	10	7.120
642	.949	7	7.102	0.956	10	7.154	.953	20	7.131
731	.924	4	7.097	.929	10	7.136	.927	10	7.120
822	.838	3	7.110	-----	--	-----	.838	5	7.110
Average unit cell for last five lines---			7.109	-----	--	7.140	-----	--	7.123

[a] Wyckoff pattern combined with that of Barth and Posnjak on ASTM card II-588.

Some of the data on the ASTM cards is confusing. The new card for the Wyckoff pattern states that the material is stable "over 275°" but does not indicate that the pattern was prepared at 290°C. The Barth and Posnjak card does not mention temperature. The combined card gives the Barth and Posnjak temperature correctly as 500°, the Wyckoff temperature erroneously as 430°, and states cryptically on the card "SiO_2 at about 450°," which is evidently meant for a rough average of the preceding values. An error occurs in the listing of intensity measurements on the Wyckoff card; the third line should read "13" rather than "7" (on the old card "0.125" rather than "0.07").

For table 21 the spacings of the ASTM patterns were reduced to angstrom units on the basis of the wavelength used for molybdenum radiation. Since, in the temperature range indicated, the coefficient of expansion is of the order 8×10^{-6} [42], the difference in the two sets of spacings due to temperature is very little. The intensities of the three patterns correlate well; in each case the three strongest lines are represented by 111, 220, and 331.

The space group of β-cristobalite, which belongs to the cubic system, is T^4 ($P2_13$) [42]. There are eight molecules in the unit cell. Published unit cell measurements, converted to angstrom units at 500°C (using the coefficient of expansion noted above) compare as follows:

Unit cell in angstroms at 500°C

1929	Wyckoff [254]	7.127
1932	Barth and Posnjak [8]	7.16
1935	Büssem, Bluth, and Grochtmann [42]	7.1282

As noted in table 21, however, an average of the last five lines of the Barth and Posnjak pattern at 500°C yields 7.140 A for the lattice constant, which is closer to the value of other workers. Because of its greater completeness, as it shows several low angle lines not given in the earlier pattern, it is recommended that the Barth and Posnjak pattern be selected as the standard ASTM pattern.

2.21. Calcium Oxide, CaO (Cubic)

The file of X-ray diffraction patterns of the ASTM includes three cards for calcium oxide (see table 1). One of these is a composite of lines from three sources, of which one was previously unpublished. The four previously published patterns are compared in table 22 with two additional patterns found in the literature by Gerlach [77], and by Natta and Passerini [157], and a pattern prepared at the NBS.

The NBS sample was obtained as calcium carbonate from the J. T. Baker Chemical Co., No. 121647, and calcined in a platinum crucible at 925°C for 1 hour. The following chemical analysis (in percent) was provided by the chemical laboratory of the NBS: insoluble in HCl and NH_4OH ppt, 0.01; chloride, <0.005; sulfate, 0.037; alkalis (as SO_4), 0.011; barium, <0.1; heavy metals (Pb, etc.), 0.001; Fe, <0.003; MgO and alkalis, 0.21. The J. T. Baker Chemical Company specified the barium content as 0.005 percent and the iron as 0.001 percent. In preparing the pattern a petrolatum mount minimized hydration.

The interplanar spacings are given in angstroms in table 22. The Gerlach [77] pattern was calculated in angstroms from published Bragg angle data. The Harrington [89] and the Brownmiller and Bogue [40] spacings were converted to angstrom units in accordance with the wavelength given for the radiation

TABLE 22. *Calcium oxide, CaO (cubic)*

hkl	1922 Gerlach Cu, 1.5405 A			1927 Harrington Mo, 0.7093 A			1929 Natta and Passerini Cu, 1.5405 A			1930 Brownmiller and Bogue Mo, 0.7093 A		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		A	A		A	A		A	A		A
111	2.772	ms	4.801	2.77	70	4.80	2.626	w	4.548	2.754	m	4.770
200	2.398	s	4.796	2.40	100	4.80	2.372	ms	4.744	2.381	ss	4.762
220	1.689	s	4.777	1.698	100	4.803	1.683	s	4.760	1.688	s	4.774
311	1.438	mw	4.769	1.448	80	4.802	1.440	ms	4.776	1.439	m	4.773
222	1.379	mw	4.777	1.387	80	4.805	1.381	ms	4.784	1.380	m	4.780
400	1.193	w	4.772	1.200	60	4.800	1.193	mw	4.772	-------	------	--------
331	1.095	w	4.773	1.100	60	4.795	1.096	mw	4.777	-------	------	--------
420	1.082	s	4.839	1.073	80	4.799	1.073	s	4.799	1.071	m	4.790
422	0.9802	ms	4.802	0.978	70	4.791	0.980	s	4.801	0.976	m	4.781
511	.9133	ms	4.746	.922	50	4.791	.926	mw	4.812	-------	------	--------
440	.8454	m	4.782	.847	30	4.791	.847	m	4.791	-------	------	--------
531	.8110	s	4.798	.810	50	4.792	-------	------	-------	-------	------	--------
600	.8003	s	4.802	.798	40	4.788	-------	------	-------	-------	------	--------
620	--------	------	-------	.756	40	4.781	-------	------	-------	-------	------	--------
533	--------	------	-------	-------	-------	--------	-------	------	-------	-------	------	--------
622	--------	------	-------	0.722	40	4.789	-------	------	-------	-------	------	--------
444	--------	------	-------	.692	10	4.794	-------	------	-------	-------	------	--------
711	--------	------	-------	.671	30	4.792	-------	------	-------	-------	------	--------
640	--------	------	-------	.665	20	[a] 4.795	-------	------	-------	-------	------	--------
Average unit cell for last five lines			4.786	-------	-------	[b] 4.779	-------	------	4.796	-------	------	4.780

[a] Eleven additional lines omitted.

[b] Averaged from lines not shown.

(Continued)

TABLE 22. *Calcium oxide, CaO (cubic)*—Con.

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A			1946 Clark Co, 1.7869 A				1953 Swanson and Tatge Cu, 1.5405 A, 27°C		
	d	*I*	*a*	*d*	*I*[c]	*I*[d]	*a*	*d*	*I*	*a*
	A		*A*	*A*			*A*	*A*		*A*
111	2.77	40	4.80	2.77	vw	20	4.80	2.778	34	4.815
200	2.39	100	4.78	2.39	s	80	4.78	2.405	100	4.810
220	1.69	63	4.78	1.69	vs	100	4.78	1.701	45	4.811
311	1.448	20	4.802	1.443	w	40	4.786	1.451	10	4.812
222	1.385	20	4.798	1.381	w	40	4.784	1.390	5	4.815
400	1.202	10	4.808	1.197	vw	20	4.788	1.203	4	4.812
331	1.102	7	4.804	1.099	vw	20	4.790	1.1036	4	4.8105
420	1.073	27	4.799	1.072	m	60	4.794	1.0755	9	4.8098
422	0.981	13	4.806	0.9794	m	70	4.798	0.9819	9	4.8103
511	.924	3	4.810	.9240	vw	20	4.810	.9258	3	4.8106
440	.849	3	4.803	----------	--------	-------	---------	.8504	4	4.8106
531	.812	3	4.804	----------	--------	-------	---------	.8131	5	4.8104
600	.802	6	4.812	----------	--------	-------	---------	.8018	6	4.8108
620	.761	2	4.813	----------	--------	-------	---------	----------	-------	----------
533	.732	1	4.800	----------	--------	-------	---------	----------	-------	----------
622	.724	2	4.802	----------	--------	-------	---------	----------	-------	----------
444	---------	---------	---------	----------	--------	-------	---------	----------	-------	----------
711	0.672	1	4.799	----------	--------	-------	---------	----------	-------	----------
640	.667	1	4.810	----------	--------	-------	---------	----------	-------	----------
Average unit cell for last five lines			4.805	----------	--------	-------	4.796	----------	-------	4.8105

[c] Published. [d] ASTM card.

used. The remaining patterns were converted from kX units. The intensity measurements of Hanawalt, Rinn, and Frevel, and of the NBS show the three strongest lines as 200, 220, and 111 in the order given.

Calcium oxide has a face-centered cubic lattice, and the space group O_h^5 (Fm3m) [61]. There are four molecules in the unit cell. Several lattice constants are listed below for comparison.

Unit cell in angstroms

--------	United Steel, England----------	4.8082
1942	Huber and Wagener [97]----------	4.811
1953	Swanson and Tatge (27°C)----------	4.8105

The density calculated from the NBS lattice constant is 3.345 at 27°C. The index of refraction was not determined on the NBS sample; it is given as $n_D = 1.837$ by Winchell [250].

2.22. Titanium Dioxide (Rutile), TiO_2 (Tetragonal)

The three patterns of the ASTM diffraction pattern file (see table 1) are compared in table 23 with an earlier pattern found in the literature, Vegard [234], and with one prepared at the NBS. One of the ASTM patterns lists five references as sources, only three of which were published; of these only two (by Kerr, and by Weiser and Milligan) appear in table 23. The third, ascribed to Boldyrev [19] (who compiled it from a Russian published source [133]), was made from a natural mineral from the Ural mountains and, possibly because of impurities, is so unlike the other patterns in the table that it was not included.

Material for the NBS pattern was obtained from the National Lead Company, Sample No. MP 559. Spectrographic analysis at the NBS shows no impurity greater than 0.001 percent.

The sample, chiefly anatase, was heated for two hours at 1,000°C and cooled slowly to obtain the rutile phase.

The interplanar spacings of all patterns were converted from kX to angstrom units except those of the Vegard pattern, which were calculated in angstroms from the published Bragg angle data, and the pattern of the United Steel Companies, which is given, apparently, in angstroms. The three strongest lines are shown by the Vegard and the Hanawalt, Rinn, and Frevel patterns as 211, 110, and 101; the Kerr, the Weiser and Milligan, and the NBS patterns show them to be 110, 211, and 101.

Rutile, which belongs to the tetragonal system, has a space group determined as D_{4h}^{14} ($P4/mnm$) by Huggins [98]. Recent unit cell determinations, converted from kX to angstrom

TABLE 23. *Titanium dioxide (rutile)*, TiO_2

hkl	1926 Vegard Cu, 1.5405 A		1932 Kerr		1934 Weiser and Milligan		1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A		---- United Steel		1953 Swanson and Tatge Cu, 1.5405 A, 26°C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*		*A*		*A*	
110	3.292	50	3.28	100	3.25	100	3.25	80	3.25	85	3.245	100
101	2.510	30	2.51	50	2.48	90	2.49	60	2.49	70	2.489	41
200	2.327	5	2.32	5	2.29	10	2.29	4	2.30	50	2.297	7
111	2.212	20	2.269	10	2.18	40	2.19	30	2.19	60	2.188	22
210	2.046	10	2.179	30	2.04	20	2.05	12	2.05	50	2.054	9
211	1.708	100	1.703	100	1.688	100	1.69	100	1.69	100	1.687	50
220	1.649	40	1.643	30	1.620	30	1.62	30	1.62	70	1.624	16
002	1.499	10	1.503	20	1.481	20	1.487	20	1.48	60	1.480	8
310	1.472	10	1.473	20	1.450	20	1.451	20	1.45	60	1.453	6
301 112	1.377	70	1.368	60	1.353	80	1.357	30	1.36 1.35	85 70	1.360 1.347	16 7
311	-------	-------	-------	-------	-------	-------	-------	-------	1.30	20	1.305	1
202	-------	-------	1.262	5	1.242	10	1.247	4	1.24	30	1.243	3
212	-------	-------	-------	-------	-------	-------	-------	-------	1.20	20	1.200	1
321	1.184	10	1.181	10	1.169	10	1.172	8	1.17	60	1.1700	4
400	1.164	10	1.162	5	1.146	10	1.149	4	1.15	50	1.1485	4
410	1.107	25	-------	-------	-------	-------	-------	-------	1.11	20	1.1329	1
222	1.093	10	1.097	20	1.094	10	1.093	8	1.09	70	1.0933	4
330	-------	-------	-------	-------	-------	-------	-------	-------	1.08	60	1.0827	4
411	1.050	20	1.048	20	1.039	10	1.042	8	1.04	60	1.0424	5
312	1.038	5	-------	-------	-------	-------	-------	-------	1.04	60	1.0361	4
420	-------	-------	-------	-------	-------	-------	-------	-------	1.03	60	1.0273	3
421	-------	-------	-------	-------	-------	-------	-------	-------	0.970	30	-------	-------
322 103	0.976	10	0.975	5			0.966	4	.964	70	0.9642	2
402	.920	10	.912	5	-------	-------	-------	2	.907	70	.9071	3
510	.913	10	.902	5	-------	-------	0.905	2	.900	70	.9007	3
213	.897	40	-------	-------	-------	-------	.892	8	-------	-------	.8892	5
431 332	.884	50	0.882	5	-------	-------	.877	4	-------	-------	.8773 .8739	6 5
422 223	.851	10	.852	5	-------	-------	.845	2	-------	-------	.8437	5
303	.837	30	-------	-------	-------	-------	.834	4	-------	-------	.8290	5
521	.826	50	0.826	5	-------	-------	-------	-------	-------	-------	.8196	8
432	-------	-------	.779	3	-------	-------	-------	-------	-------	-------	-------	-------
-------	-------	-------	.748	3	-------	-------	-------	-------	-------	-------	-------	-------

units, are compared in the following table with those of the NBS.

Unit cell in angstroms

		a	c
1942	Schossberger [203]	4.598	2.960
1946	Frevel, Rinn, and Anderson [75]	4.59	2.96
----	United Steel	4.5928	2.9582
1953	Swanson and Tatge (26°C)	4.594	2.958

In accordance with the NBS lattice constant the density is 4.250 at 26°C. The indices of refraction are very high; Schröder [204] measured them at 25°C as $\epsilon_D = 2.8893$ and $\omega_D = 2.6124$.

2.23. Titanium Dioxide (Anatase), TiO_2 (Tetragonal)

The first of the four ASTM cards listed in table 1 has no X-ray data on it except a

TABLE 24. *Titanium dioxide (anatase)*, TiO_2

hkl	1926 Vegard Cu, 1.5405 A		1934 Weiser and Milligan Mo, 0.7093 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A		---- United Steel ----------		1953 Swanson and Tatge Cu, 1.5405 A, 26°-27°C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		*A*		*A*		*A*		*A*	
101	3.58	100	3.50	100	3.53	100	3.515	100	3.51	100
103	----	----	----	----	----	----	2.430	10	2.435	9
004	2.401	35	2.38	50	2.38	24	2.377	50	2.379	22
112	----	----	----	----	----	----	2.338	10	2.336	9
200	1.911	70	1.887	80	1.88	40	1.891	90	1.891	33
105	1.717	30	1.698	60	1.70	28	1.699	70	1.699	21
211	1.681	50	1.658	60	1.66	24	1.665	70	1.665	19
213	----	----	----	----	----	----	----	----	1.494	4
204	1.499	60	1.480	50	1.483	24	1.450	70	1.480	13
116	1.382	20	1.361	20	1.365	8	1.364	60	1.367	5
220	1.351	30	1.337	20	1.338	8	1.338	60	1.337	5
215	1.275	50	1.267	40	1.265	11	1.264	70	1.264	10
301	----	----	----	----	----	----	1.250	20	1.250	3
303	----	----	----	----	----	----	1.165	60	1.171	2
312	1.173	50	1.163	30	1.166	6	1.160	10	1.1609	3
118	----	----	----	----	----	----	1.056	10	1.0598	1
217	----	----	----	----	----	----	1.0509	50	1.0510	1
321	1.055	30	1.046	20	1.047	3	1.0428	50	1.0433	3
226	----	----	----	----	----	----	1.0176	50	1.0173	2
109	1.026	10	1.017	20	----	----	1.0063	20	1.0065	2
323	----	----	----	----	----	----	0.9959	10	0.9964	1
316	0.961	20	0.953	10	0.952	2	.9547	70	.9550	4
400	----	----	----	----	----	----	.9456	60	.9461	3
325	0.922	35	0.915	10	0.915	2	.9186	70	.9189	2
411	----	----	----	----	----	----	.9132	70	.9135	1
219	0.902	50	0.894	10	0.896	2	----	----	.8960	3
228	----	----	----	----	----	----	----	----	.8894	1
332	0.883	50	0.878	10	----	----	----	----	.8794	2
318	.852	40	.845	10	----	----	----	----	.8464	2
327	----	----	----	----	----	----	----	----	.8311	1
415	0.832	40	0.826	10	----	----	----	----	.8268	3
309	.814	20	.808	10	----	----	----	----	.8100	1
424	.800	50	.797	10	----	----	----	----	.7990	3
----	----	----	.742	10	----	----	----	----	----	----
----	----	----	.703	10	----	----	----	----	----	----
----	----	----	.669	10	----	----	----	----	----	----

highly inaccurate value for the axial ratio, determined by Vegard in 1916. The second card is a composite from which only the pattern of Weiser and Milligan appears in table 24, along with the patterns of the remaining two cards, a pattern by Vegard [234] from the literature, and a pattern made at the NBS.

The NBS pattern was prepared from material supplied by the Research Laboratory of the National Lead Company, South Amboy, N.J., Sample No. MP 559. Spectrographic analysis at the NBS showed no impurity greater than 0.001 percent.

The interplanar spacings of table 24 were all recalculated to angstroms from kX units except those of Vegard, which were calculated directly in angstroms from the Bragg angle data given. All patterns agree that 101 is the strongest line and 200 second strongest. Three or four almost equally intense lines, however, provide variation in the third strongest given in different patterns; this is listed as 004 in the NBS pattern. Two very weak rutile lines appearing in the NBS X-ray diagram are omitted from the pattern given in the table.

The space group of the tetragonal anatase form of titanium dioxide is D_{4h}^{19} (I4/amd) according to Huggins [98] and Vegard [233]. The unit cell contains four molecules. The lattice constants obtained from the NBS pattern are compared in the table below with those of other workers:

Unit cell, angstroms

		a	*c*
----	United Steel	3.783	9.509
1942	Schossberger [203]	3.784	9.505
1946	Frevel, Rinn, and Anderson [75]	3.76	9.45
1953	Swanson and Tatge (26°-27°C)	3.783	9.51

The density, calculated from the NBS lattice constant, is 3.899 at 26°-27°C. The indices of refraction could not be obtained from the NBS sample, which was too finely powdered.

2.24. Nickelous Oxide (Bunsenite), NiO (Cubic)

Three cards for nickelous oxide are included in the X-ray diffraction file of the ASTM (see table 1). One of them records no pattern but only a determination of the lattice constant (card number 3-1287). One of the patterns is a composite from four sources of which one is unpublished and not represented in table 25. The X-ray patterns of the two cards, from four previously published sources, are compared in the table with those of three additional workers, Clark, Asbury, and Wick [49], Bravo [34], and Passerini [182], that were obtained from the literature, and with a pattern prepared at the NBS. An electron diffraction pattern by Darbyshire [55] is also included, for comparison.

The sample from which the NBS pattern was made was obtained from Johnson, Matthey & Co., Ltd., and was numbered 3087. They estimated the purity at 99.99 percent. This was corroborated by spectroscopic analysis at the Bureau, which showed only faint traces of Mg, Si, and Ca.

The Levi and Tachinni, the Bravo, and the Ksanda spacings (table 25) were calculated in angstrom units from Bragg angle data. The spacings of the remaining patterns were assumed given in kX units, and were converted to angstroms. The lines 200, 111, and 220 are the first, second, and third strongest index lines for the NBS and Darbyshire patterns and would be chosen in this order in selecting index lines for the Hanawalt, Rinn, and Frevel pattern, although 111 and 220 have actually the same intensity. Converting the intensity values of the Hanawalt, Rinn, and Frevel pattern to their equivalents if copper rather than molybdenum radiation had been used, ([1] page 108 of index covering original set of cards or card no. vii of introduction to 1950 file), 111 becomes considerably stronger than 220.

The lattice of nickelous oxide is face-centered cubic [61]. It has a space group O_h^5 (Fm3m), with four molecules to the unit cell.

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In 1948 Rooksby [194] showed that at 18°C most of the diffraction lines are doublets or triplets, and interpreted the structural significance as a slight distortion of the generally accepted cubic lattice. He regards the lattice as rhombohedral, a=2.9518, $\alpha = 60°4.2'$ (for a face-centered cube referred to a primitive rhombohedral lattice $\alpha = 60°$).

