EXERCISE 15

IDENTIFICATION OF AN UNKNOWN BY X-RAY POWDER DIFFRACTOMETER TRACING

PURPOSE OF EXERCISE

To understand the steps involved in the identification of an unknown mineral using the diffractometer tracing of its powder diffraction effects. As in exercise 14, you will need to refer to the Powder Diffraction File of the JCPDS.

BACKGROUND INFORMATION: If you have completed exercise 14 before beginning this assignment, you will find that identification of unknown crystalline materials is a great deal faster by diffractometer technique than it is by film. This is so because a diffractometer tracing provides you with a graphical display of each peak position relative to a direct reading 2θ scale, as well as to a reasonably quantitative, direct reading relative intensity scale.

A powder X-ray diffractometer is a great deal more complex and expensive than a powder camera mounted on an X-ray generator. A diffractometer, in conjunction with an X-ray generator, consists of a goniometer (a device that measures the angular location in terms of 2θ for a diffraction peak), an X-ray counting device (such as a Geiger, a scintillation, or a proportional counter for measurement of peak intensity), and an electronic readout system (see Fig. 15.1). On nonautomated powder diffractometers the graphical result is a diffractometer chart obtained over a 2θ region of about 6° to 80°, during a time period of about 45 minutes. On an automated diffractometer the same results are printed out on an $8\frac{1}{2} \times 11$-inch page in about 15 minutes. In either case, the final diagram shows peak locations with respect to a horizontal 2θ scale, as well as relative intensities of the peaks in terms of a vertical scale. To search the JCPDS file for identification of the unknown, an investigator needs at the minimum to convert the 2θ values of the three most intense peaks on the graph to *d* values [using the *X-ray Diffraction Tables* of Fang and Bloss (1966), or, if these are not available, by using Table 14.1, or by solving the Bragg equation as outlined in section 2 of assignment 14]. It is strongly suggested, however, that to be certain the identification is completely unambiguous, the investigator should compare the *d*s of another ten or so peaks in the pattern with the published pattern on which the identification is based. Even though the identification of an unknown is based on matching of the three most intense X-ray diffraction lines, all other lines in the unknown pattern and those of the selected matching reference pattern should show good agreement in *d* values and intensity.

MATERIALS

The diffractometer tracing in Fig. 15.2 and Table 15.1 for data tabulation. A 90° triangle is useful for locating peak positions accurately on the diffractometer tracing with respect to the horizontal 2θ scale. You need access to the 2θ-to-*d* conversion tables of Fang and Bloss (1966), *X-ray Diffraction Tables*. If these are not available, the 2θ values can be converted to their appropriate *d*s by solving the Bragg equation with the help of an electronic calculator. Figures 15.3 and 15.4 should allow for unambiguous identification of the unknown. To check the *d*s and the intensities of all the diffraction lines on the pattern, you will need access to a microfiche or card edition of the JCPDS file.

REFERENCES See listing in exercise 14.

ASSIGNMENT

1. Using the diffractometer tracing in Fig. 15.2, assign 2θ values to each of the peaks. Carefully locate each peak position with reference to the horizontal 2θ scale. Write the 2θ appropriate to the peak next to it on the figure. Number the peaks from left to right. Enter the peak numbers and 2θ values into Table 15.1.
2. Read the relative intensities of all the peaks, by measuring the height of the peak on the vertical scale and subtracting the background value in the area of the peak. Assign the value of 100 to the most intense peak. If the height of the tallest peak is *y* divisions (where *y* is some number less that 100), multiply all the other peaks by the ratio of $100/y$ to obtain their values relative to 100. Enter these relative peak heights into Table 15.1.
3. Convert the 2θ angles to *d* values using the *X-ray Diffraction Tables* of Fang and Bloss, or Table 14.1, or calculate each *d*, using the Bragg equation as outlined in section 2 of the assignment in exercise 14. Because the pattern shows no $\alpha_1 - \alpha_2$ doublets , use the CuKa column in Fang and Bloss.
4. Using the *d* values of the three most intense peaks, identify the substance with Fig. 15.3 or 15.4.
5. After identification, make sure the additional five *d* values listed in Fig. 15.3 or 15.4 show good agreement with the data from your pattern.
6. If a JCPDS file is available, locate the complete reference card on the substance and make sure *all* peaks and their intensities of both the "unknown" and the substance you identified it to be show good correspondence.