TABLE 25. *Nickelous oxide, NiO (cubic)*

hkl	1925 Levi and Tacchini Cu, 1.5405 A			1925 Clark, Asbury, and Wick Mo, 0.7093 A		1926 Bravo Cu, 1.5405 A			1929 Passerini			1930 Hendricks, Jefferson and Shultz Fe and Cu		
	d	*I*	*a*	*d*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		A	A	A	A		A	A		A	A		A
111	2.34	s	4.05	2.401	4.159	2.37	s	4.11	2.344	ms	4.06	2.411	s	4.176
200	2.03	vs	4.06	2.083	4.166	2.06	vs	4.12	2.044	vs	4.09	2.087	vs	4.174
220	1.450	vs	4.101	1.480	4.186	1.470	vs	4.158	1.459	vs	4.13	1.477	vs	4.178
311	1.243	ms	4.123	1.263	4.189	1.255	m	4.162	1.248	vs	4.14	1.259	m	4.176
222	1.191	m	4.126	1.208	4.185	1.200	w	4.157	1.198	s	4.15	1.206	m	4.178
400	1.037	m	4.148	-------	-------	1.037	vw	4.148	1.040	ms	4.16	-------	--	-------
331	0.966	m	4.211	0.959	4.180	0.953	vw	4.154	0.957	s	4.17	-------	--	-------
420	.930	s	4.159	.933	4.173	.930	s	4.159	.932	vs	4.17	-------	--	-------
422	.852	s	4.174	-------	-------	.850	vs	4.164	-------	----	-------	-------	--	-------
511	.805	vs	4.183	-------	-------	.804	m	4.178	-------	----	-------	-------	--	-------
440	-------	----	-------	-------	-------	-------	---	-------	-------	----	-------	-------	--	-------
600	-------	----	-------	-------	-------	-------	---	-------	-------	----	-------	-------	--	-------
620	-------	----	-------	-------	-------	-------	---	-------	-------	----	-------	-------	--	-------
Average unit cell for last five lines			4.175	-------	4.183	-------	---	4.161	-------	----	4.16	-------	--	4.176

hkl	1931 Ksanda Mo, 0.7093 A			1931 Darbyshire Electron diffraction			1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A			1953 Swanson and Tatge Cu, 1.5405 A, 26°C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		A	A		A	A		A	A		A
111	2.413	80	4.179	2.39	90	4.14	2.40	60	4.16	2.410	91	4.174
200	2.092	100	4.184	2.04	100	4.08	2.08	100	4.16	2.088	100	4.176
220	1.478	90	4.180	1.45	60	4.10	1.477	60	4.178	1.476	57	4.175
311	1.260	70	4.179	1.22	20	4.05	1.260	24	4.179	1.259	16	4.176
222	1.206	60	4.178	1.18	20	4.09	1.205	12	4.174	1.206	13	4.178
400	1.044	40	4.179	1.00	10	4.00	1.044	2	4.176	1.0441	8	4.176
331	0.9591	30	4.181	--------	-------	------	0.959	4	4.180	0.9582	7	4.177
420	.9346	50	4.180	0.93	25	4.16	.935	6	4.181	.9338	21	4.176
422	.8529	20	4.178	.84	20	4.12	.854	3	4.184	.8527	15	4.177
511	.8041	10	4.178	.79	10	4.10	.804	2	4.178	.8040	7	4.179
440	--------	-----	-------	.72	5	4.07	-------	-------	-------	----------	-------	-------
600	--------	-----	-------	.69	5	4.14	-------	-------	-------	----------	-------	-------
620	--------	-----	-------	.67	5	4.24	-------	-------	-------	----------	-------	-------
Average unit cell for last five lines			4.179	--------	-------	4.13	-------	-------	4.180	----------	-------	4.177

The doubling of lines could not be detected on the NBS chart. The NBS unit cell determination is compared below with other published values:

Unit cell, in angstroms

1920	Davey and Hoffman [61]	4.20
1925	Clark, Asbury, and Wick [49]	4.17
1925	Brentano [35]	4.180
1926	Bravo [34]	4.152
1927	Brentano and Dawson [36]	4.1789
1930	Hendricks, Jefferson, and Shultz [25]	4.178
1931	Ksanda [134]	4.1798
1933	Cairns and Ott [46]	4.1768
1934	Preston [188]	4.11
1936	Smith [209]	4.19
1943	Shirai [206]	4.17
1953	Swanson and Tatge (26°C)	4.177

The density, calculated from the NBS value for the lattice constant, is 6.806 at 26°C. The index of refraction is very high; Ksanda in 1931 [134] gave n_{Li} =2.73.

2.25. Cupric Oxide (Tenorite), CuO (Monoclinic)

The ASTM file contains six cards for cupric oxide (see table 1). One of these (number 2-1263) contains only lattice constants and structure data. Of the cards containing patterns, one (number 2-1037) is a composite of data from four sources, only one of which is in the literature. Two others contain patterns by Tunell, Posnjak, and Ksanda, one from molybdenum radiation, the other copper, of which the lines were indexed on the basis of single crystal data. Those ASTM patterns appearing in the literature are compared in table 26 with two additional patterns, by Waldo [242], and by Billiet and Vandendriesshe [16], and with a pattern prepared at the NBS. The Harcourt and Waldo data of card number 2-1037 were doubtless communicated to the ASTM before publication elsewhere.

The sample used at the NBS was obtained from Johnson, Matthey & Co., Ltd, and was numbered 3257. Spectrographic analysis at the NBS showed only faint traces of iron and magnesium as impurities.

All the interplanar spacings of the patterns in table 26 were converted from kX to angstrom units except the first one, by Niggli, accompanied by a wavelength value of 1.541 for copper radiation. The indexing of the lines in table 26 follows that worked out by Tunell, Posnjak, and Ksanda in 1935, differing only where a line due to a group of superimposed reflections is resolved in the NBS pattern.

The three strongest or index lines are, in all except the first pattern, the combined $\bar{1}11$-002, 111-200, and $\bar{2}02$ lines. The NBS pattern records the three strongest lines as $\bar{1}11$, 111, and 002. The $\bar{1}11$ reflection cannot be separated entirely in the NBS powder pattern, from the 002, nor can the intensity of the 111 be measured without the influence of the 200. Integrated measurements showed the total intensity of the 002, $\bar{1}11$ doublet to be about 85 percent of the 111, 200 doublet; however, because 002 and $\bar{1}11$ reflections are closer to each other than are the 200 and 111, their reinforced intensities are greater when measured as peak height above background.[3]

In 1933 Tunell, Posnjak, and Ksanda [225] assigned tenorite to the monoclinic system, with the space group C_{2h}^6 (C2/c). There are four molecules to the unit cell. Converted from kX to angstrom units, the 1935 set of data from Tunell, Posnjak, and Ksanda compare thus with the NBS measurements:

Unit cell, in angstroms

		a	b	c	β
1935	Tunell, Posnjak, and Ksanda [226]	4.662	3.417	5.118	99°29′
1953	Swanson and Tatge (26°C)	4.684	3.425	5.129	99°28′

The density, based on the NBS lattice constant, is 6.51 at 26°C.

[3] Peak height intensities are considered preferable in the ASTM card file to integrated intensities because most of those using the file for routine analyses measure peak height or its equivalent.

TABLE 26. *Cupric oxide, CuO (monoclinic)*

hkl	1922 Niggli Cu, 1.5405 A		1929 Posnjak and Tunell Mo		1935 Waldo ----------		1935 Tunell, Posnjak, and Ksanda Mo, 0.7093 A		1935 Tunell, Posnjak, and Ksanda Cu, 1.5405 A		1938 Hanawalt, Binn, and Frevel Mo, 0.7093 A		1938 Billiet and Vandendriessche Cu, 1.5405 A		1942 Harcourt Cu, 1.5405 A		1953 Swanson and Tatge Cu, 1.5405 A, 26°C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		A		A		A		A		A		A		A		A	
110	2.76	vs	-----	-----	------	--	2.75	10	2.743	20	------	-----	2.75	20	-----	-----	2.751	12
002 $\bar{1}11$	2.52	vs	2.520	100	2.54	s	2.52	90	2.518	100	2.52	100	2.52	100	2.49	100	2.530 2.523	49 100
111 200	2.31	s	2.324	100	2.33	s	2.30	100	2.312	90	2.32	100	2.31	100	2.32	100	2.323 2.312	96 30
$\bar{1}12$	------	------	-----	-----	------	--	------	-----	1.958	8	------	-----	-------	-----	-----	-----	1.959	3
$\bar{2}02$	1.84	mw	1.868	60	1.869	m	1.859	60	1.856	60	1.85	20	1.861	60	1.87	25	1.866	25
112	1.71	m	-----	-----	------	--	------	-----	-------	-----	------	-----	-------	-----	-----	-----	1.778	2
020	1.68	m-s	1.715	20	1.713	w	1.705	30	1.707	20	1.70	8	1.706	20	1.71	6	1.714	8
021	------	------	-----	-----	------	--	1.619	< 3	-------	-----	------	-----	-------	-----	-----	-----	-------	-----
202	1.56	s-vs	1.583	30	1.581	vs	1.579	50	1.578	30	1.57	8	1.579	30	1.58	13	1.581	14
$\bar{1}13$	1.50	m-s	1.506	40	1.504	m	1.501	60	1.503	50	1.50	15	1.506	50	1.51	25	1.505	20
022	------	------	-----	-----	------	--	------	-----	1.414	10	------	-----	1.416	10	-----	-----	1.418	12
$\bar{3}11$ 310	1.40	w-m	1.410	60	1.413	m	1.408	70	1.404	30	1.408	20	1.404	30	1.41	13	1.410	15
220 113	1.36	m-s	1.379	50	1.373	m	1.373	70	1.373	50	1.370	20	1.376	50	1.378	25	1.375	19
311 $\bar{3}12$ 221	1.30	v-w	1.305	10	1.305	f	1.299	30	1.301	20	1.298	5	1.298	20	1.308	6	1.304	7
004 $\bar{2}22$	1.26	m-s	1.264	30	1.263	w	1.259	50	1.261	40	1.258	10	1.256	40	1.263	25	1.265 1.262	6 7
$\bar{2}04$ $\bar{1}14$	1.20	v-w	1.197	10	------	--	1.191	10	1.190	10	------	-----	1.190	10	-----	-----	1.1961	2
$\bar{3}13$ 222	1.16	m	1.169	20	1.157	f	1.159	20	1.165	20	1.161	5	1.165	20	-----	-----	1.1697 1.1620	5 3
312 400	-----	------	-----	-----					1.151	10			1.150	10	-----	-----	1.1585 1.1556	2 4
$\bar{4}02$ $\bar{2}23$	1.12	vw	1.124	10	------	--	1.118	5	1.118	10	------	-----	1.119	10	-----	-----	1.1233	2
$\bar{1}31$	1.09	m	1.094	10	------	--	1.087	10	1.088	20	1.088	3	1.085	10	1.092	13	1.0916	6
131	------	------	1.075	10	------	--	1.071	5	1.072	5	------	-----	-------	-----	-----	-----	1.0737	2
204	1.04	m-s	-----	-----	------	--	1.040	5	1.038	10	------	-----	-------	-----	-----	-----	1.0394	< 1
024 223	-----	------	-----	-----	------	--	1.019	5	1.016	20	------	-----	-------	-----	-----	-----	1.0178	3
313	1.01	w-m	1.014	10	------	--	1.006	5	1.005	20	1.009	3	-------	-----	-----	-----	1.0074	4
402 $\bar{2}24$ $\bar{1}15$	0.981	m	0.981	20	------	--	0.979	20	0.990 .978	5 30	0.980	3	0.977	20	0.980	13	0.9921 .9808	< 1 4
$\bar{4}21$	------	------	-----	-----	------	--	------	-----	.968	3	------	-----	-------	-----	-----	-----	-------	-----
420	0.958	m	0.957	10	------	--	0.958	5	.956	10	------	-----	0.957	10	-----	-----	0.9576	3
$\bar{1}33$ $\bar{4}22$	.940	w-m	.939	10	------	--	.941	10	.947 .938	< 3 20	------	-----	-------	-----	-----	-----	.9435 .9390	< 1 4
$\bar{4}04$	------	------	-----	-----	------	--	------	-----	.931	8	------	-----	-------	-----	-----	-----	.9332	2
115 $\bar{3}31$	-----	------	-----	-----	------	--	0.923	5	.918	20	------	-----	0.921	20	0.920	6	.9209	2
133	------	------	-----	-----	------	--	.907	5	.908	8	------	-----	-------	-----	-----	-----	.9100	2
$\bar{5}11$	------	------	-----	-----	------	--			.902	8	------	-----	-------	-----	-----	-----	.9039	1
$\bar{3}15$ 331 224	0.890	------	-----	-----	------	--	.887	20	.887	40	0.887	3	0.885	30	0.889	6	.8871	6
---	.860	m-s	-----	-----	------	--	------	-----	.857	30	------	-----	.857	30	.857	4	.8576	2
---	------	------	-----	-----	------	--	------	-----	-------	-----	------	-----	-------	-----	-----	-----	.8557	5
---	0.845	m-s	-----	-----	------	--	------	-----	0.844	20	------	-----	0.843	20	----	-----	.8467	2
---	------	------	-----	-----	------	--	------	-----	.838	20	------	-----	.839	20	----	-----	.8412 .8383	3 4
---	------	------	-----	-----	------	--	------	-----	.819	10	------	-----	.818	10	-----	-----	-------	-----
---	------	------	-----	-----	------	--	------	-----	.812	8	------	-----	-------	-----	-----	-----	-------	-----
---	------	------	-----	-----	------	--	------	-----	-------	-----	------	-----	0.803	10	-----	-----	-------	-----

2.26. Germanium Dioxide, GeO_2 (Hexagonal)

The two patterns for germanium dioxide in the X-ray diffraction file of the ASTM (see table 1) are compared in table 27 with a pattern prepared at the NBS. The sample for the NBS pattern was obtained from Johnson, Matthey & Co., Ltd, and was labelled number 3662. The only impurity indicated in their spectrographic analysis was a faint trace of calcium.

In table 27 the interplanar spacings of all patterns are given in angstrom units.

TABLE 27. *Germanium dioxide, GeO_2 (hexagonal)*

hkl	1928 Zachariasen Fe, 1.9360 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A		1953 Swanson and Tatge Cu, 1.5405 A 26°C		hkl	1953 Swanson and Tatge Cu, 1.5405 A 26°C	
	d	I	d	I	d	I		d	I
	A		A		A			A	
100	4.33	20	4.32	20	4.32	21	005	1.1308	1
101	3.431	100	3.42	100	3.429	100	312	1.1026	2
110	2.486	15	2.49	14	2.496	11	105	1.0933	2
102	2.362	40	2.35	25	2.366	22	214	1.0683	3
111	2.278	15	2.28	16	2.283	13	401	1.0605	2
200	2.159	40	2.15	20	2.159	18	223	1.0397	2
201	2.014	5	2.00	2	2.018	2	115	1.0297	2
003	1.879	15	-----	---	1.884	8	402	1.0084	4
112	1.868	30	1.87	25	1.870	14	304		
103	1.727	15	-----	---	1.726	4	321	0.9759	2
202	1.717	15	1.71	12	1.716	7	006	.9419	1
210	1.634	10	1.62	2	1.633	3	322	.9352	1
211	1.564	60	1.56	25	1.568	13	224	.9345	3
113	1.500	20	1.498	8	1.303	5	411	.9294	3
203	1.420	30	1.448	4	1.420	11	412	.8943	<1
212	1.413	30	1.413	25	1.414	13	305	.8894	<1
301	1.394	30	1.389	8	1.395	7	403	.8814	<1
104	1.341	30	1.342	10	1.343	5	500	.8636	<1
---	-----	---	1.304	2	------	--	404	.8579	1
302	1.281	25	1.279	10	1.283	4	501	.8541	<1
220	1.246	5	1.256	2	1.247	1	330	.8315	1
213	1.230	25	1.230	6	1.234	4	331	.8223	1
114					1.231	4	420	.8162	1
221	1.218	20	-----	----	1.218	2	324	.8112	2
310	1.196	40	-----	----	1.1976	4	421	.8078	1
204	1.182	5	-----	----	------	--	---	------	--
311	1.172	10	-----	----	1.1720	1	---	------	--
303	1.142	10	-----	----	1.1420	1	---	-----	--
222									

One line of the Hanawalt, Rinn and Frevel pattern is extraneous to the postulated structure; it could not be indexed. The intensity measurements of the first lines of the three patterns are closely comparable. For all patterns the first, second, and third strongest lines are the 101, 100, and 110, respectively.

The lattice of germanium dioxide is hexagonal and was determined by Zachariasen [260] as D_3^4 ($C3_12$), isomorphous with low quartz. There are three molecules in the unit cell. The new file card for the Hanawalt, Rinn, and Frevel pattern is unfortunately mislabelled "Tetragonal." From table 27 the pattern is plainly identical to the hexagonal patterns of Zachariasen and the NBS. The published pattern [85] is unaccompanied by symmetry classification. Converted to angstrom units, the Zachariasen measurements compare thus with those of the NBS pattern:

Unit cell, angstroms

		a	c
1928	Zachariasen [260]	4.982	5.659
1953	Swanson and Tatge (26°C)	4.987	5.652

The density, using the NBS unit cell dimensions, is 4.280. The material was very fine-grained, which made optical examination difficult. The double refraction is very weak; the average index of refraction is $n = 1.67$.

2.27. Arsenic Trioxide, As_2O_3 (Cubic)

The ASTM file of diffraction patterns includes five cards for arsenic trioxide (see table 1); one of these (number 3-1234) does not bear a pattern, but records only a lattice constant and a space group determination. Of the remaining four, two are for synthetic compounds, and two for naturally occurring minerals. One of the latter (2-0530) represents the monoclinic form claudetite, the other (2-0531), like the two artificial forms, represents cubic arsenolite. The natural arsenolite is from Bieber, Hesse, Germany (misspelled "Hasse" on the new file card). The

TABLE 28. *Arsenic trioxide, As_2O_3 (cubic)*

hkl	1928 Passerini Cu, 1.5405 A					1931 Lihl Fe, 1.9360 A			1938 Mikheev and Dubinina Fe, 1.960 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A			1953 Swanson and Tatge Cu, 1.5405, 26°C		
	d[a]	d[b]	I[c]	I[d]	a	d	I	a	d	I	a	d	I	a	d	I	a
	A	A			A	A		A	A		A	A		A	A		A
111	5.975	6.39	w	40	10.34	------	---	------	-----	---	-----	6.3	56	10.9	6.39	63	11.07
220	3.754	3.92	ms	70	10.60	------	---	------	-----	---	-----	-----	-----	-----	3.92	<1	11.09
222	3.111	3.20	s	80	10.78	3.191	s	11.05	3.195	100	11.07	3.19	100	11.1	3.195	100	11.07
------	-----	-----	---	---	-----	------	---	------	2.944	10	-----	-----	-----	-----	------	-----	------
400	2.725	2.77	m	60	10.88	2.764	s	11.06	2.764	60	11.06	2.76	24	11.0	2.768	28	11.07
331	2.500	2.54	m	60	10.92	2.535	s	11.05	2.539	90	11.07	2.54	32	11.1	2.541	38	11.08
------	2.332	2.36	vw	20	-----	------	---	------	-----	---	-----	-----	-----	-----	------	-----	-----
422	2.235	2.26	vw	20	10.93	2.257	w	11.10	2.255	50	11.05	2.24	8	11.1	2.262	12	11.08
511	2.112	2.13	w	30	10.97	2.126	w	11.05	2.127	60	11.05	2.12	16	11.0	2.132	17	11.08
440	1.937	1.96	ms	70	10.96	1.971	s	11.15	1.955	90	11.06	1.95	24	11.0	1.958	27	11.08
531	-----	-----	---	---	-----	------	---	------	1.875	40	11.09	-----	-----	-----	1.873	6	11.08
442	1.837	1.85	mw	50	11.02	------	---	------	1.841	50	11.05	-----	-----	-----	1.846	5	11.08
------	-----	-----	---	---	-----	------	---	------	1.810	10	-----	-----	-----	-----	------	-----	------
622	1.661	1.67	ms	70	11.00	1.666	s	11.05	1.668	90	11.06	1.66	16	11.0	1.670	21	11.08
444	1.589	1.60	mw	50	11.00	------	---	------	1.596	60	11.06	1.59	8	11.0	1.599	10	11.08
711	1.541	1.55	ms	70	11.01	1.547	---	11.05	1.550	90	11.07	1.54	16	11.0	1.551	22	11.08
642	-----	-----	---	---	-----	------	---	------	1.480	40	11.08	-----	-----	-----	1.480	'2	11.08
731	1.434	1.44	ms	70	11.02	1.439	s	11.05	1.442	90	11.08	1.441	8	11.07	1.442	12	11.08
800	-----	-----	---	---	-----	------	---	------	1.383	10	11.06	-----	-----	-----	1.385	3	11.08
733	-----	-----	---	---	-----	1.350	s	11.05	1.353	90	11.07	-----	-----	-----	1.353	10	11.07
644	1.342	1.342	ms	70	11.05	------	---	------	-----	---	-----	1.346	8	11.10	1.343	1	11.07
822	1.300	1.300	w	40	11.04	1.302	w	11.04	1.305	80	11.07	1.305	8	11.06	1.305	5	11.07
751	-----	-----	---	---	-----	1.278	w	11.07	1.277	60	11.06	-----	-----	-----	1.278	3	11.07
662	1.269	1.269	w	40	11.06	------	---	------	1.270	50	11.07	1.269	8	11.06	1.271	1	11.08
840	-----	-----	---	---	-----	------	---	------	1.238	40	11.07	-----	-----	-----	1.238	2	11.07
911	-----	-----	---	---	-----	------	---	------	1.213	60	11.05	-----	-----	-----	1.216	5	11.08
842	1.206	1.206	ms	70	11.06	1.2065	m	11.058	1.208	60	11.07	1.207	8	11.06	1.208	6	11.07
664	-----	-----	---	---	-----	1.1781	w	11.052	-----	---	-----	-----	-----	-----	1.1812	1	11.081
931	1.161	1.161	w	40	11.08	1.1592	m	11.058	1.161	50	11.08	-----	-----	-----	1.1610	3	11.075
933	-----	-----	---	---	-----	------	---	------	1.113	25	11.07	-----	-----	-----	1.1132	2	11.076
------	1.108	1.108	vvw	10	-----	------	---	------	-----	---	-----	-----	-----	-----	------	-----	------
10·2·0	-----	-----	---	---	-----	------	---	------	1.086	13	11.08	-----	-----	-----	1.0859	1	11.074
951	1.068	1.068	vs	100	11.05	1.0685	s	11.053	1.070	100	11.07	1.066	8	11.03	1.0706	6	11.074
864	1.030	1.030	vw	20	11.10	1.0266	w	11.057	1.029	25	11.08	-----	-----	-----	1.0294	2	11.087
10·4·2	-----	-----	---	---	-----	------	---	------	-----	---	-----	-----	-----	-----	1.0117	<1	11.083
11·1·1	-----	-----	---	---	-----	0.9970	m	11.057	-----	---	-----	-----	-----	-----	0.9976	2	11.064
11·3·1	-----	-----	---	---	-----	------	---	------	-----	---	-----	-----	-----	-----	.9676	4	11.075
10·4·4	0.965	0.965	vs	100	11.08	------	---	------	-----	---	-----	-----	-----	-----	.9643	2	11.079
10·6·0	.950	.950	vw	20	11.07	------	---	------	-----	---	-----	-----	-----	-----	.9496	1	11.074
11·3·3	.937	.937	vw	20	11.08	------	---	------	-----	---	-----	-----	-----	-----	.9392	2	11.073
11·5·1	.915	.915	vvw	10	11.09	------	---	------	-----	---	-----	-----	-----	-----	.9135	1	11.075
12·2·2	.898	.898	s	80	11.08	------	---	------	-----	---	-----	-----	-----	-----	.8982	3	11.073
12·4·2	.865	.865	ms	70	11.08	------	---	------	-----	---	-----	-----	-----	-----	.8648	2	11.074
13·1·1	.846	.846	ms	70	11.08	------	---	------	-----	---	-----	-----	-----	-----	.8469	3	11.075
13·3·1	-----	-----	---	---	-----	------	---	------	-----	---	-----	-----	-----	-----	.8278	3	11.075
13·3·3	-----	-----	---	---	-----	------	---	------	-----	---	-----	-----	-----	-----	.8098	2	11.074
Average unit cell for last five lines					11.08	------	---	11.055	-----	---	11.08	-----	-----	11.07	------	-----	11.074

[a] Published. [b] On ASTM card; first fourteen lines recalculated (converted to angstroms). [c] Published. [d] On ASTM card.

claudetite pattern is of little value to the file inasmuch as its locality is not given and it contains a large number of arsenolite lines. The reference "RI" appearing on the ASTM card for the two patterns of naturally occurring minerals indicates a compilation of Boldyrev [19] which gives the original published source [153] of the patterns. In table 28 the natural arsenolite pattern is listed along with the remaining two ASTM patterns, a fourth from the literature, Lihle [140], and one by the NBS.

The NBS pattern was made from a sample obtained from the Mallinckrodt Chemical Works, and numbered 906487. Their spectrographic analysis indicated the following impurities in amounts of 0.001 to 0.01 percent: Ca, Fe, Mg, Pb, Sb, and Si. The material was recrystallized by sublimation before using.

The Passerini and Lihl spacings were calculated for table 28 in angstroms from published Bragg angle data; the Mikheev and Dubinina, and the Hanawalt, Rinn, and Frevel spacings were converted from kX units. On the ASTM card the first fourteen spacings of the Passerini pattern are not those originally published, but were recalculated on the basis of a lattice constant determined from the last or high angle lines of the pattern. The original intensity measurements were converted to numerical designations for the ASTM card. Both the published and the ASTM patterns are given in table 28. The Passerini pattern and that of Mikheev and Dubinina both include lines not permitted by the postulated O_h^7 space group. The intensity values of the Hanawalt, Rinn, and Frevel and the NBS patterns agree fairly closely. Both show 222, 111, and 331 as the first, second, and third strongest lines.

Arsenic trioxide was determined by Bozorth in 1923 [24] as having the diamond structure on the basis of line spectra from 100, 110, and 111, and Laue photographs. Eight As_4O_6 units are tetrahedrally arranged in a unit cell having the space group O_h^7 (Fd3m). Two recent measurements of the lattice constant are compared below with that of the NBS. All are in angstroms at 25°C, converted by means of the coefficient of expansion 37.0×10^{-6} [217].

Unit cell in angstroms at 25°C

1936	Straumanis and Ievinš [216]	11.0724
1939	Straumanis, Ievinš, and Karlsons [217]	11.07441
1953	Swanson and Tatge	11.074

The density, based on the NBS lattice constant, is 3.8654 at 25°C. The index of refraction determined for the NBS sample is $n = 1.748$.

2.28. Selenium Dioxide, SeO_2 (Tetragonal)

No patterns were found for selenium dioxide (selenolite) in the ASTM file or in the literature. The one given in table 29 was prepared at the NBS from specially purified material supplied by the Mallinckrodt Chemical Works. Spectrographic analysis at the NBS showed no impurities greater than 0.001 percent. The material is very hygroscopic and, although the sample was mixed with petrolatum, a few weak lines from the monohydrate appeared in the diagram which were omitted from the pattern in table 29.

The lines of the pattern are indexed in accordance with the structure and unit-cell dimensions determined by McCullough [145] in 1937. Although crystals of SeO_2 generally have been described as monoclinic (Waitkins and Clark [241]), the NBS pattern agrees with the structure determination of McCullough, showing a tetragonal structure. McCullough gives the probable space group as D_{4h}^{13} (P4/mbc), or C_{4v}^{8} (C4cb), with eight molecules in the unit cell. The lattice constants derived by McCullough, which were used by Frevel, Rinn, and Anderson [75] in 1946, compare with the NBS determinations as follows, after conversion to angstrom units:

Unit cell, in angstroms

		a	c
1937	McCullough [145]	8.370	5.061
1951	Swanson and Tatge (26°C)	8.35	5.08

The density is 4.16 at 26°C, based on the NBS lattice constant. The material proved too unstable for a determination of the indices of refraction.

TABLE 29. *Selenium dioxide, SeO_2 (tetragonal)*

hkl	1951 Swanson and Tatge Cu, 1.5405 A, 26°C		hkl	1951 Swanson and Tatge Cu, 1.5405 A, 26°C	
	d	I		d	I
	A			A	
110	5.92	13	322	1.711	25
200	4.17	85	500	1.673	9
210	3.73	100	510	1.640	9
201	3.227	11	431	1.588	3
211	3.009	88	511	1.559	14
220	2.998	38	332	1.556	10
300	2.789	2	213	1.538	4
310	2.640	14	422	1.503	3
002	2.533	2	440	1.478	4
311	2.343	3	530	1.437	4
112	2.320	15	313	1.421	5
202	2.252	14	432	1.394	8
321	2.105	6	512	1.379	20
400	2.090	14	522	1.324	9
330	1.973	10	620		
401	1.933	17	540	1.305	4
411	1.895	14	413	1.292	3
420	1.871	14	621	1.278	12
312	1.831	17	004	1.264	15
421	1.755	13	612	1.209	13

2.29. Stannic Oxide, SnO_2 (Tetragonal)

In addition to the seven patterns for stannic oxide (cassiterite) appearing on ASTM cards (see table 1), an eighth was found in the literature, Natta and Passerini [158]. These are compared with an NBS pattern for which a sample of tin oxide was obtained from Johnson, Matthey & Co., Ltd; the sample was numbered 2763. The report on the spectrographic examination which accompanied the sample shows no lines for impurities stronger than faintly visible.

The interplanar spacings recorded in table 30 were all converted to angstrom units except those of the United Steel Companies pattern, which were evidently calculated in angstroms originally, and of the Natta and Passerini pattern, which were calculated directly in angstroms from the sine θ data published.

Several patterns list the 211 as the strongest line, or at least equal in strength to the 110 and 101. The Hanawalt, Rinn, and Frevel, and the NBS patterns show the 110 strongest. In listing the first, second, and third strongest lines, four of the eight patterns, including those of Hanawalt, Rinn, and Frevel, and the NBS, would record them in the following order: 110, 101, 211.

Vegard [232] in 1916 recorded the space group determination of D_{4h}^{14} for tetragonal stannic oxide. There are two molecules in the unit cell. The lattice constants derived from the NBS pattern compare as follows with earlier determinations:

Unit cell, in angstroms

		a	c
1924	Davey [58]	4.728	3.167
1932	Bragg and Darbyshire [33]	4.73	3.18
----	United Steel	4.7355	3.1850
1953	Swanson and Tatge (26°C)	4.738	3.188

The density calculated from the NBS dimensions of the unit cell is 6.995.

TABLE 30. *Stannic oxide* SnO_2 *(tetragonal)*

hkl	1929 Natta and Passerini Fe, 1.9360 A		1932 Weiser and Milligan Mo, 0.7093 A		1938 Boldyrev Mo, 0.7093 A		1938 Banawalt, Rinn, and Frevel Mo, 0.7093 A		1942 Harcourt Cu, 1.5405 A		---- Harcourt; Poldyrev Mo, 0.7093 A		---- British Museum Cu, 1.5405 A		---- United Steel Co, 1.7902 [a] A		1953 Swanson and Tatge Cu, 1.5405 A, 26°C	
	d	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A		A		A		A		A		A		A		A		A	
110	3.27	mw	3.41	100	3.337	50	3.35	100	3.33	100	3.34	80	3.31	80	3.36	80	3.351	100
---	-----	----	------	---	-----	----	-----	----	-----	----	-----	----	2.92	20	-----	-----	------	---
101	2.606	s	2.68	100	2.636	50	2.65	63	2.63	100	2.64	80	2.63	80	2.65	80	2.644	81
200	-----	----	2.35	50	2.367	40	2.36	18	2.35	33	2.36	60	2.35	60	2.37	50	2.369	24
111	-----	----	------	---	-----	----	-----	----	2.28	8	2.28	30	------	---	2.31	20	2.309	5
210	-----	----	------	---	-----	----	-----	----	2.11	5	2.11	20	1.95	50	-----	-----	2.120	2
211	1.754	vs	1.77	100	1.764	100	1.75	63	1.75	100	1.75	100	1.75	100	1.76	100	1.765	63
220	-----	----	------	---	1.675	70	1.67	10	1.668	33	1.67	70	1.67	60	1.67	60	1.675	63
002	1.583	mw	------	---	1.590	20	1.58	5	1.58	17	1.58	50	1.59	50	1.59	50	1.593	8
---	-----	----	------	---	1.529	10	-----	----	-----	----	-----	----	1.57	40	-----	-----	------	---
310	1.491	----	------	---	1.500	80	1.495	10	1.49	33	1.49	70	1.50	60	1.50	60	1.498	13
112	1.430	s	1.43	70	1.438	70	1.438	10	1.43	33	1.43	70	1.44	60	1.44	60	1.439	17
301	1.409	s	------	---	1.413	70	1.415	15	1.408	33	1.411	70	1.41	60	1.41	60	1.415	15
---	-----	----	------	---	-----	----	-----	----	-----	----	-----	----	1.35	20	-----	-----	------	---
202	-----	----	1.32	20	1.323	40	1.318	6	1.318	17	1.321	50	1.32	40	1.32	50	1.322	7
321	1.211	vs	1.21	70	1.216	80	1.215	10	1.211	33	1.213	80	1.22	70	1.21	60	1.215	11
400	-----	----	------	---	1.185	30	1.182	2	1.181	8	1.183	40	1.19	20	1.18	40	1.184	3
222	1.150	s	1.16	20	1.155	70	1.152	6	1.151	17	1.153	60	1.16	60	1.15	60	1.155	8
---	-----	----	------	---	-----	----	-----	----	-----	----	1.141	30	------	---	-----	-----	------	---
330	1.114	ms	------	---	1.118	60	1.112	3	1.113	17	1.115	60	1.12	60	1.12	50	1.117	3
312	1.087	s	1.10	40	1.092	70	1.087	8	1.088	33	1.090	80	1.09	80	1.09	60	1.092	8
411	1.078	s	------	---	1.081	80	-----	----	1.077	33	1.079	80	1.08	80	1.08	60	1.081	8
420	1.058	ms	------	---	1.060	70	1.059	3	1.057	17	1.059	70	1.06	50	1.06	50	1.059	3
---	1.049	mw	1.05	10	-----	----	-----	----	-----	----	1.047	70	1.05	40	-----	-----	------	---
103	1.035	ms	------	---	1.037	40	1.037	2	1.033	17	1.035	50	1.04	40	1.04	50	1.036	4
---	-----	----	------	---	-----	----	-----	----	-----	----	-----	----	1.01	20	-----	-----	------	---
402	-----	----	------	---	-----	----	0.950	8	0.947	50	0.947	80	------	---	0.951	80	0.9505	8
510	-----	----	------	---	-----	----	.931	1	.928	17	.928	60	------	---	.931	70	.9291	3
332	-----	----	------	---	-----	----	-----	----	.914	17	.914	60	------	---	.916	70	.9143	3
501	-----	----	------	---	-----	----	0.907	4	.907	33	.907	70	------	---	.910	80	.9081	8
422	-----	----	------	---	-----	----	.882	4	.881	50	.881	80	------	---	-----	-----	.8819	7
303	-----	----	------	---	-----	----	-----	----	-----	----	-----	----	------	---	-----	-----	.8814	6
521	-----	----	------	---	-----	----	0.847	2	0.848	50	0.848	80	------	---	-----	-----	.8480	6
440	-----	----	------	---	-----	----	-----	----	.838	17	-----	----	------	---	-----	-----	.8375	1
323	-----	----	------	---	-----	----	-----	----	.826	33	-----	----	------	---	-----	-----	.8261	4
530	-----	----	------	---	-----	----	-----	----	.813	8	-----	----	------	---	-----	-----	.8125	2
441	-----	----	------	---	-----	----	-----	----	.807	33	-----	----	------	---	-----	-----	------	---
512	-----	----	------	---	-----	----	-----	----	-----	----	-----	----	------	---	-----	-----	0.8026	6

[a] Weighted $K\alpha$.

2.30. Ceric Oxide, CeO_2 (Cubic)

Two patterns for ceric oxide in the ASTM file (see table 1) are compared in table 31 with a pattern prepared at the NBS. The sample used, of unknown origin, was obtained from the NBS spectrographic laboratory, and was labeled number 41-9100. It is approximately 99.99 percent pure, showing only spectrographic traces of praseodymium and copper.

The three patterns are compared in table 31. The spacings of the Hanawalt, Rinn, and Frevel pattern were converted from kX units to angstroms. The Passerini pattern was derived directly in angstroms from the Bragg angles published. As shown in table 31 by comparing the unit cell values in column a, the first six spacings are not in very good agreement with the last four. For this reason they had been replaced on the ASTM card with values calculated from the smaller interplanar spacings in the last three lines of column d.

The intensity measurements by Passerini were published as visual estimates which were given numerical values for the ASTM card. The first, second, and third strongest lines are 111, 220, and 311, respectively.

Ceric oxide has the fluorite structure, a face-centered cubic lattice, space group O_h^5 ($Fm3m$), and four molecules to the unit cell [80]. Several determinations of the unit cell have been made but temperature data have not been published with them. McCullough used angstrom units. Assuming that the other

TABLE 31. *Ceric oxide, CeO_2 (cubic)*

hkl	1930 Passerini Fe, 1.9360 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A			1953 Swanson and Tatge Cu, 1.5405 A, 26°C		
	d	I	a	d	I	a	d	I	a
	A		A	A		A	A		A
111	3.083	70	5.340	3.12	100	5.40	3.124	100	5.411
200	2.678	40	5.356	2.70	25	5.40	2.706	29	5.412
220	1.907	100	5.394	1.90	80	5.37	1.913	51	5.411
311	1.627	100	5.396	1.62	60	5.37	1.632	44	5.413
222	1.559	50	5.401	1.55	10	5.37	1.562	5	5.411
400	1.350	40	5.400	1.350	10	5.400	1.353	5	5.412
331	1.242	80	5.414	1.239	25	5.401	1.241	15	5.409
420	1.212	80	5.420	1.209	16	5.407	1.210	6	5.411
422	1.107	100	5.423	1.103	20	5.404	1.1044	12	5.4104
511	1.044	100	5.425	1.039	18	5.399	1.0412	9	5.4102
440	----------	---------	----------	0.956	4	5.408	0.9565	5	5.4108
531	----------	---------	----------	.914	14	5.407	.9146	13	5.4108
600	----------	---------	----------	.901	2	5.406	.9018	7	5.4108
620	----------	---------	----------	.855	4	5.407	.8556	7	5.4113
533	----------	---------	----------	----------	---------	----------	.8251	6	5.4105
622	----------	---------	----------	0.818	2	5.426	.8158	5	5.4114
711	----------	---------	----------	.758	4	5.413	----------	---------	----------
642	----------	---------	----------	.723	4	5.410	----------	---------	----------
731	----------	---------	----------	.704	2	5.407	----------	---------	----------
Average unit cell for last five lines			5.416	----------	---------	5.413	----------	---------	5.4110

workers used kX units, the following table makes a comparison of their values with the NBS determination, in angstroms:

Unit cell, angstroms

1923	Goldschmidt and Thomassen [80]	5.42
1925	Goldschmidt, Ulrich, and Barth [81]	5.413
1930	Passerini [183]	5.426
1939	Zintl and Croatto [262]	5.407
1950	McCullough [146]	5.411
1953	Swanson and Tatge (26°C)	5.4110

The density calculated from the NBS lattice constant is 7.215 at 26°C.

2.31. Thorium Oxide, ThO_2 (Cubic)

Two patterns for thorium oxide (thorianite) from the ASTM file (see table 1) are supplemented by three from the literature, Van Arkel [229], Levi and Reina [138], and Burgers and Van Liempt [45], and compared in table 32 with a pattern recently prepared at the NBS. The NBS pattern was made by the use of material obtained from the Lindsay Light and Chemical Company of West Chicago, who stated a purity of 99.99 percent.

Interplanar spacings for the first three patterns of table 32 were obtained directly in angstrom units from the published Bragg angle data. At the time the Passerini pattern was transferred to the ASTM card only the last four of the interplanar spacings were copied from his data; the first six were recalculated on the basis of the unit cell derived from the remaining lines. In table 32 the original values are given instead of the ASTM values for all lines, after con-

TABLE 32. *Thorium oxide, ThO_2 (cubic)*

hkl	1924 Van Arkel Cu, 1.5405 A		1927 Levi and Reina Cu, 1.5405 A		1930 Burgers and Van Liempt Cu, 1.5405 A		1930 Passerini Fe, 1.9360 A				1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A			1953 Swanson and Tatge Cu, 1.5405 A, 26°C		
	d	*a*	*d*	*a*	*d*	*a*	*d*	*I*[a]	*I*[b]	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A	*A*	*A*	*A*	*A*	*A*	*A*			*A*	*A*		*A*	*A*		*A*
111	3.14	5.44	-----	-----	3.24	5.61	3.166	ms	70	5.485	3.23	100	5.59	3.234	100	5.602
200	2.73	5.46	-----	-----	2.80	5.60	2.764	w	40	5.528	2.81	38	5.62	2.800	35	5.600
220	1.94	5.49	1.930	5.459	1.98	5.60	1.960	vs	100	5.542	1.97	75	5.57	1.980	58	5.600
311	1.66	5.51	1.658	5.499	1.69	5.61	1.675	vs	100	5.555	1.68	88	5.57	1.689	64	5.602
222	1.59	5.51	-----	-----	1.61	5.58	1.609	mw	50	5.572	-----	-----	-----	1.616	11	5.598
400	1.38	5.52	1.392	5.568	1.40	5.60	1.393	w	40	5.573	1.402	13	5.608	1.400	8	5.600
331	1.27	5.54	1.272	5.545	1.30	5.67	1.282	s	80	5.589	1.283	38	5.592	1.284	26	5.597
420	1.24	5.55	1.242	5.554	1.25	5.59	1.250	s	80	5.592	1.248	25	5.581	1.252	17	5.599
422	1.132	5.546	1.133	5.551	1.14	5.58	1.141	vs	100	5.591	1.142	38	5.595	1.1432	20	5.6005
511	1.070	5.560	1.071	5.565	1.076	5.591	1.077	vs	100	5.597	1.076	38	5.591	1.0779	19	5.6010
440	-----	-----	0.983	5.561	0.988	5.589	-----	----	-----	-----	0.989	13	5.595	0.9900	6	5.6003
531	0.940	5.561	.941	5.567	.945	5.591	-----	----	-----	-----	.945	25	5.591	.9465	18	5.5996
600	.929	5.574	.931	5.588	.933	5.598	-----	----	-----	-----	.933	25	5.598	.9333	8	5.5998
620	.884	5.591	.883	5.582	.884	5.591	-----	----	-----	-----	-----	-----	-----	.8854	14	5.5998
533	.852	5.587	.851	5.582	.853	5.593	-----	----	-----	-----	-----	-----	-----	.8540	9	5.6001
622	.843	5.592	.843	5.592	.843	5.592	-----	----	-----	-----	-----	-----	-----	.8441	9	5.5991
444	.809	5.605	-----	-----	.807	5.591	-----	----	-----	-----	-----	-----	-----	------	-----	------
711	.784	5.600	-----	-----	.783	5.592	-----	----	-----	-----	-----	-----	-----	------	-----	------
640	-----	-----	-----	-----	.780	5.625	-----	----	-----	-----	-----	-----	-----	------	-----	------
Average unit cell for last five lines		5.595	-----	5.582	-----	5.986	-----	----	-----	5.588	-----	-----	5.594	------	-----	5.5997

[a] Published. [b] ASTM card.

version from kX to angstrom units. The interplanar spacings listed by Hanawalt, Rinn, and Frevel were likewise converted from kX units to angstroms for the table. The intensity data of Hanawalt, Rinn, and Frevel agree well with those of the NBS. The three strongest lines of both patterns are 111, 311, and 220.

Thorium oxide has the fluorite structure (Goldschmidt and Thomassen [80]), a face-centered cubic lattice, space group O_h^5 (Fm3m). The unit cell contains four molecules. W. H. Zachariasen gave 5.5859 kX units for the lattice constant at the New Haven meeting of the American Society for X-ray and Electron Diffraction in 1948. This measurement and others published since 1929 (all probably in kX units and converted to angstroms) may be compared with the NBS determination thus:

Unit cell, angstroms

1929	Ruff, Ebert, and Woitinek [197]	5.58
1930	Passerini [183]	5.596
1930	Burgers and Van Liempt [45]	5.601
1944	Palache, Berman, and Frondel [180]	5.62
1948	Zachariasen	5.5972
1953	Swanson and Tatge (26°C)	5.5997

In the new (1950) ASTM file the Hanawalt, Rinn, and Frevel card (1-0731) states the lattice constant as 5.61, ascribed correctly to "D_7," that is, Dana's Mineralogy, 7th edition [180]; the Passerini card (2-1278) gives it as 5.590, ascribed to Dana, although in this case the value is actually that of Passerini. Temperature data are not available for the comparison patterns. The density calculated from the NBS lattice constant is 9.991 at 26°C.