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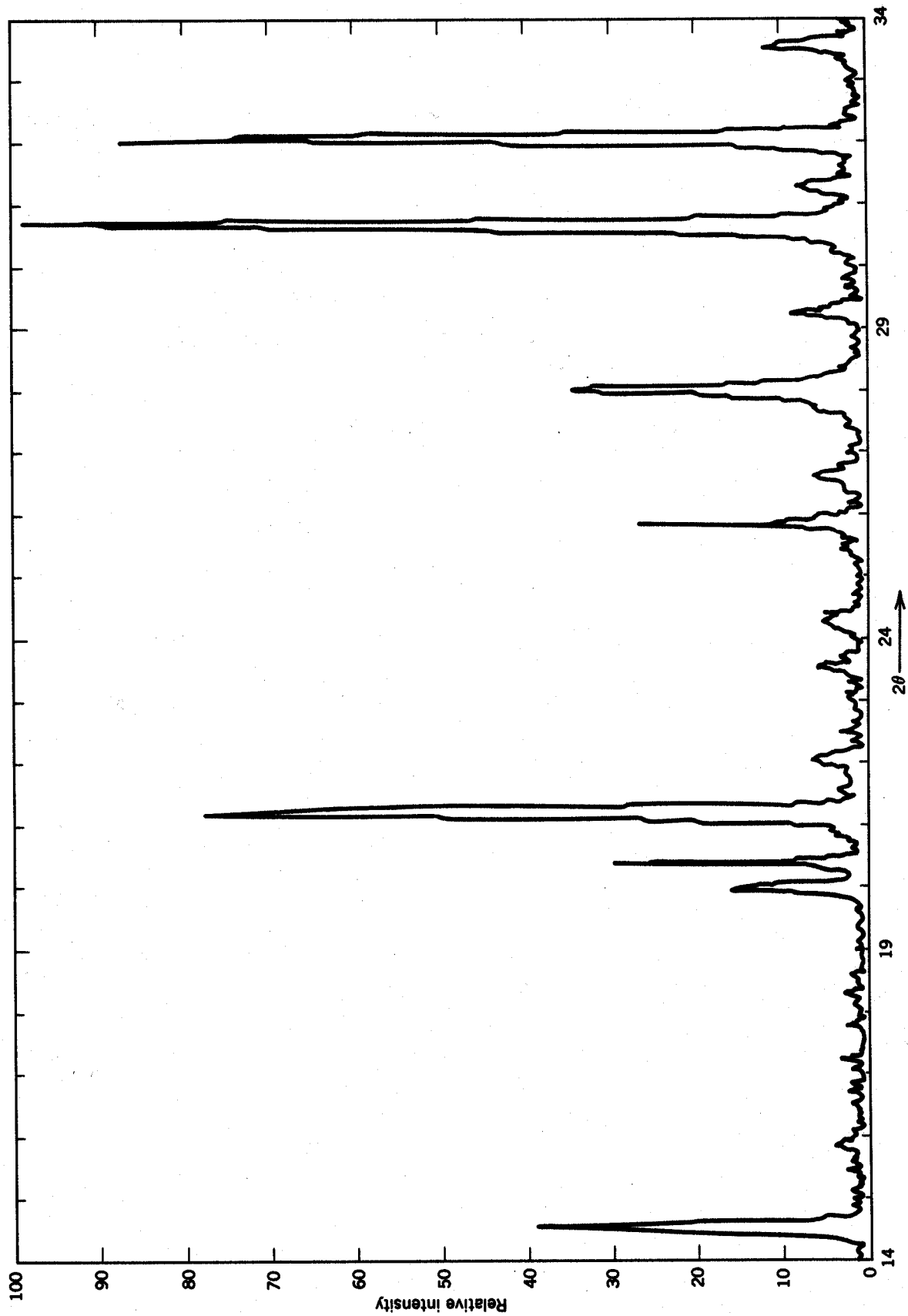

FIGURE 15.2 Diffractometer tracing for the unknown that is to be identified in this exercise. The X-ray radiation was produced by a Cu target X-ray tube. The 2θ-angle scale is horizontal. The relative intensity scale is vertical.

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TABLE 15.1 Record of Measurements Obtained from the Diffractogram in Fig. 15.2.
Refer to the diffractogram in Fig. 15.2.

Line Number [a]	*2θ angle*	*d*	*I*

Published 2θ values for the three most intense lines in the pattern of Fig. 15.2.

2θ	I
30.62	100
31.97	90
21.06	75

[a] Line numbers go consecutively from left to right.

Mineral identified as: _____

JCPDS file no.: _____

FIGURE 15.3 A page from the *Search Manual* (Hanawalt Section) of the *Powder Diffraction File*, for Inorganic Phases, 1986. The *d* values for families of planes that produce the eight strongest diffraction lines from a specific substance are listed. The number of the complete reference file card is given in the right column. (Reproduced by permission of JCPDS-International Center for Diffraction Data.)