2.32. Calcium Hydroxide, $Ca(OH)_2$ (Hexagonal)

The ASTM file of X-ray diffraction patterns contains four cards for calcium hydroxide (portlandite) (see table 1). The four patterns are compared in table 33 with two from the literature (Levi [136] and Natta and Passerini [156]), and with a pattern prepared at the NBS.

The NBS sample was obtained as calcium carbonate from the J. T. Baker Chemical Company; it was numbered 121647. At the NBS laboratory it was heated in a platinum crucible at 925°C for one hour, and water added to the resulting calcium oxide in a nitrogen atmosphere.

The following chemical analysis (in percent) was provided by the chemical laboratory of the NBS: Insoluble in HCl and NH_4OH ppt, 0.01; chloride, <0.005; sulfate, 0.037; alkalis (as SO_4), 0.011; barium, <0.1; heavy metals (as Pb), 0.001; Fe, 0.003; MgO and alkalis, 0.21. The laboratory of the J. T. Baker Chemical Company specified the barium content as 0.005 percent and the iron as 0.001 percent.

For table 33 the Levi and Natta and Passerini patterns were calculated directly in angstroms from Bragg angle data given. The spacings of the ASTM patterns were all converted to angstroms from kX units. The fifth pattern in the table appeared in the old ASTM file with the source for it omitted; it was tentatively ascribed to the United Steel Companies, England, in the 1950 file. The Hanawalt, Rinn, and Frevel pattern and the two of the United Steel Companies agree with that of the NBS in showing the three strongest lines as 101, 001, and 102.

The space group assigned to hexagonal calcium hydroxide [23] is D_{3d}^3 (C3mi); there is one molecule in the unit cell. Lattice constants of several investigators are compared in the table below. All are from the literature except the two values of the United Steel Companies, which were taken from the ASTM cards, and are in angstrom units.

Unit cell, in angstroms

		a	c
1927	Harrington [89]	3.587	5.040
1933	Tilley [222]	3.592	4.905
1935	Bunn, Clark, and Clifford [44]	3.5916	4.9061
----	United Steel	3.588	4.903
----	United Steel (?)	3.584	4.916
1953	Swanson and Tatge (27°C)	3.593	4.909

The density calculated from the NBS data is 2.241. Because of the platy nature and fine grain of the material the index of refraction was determined only for the ordinary ray, $\omega = 1.573$. Ashton and Wilson [3] give $\omega_D = 1.574$, $\epsilon_D = 1.545$.

TABLE 33. *Calcium hydroxide, $Ca(OH)_2$ (hexagonal)*

hkl	1924 Levi Cu, 1.5405 A		1927 Harrington Mo, 0.7093 A		1928 Natta and Passerini Cu, 1.5405 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A		---- United Steel(?) ----------		---- United Steel ----------		1953 Swanson and Tatge Cu, 1.5405 A, 27°C	
	d	I	d	I	d	I	d	I	d	I	d	I	d	I
	A		A		A		A		A		A		A	
001	4.45	m	-------	-----	3.770	ms	4.94	50	4.92	70	4.90	90	4.90	74
100	2.94	mw	3.11	40	-------	----	3.12	25	3.11	50	3.108	60	3.112	23
101	2.50	vs	2.63	100	2.502	s	2.64	100	2.63	100	2.625	100	2.628	100
002	-------	----	-------	-----	-------	----	-------	-------	-------	-----	--------	-----	2.447	3
102	1.906	s	1.928	80	1.902	ms	1.93	50	1.927	60	1.925	90	1.927	42
110	1.746	s	1.793	90	1.748	s	1.79	40	1.793	50	1.795	70	1.796	36
111	1.645	ms	1.683	60	1.640	ms	1.69	30	1.683	50	1.688	60	1.687	21
003	-------	----	-------	-----	-------	----	-------	-------	-------	-----	--------	-----	1.634	1
200	-------	----	1.553	10	-------	----	1.55	2	-------	-----	1.554	20	1.557	3
201	1.446	m	1.478	60	1.471	mw	1.488	20	1.480	50	1.481	60	1.484	13
112 103	1.418	m	1.453	50	1.434	ms	1.453	20	1.448	50	1.447	60	1.449	13
202	1.286	m	1.311	50	1.293	mw	1.318	20	1.313	50	1.313	60	1.314	8
004	-------	----	-------	-----	-------	----	-------	-------	-------	-----	1.249	10	1.228	1
113	-------	----	-------	-----	-------	----	-------	-------	-------	-----	1.208	20	1.211	1
210	-------	----	1.174	5	-------	----	1.180	2	-------	-----	1.174	20	1.1762	3
211 104	1.128	ms	1.143	40	1.138	w	1.147	15	1.141	50	1.142	60	1.1432	11
203	-------	----	1.127	10	-------	----	-------	-------	-------	-----	1.126	50	1.1275	2
212	1.046	ms	1.060	40	1.047	w	1.065	10	1.059	50	1.059	60	1.0599	12
300	1.004	m	1.037	20	-------	----	1.037	5	1.035	40	1.036	50	1.0366	5
301 114	------	----	1.012	20	1.003	mw	1.014	8	1.013	50	1.0135	60	1.0143	7
302 213	0.951	mw	0.953	10	0.952	mw	0.957	5	0.954	40	0.9624 .9543	10 70	0.9551	4
105	.892	w	-------	-----	-------	----	-------	-------	-------	-----	.9351	20	.9379	1
220	-------	----	0.897	10	-------	----	-------	-------	-------	-----	--------	-----	.8979	1
221	-------	----	.882	5	-------	----	-------	-------	-------	-----	--------	-----	.8838	2
303	-------	----	-------	-----	-------	----	-------	-------	-------	-----	--------	-----	.8760	1
310 115 222	0.861	w	0.860	3	-------	----	-------	-------	-------	-----	--------	-----	.8623	2
311 214	.841	ms	.847	5	-------	----	0.852	2	-------	-----	--------	-----	.8495	6
006	.813	ms	.813	5	-------	----	-------	-------	-------	-----	--------	-----	.8140	5
223	.792	m	.789	[a]3	-------	----	-------	-------	-------	-----	--------	-----	----------	-------

[a] Nine lines following are omitted.

2.33. Ammonium Chloride, NH_4Cl (Cubic)

Four patterns from ASTM cards (see table 1) are compared in table 34 for ammonium chloride (sal-ammoniac) with a fifth pattern made at the NBS. The NBS sample was obtained from the J. T. Baker Chemical Company. It was tested by the NBS chemical laboratory and was found to conform with ACS standards;

it was recrystallized by sublimation before exposure to X rays.

The interplanar spacings of table 34 were changed to angstrom units on the basis of the wavelengths given for the radiation used in preparing the patterns, except for the Wyckoff and Armstrong spacings, which were calculated in angstroms from Bragg angle data given.

All patterns agree upon the 110 line as the strongest. For all except the NBS pattern the second strongest line is 211, and the third strongest 100; for the NBS pattern these are of the same intensity. This is in part due to the use of different radiation; however, recalculation of the intensities to a common basis by the use of the ASTM conversion scale ([1] p. 108 of index covering original set of cards, or card no. vii of introduction to 1950 file) preserves the same choice of the three strongest lines although reducing the discrepancies in intensity between patterns. Bartlett and Langmuir missed the 100 line of the pattern, and weak lines are missing from other patterns.

An error has been carried over from the old ASTM card to the new one for the Bartlett and Langmuir pattern; in column d the second interplanar spacing was originally published as 2.238 rather than the 2.338 of the ASTM card. The radiation wavelength is given on

TABLE 34. *Ammonium chloride*, NH_4Cl *(cubic)*

hkl	1921 Bartlett and Langmuir Mo, 0.7093 A			1924 Havighurst, Mack and Blake Mo, 0.7093 A			1929 Wyckoff and Armstrong Mo, 0.7093 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A			---- United Steel Companies, England Mo, 0.7093 A			1953 Swanson and Tatge Cu, 1.5405 A, 26°C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*	*A*		*A*	*A*		*A*	*A*		*A*
100	-----	---	-----	3.87	30	3.870	3.85	8	3.85	3.86	15	3.86	3.87	60	3.87	3.87	23	3.87
110	2.708	100	3.829	2.731	100	3.862	2.728	100	3.857	2.73	100	3.86	2.74	100	3.87	2.740	100	3.875
111	2.229	10	3.861	2.231	7	3.864	2.226	3	3.856	2.22	5	3.85	2.24	50	3.88	2.238	4	3.876
200	1.917	20	3.834	1.932	15	3.864	1.928	11	3.856	1.92	12	3.84	1.94	60	3.88	1.939	7	3.878
210	1.716	15	3.842	1.726	12	3.859	1.724	6	3.855	1.72	8	3.85	1.73	50	3.87	1.733	5	3.875
211	1.562	30	3.826	1.556	40	3.811	1.575	21	3.858	1.57	25	3.85	1.58	70	3.87	1.582	23	3.875
220	1.357	15	3.838	1.365	10	3.862	1.363	6	3.855	1.373	5	3.883	1.37	60	3.87	1.370	5	3.875
300	1.282	10	3.846	1.288	12	3.863	1.286	3	3.858	1.291	3	3.873	1.29	50	3.87	1.292	3	3.876
310	1.209	15	3.823	1.221	15	3.861	1.220	6	3.858	1.223	7	3.867	1.22	60	3.86	1.225	5	3.874
311	1.158	8	3.841	1.165	3	3.863	1.163	2	3.857	1.167	1	3.871	1.17	50	3.88	1.1687	4	3.8761
222	1.107	8	3.835	1.116	2	3.865	1.113	2	3.856	1.117	1	3.869	1.12	50	3.88	1.1188	2	3.8576
320	1.069	6	3.854	1.070	2	3.859	1.069	1	3.854	-----	---	-----	1.07	50	3.86	1.0751	1	3.8764
321	1.020	18	3.816	1.032	20	3.860	1.031	6	3.858	1.035	4	3.873	1.03	80	3.85	1.0357	3	3.8753
400	0.954	3	3.816	0.965	1	3.858	0.964	1	3.856	-----	---	-----	0.968	50	3.872	0.9680	1	3.8720
410	.931	6	3.839	.937	1	3.862	.935	1	3.855	-----	---	-----	.939	70	3.872	.9400	2	3.8757
411	.908	8	3.852	.910	6	3.860	.909	2	3.857	0.914	1	3.878	.913	85	3.873	.9134	3	3.8752
331	.888	5	3.871	-----	---	-----	.885	1	3.857	-----	---	-----	-----	---	------	.8890	1	3.8751
420	.864	5	3.864	0.864	3	3.863	-----	---	-----	0.866	1	3.873	-----	---	------	.8667	2	3.8760
421	.841	5	3.854	.844	2	3.866	-----	---	-----	-----	---	-----	-----	---	------	.8457	3	3.8755
332	.819	5	3.841	.823	1	3.858	-----	---	-----	-----	---	-----	-----	---	------	.8263	4	3.8757
422	.784	4	3.841	.788	2	3.860	-----	---	-----	-----	---	-----	-----	---	------	.7911	3	3.8756
500	.769	3	3.845	.774	4	3.869	-----	---	-----	-----	---	-----	-----	---	------	------	---	------
510	.752	7	3.834	.757	7	3.863	-----	---	-----	-----	---	-----	-----	---	------	------	---	------
521	-----	---	-----	.706	1	3.866	-----	---	-----	-----	---	-----	-----	---	------	------	---	------
Average unit cell for last five lines-----			3.843	-----	---	3.863	-----	---	3.857	-----	---	3.873	-----	---	[a]3.872	------	---	3.8756

[a]Average for last three lines only.

the old card as 0.708, on the new one 0.709, while 0.712 was actually used. On the old card for the Havighurst, Mack, and Blake pattern the interplanar spacings 1.221 and 0.7748 should read 1.2221 and 0.7745; these errors were eliminated from the new card in reducing the values to two decimal places only. The radiation wavelength was changed on the cards from 0.708 to 0.709; actually 0.710 was used. The Wyckoff and Armstrong reference is given incorrectly on both old and new cards; it should read "Z. Krist. 72, 319 (1929)" rather than "320 (1930)." The interplanar spacings and intensity measurements check with those of the reference given; it is not understood why reference is given also to Greenberg and Walden [82] (misspelled "Walder" on the new card) with the notation "intensities by ionization spectrometer," since the intensity data of this paper seem of little value and are apparently not recorded on the ASTM card at all.

The structure of ammonium chloride [54] is based on a simple cubic lattice, space group O_h^1 (Pm3m). There is one molecule to the unit cell. The early lattice constant determinations (Bragg [28], Vegard [235], and Bartlett and Langmuir [9]) vary considerably, and uncertainty exists as to the correction to apply to convert their units to angstroms. In the table below a value of Havighurst, Mack, and Blake [92] is compared with an electron diffraction determination of Trillat and Laloeuf [223], and the NBS lattice constant. The two former are converted from assumed kX units to angstroms.

Unit cell, angstroms

1924	Havighurst, Mack, and Blake [92]	3.874
1948	Trillat and Laloeuf [223]	3.871
1953	Swanson and Tatge (26°C)	3.8756

The density of ammonium chloride based on the unit cell of the NBS is 1.527 at 26°C. The index of refraction of the sample was determined as $n = 1.641$.

2.34. Lithium Fluoride, LiF (Cubic)

Six patterns are compared in table 35; besides the three from the ASTM file (see table 1), there is one from Debye and Scherrer [63], one from Bruni and Levi [41], and an NBS pattern. In their same publication Debye and Scherrer give a second pattern which closely corresponds to the first and is not reproduced in table 35.

The sample of lithium fluoride used for the NBS pattern was obtained from the Harshaw Chemical Co. Spectrographic analysis at the NBS showed (in percent): Sr, 0.01 to 0.1; Pb, Si, 0.001 to 0.01; Al, Ba, Ca, Cu, Fe, Mg, Sn, <0.001.

The interplanar spacings of the ASTM patterns in table 35 were converted from kX to angstrom units. The data of Debye and Scherrer and of Bruni and Levi were published in Bragg angles, from which the interplanar spacings were derived directly in angstroms. Most of the relative intensity measurements of the various patterns bear out the choice of the three strongest lines as given in the NBS pattern; 200, 111, and 220 are the first, second, and third strongest lines, respectively.

Lithium fluoride has the well-known NaCl structure, space group O_h^5 (Fm3m), with four molecules to the unit cell. Published lattice constants after converting from kX to angstrom units and allowing for temperature differences (the coefficient of expansion was determined by Straumanis, Ievinš and Karlsons [217] as 34.17×10^{-6}) compare with the NBS value thus:

Unit cell at 25°C, angstroms

1937	Moeller [155]	4.0286
1939	Straumanis, Ievinš, and Karlsons [217]	4.02620
1940	Hutchison and Johnston [110]	4.0255
1953	Swanson and Tatge	4.0269

The density based on the NBS lattice constant is 2.638 at 25°C. The refractive index of lithium fluoride determined by Spangenberg [211] is $n_D = 1.3915$.

TABLE 35. *Lithium fluoride, LiF (cubic)*

hkl	1916 Debye and Scherrer Cu, 1.5405 A			1923 Davey Mo, 0.7093 A			1924 Bruni and Levi Cu, 1.5405 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A			---- Crystallographic Laboratory, England Mo, 0.7093 A			1953 Swanson and Tatge Cu, 1.5405 A, 26°C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*	*A*		*A*	*A*		*A*	*A*		*A*
111	2.38	s	4.04	2.31	67	4.00	2.27	vs	3.93	2.32	67	4.02	2.32	100	4.02	2.325	95	4.027
200	2.05	s	4.02	2.00	100	4.00	1.97	vs	3.94	2.00	100	4.00	2.01	100	4.02	2.013	100	4.027
220	1.46	s	4.076	1.425	67	4.031	1.41	s	3.99	1.422	23	4.022	1.42	80	4.02	1.424	48	4.027
311	1.24	m	4.013	1.213	5	4.023	1.21	m	4.01	1.213	3	4.023	1.212	40	4.020	1.214	10	4.027
222	1.188	m	4.005	1.163	5	4.029	1.16	m	4.02	1.162	3	4.025	1.162	40	4.025	1.1625	11	4.0270
400	1.022	m	4.012	1.008	3	4.032	1.008	m-w	4.032	-----	---	------	1.006	20	4.024	1.0068	9	4.0272
331	0.935	w	4.028	0.922	2	4.019	0.926	m-w	4.036	-----	---	------	0.924	20	4.028	0.9239	8	4.0270
420	.908	s	4.029	.901	4	4.029	.902	s	4.034	-----	---	------	.900	60	4.025	.9005	14	4.0270
422	.826	s	4.032	.823	3	4.032	.825	s	4.042	-----	---	------	-------	---	-----	.8220	13	4.0270
511	.776	s	4.037	-----	---	-----	-----	---	-----	-----	---	------	-------	---	-----	------	---	------
440	-----	--	-----	0.711	1	4.022	-----	---	-----	-----	---	------	-------	---	-----	------	---	------
531	-----	--	-----	.680	1	4.023	-----	---	-----	-----	---	------	-------	---	-----	------	---	------
600	-----	--	-----	.671	2	4.026	-----	---	-----	-----	---	------	-------	---	-----	------	---	------
620	-----	--	-----	.637	1	4.029	-----	---	-----	-----	---	------	-------	---	-----	------	---	------
Average unit cell for last five lines---			4.032	-----	---	4.026	-----	---	4.033	-----	---	[a]4.023	-------	---	4.024	------	---	4.0270

[a] Average for last three lines only.

2.35. Lithium Chloride, LiCl (Cubic)

In table 36 the three patterns for lithium chloride included in the ASTM diffraction pattern file (see table 1) are compared with a pattern prepared at the NBS. The material for the NBS sample was obtained from the Mallinckrodt Chemical Works, labelled with their number SDD, and was accompanied by the following chemical analysis (in percent): N_2O_5, 0.001; SO_3, 0.01; heavy metals, 0.005; Fe, 0.001; other alkalis, 0.02; Cl_2O_5, trace.

The interplanar spacings were converted for the table from kX units to angstroms. The intensity measurements of all four patterns yield 111, 200, and 220 as the three strongest lines to be used as the ASTM index lines. It should be noted that in the flat packed sample used with Geiger counter apparatus the powder easily orients so that the 200 line is strongest. The NBS intensity measurements were made as usual on a loosely packed sample expressly prepared to avoid orientation.

Lithium chloride crystallizes with the NaCl lattice, has the space group O_h^5 ($Fm3m$), and has four molecules in the unit cell. A recent value for the lattice constant is compared with that of the NBS in the following table after conversion to angstrom units at 25°C. The coefficient of expansion of 44.76×10^{-6} [113] was employed in making the corrections.

Unit cell in angstroms at 25°C

1938	Ievinš, Straumanis, and Karlsons [113]	5.13988
1953	Swanson and Tatge	5.1396

The density, calculated from the NBS lattice constant, is 2.074 at 25°C. The index of refraction determined on the material used for the NBS pattern is $n = 1.663$.

TABLE 36. *Lithium chloride, LiCl (cubic)*

hkl	1923 Davey Mo, 0.7093 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A			---- Crystallographic Laboratory Mo, 0.7093 A			1953 Swanson and Tatge Cu, 1.5405 A, 25°C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*	*A*		*A*
111	2.97	100	5.13	2.97	100	5.14	3.02	100	5.31	2.967	100	5.139
200	2.56	100	5.11	2.57	100	5.13	2.60	100	5.19	2.570	86	5.140
220	1.818	70	5.141	1.81	60	5.13	1.83	8	5.19	1.817	58	5.140
311	1.552	38	5.147	1.55	32	5.15	1.56	8	5.18	1.550	29	5.141
222	1.485	8	5.144	1.485	12	5.144	1.489	4	5.158	1.484	16	5.140
400	1.284	4	5.134	1.286	5	5.142	1.287	2	5.146	1.285	4	5.140
331	1.180	5	5.145	1.180	12	5.145	1.181	4	5.149	1.1791	10	5.1396
420	1.149	8	5.140	1.150	14	5.144	1.151	6	5.148	1.1493	12	5.1398
422	1.046	5	5.125	1.050	6	5.144	1.049	6	5.139	1.0491	8	5.1395
511	0.987	5	5.128	0.991	5	5.149	0.989	6	5.139	0.9892	9	5.1399
440	---	---	---	.911	2	5.152	.908	2	5.135	.9086	2	5.1396
531	0.868	3	5.133	.871	3	5.151	---	---	---	.8688	10	5.1397
600	.856	4	5.134	.839	2	5.152	---	---	---	.8566	6	5.1397
620	.812	1	5.133	---	---	---	---	---	---	.8126	4	5.1393
711	.719	1	5.138	---	---	---	---	---	---	---	---	---
Average unit cell for last five lines			5.133	---	---	5.149	---	---	5.144	---	---	5.1396

2.36. Sodium Fluoride, NaF (Cubic)

Three patterns for sodium fluoride (villiaumite) recorded on the ASTM file cards (see table 1) are compared in table 37 with two patterns obtained from the literature and one made at the NBS. Those from the literature are by Debye and Scherrer [64] and by Wasastjerna [244]. A fourth ASTM pattern, from the Crystallographic Laboratory, Cambridge, England, had not been published prior to the ASTM compilation, and as the data were combined on the file card with those of Wyckoff and Armstrong, it is impossible to reproduce it as a separate pattern for comparison in table 37.

The NBS pattern was obtained from a sample numbered 7445 furnished by the J. T. Baker Chemical Company. The NBS chemical laboratory found that the sample complied with ACS specifications. The spectrographic laboratory reported the presence of silicon, 0.001 to 0.01 percent, and no other impurity greater than 0.001 percent. The sample was recrystallized by sublimation before using.

The spacings of the Debye and Scherrer and the Wyckoff and Armstrong patterns of table 37 were calculated directly in angstrom units from the published Bragg angle data. The Davey, the Hanawalt, Rinn, and Frevel, and the Wasastjerna patterns were converted from the kX units of the published data. Thus, the entire table is in angstroms.

The patterns of table 37 agree in showing the 200, 220, and 222 lines as the first, second, and third strongest, respectively. The Wyckoff and Armstrong intensity measurements in their original publication differ considerably from those on either the old or new ASTM cards. They were recalculated for

table 37 directly from the published photometric measurements, which have lost much of their original precision in the versions used on the ASTM cards.

Sodium fluoride has the NaCl structure, space group O_h^5 (Fm3m), with four molecules in the unit cell. In 1939 Straumanis, Ieviņš, and Karlsons [217] found a lattice constant of 4.62345 kX units at 25°C. Converting to angstroms at 25°C, this compares with the NBS value:

Unit cell at 25°C, angstroms

1939	Straumanis, Ieviņš, and Karlsons [217]	4.63279
1953	Swanson and Tatge	4.6342

The coefficient of expansion 36.0×10^{-6} [217] was used. The density of sodium fluoride based on the NBS cell value of the lattice constant is 2.799. The index of refraction was given by Spangenberg [211] as $n_D = 1.3258$.

TABLE 37. *Sodium fluoride, NaF (cubic)*

hkl	1918 Debye and Scherrer Cu, 1.5405 A			1923 Davey Mo, 0.7093 A			1929 Wyckoff and Armstrong Mo, 0.7093 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A			1944 Wasastjerna Cu, 1.5405 A		1953 Swanson and Tatge Cu, 1.5405 A, 26°C		
	d	I	a	d	I	a	d	I	a	d	I	a	d	a	d	I	a
	A		A	A		A	A		A	A		A	A	A	A		A
111	-----	----	-----	-----	----	-----	2.67	4	4.62	-----	----	-----	2.672	4.628	2.680	1	4.692
200	2.35	s	4.70	2.33	100	4.66	2.32	100	4.64	2.32	100	4.64	2.315	4.629	2.319	100	4.638
220	1.66	s	4.70	1.639	67	4.636	1.64	62	4.64	1.64	60	4.64	1.636	4.628	1.639	56	4.636
311	1.42	w	4.71	-----	----	-----	1.396	2	4.630	-----	----	-----	1.396	4.629	1.399	1	4.640
222	1.35	s	4.68	1.338	13	4.635	1.338	16	4.635	1.339	16	4.638	1.336	4.627	1.338	10	4.635
400	1.170	m	4.680	1.160	7	4.640	1.159	5	4.636	1.160	3	4.640	1.157	4.629	1.1588	3	4.6352
331	-----	----	-----	-----	----	-----	-----	----	-----	-----	----	-----	1.062	4.629	1.0633	1	4.6348
420	1.049	s	4.691	1.035	13	4.629	1.037	12	4.638	1.037	8	4.638	1.035	4.629	1.0363	8	4.6345
422	0.958	s	4.693	0.945	7	4.630	0.943	7	4.620	0.948	3	4.644	0.945	4.628	0.9458	7	4.6335
511	.903	vw	4.692	-----	----	-----	.889	1	4.619	-----	----	-----	-----	-----	.8920	1	4.6350
440	.828	m	4.684	0.817	3	4.622	.821	1	4.644	0.823	1	4.656	0.818	4.628	.8192	2	4.6341
531	.788	w	4.662	-----	----	-----	-----	----	-----	-----	----	-----	-----	-----	------	----	------
600	-----	----	-----	0.771	5	4.626	0.774	2	4.644	0.776	1	4.656	-----	-----	------	----	------
620	-----	----	-----	.731	5	4.623	.731	1	4.623	-----	----	-----	-----	-----	------	----	------
622	-----	----	-----	.697	3	4.623	-----	----	-----	-----	----	-----	-----	-----	------	----	------
Average unit cell for last five lines			4.684	-----	----	4.625	-----	----	4.630	-----	----	4.647	-----	4.629	------	----	4.6344

2.37. Potassium Fluoride, KF (Cubic)

Three diffraction patterns, all in the ASTM file, for potassium fluoride (see table 1) are compared with a pattern prepared at the NBS in table 38. The NBS sample was obtained from the J. T. Baker Chemical Company, and accompanied by the following analysis (in percent): insoluble, 0.05; Cl, 0.005; HF (free acid), 0.05; alkali (K_2CO_3), 0.1; K_2SiF_6, 0.05; SO_4, 0.02; SO_3, 0.005; heavy metals (as Pb), 0.003; Fe, 0.001. A spectrographic analysis made at the NBS indicates approximately 0.1 percent sodium present, the only extraneous element recognized greater than 0.01 percent. The presence of 0.1 percent sodium fluoride in solid solution with potassium fluoride decreases the unit-cell size approximately 0.0007 A. As potassium fluoride is very deliquescent, the sample was first dried at 220°C, then mixed with petrolatum before mounting on the X-ray spectrometer.

The spacings of the Davey pattern were converted to angstrom units by recalculating them to agree with a molybdenum wavelength of 0.7093 angstroms rather than the 0.712 used to obtain the published data. The spacings of the remaining ASTM patterns were converted to angstroms from kX units. The Hanawalt, Rinn, and Frevel, and the NBS patterns show the 200, 220, and 111 lines as the three strongest. The 420 and 422 are strong lines also, and, due to focusing and absorption effects, appear in the other two patterns as strong or stronger than the 111 line.

Potassium fluoride has the well known face-centered cubic structure of NaCl, space group O_h^5 (Fm3m), with four molecules in the unit cell. The lattice constants found in the literature are not in close agreement. Several, converted to angstrom units, are compared with that of the NBS in the table below:

Unit cell, in angstroms

1922	Posnjak and Wyckoff [187]	5.37
1929	Broch, Oftedal, and Pabst [38]	5.344
1938	Finch and Fordham[a] [68]	5.367
1948	Mehmel [150]	5.34
1953	Swanson and Tatge (26°C)	5.347

[a]By electron diffraction.

The density, calculated from the NBS lattice constant, is 2.524 at 26°C. The index of refraction was not determined because of the fineness of the sample; it is given by Spangenberg [211] as $n_D = 1.361$.

TABLE 38. *Potassium fluoride, KF (cubic)*

hkl	1923 Davey Mo, 0.7093 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A			---- Crystallographic Laboratory Mo, 0.7093 A			1953 Swanson and Tatge Cu, 1.5405 A, 26°C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*	*A*		*A*
111	3.10	15	5.37	3.09	27	5.35	3.02	40	5.23	3.087	29	5.347
200	2.68	100	5.36	2.67	100	5.34	2.64	100	5.28	2.671	100	5.342
220	1.88	80	5.317	1.88	83	5.32	1.87	80	5.29	1.890	63	5.346
311	1.603	10	5.317	1.60	10	5.31	1.599	20	5.303	1.612	10	5.346
222	1.533	20	5.310	1.54	27	5.33	1.533	40	5.310	1.542	17	5.342
400	1.328	10	5.312	1.336	8	5.344	1.330	40	5.320	1.337	8	5.348
331	1.217	8	5.305	1.225	4	5.340	1.219	20	5.313	1.227	2	5.348
420	1.187	25	5.308	1.193	20	5.335	1.190	80	5.322	1.1946	14	5.342
422	1.083	15	5.306	1.091	10	5.345	1.091	80	5.345	1.0912	8	5.346
511	1.020	5	5.300	1.029	1	5.347	---	---	---	1.0297	3	5.350
440	0.935	5	5.289	0.945	1	5.346	0.945	20	5.346	0.9452	3	5.347
531	.897	5	5.307	.903	1	5.342	.904	40	5.348	.9037	4	5.346
600	.884	8	5.304	.891	2	5.346	---	---	---	.8915	5	5.349
620	.839	8	5.306	.845	1	5.344	---	---	---	.8455	5	5.347
622	.800	8	5.307	---	---	---	---	---	---	.8060	4	5.346
642	.708	8	5.298	---	---	---	---	---	---	---	---	---
Average unit cell for last five lines			5.304	---	---	5.345	---	---	5.335	---	---	5.347

2.38. Potassium Chloride, KCl (Cubic)

The two patterns of potassium chloride (sylvite) in the ASTM file (see table 1), supplemented by two found in the literature, Wasastjerna [244a] and Sidhu [207], are compared in table 39 with a pattern made at the NBS.

The sample used by the NBS was obtained from the Mallinckrodt Chemical Works, and bore the label KYD-1. The following chemi-

cal analysis accompanied it (in percent): Ba, 0.001; Ca, Mg, and NH_4OH ppt, 0.005; Chlorate (ClO_3), 0.001; insoluble, 0.005; Fe, 0.0003; heavy metals, 0.0005; neutrality OK; NO_3, 0.003; N, 0.001; PO_4, 0.002; Na, 0.02; SO_4, 0.005.

The conversion of the interplanar spacings of the patterns of table 39 to angstrom units was made from kX units except in the case of Wasastjerna, from whose data published as $\frac{\sin\theta}{\lambda}$, values were calculated directly in angstrom units. For each pattern the three strongest lines are 200, 220, and 222.

Apparently Bragg [29] is responsible for the original structure determination; he referred to the structure as "simple cubic," that is, face-centered cubic, having the space group O_h^5 (Fm3m). Tu [224] in 1936 determined the coefficient of expansion of potassium chloride as 3.65×10^{-5}. Four measurements of the lattice constant made at specified temperatures are compared, after conversion to angstrom units at 25°C, with the NBS value in the following table:

Unit cell in angstroms at 25°C

1936	Tu [224]	6.29229
1942	Batuecas and Fernandez-Alonso [10]	6.307
1944	Hutchinson [111]	6.30511
1947	Vegard [237]	6.289
1953	Swanson and Tatge	6.2931

Hutchinson, and Batuecas and Fernandez-Alonso did not obtain their lattice constants from X-ray measurements but from precision density determinations. The density calculated from the NBS unit cell is 1.9865 at 25°C. An index of refraction of $n = 1.490$ was obtained for the NBS sample of potassium chloride.

TABLE 39. *Potassium chloride, KCl (cubic)*

hkl	1923 Davey Mo, 0.7093 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A			1944 Wasastjerna Cu, 1.5405 A		1948 Sidhu Cu, 1.5405 A			1953 Swanson and Tatge Cu, 1.5405 A, 25°C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		A	A		A	A	A	A		A	A		A
200	3.1	100	6.24	3.14	100	6.28	3.147	6.294	3.13	vs	6.26	3.146	100	6.292
220	2.21	67	6.25	2.21	60	6.25	2.224	6.290	2.21	s	6.25	2.224	59	6.290
222	1.812	20	6.277	1.81	14	6.27	1.817	6.294	1.81	m	6.27	1.816	23	6.291
400	1.567	7	6.268	1.57	6	6.28	1.573	6.292	1.57	w	6.28	1.573	8	6.292
420	1.403	17	6.274	1.404	12	6.279	1.407	6.292	1.41	m	6.31	1.407	20	6.292
422	1.281	10	6.275	1.283	6	6.285	1.285	6.295	1.28	m	6.27	1.284	13	6.290
440	1.110	3	6.279	1.110	2	6.279	1.112	6.294	1.11	w	6.28	1.1126	2	6.2938
600	1.045	7	6.270	1.049	2	6.294	1.049	6.294	1.05	w	6.30	1.0490	6	6.2940
620	0.991	3	6.268	0.993	2	6.280	0.9948	6.2917	0.994	w	6.287	0.9951	2	6.2936
622	.994	3	6.261	-------	---	-------	.9485	6.2930	.950	w	6.302	.9486	3	6.2923
444	.905	3	6.270	-------	---	-------	.9083	6.2929	.912	vw	6.319	.9083	1	6.2929
640	.869	3	6.266	-------	---	-------	.8727	6.2931	.875	w	6.310	.8727	2	6.2931
642	.840	3	6.271	-------	---	-------	.8409	6.2927	.843	m	6.308	.8410	6	6.2934
Average for last five lines			6.267	-------	---	6.283	--------	6.2927	-------	--	6.305	--------	---	6.2931

2.39. Potassium Bromide, KBr (Cubic)

The two ASTM patterns of potassium bromide (see table 1), one from the literature (Wasastjerna [243]), and a pattern prepared at the NBS are compared in table 40. The material for the NBS pattern was obtained from the J. T. Baker Chemical Company, numbered 111642, and accompanied by the following analysis (in percent): insoluble, 0.001; PO_4, 0.000; SO_4, 0.003; heavy metals, 0.0001; KOH, 0.002; N,

0.0001; Ca, Mg, and NH_4OH ppt, 0.003; Cl, 0.1; BrO_3, 0.001; Ba, 0.002; Fe, 0.0001. It was checked at the NBS and found to comply with ACS reagent standards.

After the calculation of the Wasastjerna spacings from the given $\frac{\sin\theta}{\lambda}$ data, the interplanar spacings of the three published patterns were converted from kX to angstrom units. Two errors in entering intensity measurements on the Davey ASTM card were corrected for the 1950 file. The three lines 200, 220, and 420 are recognized as the first, second, and third strongest lines, respectively, in each of the four patterns.

Potassium bromide has a face-centered cubic lattice [29], space group O_h^5 (Fm3m), and four molecules to the unit cell. Three determinations of the lattice constant, given at specified temperatures, are compared below with the NBS determination, all reduced to angstrom units at 25°C. A recent determination of the coefficient of expansion is 40.5×10^{-6} [52].

Unit cell in angstroms at 25°C

1926	Ott [172]	6.600
1942	Batuecas and Fernandez-Alonso [10]	6.616
1947	Vegard [237]	6.593
1953	Swanson and Tatge	6.6000

Batuecas and Fernandez-Alonso did not obtain their lattice constant from X-ray measurements but calculated it from a pycnometric density determination of high precision. The density, calculated from the NBS diffraction data, is 2.7533 at 25°C. The index of refraction of the specimen used for the NBS pattern was determined as $n = 1.559$.

TABLE 40. *Potassium bromide,* KBr *(cubic)*

hkl	1923 Davey Mo, 0.7093 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A			1944 Wasastejerna Cu, 1.5405 A		1953 Swanson and Tatge Cu, 1.5405 A, 25°C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*a*	*d*	*I*	*a*
	A		A	A		A	A	A	A		A
111	3.79	20	6.56	----	----	----	3.804	6.589	3.81	15	6.60
200	3.28	100	6.55	3.30	100	6.59	3.296	6.592	3.300	100	6.600
220	2.33	90	6.57	2.34	42	6.60	2.330	6.590	2.333	57	6.599
311	1.961	15	6.563	----	----	----	1.987	6.590	1.990	7	6.600
222	1.899	50	6.577	1.89	10	6.56	1.903	6.592	1.905	16	6.599
400	1.641	15	6.565	1.64	7	6.57	1.648	6.592	1.650	10	6.600
331	1.513	8	6.595	----	----	----	1.512	6.591	1.514	2	6.599
420	1.468	60	6.565	1.471	17	6.578	1.474	6.592	1.476	17	6.601
422	1.346	30	6.592	1.346	7	6.592	1.345	6.589	1.347	8	6.599
511	----	----	----	----	----	----	1.268	6.589	1.270	2	6.599
440	1.164	8	6.586	1.166	3	6.598	1.1651	6.5909	1.1666	3	6.5993
531	----	----	----	----	----	----	1.1141	6.5911	1.1157	1	6.6006
600	1.098	10	6.589	1.097	3	6.583	1.0984	6.5904	1.1000	5	6.6000
620	1.038	10	6.565	1.042	3	6.591	1.0422	6.5915	1.0437	4	6.6009
533	----	----	----	----	----	----	1.0052	6.5915	----	----	----
622	0.991	5	6.573	----	----	----	0.9937	6.5915	0.9949	4	6.5994
444	----	----	----	----	----	----	.9514	6.5915	.9527	2	6.6002
711	----	----	----	----	----	----	.9230	6.5915	.9241	1	6.5997
640	----	----	----	----	----	----	.9141	6.5917	.9153	2	6.6003
642	----	----	----	----	----	----	.8808	6.5913	.8819	3	6.5995
731	----	----	----	----	----	----	.8582	6.5919	.8594	1	6.6002
Average unit cell for last five lines	----		6.581	----	----	6.588	----	6.5916	----	----	6.6000

2.40. Potassium Iodide, KI (Cubic)

Three patterns for potassium iodide included in the ASTM file of powder diffraction patterns (see table 1) are compared in table 41 with a pattern found in the literature, Wasastjerna [244], and one prepared at the NBS. The specimen used for the NBS pattern was obtained from B. R. Elk & Company, sample No. E-PF-3, accompanied by the following analysis, denoting higher purity than required by ACS specifications (in percent): alkali, 0.04; Ba, 0.002; Ca, Mg, and NH_4OH ppt, 0.005; Cl and Br, 0.01; insoluble, 0.005; IO_3, 0.0003; Fe, 0.0003; heavy metals (as Pb), 0.0005; H_2O, 0.20; N, 0.002; PO_4, 0.005; Na, 0.03; SO_4, 0.01. Annealing at 450°C for a half hour presumably was accompanied by elimination of the water.

The spacings of the patterns were either calculated directly in angstrom units from the Bragg angle data given or were converted from kX to angstrom units. There is general agreement that the first two strongest lines are 200 and 220, but the Davey and the Olshausen patterns show 420 as third strongest, while the Hanawalt, Rinn, and Frevel pattern agrees with that of the NBS in showing the 111 line as third strongest.

TABLE 41. *Potassium iodide, KI (cubic)*

hkl	1923 Davey Mo, 0.7093 A			1925 Olshausen Cu, 1.5405 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A			1944 Wasastjerna Cu, 1.5405 A		1953 Swanson and Tatge Cu, 1.5405 A, 25°C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*	*A*	*A*	*A*		*A*
111	4.08	30	7.06	4.02	m	6.97	4.09	40	7.08	4.08	7.07	4.08	42	7.07
200	3.54	100	7.07	3.58	s	7.15	3.54	100	7.07	3.533	7.066	3.53	100	7.06
220	2.50	80	7.05	2.49	s	7.03	2.51	80	7.08	2.499	7.067	2.498	70	7.065
311	2.13	30	7.07	2.13	m	7.05	2.13	24	7.07	2.130	7.050	2.131	29	7.065
222	2.04	40	7.08	2.04	m	7.07	2.03	32	7.04	2.040	7.066	2.039	27	7.063
400	1.767	20	7.052	1.75	m	7.01	1.76	16	7.05	1.765	7.061	1.767	15	7.068
331	1.623	10	7.075	1.62	w	7.05	1.62	8	7.07	1.621	7.067	1.621	7	7.066
420	1.581	70	7.071	1.58	s	7.06	1.58	32	7.08	1.580	7.066	1.580	24	7.066
422	1.445	40	7.078	1.44	m	7.08	1.445	24	7.078	1.443	7.067	1.442	14	7.064
511	1.359	9	7.060	1.36	w	7.07	1.361	5	7.070	1.360	7.067	1.360	3	7.067
440	1.250	10	7.068	1.25	w	7.06	1.240	3	7.068	1.249	7.065	1.249	2	7.065
531	1.196	6	7.078	1.19	w	7.06	1.196	3	7.078	1.1943	7.0656	1.1944	3	7.0662
600	1.174	10	7.046	1.18	m	7.11	1.178	8	7.070	1.1778	7.0666	1.1776	5	7.0656
620	1.116	10	7.060	1.12	w	7.09	1.119	5	7.079	1.1173	7.0668	1.1167	3	7.0626
------	-------	----	-------	-------	--	------	1.097	2	-------	--------	--------	--------	----	--------
533	-------	----	-------	-------	--	------	1.082	2	7.096	1.0777	7.0667	1.0779	1	7.0683
622	1.063	9	7.052	1.07	w	7.07	1.069	3	7.092	1.0653	7.0666	1.0650	3	7.0641
444	-------	----	-------	1.02	vw	7.05	-------	----	-------	1.0199	7.0664	1.0195	1	7.0633
711	-------	----	-------	0.985	vw	7.03	0.992	2	7.084	0.9896	7.0670	0.9895	2	7.0664
640	-------	----	-------	-------	--	------	.982	2	7.081	.9799	7.0659	.9800	3	7.0668
642	0.942	10	7.048	0.949	m	7.10	-------	----	-------	.9442	7.0657	.9442	4	7.0657
731	-------	----	-------	.927	w	7.12	-------	----	-------	.9199	7.0662	.9199	1	7.0659
800	-------	----	-------	-------	--	------	-------	----	-------	.8833	7.0662	.8831	2	7.0648
820	-------	----	-------	-------	--	------	-------	----	-------	.8568	7.0655	.8569	3	7.0662
822	-------	----	-------	0.842	s	7.14	-------	----	-------	.8328	7.0663	.8326	1	7.0648
Average unit cell for last five lines-----			7.057	-------	--	7.09	-------	----	7.086	--------	7.0660	-------	-----	7.0655

Potassium iodide has the NaCl structure [253], face-centered cubic, with four molecules to the unit cell, and space group O_h^5 (Fm3m). Lattice constants of several investigators are compared as follows (Finch and Fordham obtained theirs from electron diffraction measurements):

Unit cell in angstroms

1922	Clark and Duane [50]	7.064
1923	Davey [57]	7.050
1924	Havighurst, Mack, and Blake [92]	7.052
1925	Olshausen [170]	7.040
1936	Finch and Fordham [68]	7.078
1953	Swanson and Tatge (25°C)	7.0655

The density calculated from the NBS lattice constant is 3.1257 at 25°C. The index of refraction of the sample used by the Bureau was determined as $n = 1.668$.

2.41. Calcium Fluoride, CaF_2 (Cubic)

Calcium fluoride (fluorite) is represented in table 42 by four patterns reproduced in the ASTM file (see table 1), one appearing in the literature, Gerlach [78], and one prepared at the NBS.

The sample of calcium fluoride used for the NBS pattern was prepared by D. C. Stockbarger at the Massachusetts Institute of Technology. Spectrographic analysis at the NBS showed arsenic, boron, iron, magnesium, silicon, and strontium less than 0.001 percent each, and silver and copper less than 0.0001 percent.