2.94 – 2.90 (± .01)

										File No.	I/Ic
	2.90$_8$	2.82$_7$	2.80$_7$	3.98$_6$	3.47$_6$	2.68$_6$	1.88$_6$	2.03$_5$	$Ca_3(AsO_4)_3(OH)$ Johnbaumite	33– 265	
i	2.90$_8$	2.82$_8$	2.58$_8$	2.23$_6$	1.69$_6$	4.47$_5$	3.81$_5$	3.16$_5$	Tl_3Te_3	24–1310	
	2.90$_8$	2.82$_7$	2.33$_7$	1.21$_7$	1.49$_6$	1.34$_6$	1.32$_6$	2.78$_4$	GaSm	20– 436	
	2.90$_8$	2.82$_8$	2.31$_8$	2.48$_6$	3.11$_5$	3.00$_5$	2.61$_5$	2.36$_5$	$K_4H_2(CO_3)_3 \cdot 1.5H_2O$	20– 886	
	2.89$_9$	2.82$_8$	3.06$_8$	2.86$_8$	2.29$_8$	2.98$_6$	2.55$_6$	2.71$_4$	$Ca_4Si_3O_{12} \cdot H_2O$	14– 35	
	2.89$_9$	2.82$_8$	2.84$_7$	2.01$_6$	1.66$_4$	1.72$_3$	2.47$_2$	1.78$_2$	CaY_2O_4	19– 265	
	2.89$_8$	2.82$_8$	2.78$_8$	2.14$_8$	2.05$_8$	1.99$_8$	1.84$_8$	1.83$_8$	$(Ca,Sr)_2B_3O_6(OH)_2Cl$/Hilgardite-1Tc, strontian	11– 405	
	2.89$_9$	2.82$_8$	2.75$_8$	2.80$_8$	4.69$_6$	4.53$_6$	2.07$_6$	1.96$_6$	La_2CuIrO_6	18– 673	
	2.89$_8$	2.82$_8$	2.02$_7$	1.66$_7$	2.55$_6$	5.16$_5$	5.02$_5$	1.47$_5$	K_3As	4– 676	
*	2.95$_8$	2.81$_8$	4.23$_8$	2.69$_8$	8.47$_7$	2.56$_7$	1.71$_6$	1.93$_5$	$LuFeMgO_4$	36– 965	
	2.95$_8$	2.81$_8$	3.39$_8$	2.90$_8$	2.17$_8$	1.99$_8$	1.62$_8$	3.06$_7$	$K_4CaSi_3O_9$	27–1346	
c	2.95$_8$	2.81$_8$	2.79$_8$	1.92$_8$	3.06$_7$	2.18$_7$	2.16$_7$	3.17$_7$	Bi_2Rh	28– 172	
*	2.95$_8$	2.81$_8$	2.14$_8$	1.99$_8$	2.19$_7$	2.59$_4$	1.47$_4$	6.57$_3$	K_2MgF_4	23– 469	
o	2.94$_8$	2.81$_8$	2.55$_8$	2.75$_3$	2.45$_3$	2.34$_3$	2.26$_3$	1.96$_3$	Ba_2MgCl_6	15– 292	
c	2.94$_8$	2.81$_8$	1.88$_8$	5.63$_3$	1.72$_3$	1.47$_2$	3.45$_2$	1.27$_2$	Bi_2Cs	27– 323	
	2.93$_8$	2.81$_8$	8.43$_3$	2.23$_2$	6.18$_1$	4.22$_1$	2.10$_1$	3.32$_1$	$K_4Fe(CN)_6 \cdot 3H_2O$/Kafehydrocyanite, syn	14– 695	1.80
o	2.93$_8$	2.81$_8$	4.05$_7$	2.03$_7$	2.31$_6$	1.64$_5$	1.84$_4$	2.43$_4$	$Ba_2MgSi_2O_8$	10– 74	
	2.93$_8$	2.81$_8$	3.05$_7$	1.72$_4$	3.11$_4$	2.85$_4$	1.87$_4$	2.50$_3$	$Pb_2Sr_2SiO_7$	30– 728	
*	2.92$_8$	2.81$_8$	4.16$_8$	2.43$_6$	2.63$_3$	3.03$_3$	3.80$_2$	2.49$_2$	Li_2CO_3	22–1141	0.90
*	2.91$_8$	2.81$_7$	4.05$_8$	5.30$_5$	2.44$_4$	4.48$_4$	3.39$_3$	2.57$_3$	$Na_2CO_3 \cdot 7H_2O$	25– 816	
*	2.91$_8$	2.81$_8$	4.04$_8$	2.02$_5$	2.31$_3$	1.83$_3$	1.64$_2$	2.42$_2$	$NaBaPO_4$	33–1210	
i	2.91$_8$	2.81$_8$	3.33$_8$	3.18$_8$	4.21$_7$	1.93$_7$	1.82$_7$	2.02$_7$	$Eu_5(PO_4)_3F$	26– 627	