The spacings of the Gerlach pattern were computed for table 42 in angstrom units directly from the published Bragg angle data. Those of the four remaining patterns, which appear on the ASTM cards, were converted from kX units to angstroms. Of these, only the Hanawalt, Rinn, and Frevel pattern is known to be previously published. As can readily be seen from the unit-cell calculations of the table, the precision of the Jessop-United Steel Companies and the United Steel Companies patterns fully justifies the use of four decimal places in the high-angle part of the patterns, arbitrarily abbreviated in the version of the pattern given on the 1950 edition of the ASTM cards. The British Museum pattern, appearing only in the 1950 edition, is possibly abbreviated also. In performing this abbreviation, the 444 interplanar spacings of the Hanawalt, Rinn, and Frevel pattern should be given 0.79 rather than the 0.80 appearing on the card (the published value appearing on the original ASTM card is 0.789). The Gerlach pattern of 1922 is the only one to show a line for the 200 plane; this, marked very very weak, may well be in error.

All patterns give the strongest line as 220. Two of the British patterns give the 111 and 311 lines the same intensity, recording these as second and third strongest lines; the United Steel Companies pattern is completely at variance here, with 422 and 531 listed second and third strongest. The Hanawalt, Rinn, and Frevel pattern and that of the NBS list the three strongest lines as 220, 111, and 311.

It is difficult to get unoriented intensity measurements for CaF_2. The perfect cleavage of the 111 plane caused considerable variation in the first few of several patterns made at the NBS. Only after diluting the sample with finely ground silica gel and drifting it very carefully into the specimen holder were consistent values obtained. CaF_2 is one of the few materials in which the question of orientation is critical in determining the strongest line for indexing, as in most cases cleavage plane reflections are inherently the strongest. With CaF_2 the planes of the 111 form, which bound the eight sides of a cleavage particle, are easily oriented to produce the strongest reflections. The 220 is the strongest reflection in an unoriented sample. Flat specimens prepared for Geiger-counter equipment will without extraordinary precaution invariably show the 111 as the strongest indexing line.

The structure was determined by W. H. Bragg [30] in 1914. The lattice is face-centered cubic, the space group O_h^5 (Fm3m), with four molecules to the unit cell. Published lattice constants, supposedly in kX units, were converted to angstroms and are compared with the NBS value.

Unit cell, angstroms

1922	Gerlach [78]	5.466
1927	Thilo [221]	5.55
1930	Rumpf [198]	5.460
1933	Schumann [205]	5.462
1939	Zintl and Udgard [263]	5.479
1953	Swanson and Tatge (25°C)	5.4626

The density of calcium fluoride, in accordance with the NBS lattice constant, is 3.181 at 25°C. The index of refraction of the sample used for the NBS pattern is $n = 1.433$.

TABLE 42. *Calcium fluoride, CaF_2 (cubic)*

hkl	1922 Gerlach Cu, 1.5405 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A			---- Jessop United Steel Mo, 0.7093 A			---- United Steel Mo, 0.7093 A			---- British Museum Cu, 1.5405 A			1953 Swanson and Tatge Cu, 1.5405 A, 25°C		
	d	I	a	d	I	a	d	I	a	d	I	a	d	I	a	d	I	a
	A		A	A		A	A		A	A		A	A		A	A		A
111	3.15	m	5.46	3.17	67	5.49	3.154	70	5.463	3.153	70	5.461	3.11	80	5.39	3.153	94	5.461
200	2.74	vvw	5.48	-----	---	-----	------	---	------	------	---	------	----	---	----	------	---	------
220	1.94	s	5.49	1.93	100	5.46	1.932	100	5.465	1.931	100	5.462	1.90	100	5.37	1.931	100	5.462
311	1.65	s	5.47	1.65	50	5.47	1.647	70	5.462	1.646	70	5.459	1.63	80	5.41	1.647	35	5.462
222	-----	---	-----	-----	---	-----	------	---	------	------	---	------	----	---	----	1.577	2	5.463
400	1.37	m	5.48	1.37	23	5.48	1.366	40	5.464	1.365	60	5.460	1.36	60	5.44	1.366	12	5.464
331	1.25	ms	5.45	1.259	23	5.488	1.254	50	5.466	1.253	60	5.462	1.25	60	5.45	1.253	10	5.462
422	1.12	s	5.49	1.119	30	5.482	1.1153	70	5.4639	1.114	90	5.457	1.11	80	5.44	1.1150	16	5.4624
511	1.050	ms	5.456	1.052	10	5.466	1.0515	50	5.4638	1.0510	70	5.4612	1.05	50	5.46	1.0512	7	5.4622
440	0.964	ms	5.453	0.970	6	5.487	0.9659	50	5.4640	0.9654	70	5.4611	----	---	----	0.9657	5	5.4628
531	.924	s	5.466	.927	7	5.484	.9236	60	5.4641	.9231	90	5.4611	----	---	----	.9233	7	5.4623
600	-----	---	-----	-----	---	-----	------	---	------	.9101	50	5.4606	----	---	----	.9105	1	5.4630
620	0.863	ms	5.458	0.868	5	5.490	------	---	------	------	---	------	----	---	----	.8637	9	5.4625
533	.833	ms	5.462	.837	2	5.489	------	---	------	------	---	------	----	---	----	.8330	3	5.4623
444	-----	---	-----	.791	1	5.480	------	---	------	------	---	------	----	---	----	------	---	------
711	-----	---	-----	.769	2	5.491	------	---	------	------	---	------	----	---	----	------	---	------
642	-----	---	-----	.732	5	5.478	------	---	------	------	---	------	----	---	----	------	---	------
731	-----	---	-----	.714	3	5.484	------	---	------	------	---	------	----	---	----	------	---	------
822	-----	---	-----	.645	1	5.473	------	---	------	------	---	------	----	---	----	------	---	------
Average unit cell for last five lines	5.459			-----	---	5.481	------	---	[1]5.4640	------	---	[1]5.4610	----	---	5.44	------	---	5.4626

[1] Average for last four lines only.

2.42. Barium Fluoride, BaF_2 (Cubic)

The two ASTM patterns of barium fluoride (see table 1) are compared in table 43 with one of two published by Broch, Oftedal, and Pabst [37], of which the more nearly complete is given in the table, along with a pattern made at the NBS.

The NBS sample was a specially purified material supplied by the Mallinckrodt Chemical Works. Their spectrographic analysis showed 0.01 to 0.1 percent of sodium and strontium.

The interplanar spacings for the Thilo and for the Broch, Oftedal, and Pabst patterns

were computed for table 43 directly in angstroms from the published Bragg angle data. The Hanawalt, Rinn, and Frevel values were converted to angstroms from kX units. For the Thilo pattern the values of the unit cell for the last ten lines are within 0.005 of each other, indicating that the interplanar spacings are accurate to the third decimal place in this part of the pattern. Only the second place is recorded on the ASTM cards of both the old and new (1950) files. The first three spacings of the Thilo pattern as they appear on the ASTM card are calculated values to fit the unit cell dimension based on the high angle diffraction lines. The intensity measurements published by Thilo and those recorded on the ASTM card are both given in the table (columns I^a and I^b). The Hanawalt, Rinn, and Frevel, and the NBS measurements agree relatively well; the three strongest lines of both patterns are 111, 220, and 311.

Barium fluoride has the fluorite structure, a face-centered cubic lattice, space group O_h^5 (Fm3m), and four molecules to the unit cell. Several published lattice constants, assumed to be in kX units, compare with the NBS value thus:

Unit cell, angstroms

1922	Davey [56]	6.21
1927	Thilo [221]	6.21
1933	Schumann [205]	6.199
1953	Swanson and Tatge (26°C)	6.2001

TABLE 43. *Barium fluoride*, BaF_2 *(cubic)*

hkl	1927 Thilo Cu, 1.5405 A				1929 Broch, Oftedal, and Pabst Cu, 1.5405 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A			1953 Swanson and Tatge Cu, 1.5405 A, 26°C		
	d	I^a	I^b	*a*	*d*	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A			*A*	*A*		*A*	*A*		*A*	*A*		*A*
111	3.61	m	70	6.25	-------	-----	-------	3.59	100	6.22	3.58	100	6.20
200	3.12	w	50	6.24	-------	-----	-------	3.10	25	6.20	3.100	30	6.200
220	2.206	s	100	6.240	2.194	s	6.205	2.19	100	6.19	2.193	79	6.203
311	1.875	s	100	6.219	1.868	s	6.195	1.86	80	6.17	1.870	51	6.202
222	1.798	w	50	6.228	1.789	m	6.197	1.78	15	6.17	1.790	3	6.201
400	1.553	w	50	6.212	-------	-----	-------	1.55	15	6.20	1.550	6	6.2000
331	1.426	s	100	6.216	1.420	s	6.190	1.423	32	6.203	1.423	13	6.2027
420	1.392	m	70	6.225	1.385	m	6.194	1.385	18	6.194	1.386	6	6.1983
422	1.268	s	100	6.212	1.264	m	6.192	1.265	32	6.197	1.266	14	6.2021
511	1.195	s	100	6.209	1.192	m	6.194	1.192	20	6.194	1.1933	6	6.2006
440	1.098	w	50	6.211	1.094	w	6.198	1.097	5	6.206	1.0959	2	6.1993
531	1.050	s	100	6.212	-------	-----	-------	1.047	15	6.194	1.0481	6	6.2006
600	1.035	m	70	6.210	-------	-----	-------	1.033	3	6.198	1.0332	1	6.1992
620	0.981	s	100	6.204	-------	-----	-------	0.980	6	6.198	0.9803	2	6.2000
533	.947	m	70	6.212	-------	-----	-------	.946	3	6.203	.9455	1	6.2001
622	.937	m	70	6.213	-------	-----	-------	.935	2	6.202	.9347	3	6.2001
444	-------	-----	-----	-------	-------	-----	-------	-------	-----	-------	.8948	1	6.1994
711	0.869	s	100	6.204	-------	-----	-------	0.868	3	6.199	.8682	4	6.2002
640	.861	m	70	6.209	-------	-----	-------	.861	2	6.209	.8599	1	6.2008
642	-------	-----	-----	-------	-------	-----	-------	.829	5	6.204	.8285	5	6.1999
731	-------	-----	-----	-------	-------	-----	-------	-------	-----	-------	.8072	6	6.2002
Average unit cell for last five lines				6.208	-------	-----	6.191	-------	-----	6.203	-------	-----	6.2001

[a] Published. [b] ASTM card.

The lattice constant (6.20) given on the ASTM card for the Thilo pattern is that of Thilo and not, as designated, of Wyckoff (written "Wys" in error for "Wy_2", Wyckoff, vol. 2). The density calculated from the NBS lattice constant is 4.886 at 26°C. The index of refraction obtained for the sample used is $n = 1.472$.

2.43. Mercurous Chloride, Hg_2Cl_2 (Tetragonal)

Four ASTM patterns of mercurous chloride (calomel) (see table 1) are compared in table 44 with a pattern prepared at the NBS using a sample from the General Chemical Company, labelled No. 1891. The spectrographic analysis made at the Bureau indicated only traces

TABLE 44. *Mercurous chloride, Hg_2Cl_2 (tetragonal)*

hkl	1925 Havighurst Mo, 0.7093 A		1926 Hylleraas Fe, 1.9360 A		1928 Ruff, Ebert, and Luft Cu, 1.5405 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A		1953 Swanson and Tatge Cu, 1.5405 A, 26°C	
	d	*I*	*d*	*I*	*d*	*I*[a]	*I*[b]	*d*	*I*	*d*	*I*
	A		A		A			A		A	
101	4.13	90	4.13	80	4.05	s	80	4.17	100	4.14	97
110	3.15	100	3.163	100	3.129	vs	100	3.18	100	3.164	100
103	2.806	10	2.849	15	----------	------	------	2.84	8	2.824	9
004	2.718	30	2.717	40	2.688	vw	20	2.73	30	2.727	28
200	2.234	20	2.233	40	2.215	ms	70	2.24	30	2.242	23
114	2.061	50	2.071	80	2.043	m	60	2.06	60	2.065	53
211	1.959	70	1.959	100	1.940	vs	100	1.97	80	1.970	38
105										1.962	47
213	----------	------	1.748	10	----------	------	------	----------	------	1.755	1
204	1.731	20	1.728	50	1.714	m	60	1.73	35	1.731	16
220	1.578	15	1.579	30	1.562	s	80	1.58	8	1.584	10
301	1.472	25	1.473	80	1.460	m	60	1.481	40	1.475	15
215											
310	1.413	8	1.411	40	1.403	m	60	1.420	16	1.417	4
224	1.366	15	1.367	50	1.356	m	60	1.369	16	1.380	8
008										1.365	4
314	1.254	20	1.253	80	1.246	mw	50	1.263	20	1.257	5
118										1.253	6
321	1.231	8	1.231	50	1.220	mw	50	1.239	6	1.233	3
305											
109	1.167	15	1.168	80	1.160	w	40	1.173	16	1.1694	5
208											
400	----------	------	1.122	10	----------	------	------	1.129	2	1.1179	<1
411	1.079	6	1.079	60	1.071	mw	50	1.085	6	1.0801	1
325											
330	----------	------	1.054	10	1.050	mw	50	1.062	2	1.0552	<1
219	1.035	15	1.036	100	1.028	m	60	1.040	14	1.0362	6
404											
228											
420	----------	------	----------	------	----------	------	------	1.005	2	----------	-----
334	0.983	4	----------	------	0.978	mw	50	0.989	2	0.9823	1
318											
415	----------	------	----------	------	----------	------	------	----------	------	.9723	1
309	0.938	6	----------	------	0.936	mw	50	0.944	2	.9404	1
424											

[a] Published. [b] ASTM card.

of Cu and Fe, and faint traces of Al, Mg, and Si; the limit of detection of the alkali elements is about 0.05 percent.

The Havighurst [90] pattern was made with molybdenum radiation for which a wavelength of 0.710 angstrom was given. The interplanar spacings were converted to the angstrom unit used here in accordance with the change in wavelength assigned to the radiation. The Hylleraas [112] spacings were published as Bragg angle measurements, and were converted to interplanar spacings directly in angstroms for table 44. The spacings of the Ruff, Ebert, and Luft [196] and the Hanawalt, Rinn, and Frevel [85] patterns were measured in kX units, and were converted to angstroms. The NBS pattern resolves three lines not separated in previous patterns, resulting in a different selection of the three strongest lines. Where previous patterns had always included the combined 211-105 among the ASTM index lines, although not always in the same position, the NBS pattern shows the 110, 101, and 114 lines first, second, and third strongest, respectively.

Mercurous chloride has a tetragonal lattice, space group D_{4h}^{17} (I4/mm) [143], and two molecules of Hg_2Cl_2 in the unit cell. The lattice constant a was determined for the NBS sample from an average of five calculations from $hk0$ planes, c from an average of five calculations from hkl planes with 0 or low h and k values. These are compared with earlier determinations thus:

Unit cell in angstroms

		a	c
1925	Havighurst [90]	4.48	10.91
1926	Mark and Steinbach [143]	4.46	10.91
1946	Frevel, Rinn, and Anderson [75]	4.47	10.91
1953	Swanson and Tatge (26°C)	4.478	10.91

The density from the NBS lattice constant is 7.176 at 26°C. The indices of refraction were not measured on the NBS sample. Havighurst refers to the birefringence as the strongest known, and quotes values for the indices: $\omega_D = 1.97325$ (which is miscopied on the ASTM card as 1.97525) and $\epsilon_D = 2.6559$.

2.44. Mercuric Chloride, $HgCl_2$ (Orthorhombic)

The two patterns for mercuric chloride in the X-ray diffraction file of the ASTM (see table 1) are compared in table 45 with one recently prepared at the Bureau. The Hanawalt, Rinn, and Frevel pattern, omitted from the original ASTM index, is included in the 1950 index. In the original index the index lines of this pattern (the three strongest lines 4.35, 3.00, 2.70) are mistakenly assigned to mercuric chlorate [1]. The NBS pattern was obtained from a J. T. Baker Chemical Co. sample numbered 101742. Spectrographic analysis at the NBS showed no impurity greater than 0.01 percent.

The data of Bräkken and Harang were published as a table of hkl indices, $\sin^2\theta$ values, and intensity values visually estimated. For table 45 the $\sin^2\theta$ values were converted to interplanar spacings, using the iron radiation wavelength 1.93597 A. The spacings of Hanawalt, Rinn, and Frevel were converted from kX units to angstroms. The 120 line is the strongest for all three patterns. The second strongest is the 200, but this line is not resolved from the 031 line by Hanawalt, Rinn, and Frevel, so that their intensity measurement is a combination of the two intensities. The 011 and 111 are third and fourth strongest in the Hanawalt, Rinn, and Frevel pattern, reversed for the NBS pattern. The difference in intensity is probably too small to be significant; it is not due to the radiation used, as the conversion factor for molybdenum to copper radiation is close to 1 in this range ([1] page 108 of index covering original set of cards, or card no. vii of introduction to 1950 file).

In indexing the pattern the unit-cell dimensions were taken in the Dana convention, c<a<b, although the reverse order is sometimes given. The unit cell dimensions published in 1934 by Braekken and Scholten [27] converted from kX units to angstroms compare

thus with those derived from the NBS pattern:

Unit cell, angstroms

		a	b	c
1934	Braekken and Scholten [27]	5.975	12.761	4.334
1951	Swanson and Tatge (26°C)	5.96	12.76	4.32

The presence of hkO lines only if k is even, and hOl lines only if h + l is even, agrees with the generally accepted orthorhombic space group determination D_{2h}^{16} (Pmnb) for the crystal orientation used here. The density of the material, calculated from the NBS lattice constant, is 5.49 at 26°C. The indices of refraction are higher than 1.75.

TABLE 45. *Mercuric chloride,* $HgCl_2$ *(orthorhombic)*

hkl	1928 Brakken and Harang Fe, 1.936 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A		1953 Swanson and Tatge Cu, 1.5405 A, 26°C	
	d	I	d	I	d	I
	A		A		A	
120	4.34	vs	4.36	100	4.35	100
011	4.08	s	4.11	25	4.10	38
021	3.57	w	-------	-----	3.58	3
101	3.488	w	-------	-----	3.51	1
111	3.368	s	3.41	38	3.383	31
040	3.172	w	3.21	13	3.188	11
121	3.056	vw	-------	-----	3.066	2
031	3.019	w	3.01	75	3.033	21
200	2.976	s			2.986	48
131	2.692	s	2.70	50	2.707	36
220						
211	2.403	m	2.41	25	2.420	14
141	2.348	w	-------	-----	2.366	2
221	2.281	vw	-------	-----	2.297	4
051	2.194	w	-------	-----	2.202	2
002	2.158	vw	2.18	13	2.182	6
012	2.120	m	2.12	25	2.132	9
231						
060						
151	2.056	m	2.06	25	2.065	13
112	1.997	m	2.00	50	2.004	16
241	1.929	m	1.94	25	1.940	11
061	1.895	w	1.90	13	1.902	8
132	1.829	w	-------	-----	1.837	1
301	1.806	vw	-------	-----	1.810	1
042	1.784	m	1.79	13	1.791	6
311						
251	1.762	w	-------	-----	1.769	4

TABLE 45. *Mercuric chloride,* $HgCl_2$ *(orthorhombic)*—Con.

hkl	1928 Brakken and Harang Fe, 1.936 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.709 A		1953 Swanson and Tatge Cu, 1.5405 A, 26°C	
	d	I	d	I	d	I
	A		A		A	
202	1.745	vw	-------	-----	1.765	1
071	1.674	vw	-------	-----	1.681	<1
331	1.658	w	1.67	13	1.666	4
052	1.643	m	-------	-----	1.653	<1
232	-------	-----	1.62	13	1.619	3
080	1.589	m	1.59	13	1.595	1
341	1.569	vw	-------	-----	1.572	1
180	1.531	m	1.54	13	1.539	2
081	1.489	w	-------	-----	1.496	1
312	-------	-----	1.455	13	1.454	4
013	-------	-----	-------	-----	1.431	1
023	-------	-----	-------	-----	1.406	3

2.45. Mercuric Iodide, HgI_2 (Tetragonal)

The ASTM file of diffraction patterns contains three cards for mercuric iodide (see table 1) of which one (No. 3-1281) records only unit cell measurements. The patterns of the other two are compared in table 46 with a pattern prepared at the NBS.

The sample used for the NBS pattern was from Mallinckrodt Chemical Works, and was stated to be of ACS purity. Spectrographic analysis at the NBS shows a trace of iron and faint traces of calcium, chromium, magnesium, and silicon.

The interplanar spacings of the Havighurst pattern were reduced to angstroms in accordance with the wavelength given for the X radiation. The spacings of the Hanawalt, Rinn, and Frevel pattern were converted to angstroms from kX units. The line 200-114-201 is not resolved in the ASTM patterns, and appears very strong—even stronger than the 200-114 and 201 combined for the NBS pattern. Thus in the Havighurst pattern this is the strongest line, and in the Hanawalt, Rinn, and Frevel pattern it is equally as strong as the 102. The NBS pattern shows the three strongest lines as 102, 101, and the combination 200-114.