i	2.91$_8$	2.81$_8$	3.03$_8$	1.80$_7$	2.63$_6$	2.55$_6$	1.77$_6$	1.75$_6$	$Ge_{58}P_8I_8$	26– 689	
	2.91$_8$	2.81$_8$	2.96$_8$	2.25$_8$	3.97$_6$	3.48$_6$	2.56$_6$	2.46$_6$	$KBF(OH)_3$	30– 918	
	2.91$_8$	2.81$_8$	2.62$_8$	2.43$_8$	1.70$_6$	1.63$_5$	1.31$_5$	1.30$_5$	$AuPb_3$	26– 711	
	2.90$_8$	2.81$_8$	3.39$_8$	2.95$_8$	2.17$_8$	1.99$_8$	1.62$_8$	3.06$_7$	$K_4CaSi_3O_9$	27–1346	
	2.90$_8$	2.81$_8$	3.18$_8$	3.31$_7$	2.16$_7$	4.20$_7$	2.01$_7$	4.04$_7$	$Eu_5(PO_4)_3OH$	22– 613	
	2.90$_8$	2.81$_8$	2.65$_8$	1.59$_8$	1.47$_8$	1.09$_8$	0.83$_8$	1.73$_5$	Am	15– 657	
i	2.90$_8$	2.81$_8$	2.02$_8$	3.45$_5$	1.66$_3$	2.45$_2$	2.20$_2$	1.64$_2$	$Ba_2Sc_4O_9$	31– 161	
	2.89$_8$	2.81$_8$	4.46$_7$	3.36$_5$	2.09$_4$	1.92$_3$	4.21$_2$	3.14$_2$	$CsAl(SeO_4)_2 \cdot 12H_2O$	28– 278	
	2.89$_8$	2.81$_8$	3.22$_5$	6.79$_3$	3.99$_3$	2.41$_3$	2.01$_3$	1.79$_3$	$(Na,Ca,Mn)_2Zr(SiO_4)_2F$/Lavenite	14– 586	
c	2.94$_8$	2.80$_8$	2.51$_8$	2.20$_6$	2.65$_5$	1.47$_3$	2.72$_3$	2.48$_3$	$Ba_2Zn_2Fe_{12}O_{22}$	25–1193	
	2.93$_8$	2.80$_8$	2.64$_8$	3.91$_7$	2.95$_6$	5.88$_4$	2.86$_3$	2.43$_3$	$PbFe_6O_{10}$	33– 757	
i	2.91$_8$	2.80$_8$	1.98$_8$	1.63$_5$	3.78$_4$	1.70$_4$	2.14$_3$	1.45$_2$	K_2NiO_2	27– 423	
	2.90$_8$	2.80$_8$	4.23$_8$	2.82$_7$	5.60$_6$	2.28$_5$	2.02$_4$	1.79$_4$	Al_4Ba	10– 250	
	2.90$_8$	2.80$_8$	2.95$_5$	2.03$_4$	1.67$_3$	1.66$_3$	2.01$_2$	1.70$_2$	$SrYb_2O_4$	20–1222	
o	2.90$_8$	2.80$_4$	1.90$_3$	3.61$_2$	3.19$_2$	2.03$_2$	1.81$_2$	1.85$_2$	$Ca_4Nd_2Sr_4(PO_4)_4(SiO_4)_2F_2$	30– 268	
	2.89$_8$	2.80$_8$	3.21$_8$	2.60$_8$	4.41$_6$	3.58$_6$	3.51$_6$	3.26$_6$	K_2S_4	30– 992	
i	2.95$_8$	2.79$_8$	2.66$_8$	4.12$_6$	2.69$_6$	3.47$_5$	3.39$_5$	3.11$_5$	$Ba_{1.4}Sb_{10}O_{10}S_{6.4}$	31– 119	
o	2.95$_8$	2.79$_8$	2.03$_8$	1.74$_6$	1.64$_6$	4.37$_5$	3.73$_5$	3.12$_5$	$BaLa_2Ti_2O_8$	35– 164	
c	2.94$_8$	2.79$_8$	2.96$_8$	3.16$_5$	2.16$_3$	1.53$_2$	1.91$_2$	1.61$_2$	CaD_2	31– 266	3.08
c	2.93$_8$	2.79$_8$	4.60$_8$	5.05$_6$	2.91$_5$	3.23$_5$	3.97$_4$	3.78$_4$	Ba_3P_{14}	33– 172	1.88
*	2.92$_8$	2.79$_8$	4.21$_8$	6.12$_4$	4.36$_4$	3.44$_4$	3.19$_4$	2.45$_3$	α-$LiAlSi_2O_6$/Spodumene	33– 786	
	2.92$_8$	2.79$_8$	2.57$_8$	2.30$_8$	3.60$_8$	3.18$_8$	2.83$_8$	2.62$_8$	$Ca_2SiO_4 \cdot CaCl_2$	36– 558	
*	2.92$_8$	2.79$_8$	2.02$_7$	2.06$_3$	1.48$_2$	1.44$_2$	1.21$_2$	1.66$_2$	Sn/Tin, syn	4– 673	