TABLE 46. *Mercuric iodide, HgI_2 (tetragonal)*

hkl	1925 Havighurst Mo, 0.7093 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A		1953 Swanson and Tatge Cu, 1.5405 A, 26°C	
	d	*I*	*d*	*I*	*d*	*I*
	A		A		A	
002	6.186	40	6.2	30	6.20	28
101	4.112	40	4.12	80	4.12	83
102	3.559	50	3.57	100	3.57	100
004	-------	---	-------	-------	3.091	8
103	3.003	20	3.01	30	3.006	39
112	2.753	25	2.77	40	2.766	42
104	2.520	2	-------	-------	2.533	4
200, 114, 201	2.181	100	2.18	100	2.190	73
					2.165	9
202, 006	2.061	8	2.05	12	2.075	7
					2.064	6
211, 203	1.923	10	1.92	14	1.932	13
212, 106	1.861	25	1.86	25	1.873	12
					1.864	17
213	1.761	8	1.76	10	1.770	8
116	-------	---	-------	-------	1.719	1
214, 205, 107	1.645	6	1.65	6	1.654	3
					1.648	3
					1.644	1
220, 008, 215	1.539	10	1.54	12	1.556	5
					1.545	9
					1.540	6
222, 206	1.498	7	1.50	8	1.504	5
300, 108, 301	1.453	3	-------	-------	1.465	2
					1.447	2
302, 216	1.415	9	1.421	6	1.423	5
311, 303, 207	1.374	3	1.374	4	1.374	2
312	1.342	6	1.349	4	1.349	4
313, 217, 109	1.312	5	1.317	4	1.317	1
					1.315	4
314, 208, 305	1.259	10	1.263	14	1.267	4
					1.263	8
					1.260	5
226, 0·0·10	1.235	3	-------	-------	1.239	2
218					1.217	1
321, 315	1.215	2	-------	-------	1.206	1

TABLE 46. *Mercuric iodide, HgI_2 (tetragonal)*—Con.

hkl	1925 Havighurst Mo, 0.7093 A		1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A		1953 Swanson and Tatge Cu, 1.5405 A, 26°C	
	d	*I*	*d*	*I*	*d*	*I*
	A		A		A	
322	-------	---	-------	-------	1.1914	1
306, 1·0·10	1.187	6	-------	-------	1.1898	3
323, 209	-------	---	-------	-------	1.1631	2
316	1.155	6	-------	-------	1.1539	3
1·1·10	-------	---	-------	-------	1.1423	1
324	-------	---	-------	-------	1.1309	1
307, 219	1.124	5	-------	-------	1.1283	<1
400, 228	-------	---	-------	-------	1.0954	4
401, 325, 317, 1·0·11	1.088	8	-------	-------	1.0924	3
411, 403	-------	---	-------	-------	1.0562	1
412, 326, 2·1·10	1.044	5	-------	-------	1.0456	2
413	-------	---	-------	-------	1.0272	1
332	-------	---	-------	-------	1.0169	1
420, 334, 1·1·12	0.976	7	-------	-------	0.9776	2
422, 406, 2·2·10	-------	---	-------	-------	.9661	1
336, 3·1·10	0.920	3	-------	-------	---------	---
505, 339, 3·2·11, 4·0·10, 2·0·14	.821	4	-------	-------	---------	---

Mercuric iodide belongs to the tetragonal system. It has a space group of D_{4h}^{15} ($P4_2/nmc$) [15], with two molecules in the unit cell. The unit cell measurements derived from the NBS powder pattern are compared below with those of other workers after conversion to angstroms from kX units:

Unit cell, in angstroms

		a	c
1926	Bijvoet, Claassen, and Karssen [15]	4.366	12.38
1927	Huggins and Magill [99]	4.35	12.36
1953	Swanson and Tatge (26°C)	4.390	12.38

The density on the basis of the NBS determined unit cell is 6.325 at 26°C.

2.46. Lead Fluochloride, PbFCl (Tetragonal)

The 1950 ASTM X-ray diffraction file includes two patterns for lead fluochloride (see table 1); one, of natural matlockite, is from the mineral type locality of Matlock, Derbyshire, England, furnished by the British Museum (Natural History), London; the other, from synthetic material, was first published in 1932 by Nieuwenkamp and Bijvoet. In 1933 Nieuwenkamp [162] compared patterns of matlockite, whose formula was then given as Pb_2OCl_2, and synthetic PbFCl, showing their identity. In table 47 the two ASTM patterns are compared with one prepared at the Bureau from material of high purity obtained from the NBS chemical laboratory. The sample had been prepared as part of a project for the precise determination of fluorine.

The data published on the Nieuwenkamp and Bijvoet pattern do not include interplanar spacings; for table 47 they were calculated directly in angstroms from the $\sin^2\theta$ values listed. The interplanar spacings of the British Museum pattern, presumably in kX units, were converted to angstroms. Although the interplanar spacings of the patterns check closely, the intensity measurements vary. The NBS and British Museum patterns agree that 101 is the strongest line, but the Nieuwenkamp and Bijvoet pattern shows the last line (312) strongest, with the second and third strongest in close proximity. The 002, the second strongest line of the NBS pattern, is unresolved in the others. The third and fourth strongest lines of the NBS pattern appear as second and third strongest in the British Museum pattern.

Bannister [5] in 1934 gave the structure as tetragonal, space group D^7_{4h} (P4/nmm), and postulated two molecules in the unit cell. A Nieuwenkamp and Bijvoet determination of the lattice constant, converted to angstroms, compares thus with the NBS value:

Unit cell angstroms

		a	c
1932	Nieuwenkamp and Bijvoet [164]	4.09	7.21
1951	Swanson and Tatge (25°C)	4.106	7.23

The density, in accordance with the NBS lattice constant, is 7.13 at 26°C. The NBS sample was too finely powdered to determine the indices of refraction; Bannister found $\omega_D = 2.145$, $\epsilon_D = 2.006$.

TABLE 47. *Lead fluochloride, PbFCl (tetragonal)*

hkl	1932 Nieuwenkamp and Bijvoet Cr, 2.2896 A		---- British Museum ----		1953 Swanson and Tatge Cu, 1.5405 A, 26°C	
	d	I	d	I	d	I
	A		A		A	
001	-------	-----	7.2	40	7.22	20
002	-------	-----	-------	-----	3.61	70
101	3.58	48	3.55	100	3.56	100
110	2.905	28	2.90	70	2.904	47
102	2.719	28	2.70	70	2.714	35
003	2.410	6	2.40	20	2.409	6
112	2.262	51	2.25	80	2.263	38
103	2.074	20	2.07	70	2.079	14
200	2.052	34	1.99	60	2.053	24
201	1.954	23	1.96	40	1.974	1
113	1.852	17	1.84	60	1.855	4
004	-------	-----	-------	-----	1.808	1
211	1.780	66	1.77	80	1.780	36
104	1.654	40	1.65	70	1.654	11
212	1.635	28	1.63	60	1.637	7
203	1.560	14	1.558	20	1.564	1
213	1.462	31	1.461	60	1.461	4
220	-------	-----	-------	-----	1.452	3
005	1.447	34	1.443	60	1.448	1
221	1.417	37	-------	-----	--------	------
105	1.363	23	-------	-----	--------	------
222, 301	1.344	66	1.343	60	1.346	3
310	1.298	68	-------	-----	1.299	4
115	-------	-----	-------	-----	1.293	3
214	1.285	89	-------	-----	1.289	5

TABLE 47. *Lead fluochloride, PbFCl (tetragonal)*—Con.

hkl	1932 Nieuwenkamp and Bijvoet Cr, 2.2896 A		---- British Museum ----------		1953 Swanson and Tatge Cu, 1.5405 A, 26°C	
	d	I	d	I	d	I
	A		A		A	
302 311	1.281	17	1.276	70	1.281	1
223	-------	-----	1.240	20	1.244	1
312	1.220	100	1.222	60	1.223	2
006	-------	-----	-------	-----	1.2041	1
303	-------	-----	-------	-----	1.1911	2
205	-------	-----	1.181	60	1.1826	2
106	-------	-----	1.156	60	1.1565	2
313	-------	-----	1.142	40	1.1443	1
215	-------	-----	-------	-----	1.1386	1
321	-------	-----	1.126	50	1.1254	1
304	-------	-----	-------	-----	1.0922	1
322	-------	-----	1.089	50	1.0863	1
323	-------	-----	-------	-----	1.0300	1
400	-------	-----	1.027	60	1.0265	1
216	-------	-----	1.008	60	1.0078	2
402	-------	-----	-------	-----	0.9872	2
117	-------	-----	-------	-----	.9735	1
330	-------	-----	-------	-----	.9664	2
324	-------	-----	-------	-----	.9639	3
412	-------	-----	-------	-----	.9608	2
207	-------	-----	-------	-----	.9223	1
413	-------	-----	-------	-----	.9203	1
420	-------	-----	-------	-----	.9185	1

2.47. Potassium Cyanide, KCN (Cubic)

The card file of diffraction patterns of the ASTM contains three cards for potassium cyanide (see table 1). Only two of these give patterns, the third [3-1299] recording only a unit cell dimension. In table 48 the two patterns are compared with one produced at the NBS. The NBS pattern was obtained from a Mallinckrodt Chemical Works sample marked lot GNB. An analysis furnished by the chemical laboratory of the NBS follows (in percent): Cl, 0.05; PO_4, 0.005; SO_4 (total S), 0.005; Fe, 0.03; Pb, 0.0000; Na, <0.05.

For table 48 the spacings of both ASTM patterns were converted from kX to angstrom units. The table shows the published inter-

TABLE 48. *Potassium cyanide, KCN (cubic)*

hkl	1931 Natta and Passerini Fe, 1.9360 A				
	d^a	d^b	I^a	I^b	a
	A	A			A
111	3.656	3.77	m	60	6.333
200	3.177	3.27	vs	100	6.355
-------	2.598	2.67	vw	20	--------
220	2.263	2.31	vs	100	6.400
-------	2.137	2.17	vw	20	--------
311	1.939	1.970	ms	70	6.431
222	1.862	1.886	ms	70	6.449
400	1.618	1.633	mw	50	6.473
331	1.486	1.498	m	60	6.477
420	1.454	1.461	m	60	6.502
422	1.330	1.334	m	60	6.514
511	1.255	1.255	m	60	6.519
531	1.102	1.102	m	60	6.521
600	---------	---------	-------	-------	--------
620	---------	---------	-------	-------	--------
622	---------	---------	-------	-------	--------
711	---------	---------	-------	-------	--------
Average unit cell for last five lines----------					6.507

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A			1953 Swanson and Tatge Cu, 1.5405 A, 25°C		
	d	I	a	d	I	a
	A		A	A		A
111	3.78	10	6.54	3.77	17	6.53
200	3.27	100	6.53	3.260	100	6.520
-------	---------	------	---------	------	---	-----
220	2.31	63	6.52	2.307	39	6.525
-------	---------	------	---------	------	---	-----
311	1.96	13	6.51	1.968	11	6.527
222	1.88	10	6.52	1.885	10	6.529
400	1.63	6	6.53	1.630	2	6.520
331	1.496	6	6.521	1.496	4	6.523
420	1.461	9	6.530	1.458	4	6.522
422	1.330	5	6.514	1.332	2	6.524
511	1.255	3	6.519	1.256	1	6.527
531	1.102	1	6.521	1.1036	1	6.529
600	---------	------	---------	1.0880	1	6.528
620	---------	------	---------	1.0321	1	6.528
622	---------	------	---------	0.9837	1	6.525
711	---	------	---------	.9140	1	6.527
Average unit cell for last five lines----------			6.521	------	---	6.527

[a] Published data. [b] As recorded on ASTM card.

planar spacings of the Natta and Passerini pattern as well as the version given on the ASTM card, which is recalculated from a unit cell derived from the last two lines. Two of the lines of this pattern are extraneous to the NaCl structure postulated for potassium cyanide and are not indexed. The three strongest lines are the same for all patterns—200, 220, and 311.

Potassium cyanide has the NaCl structure [159] with a disordered CN group, a face-centered cubic lattice, and four molecules to the unit cell. Unit cell measurements have not been of very high accuracy. A few, converted to angstrom units, are given below:

Unit cell in angstroms

1921	Cooper [53]	6.55
1922	Bozorth [22]	6.56
1931	Natta and Passerini [159]	6.51
1953	Swanson and Tatge (25°C)	6.527

The density calculated from the NBS unit cell value is 1.555 at 25°C. The index of refraction determined on the NBS sample is $n = 1.413$.

2.48. Sodium Cyanide, NaCN (Cubic)

The ASTM file contains two cards for the cubic form of sodium cyanide (see table 1), the patterns of which are compared in table 49 with a pattern prepared at the NBS. The NBS sample was obtained from the J. T. Baker Chemical Company; it was numbered 121444. The chemical laboratory of the NBS reports that the material satisfies ACS standards, and gives the following analysis (in percent): NaCN, 96.2; Cl, 0.02; FeCN, 0.00; SO_4, 0.00; S, 0.003; Thiocyanite, 0.02; Remainder CO_3 and H_2O.

The spacings of the ASTM patterns were corrected from kX to angstrom units for the table. The Natta and Passerini pattern lists several reflections extraneous to the face-centered cubic structure postulated for sodium cyanide. In order to record this pattern on the ASTM card, a unit cell of 5.83 was calculated from the interplanar spacings of the

TABLE 49. *Sodium cyanide, NaCN (cubic)*

hkl	1931 Natta and Passerini Fe, 1.9360 A					1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A			1953 Swanson and Tatge Cu, 1.5405 A, 26°C		
	d^a	d^b	I^a	I^b	a^c	d	I	a	d	I	a
	A	*A*			*A*	*A*		*A*	*A*		*A*
111	3.300	3.38	m	60	5.715	---	---	---	3.41	1	5.90
200	2.872	2.93	vs	100	5.743	2.95	100	5.89	2.951	100	5.902
---	2.572	2.62	vvw	10	---	---	---	---	---	---	---
---	2.352	2.39	vw	20	---	---	---	---	---	---	---
220	2.044	2.06	vs	100	5.782	2.07	53	5.86	2.085	35	5.898
---	1.930	1.949	vw	20	---	---	---	---	---	---	---
---	1.835	1.850	vw	20	---	---	---	---	---	---	---
311	1.752	1.762	mw	50	5.809	1.77	7	5.88	1.779	10	5.901
222	1.677	1.686	m	60	5.811	1.69	9	5.86	1.702	6	5.897
---	1.609	1.619	vvw	10	---	---	---	---	---	---	---
400	1.455	1.462	mw	50	5.820	1.47	5	5.89	1.472	3	5.888
331	1.339	1.341	mw	50	5.835	1.352	3	5.892	1.352	2	5.895
420	1.306	1.306	m	60	5.839	1.318	5	5.893	1.318	4	5.895
422	1.191	1.191	mw	50	5.837	1.202	1	5.891	1.202	1	5.890
511	1.126	1.126	mw	50	5.852	1.135	1	5.899	1.1347	1	5.8961
Average unit cell for last five lines					5.837	---	---	[d]5.894	---	---	5.893

[a] Published data. [b] As recorded on ASTM card. [c] Refers to spacings of d^a column. [d] Average for last four lines only.

last three planes, and from this value the remaining spacings were recalculated, including the five lines which do not belong to the NaCN pattern. In the table both the originally published and the ASTM versions of the pattern are given. The NBS Geiger-counter diagram for sodium cyanide showed extraneous lines due to sodium carbonate and the strong line of the orthorhombic form of NaCN. These were not listed in the table. All three patterns list 200 and 220 as the first and second strongest lines. The intensities of 311 and 222 are very close—the earlier patterns show 222 as the third strongest line, while the NBS pattern shows 311 third strongest.

The room temperature form of sodium cyanide is face-centered cubic and has four molecules to the unit cell—that is, NaCl structure [159] with disordered CN group. Some recent lattice constants, corrected from kX to angstrom units, compare with that determined at the NBS as follows:

Unit cell in angstroms

1931	Natta and Passerini [159]	5.84
1938	Verweel and Bijvoet [240]	5.88
1953	Swanson and Tatge [26°C]	5.893

The density was calculated from the NBS lattice constant as 1.591 at 26°C. The index of refraction of the NBS material was determined as $n = 1.453$.

2.49. Sodium Cyanide, NaCN (Orthorhombic)

Sodium cyanide has a reversible inversion point from the cubic form at room temperature to an orthorhombic form at 10°C. A pattern was made at the NBS with the temperature maintained between 6° and 7°C. This is compared in table 50 with a pattern in the ASTM file (see table 1), made at -10°C by Verweel and Bijvoet [240]. The NBS sample is described in section 2.48. on the cubic form of sodium cyanide.

The spacings in table 50 for the Verweel and Bijvoet pattern were calculated in angstrom units from published $\sin^2\theta$ values. The NBS diagram showed lines due to carbonate contamination as well as weak lines due to the presence of the cubic form, which are not given in the pattern of table 50. The three strongest lines are recorded in the NBS pattern as 110, 002, and 112.

The space group C_{2v}^{20} (Imm) has been repeatedly assigned to the orthorhombic form of sodium cyanide on the basis of the determination

TABLE 50. *Sodium cyanide, NaCN (orthorhombic)*

hkl	1939 Verweel and Bijvoet Cu, 1.5405 A, -10°C		1953 Swanson and Tatge Cu, 1.5405 A, 6° to 7°C	
	d	*I*	*d*	*I*
	A		*A*	
011	----------	---------	3.60	<1
101	----------	---------	3.039	<1
110	2.962	vvs	2.947	100
002	2.852	s	2.822	70
020	2.363	m	2.379	14
112	2.027	vs	2.039	45
121, 200	1.879	ms	1.889	15
022	1.813	mw	1.810	4
013	1.735	vvw	1.750	2
103, 211	1.671	w	1.675	1
202	1.562	m	1.569	12
031	1.513	mw	1.515	5
220	1.473	w	1.473	8
130	----------	---------	1.454	1
004	1.408	w	1.410	4
123	1.368	w	1.372	2
222	1.303	w	1.306	3
213	----------	---------	1.280	2
114	1.269	mw	1.273	1
310	1.209	mw	1.214	3
033			1.206	1
040, 231	1.1795	mw	1.1805	1
204	1.1228	vw	1.1294	1
312	1.1066	mw	1.1151	3
141			1.1027	<1
015, 042, 321	1.0863	vvw	----------	---------
303	----------	---------	1.0530	<1
224, 233	1.0161	w	----------	---------

of Verweel and Bijvoet, who, however, suggest the possible alternatives of D_2^8 (I222) or D_{2h}^{25} (Immm). There are two molecules in the unit cell. The NBS pattern as indexed satisfies the requirements of any one of these three groups. The Verweel and Bijvoet unit cell determination compares thus with that of the NBS:

Unit cell, in angstroms

		a	b	c
1938	Verweel and Bijvoet (-10°C) [240]	3.75	4.72	5.62
1953	Swanson and Tatge (6° to 7°C)	3.774	4.719	5.640

The density on the basis of the unit cell dimensions determined from the NBS pattern is 1.620 at 6° to 7°C.

2.50. Strontium Nitrate, $Sr(NO_3)_2$ (Cubic)

A pattern for strontium nitrate is compared in table 51 with two previously published patterns. The first, by Vegard [236] in 1922, was well indexed and misses few lines, although it is of less precision than the later patterns. The data were published as sin θ values and estimated intensities. The former were converted to interplanar spacings in angstrom units for table 51. The second pattern, by Hanawalt, Rinn, and Frevel, included in the diffraction pattern file of the ASTM (see table 1), was converted from kX to angstrom units.

The sample for the NBS pattern was a specially purified material supplied by the Mallinckrodt Chemical Works. Their spectro-

TABLE 51. *Strontium nitrate, $Sr(NO_3)_2$ (cubic)*

hkl	1922 Vegard Cu, 1.5405 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A			1951 Swanson and Tatge Cu, 1.5405 A, 26°C		
	d	I	a	d	I	a	d	I	a
	A		A	A		A	A		A
111	4.54	m	7.86	4.51	100	7.81	4.48	100	7.76
200	3.92	m	7.84	3.92	33	7.84	3.88	13	7.76
210	3.53	w	7.89	3.49	33	7.80	3.474	21	7.768
211	3.22	w	7.89	----	----	----	3.175	14	7.777
220	2.78	w	7.87	----	----	----	2.749	19	7.775
311	2.37	s	7.86	2.36	100	7.83	2.346	72	7.781
222	2.27	s	7.85	2.24	100	7.76	2.246	54	7.780
400	1.96	m	7.84	1.94	17	7.76	1.945	12	7.780
411	----	----	----	----	----	----	1.836	2	7.789
331	1.80	m	7.86	1.78	17	7.76	1.785	16	7.781
420	1.75	m	7.84	1.75	17	7.83	1.740	12	7.782
422	1.60	m	7.81	1.58	17	7.74	1.589	10	7.784
333	1.51	m	7.84	1.50	17	7.79	1.498	12	7.784
521	----	----	----	----	----	----	1.420	2	7.778
440	1.39	m	7.84	1.379	17	7.801	1.376	11	7.784
531	1.32	s	7.83	1.318	17	7.797	1.315	10	7.780
600	1.30	w	7.81	----	----	----	1.296	4	7.776
620	1.24	w	7.82	----	----	----	1.231	2	7.786
533	1.20	m	7.84	----	----	----	1.1867	4	7.782
622	1.176	m	7.80	----	----	----	1.1736	1	7.785
444	1.128	w	7.82	----	----	----	1.1235	2	7.784
711	1.094	m	7.81	----	----	----	1.0893	3	7.779
642	1.045	m	7.82	----	----	----	1.0396	3	7.780
731	1.017	s	7.81	----	----	----	1.0128	5	7.780
732	----	----	----	----	----	----	0.9878	2	7.778
820	0.951	s	7.84	----	----	----	.9435	4	7.780
422	.927	s	7.86	----	----	----	.9168	4	7.779

TABLE 51. *Strontium nitrate, $Sr(NO_3)_2$ (cubic)*—Con.

hkl	1922 Vegard Cu, 1.5405 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A			1951 Swanson and Tatge Cu, 1.5405 A, 26°C		
	d	I	a	d	I	a	d	I	a
	A		A	A		A	A		A
751	0.902	s	7.81	----------	---------	----------	0.8983	5	7.780
840	.873	m	7.80	----------	---------	----------	----------	---------	----------
911	.857	s	7.81	----------	---------	----------	----------	---------	----------
842	.851	s	7.80	----------	---------	----------	----------	---------	----------
664	.833	w	7.81	----------	---------	----------	----------	---------	----------
Average unit cell for last five lines			7.81	----------	---------	[a] 7.799	----------	---------	7.779

[a] Average of last two lines only.

graphic analysis shows Ba <0.01 percent and Na <0.01 percent as the only impurities greater than traces.

From the intensity measurements of the NBS pattern, the three strongest lines are the 111, 311, and 222, consistent with the index lines of the ASTM card for the Hanawalt, Rinn, and Frevel pattern.