	2.91$_8$	2.79$_7$	2.94$_3$	2.81$_2$	3.16$_1$	2.58$_1$	0.00$_1$	0.00$_1$	$Sr_4Ga_2O_7$	21–1181	
	2.91$_8$	2.79$_8$	2.74$_8$	3.74$_8$	5.96$_7$	3.93$_6$	2.09$_6$	2.01$_6$	$Pb_3O_2Cl_6$	6– 475	
	2.91$_8$	2.79$_8$	1.96$_8$	1.57$_8$	1.48$_6$	1.27$_6$	2.58$_3$	1.65$_3$	Sr_6Nl_2	17– 797	
i	2.90$_8$	2.79$_8$	2.78$_8$	1.45$_3$	2.94$_3$	2.02$_3$	2.00$_3$	1.66$_3$	$SrLu_2O_4$	32–1242	1.90
i	2.90$_8$	2.79$_8$	1.91$_8$	2.01$_4$	3.17$_4$	3.30$_3$	3.60$_3$	1.95$_3$	$Ca_2Sr_8(PO_4)_6(OH)_2$	34– 477	
	2.89$_8$	2.79$_8$	10.8$_8$	4.10$_8$	2.67$_8$	2.48$_8$	2.36$_8$	1.67$_8$	α_2-$Ca_4Al_2O_7 \cdot 19H_2O$	14– 628	
i	2.89$_8$	2.79$_8$	2.59$_7$	2.68$_6$	2.67$_6$	2.40$_6$	2.29$_6$	2.10$_6$	$Ca_2(Al,Fe)Al_2(SiO_4)_3OH$/Clinozoisite	21– 128	
	2.89$_8$	2.79$_8$	2.15$_7$	2.75$_7$	1.63$_7$	1.61$_7$	1.70$_7$	2.84$_4$	$Sr_9Al_2O_8$	10– 65	
i	2.89$_8$	2.79$_7$	1.98$_3$	1.63$_3$	6.34$_2$	1.68$_2$	2.11$_2$	1.44$_2$	$Sr_2Fe_{0.5}Ta_{0.5}O_4$	32–1238	
i	2.89$_8$	2.79$_8$	1.91$_8$	3.58$_8$	3.16$_7$	2.00$_7$	3.29$_6$	1.95$_5$	$Ca_3Sr_7(PO_4)_6(OH)_2$	34– 478	
	2.95$_8$	2.78$_8$	2.89$_8$	3.11$_8$	4.44$_7$	3.30$_5$	2.42$_5$	5.57$_3$	$Ba_2NaCe_2Fe(Ti,Nb)_2Si_8O_{26}(OH,F) \cdot H_2O$/Joaquinit	36– 385	
i	2.93$_8$	2.78$_8$	3.84$_8$	2.81$_8$	5.00$_7$	4.79$_7$	2.80$_7$	8.51$_6$	$Na_2SiO_3 \cdot 9H_2O$	19–1239	
i	2.93$_8$	2.78$_8$	2.92$_8$	2.89$_7$	3.33$_5$	3.76$_4$	2.15$_3$	1.91$_3$	$Pb_2Mn_2Ge_2O_9$	34–1362	
	2.92$_8$	2.78$_8$	2.57$_8$	2.13$_8$	2.00$_8$	5.71$_8$	4.21$_7$	2.27$_7$	$PtSn_4$	4– 744	
c	2.92$_8$	2.78$_8$	2.41$_8$	2.55$_5$	3.56$_5$	3.20$_5$	3.17$_4$	2.15$_3$	CeCu	25–1138	
*	2.92$_8$	2.78$_8$	2.02$_4$	2.94$_3$	3.26$_3$	2.12$_2$	4.81$_2$	2.37$_2$	$KSrPO_4$	33–1045	
c	2.89$_8$	2.78$_8$	2.99$_4$	2.44$_3$	2.14$_2$	4.78$_2$	3.67$_2$	3.10$_2$	Sb_2Sr	30– 98	6.03
	2.89$_8$	2.78$_8$	2.95$_8$	3.11$_8$	4.44$_7$	3.30$_5$	2.42$_5$	5.57$_3$	$Ba_2NaCe_2Fe(Ti,Nb)_2Si_8O_{26}(OH,F) \cdot H_2O$/Joaquinit	36– 385	
i	2.89$_8$	2.78$_8$	2.66$_8$	2.17$_7$	2.32$_5$	1.87$_4$	2.54$_3$	1.67$_3$	$Na_7AlH_2(CO_3)_4F_4$/Barentsite	35– 693	
	2.89$_8$	2.78$_8$	2.19$_8$	3.10$_6$	2.68$_6$	2.62$_6$	3.46$_5$	3.26$_5$	KCa_2FSiO_4	27–1343	
	2.95$_8$	2.77$_8$	4.72$_8$	2.53$_6$	2.46$_6$	2.36$_6$	2.27$_5$	2.24$_5$	K_2MnO_4	24– 875	
	2.95$_8$	2.77$_8$	3.51$_8$	2.48$_5$	1.20$_5$	1.17$_5$	1.76$_3$	1.72$_3$	La_2Si_2	19– 660	
	2.94$_8$	2.77$_8$	4.01$_7$	2.17$_7$	1.63$_7$	3.44$_7$	2.61$_7$	2.40$_7$	$Ba(BrO_2)_2$	20– 120	
	2.93$_8$	2.77$_8$	3.69$_8$	2.69$_8$	4.68$_5$	2.55$_5$	2.52$_5$	3.51$_4$	$H_2Ag_2NO_3P$	16– 511	
	2.92$_8$	2.77$_8$	3.75$_7$	3.43$_7$	3.08$_7$	2.33$_7$	1.78$_7$	1.54$_7$	$Ag_2V_4O_{11}$	20–1385	
*	2.92$_8$	2.77$_8$	2.01$_7$	1.62$_6$	2.20$_4$	1.60$_3$	1.38$_3$	1.29$_3$	$CaLa_4Ti_4O_{15}$	36–1278	
	2.92$_8$	2.77$_8$	2.01$_8$	1.46$_7$	1.66$_1$	1.43$_1$	2.06$_1$	0.00$_1$	InSb	19– 579	
c	2.90$_8$	2.77$_7$	5.55$_3$	1.85$_3$	1.70$_3$	2.40$_2$	1.45$_2$	1.25$_2$	Bi_2Rb	28– 175	
i	2.90$_8$	2.77$_8$	3.22$_8$	4.33$_7$	5.87$_5$	3.00$_4$	2.67$_4$	2.51$_4$	$K_2Ba(Ge_4O_9)_2$	31– 975	
	2.94$_8$	2.76$_8$	4.26$_7$	2.09$_7$	1.82$_7$	3.38$_6$	1.29$_6$	5.80$_5$	$DyPO_4 \cdot 1.5H_2O$	21– 316	
o	2.94$_8$	2.76$_8$	2.62$_8$	2.33$_8$	3.23$_6$	3.18$_6$	3.03$_6$	2.90$_6$	Rb_3BiBr_6	20– 986	
	2.93$_8$	2.76$_8$	3.05$_7$	2.40$_7$	2.30$_7$	2.16$_7$	2.85$_7$	2.58$_7$	$Ca_2Yb_2O_5$	19– 262	
	2.91$_8$	2.76$_7$	3.06$_8$	2.94$_5$	2.56$_5$	3.12$_5$	4.06$_4$	3.68$_4$	$Cu_3(PO_4)_2$	21– 298	
o	2.91$_8$	2.76$_8$	2.00$_8$	3.23$_6$	3.11$_6$	2.26$_6$	2.22$_6$	1.96$_6$	$SrLa_2Ti_2O_8$	36– 211	
	2.91$_8$	2.76$_8$	1.52$_8$	3.13$_6$	2.14$_6$	1.90$_6$	1.69$_6$	1.66$_6$	YbD_2	9– 256	
	2.90$_8$	2.76$_8$	2.01$_8$	3.93$_6$	3.62$_4$	2.18$_4$	1.64$_4$	1.61$_4$	$NaCaVO_4$	14– 54	
i	2.90$_8$	2.76$_8$	2.00$_7$	2.27$_6$	3.65$_5$	1.62$_5$	1.83$_4$	1.60$_2$	Ca_2SiO_4	23–1045	
	2.90$_8$	2.76$_8$	1.62$_8$	2.00$_8$	1.70$_8$	1.60$_8$	1.45$_8$	1.28$_8$	β-$TlFeO_2$	22– 490	
i	2.95$_8$	2.75$_8$	3.52$_8$	3.46$_8$	2.33$_7$	3.86$_6$	2.63$_6$	4.13$_5$	$PbAs_2S_4$/Sartorite	11– 76	
*	2.95$_8$	2.75$_8$	2.01$_4$	2.27$_2$	1.63$_1$	3.75$_1$	1.59$_1$	1.55$_1$	$KCaPO_4$	33–1002	
	2.95$_8$	2.75$_8$	2.00$_8$	1.47$_5$	1.29$_5$	1.60$_4$	2.06$_2$	1.38$_2$	InSb	22– 67	
	2.94$_8$	2.75$_7$	3.31$_8$	1.95$_5$	1.82$_5$	2.00$_4$	3.64$_3$	3.07$_3$	$Cd_3Cl(VO_4)_3$	19– 185	
i	2.94$_8$	2.75$_7$	2.67$_8$	3.87$_6$	3.14$_6$	3.20$_5$	1.84$_5$	4.55$_4$	$Pb_8Mg(Si_2O_7)_3$	32– 525	1.50
*	2.94$_8$	2.75$_7$	2.67$_8$	3.14$_8$	3.20$_5$	4.54$_5$	1.84$_5$	2.81$_4$	$Pb_8Ni(Si_2O_7)_3$	32– 527	1.60
	2.93$_8$	2.75$_8$	3.64$_8$	2.57$_7$	3.40$_4$	2.88$_3$	1.83$_3$	1.74$_3$	Al_2Th_3	7– 308	