The lattice of strontium nitrate is simple cubic, four molecules to the unit cell. The space group according to Jaeger and Van Melle [115] is T_h^6(Pa3); Vegard and Bilberg [238] confirm this, but indicate the possibility of T^4 ($P2_13$). The patterns of table 51 show hk0 only if h is even, adding confirmation of the T_h^6(Pa3) group. Three published lattice constants are converted from kX to angstrom units and compared with the NBS determination in the table below. Vegard and Boer [239] present a coefficient of expansion between 10° and 70°C of 2.58×10^{-5}. This was used to modify their lattice constant determination to correspond to that of the NBS made at 26°C.

Unit cell dimensions, angstroms

1922	Vegard [236]	7.81
1932	Ringdal [192]	7.827
1942	Vegard and Boer (26°C) [239]	7.7818
1951	Swanson and Tatge (26°C)	7.779

The density from the NBS lattice constant is 2.986 at 26°C. The index of refraction is $n = 1.587$.

2.51. Barium Nitrate, $Ba(NO_3)_2$ (Cubic)

The pattern for barium nitrate (nitrobarite) closely parallels that for strontium nitrate. Vegard [236] and Hanawalt, Rinn, and Frevel published patterns of which the latter is included in the ASTM file (see table 1).

The NBS sample was specially purified material supplied by the Mallinckrodt Chemical Works. Their spectrographic analysis indicates the following impurities: Al <0.01 percent, Na <0.01 percent, and Sr <0.01 percent.

In Vegard's paper the data were published as sin θ values. For comparison with the data in table 52, they were converted to interplanar spacings in angstroms. The pattern of Hanawalt, Rinn, and Frevel was converted from kX to angstrom units for this table. The three strongest lines, used as index lines for the ASTM cards, are the same for the NBS and the Hanawalt, Rinn, and Frevel patterns: 311, 111, and 222.

The lattice of barium nitrate is simple cubic, four molecules to the unit cell. The patterns of table 52 confirm the determination of the space group T_h^6(Pa3) by Jaeger and Van Melle [115] and by Vegard and Bilberg [238].

Three published lattice constants are converted from kX to angstrom units and compared with the NBS determination in the table below. Vegard and Boer [239] present a coefficient of expansion between 10° and 70°C of

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TABLE 52. *Barium nitrate, $Ba(NO_3)_2$ (cubic)*

hkl	1922 Vegard Cu, 1.5405 A			1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A			1951 Swanson and Tatge Cu, 1.5405 A, 26°C		
	d	*I*	*a*	*d*	*I*	*a*	*d*	*I*	*a*
	A		*A*	*A*		*A*	*A*		*A*
111	4.70	s	8.14	4.70	75	8.14	4.68	95	8.11
200	3.93	s	7.86	4.07	30	8.14	4.06	40	8.12
210	----------	----------	----------	3.63	15	8.12	3.63	11	8.12
211	----------	----------	----------	3.32	10	8.13	3.313	14	8.115
220	2.87	m	8.12	2.88	40	8.15	2.870	35	8.118
311	2.45	vs	8.13	2.45	100	8.13	2.448	100	8.119
222	2.34	s	8.11	2.35	50	8.14	2.343	55	8.116
400	2.03	m	8.12	2.02	20	8.08	2.029	17	8.116
411	----------	----------	----------	----------	----------	----------	1.914	21	8.120
331	1.86	m	8.11	1.86	40	8.11	1.862	21	8.116
420	1.81	m	8.09	1.81	30	8.09	1.815	20	8.117
422	1.66	m	8.13	1.65	30	8.08	1.657	15	8.118
333	1.56	m	8.11	1.56	30	8.11	1.562	15	8.116
440	1.44	m	8.15	1.436	15	8.123	1.435	5	8.118
531	1.37	vs	8.11	1.373	40	8.123	1.372	18	8.117
600	----------	----------	----------	1.354	10	8.124	1.353	7	8.118
611	----------	----------	----------	1.321	1	8.143	----------	----------	----------
620	1.29	w	8.16	1.283	8	8.114	1.284	1	8.121
533	----------	----------	----------	1.240	13	8.131	1.238	1	8.118
622	1.23	m	8.16	1.224	13	8.119	1.224	2	8.119
444	1.17	w	8.11	1.172	4	8.120	1.1721	2	8.121
711	----------	----------	----------	1.139	10	8.134	1.1370	3	8.120
640	----------	----------	----------	1.128	6	8.134	1.1261	1	8.120
642	----------	----------	----------	1.087	13	8.134	1.0849	1	8.119
731	----------	----------	----------	1.058	20	8.127	1.0566	5	8.116
800	----------	----------	----------	----------	----------	----------	1.0150	1	8.120
733	----------	----------	----------	----------	----------	----------	0.9918	1	8.118
820	----------	----------	----------	----------	----------	----------	.9843	1	8.117
822	----------	----------	----------	----------	----------	----------	.9567	1	8.118
751	----------	----------	----------	----------	----------	----------	.9374	3	8.118
662	----------	----------	----------	----------	----------	----------	.9312	1	8.118
840	----------	----------	----------	----------	----------	----------	.9078	1	8.120
911	----------	----------	----------	----------	----------	----------	.8911	7	8.118
842	----------	----------	----------	----------	----------	----------	.8858	3	8.119
931	----------	----------	----------	----------	----------	----------	.8512	4	8.120
933	----------	----------	----------	----------	----------	----------	.8159	5	8.118
10·2·0	----------	----------	----------	----------	----------	----------	.7960	3	8.118
Average unit cell for last five lines			8.14			8.130			8.119

1.75×10^{-5}. This was used to modify their lattice constant determination to correspond to that of the NBS made at 26°C.

The density calculated from the NBS lattice constant is 3.244 at 26°C. The index of refraction is $n = 1.570$.

Unit cell, angstroms

1922	Vegard [236]	8.11
1932	Ringdal [192]	8.127
1942	Vegard and Roer (26°C) [239]	8.1172
1951	Swanson and Tatge (26°C)	8.119

2.52. Zinc Borate, ZnB_2O_4 (Cubic)

No published pattern for zinc borate was found. The following pattern is offered by the NBS as an addition to the ASTM file. The sample used for the pattern of table 53 was one of the phosphor preparations of the Radio Corporation of America [135], sample XII-17, of high purity. The unit cell derived from an average of the values obtained from the last five lines is 7.4726 A, at 26°C. The lattice derived from the powder pattern is body-centered cubic, with six molecules in the unit cell. The density based on the NBS lattice constant is 3.605 at 26°C. The index of refraction for the sample was determined as $n = 1.739$.

TABLE 53. *Zinc borate, ZnB_2O_4 (cubic)*

hkl	1951 Swanson and Tatge Cu, 1.5405 A, 26°C			hkl	1951 Swanson and Tatge Cu, 1.5405 A, 26°C		
	d	I	a		d	I	a
	A		A		A		A
110	5.29	6	7.48	710	1.0568	1	7.473
200	3.74	3	7.48	640	1.0365	1	7.474
211	3.048	100	7.466	721	1.0169	3	7.473
310	2.364	23	7.476	642	0.9991	1	7.477
222	2.158	1	7.476	730	.9812	2	7.4726
321	1.997	20	7.472	732	.9490	1	7.4724
400	1.869	13	7.476	811	.9198	3	7.4725
411	1.761	38	7.471	820	.9062	1	7.4727
420	1.672	2	7.477	653	.8932	1	7.4730
332	1.594	3	7.477	822	.8807	1	7.4730
422	1.526	25	7.476	831	.8687	3	7.4728
510	1.466	5	7.475	662	.8573	1	7.4738
521	1.364	8	7.471	752	.8462	1	7.4734
440	1.321	4	7.473	910	.8252	1	7.4725
530	1.282	3	7.475	842	.8153	1	7.4723
600	1.246	1	7.476	921	.8058	1	7.4727
611	1.213	2	7.477	664	.7966	1	7.4728
620	1.1817	1	7.474	930	.7877	1	7.4728
541	1.1531	3	7.473				
631	1.1025	1	7.478	Average for last five lines			7.4726
444	1.0788	1	7.474				

2.53. Magnesium Silicate, Mg_2SiO_4 (Orthorhombic)

Two patterns for magnesium silicate (forsterite) in the ASTM file (see table 1) are compared in table 54 with a pattern prepared at the NBS. The NBS was furnished with a sample of high purity, labeled X-9, by the Radio Corporation of America. The material had been prepared in connection with a phosphor project [135] as a solid state reaction, at 1,500°C. The large unit cell of magnesium silicate furnishes a large number of the possible planar reflections for an X-ray diagram with copper radiation. Thus, indexing becomes increasingly difficult with increasing Bragg angle. As θ increases, Clark's interplanar spacings diverge more and more widely from the values calculated for indexing the NBS pattern. The last 20 lines of his pattern were omitted from the table because the divergence combined with the multiplicity of possible lines makes indexing purely arbitrary. The Geiger counter intensity measurements of the NBS pattern show 112 to be the strongest line, 131 second, and 222 third, rather than the order 222, 131, and 112 estimated by Clark himself, 222, 112, 131 given on the ASTM card for Clark, or 222, 021, 130 on the pattern of Hanawalt, Rinn, and Frevel.

Forsterite is orthorhombic with a space group presumably the same as that specified by Bragg and Brown [32] for olivine, V_h^{16}, or D_{2h}^{16} (Pbnm). There are four molecules in the unit cell. Although several sets of unit-cell dimensions are available for the closely related mineral olivine (iron-bearing), only one was found for forsterite. Rinne [193] in 1923 examined a natural forsterite from Vesuvius, for which he found dimensions which agree very closely with olivine measurements. Converting from kX to angstrom units, his values compare with those derived from the NBS pattern thus:

Unit cell, angstroms

		a	b	c
1923	Rinne [193]	4.75	10.28	6.00
1951	Swanson and Tatge (26°C)	4.76	10.20	5.99

From the NBS data the cell dimensions were calculated from spacings only of planes parallel to one or more axes. The density

calculated from the cell dimensions of the NBS determination is 3.213 at 26°C. The material was too finely powdered to determine the indices of refraction.

TABLE 54. *Magnesium silicate, Mg_2SiO_4 (orthorhombic)*

hkl	1938 Hanawalt, Rinn, and Frevel Mo, 0.7093 A		1946 Clark Co, 1.7889 A			1953 Swanson and Tatge Cu, 1.5405 A, 26°C	
	d	I	d	I[a]	I[b]	d	I
	A		A			A	
020	5.1	11	5.1	vvw	10	5.11	26
021	3.90	40	3.86	ms	70	3.88	69
101	3.73	5	3.71	vw	20	3.73	25
111 } 120	3.50	20	3.49	vw	20	3.487	21
121	3.00	13	2.98	vw	20	3.000	17
002	---	---	2.87	vvw	10	---	---
130	2.78	40	2.75	ms	70	2.768	53
131	2.52	32	2.50	s	80	2.513	73
112	2.45	40	2.45	s	90	2.458	100
041	---	---	2.34	vvw	10	2.348	9
210	---	---	2.31	vvw	10	2.316	9
122	2.26	40	2.26	w	40	2.268	59
140	---	---	2.24	w	40	2.250	33
211	2.15	11	2.15	vw	20	2.161	15
132	2.02	2	2.03	vvw	10	2.034	5
042	1.95	2	1.934	vvw	10	1.945	4
150	1.88	3	1.864	vvw	10	1.878	5
113	1.81	3	1.798	vvw	10	1.811	2
151	---	---	1.776	vvw	10	1.792	3
222	1.74	100	1.737	vs	100	1.748	60
240	---	---	1.729	vvw	10	---	---
241	1.67	10	1.661	vw	20	1.670	13
061	1.62	11	1.624	vw	20	1.636	12
133	---	---	1.607	vw	20	1.618	15
152	1.57	8	1.579	vvw	10	1.589	2
043	---	---	1.560	vvw	10	1.572	10
301	---	---	1.523	vvw	10	1.531	1
311 } 213 } 320	---	---	1.504	vvw	10	1.514	10
004	1.493	32	1.487	w	40	1.497	27
062	---	---	1.471	ms	70	1.479	30
330	---	---	1.424	vvw	10	1.438	4
170	1.398	20	1.385	vw	20	1.396	13
233	---	---	---	---	---	1.394	9
322	1.353	28	1.341	w	40	1.351	17
134	1.318	10	1.305	vw	20	1.316	9
332	---	---	1.285	vvw	[c]10	1.295	2
204	---	---	---	---	---	1.266	1

[a] Published.
[b] ASTM card.
[c] Twenty additional lines omitted.

2.54. Magnesium Tungstate, $MgWO_4$ (Monoclinic)

Four patterns, all from the literature, of magnesium tungstate are compared in table 55 with a pattern prepared at the NBS. Two of these are by Broch [39], one by Fonda [70], and one by Dunning and Megaw [65]. Broch supplied most of the indices. In addition to the indices his data include diffraction angles and, for the second pattern, estimated intensities. The interplanar spacings listed in table 55 were computed from his reflection angles so that they appear in angstroms. The Fonda and the Dunning and Megaw interplanar spacings were converted from presumed kX units to angstroms.

For the NBS pattern, material of exceptionally high purity was obtained from the Radio Corporation of America, marked No. 4, prepared at 1,000°C.

There is not notable agreement among the patterns on the strongest lines, chiefly because of the large number of lines of high intensity and the fact that the intensities are only estimated except for the NBS pattern. For the pattern of the Bureau the three strongest lines are the 111, 011, and 100.

Broch's 1930 paper [39] gives the space group as C_{2h}^4 (P2/c), two molecules in the unit cell. The unit-cell constants of the monoclinic magnesium tungstate crystals were given by Broch from his first pattern as $a=4.67$, $b=5.66$, $c=4.92$, $\beta=89°35'$, from his second pattern as $a=4.68$, $b=5.66$, $c=4.93$, $\beta=89°40'$. Converted from kX units to angstroms, the later values compare with those derived from the NBS pattern thus:

Unit cell, angstroms

		a	b	c	β
1930	Broch [39]	4.69	5.67	4.94	89°40'
1951	Swanson and Tatge (26°C)	4.69	5.68	4.92	89°40'

The density calculated from the NBS lattice constant is 6.897 at 26°C. The material was too finely powdered to determine the indices of refraction; it is known that they are higher than 1.75.

TABLE 55. *Magnesium tungstate, $MgWO_4$ (monoclinic)*

hkl	1928 Broch Cu, 1.5405 A	1930 Broch Fe, 1.9360 A		1944 Fonda Mo, 0.7093 A		1946 Dunning and Megaw Cu, 1.5405 A		1953 Swanson and Tatge Cu, 1.5405 A, 26°C	
	d	*d*	*I*	*d*	*I*	*d*	*I*	*d*	*I*
	A	*A*		*A*		*A*		*A*	
010	6.24	5.69	s	5.60	s	5.66	w	5.68	21
100	4.64	4.69	s	4.65	s	4.68	s	4.68	91
011	3.72	3.71	s	3.72	s	3.70	ms	3.70	97
110	3.60	3.60	m	3.61	f	3.60	m	3.607	39
111	2.91	2.91	s	2.91	s	2.94	ms	2.928	100
$\bar{1}11$	----------	2.90	s	----------	---------	2.92	ms	2.902	86
020	2.84	2.69	m	----------	---------	2.84	m	2.841	20
002	2.46	2.47	s	2.46	m	2.46	ms	2.462	47
021		2.45	s						
120	2.43	2.42	vw	----------	---------	2.42	mw	2.426	11
200	2.34	2.34	w	2.34	m	2.34	m	2.346	10
012	2.26	2.27	w	----------	---------	2.26	vvw	2.260	1
102	2.18	2.19	s	----------	---------	2.20	mw	2.194	26
121	2.17	2.17	s	2.18	m	2.17	ms	2.173	28
$\bar{1}21$								2.170	27
----------	2.16	2.15	vvw	----------	---------	----------	---------	----------	---------
112	2.03	2.04	vw	----------	---------	2.05	w	2.047	5
$\bar{1}12$		2.03	vw	----------	---------	2.02	w	2.026	4
211	1.98	1.99	m	----------	---------	1.991	mw	1.993	13
$\bar{2}11$	1.97	1.97	m	1.97	w	1.975	m	1.975	15
030	1.89	1.89	s	----------	---------	1.892	mw	1.892	3
022	1.86	1.86	m	1.88	w	1.860	m	1.862	5
220	1.81	1.81	s	1.80	w	1.813	m	1.806	10
130	1.75	1.75	vvs	1.75	m	1.754	ms	1.754	21
122	----------	---------	---------	----------	---------	1.738	w	1.735	2
$\bar{1}22$	1.73	---------	---------	----------	---------	1.726	vw	1.724	3
202	----------	1.71	---------	----------	---------	1.712	ms	1.708	16
221						1.705	ms	1.702	16
$\bar{2}21$	1.69	1.69	vs	1.696	m	1.692	s	1.689	22
$\bar{2}02$									
131	1.65	---------	---------	----------	---------	1.659	vw	1.652	1
$\bar{1}31$									
003	----------	---------	---------	----------	---------	1.639	vw	1.639	1
212	1.62	---------	---------	----------	---------	1.622	vw	1.617	1
$\bar{2}12$									
013	1.58	---------	---------	1.574	f	1.581	mw	1.578	4
300	----------	---------	---------	----------	---------	1.566	w	1.565	1
032	1.50	---------	---------	----------	---------	1.505	ms	1.502	10
113	1.493	---------	---------	1.497	m	1.494	m	1.499	5
$\bar{1}13$	1.489	---------	---------	----------	---------	1.477	m	1.491	1
230	1.470	---------	---------	----------	---------	1.466	w	1.473	2
222	----------	---------	---------	----------	---------	1.465	w	1.465	3
$\bar{2}22$	1.454	---------	---------	----------	---------	1.451	ms	1.448	8
311	1.438	---------	---------	----------	---------	1.438	ms	1.434	13
$\bar{3}11$									
132	1.428	---------	---------	1.427	m	1.427	ms	1.426	10
$\bar{1}32$	1.426	---------	---------	----------	---------	----------	---------	1.423	12
320	[a] 1.365	---------	---------	[b] 1.365	w	----------	---------	1.364	5

[a] 18 additional lines have been omitted.

[b] 7 additional lines have been omitted.

3. References

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4. Cumulative Index to Volumes I and II

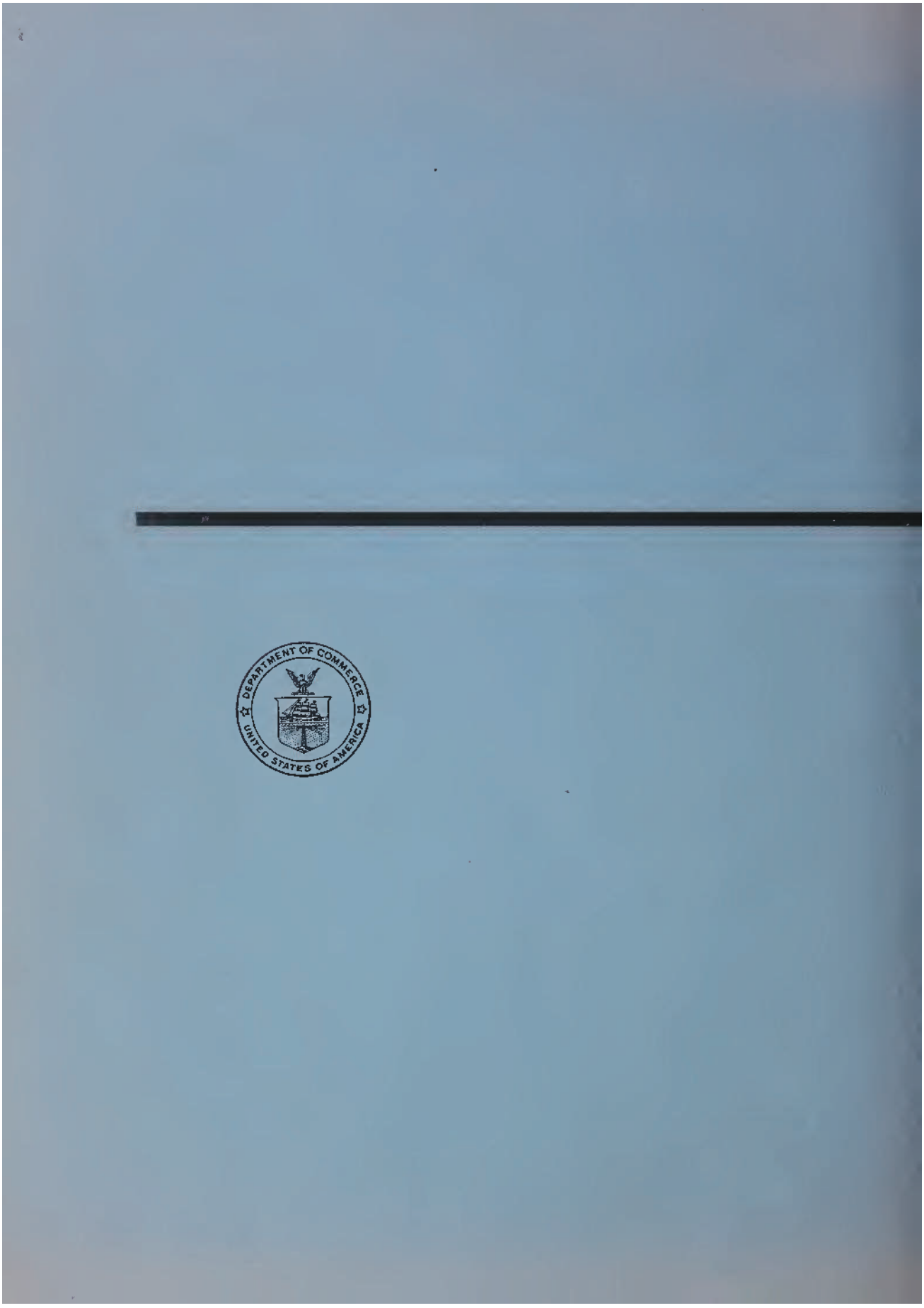
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