FIGURE 15.4 A page from the *Search Manual* (Hanawalt Section) of the *Mineral Powder Diffraction File*. The information here is similar to that in Fig. 15.3, except that here all data entries are for minerals only. (Reproduced by permission of JCPDS—International Center for Diffraction Data.)

2.94 – 2.90 (± .01)

											File No.
*	2.93$_8$	3.32$_x$	3.60$_7$	3 04$_7$	3.56$_6$	2 35$_5$	3.75$_5$	4.69$_4$	Carnallite	$KMgCl_3 \cdot 6H_2O$	24- 869
i	2.93$_8$	3.31$_x$	3.13$_8$	1 91$_7$	1.76$_6$	1.63$_5$	2 27$_5$	1.30$_5$	Wurtzite-2H, syn	rr-ZnS	5- 492
	2.93$_8$	3.31$_x$	1.91$_7$	1 76$_6$	3.13$_5$	1.63$_5$	2 27$_4$	1.60$_2$	Wurtzite-2H, syn	ZnS	10- 434
i	2.91$_7$	3.30$_x$	3.44$_7$	2 75$_7$	3.76$_6$	3.02$_6$	2 28$_6$	2.07$_5$	Anderite	$AgPbSb_3S_6$	35- 596
i	2.91$_8$	3.30$_x$	2.76$_8$	3.02$_7$	1 77$_7$	2.02$_6$	1.73$_6$	4.26$_5$	Paulmoorelte	$Pb_2As_2O_5$	33- 736
i	2.89$_8$	3.30$_x$	3.42$_8$	2 74$_7$	3.72$_6$	3.00$_4$	2.86$_4$	1.88$_4$	Andorite, cuprian	$Ag_3CuPb_6Sb_{12}S_{24}$	13- 462
	2.90$_8$	3.28$_8$	4.15$_7$	3 93$_7$	3.82$_7$	1.94$_7$	7.80$_7$	5.84$_7$	Chiavennite	$CaMnBe_2Si_5O_{13}(OH)_2 \cdot 2H_2O$	35- 602
o	2.89$_8$	3.28$_8$	2.79$_8$	2 59$_8$	1 91$_8$	1.53$_8$	4.46$_7$	3.57$_6$	Unnamed mineral	Ba-Ti-Si-O	17- 504
i	2.92$_8$	3.27$_x$	3.74$_8$	3.49$_x$	4.13$_7$	2 74$_7$	3.08$_7$	2.77$_7$	Meneghinite	$CuPb_{13}Sb_7S_{24}$	29- 559
*	2.92$_8$	3.27$_x$	3.03$_8$	3.96$_8$	2.07$_x$	2.03$_8$	2.62$_7$	1.94$_5$	Fabianite	$CaB_2O_5(OH)$	15- 631
	2.90$_8$	3.27$_x$	2.98$_x$	1.93$_x$	1.97$_8$	3.58$_7$	3.41$_5$	3.40$_5$	Juanite	$Ca_4(Mg,Fe)_3(Si,Al)_{12}(O,OH)_{36} \cdot 7H_2O$	29- 335
i	2.95$_8$	3.26$_x$	3.81$_8$	2 86$_8$	3.35$_7$	3.88$_6$	2.15$_5$	4.22$_4$	Semseyite	$Pb_9Sb_8S_{21}$	22-1130
o	2.94$_8$	3.26$_x$	1.70$_8$	2.50$_8$	3.63$_x$	1.63$_x$	1.36$_x$	2.19$_x$	Ilmenorutile	$Fe_x(Nb,Ta)_{2x}Ti_{1-3x}O_2$	31- 646
i	2.91$_x$	3.25$_x$	2.19$_x$	2 97$_x$	4.93$_x$	2.61$_x$	2.98$_x$	1.93$_x$	Viitaniemiite	$NaCaAl(PO_4)(F,OH)_3$	35- 598
c	2.90$_8$	3.24$_x$	3.02$_x$	3 44$_x$	2.25$_x$	3.73$_x$	2.14$_x$	3.62$_x$	Bustamite, ferroan	$(Ca,Mn)_3Si_3O_9$	33- 292
o	2.92$_x$	3.23$_x$	4.38$_8$	3.73$_x$	2.76$_8$	5.06$_8$	4.13$_8$	3.57$_8$	Roedderite	$(Na,K)_2(Mg,Fe)_5(Al,Si)_{12}O_{30}$	23- 76
i	2.92$_x$	3.23$_x$	2.77$_8$	4.13$_8$	3.75$_8$	7.13$_x$	5.09$_x$	5.53$_6$	Osumilite	$(K,Na,Ca)(Mg,Fe)_2(Al,Fe)_3(Si,Al)_{12}O_{30} \cdot H_2O$	25- 658
	2.90$_8$	3.23$_x$	5.12$_8$	2.69$_8$	2.62$_8$	1.65$_8$	4.25$_6$	2.30$_6$	Descloizite	$(Zn,Cu)PbVO_4(OH)$	12- 537
	2.95$_x$	3.21$_x$	2.44$_8$	2.14$_x$	1.57$_x$	4.20$_x$	5.17$_x$	1.37$_x$	Rusakovite	$(Fe,Al)_5(VO_4,PO_4)_2(OH)_9 \cdot 3H_2O$	14- 60
i	2.92$_8$	3.21$_x$	3.02$_8$	2.91$_x$	2.49$_x$	1.63$_x$	2.57$_x$	2.14$_x$	Kanoite	$(Mn,Mg)_3(Si_2O_6)$	29- 865
i	2.91$_8$	3.21$_x$	3.26$_8$	3.87$_8$	3.77$_7$	2.62$_6$	3.61$_5$	5.87$_4$	Plagionite	$Pb_5Sb_8S_{17}$	22-1129
i	2.91$_8$	3.21$_x$	3.02$_8$	2.92$_8$	2.49$_x$	1.63$_x$	2.57$_x$	2.14$_x$	Kanoite	$(Mn,Mg)_3(Si_2O_6)$	29- 865
*	2.94$_x$	3.20$_7$	3.69$_8$	2.36$_7$	2.11$_x$	3.04$_x$	1.67$_5$	2.38$_5$	Topaz	$Al_2SiO_4(F,OH)_2$	12- 765
	2.93$_8$	3.20$_x$	2.58$_8$	1.80$_8$	3.50$_7$	2.71$_7$	2.15$_7$	4.54$_6$	Carminite	$PbFe_2(AsO_4)_2(OH)_2$	12- 278
	2.91$_x$	3.20$_8$	3.40$_8$	2.63$_7$	2.19$_6$	2.10$_6$	1.68$_6$	1.57$_6$	Shcherbakovite	$NaK(Ba,K)Ti_2(Si_2O_7)_2$	31-1324
o	2.90$_8$	3.20$_x$	6.11$_8$	2.37$_x$	2.31$_x$	1.92$_5$	2.49$_4$	3.86$_1$	Unnamed mineral	$K\text{-}Ca\text{-}CO_3$	25- 627
	2.90$_8$	3.20$_x$	4.09$_8$	1.84$_8$	1.33$_8$	1.52$_7$	4.51$_6$	3.52$_5$	Sogdianite	$(K,Na)_2Li_2(Li,Fe,Al)_2ZrSi_{12}O_{30}$	21- 501
c	2.95$_8$	3.19$_x$	3.22$_x$	2.88$_8$	2.93$_8$	3.70$_6$	3.05$_6$	3.03$_5$	Baratovite	$Li_3KCa_2(Ti,Zr)_2(Si_4O_{18})_2F_2$	33- 811
	2.90$_x$	3.18$_6$	1.78$_5$	2.22$_7$	2.51$_7$	2.40$_7$	1.46$_7$	1.05$_7$	Leightonite	$K_2Ca_2Cu(SO_4)_4 \cdot 2H_2O$	15- 128
	2.90$_x$	3.17$_7$	2.79$_7$	2.01$_7$	1.91$_7$	1.47$_6$	2.32$_5$	2.15$_5$	Belovite	$Sr_3(Ce,Na,Ca)_2(PO_4)_3OH$	31-1350
i	2.93$_8$	3.15$_x$	3.23$_7$	4.52$_7$	2.72$_6$	2.66$_6$	2.26$_6$	2.70$_5$	Bayldonite	$Cu_3Pb(AsO_4)_2(OH)_2$	26-1410
	2.93$_8$	3.13$_x$	1.90$_7$	1.64$_7$	1.57$_7$	2.72$_6$	1.22$_6$	1.19$_6$	Formanite, heated	$LnTaO_4$	26-1478
	2.92$_7$	3.13$_8$	2.69$_7$	4.06$_7$	1.78$_6$	5.29$_5$	2.49$_5$	4.32$_5$	Kermesite	Sb_2OS_2	11- 91
i	2.95$_x$	3.11$_5$	2.93$_x$	1.78$_x$	4.35$_x$	1.98$_4$	2.68$_3$	2.14$_3$	Okanoganite	$(Na,Ca)_3Ln_{12}Si_6B_2O_{27}F_{14}$	35- 483
c	2.94$_x$	3.11$_8$	3.22$_7$	2.84$_6$	3.67$_4$	3.41$_3$	2.58$_3$	2.89$_2$	Triploidite	$Mn_{1.5}Fe_{0.5}PO_4(OH)$	26-1239
i	2.93$_8$	3.11$_x$	3.04$_7$	2.66$_7$	8.84$_6$	2.69$_6$	4.51$_5$	3.58$_5$	Kulanite	$Ba(Fe,Mn,Mg)_2Al_2(PO_4)_3(OH)_3$	29- 170
	2.94$_x$	3.10$_8$	3.19$_8$	1 80$_6$	3.41$_5$	2.58$_5$	2.31$_5$	2.15$_5$	Triploidite	$(Mn,Fe)_3PO_4(OH)$	26-1240
	2.94$_x$	3.10$_x$	3.00$_x$	2.16$_x$	3.44$_8$	1.65$_7$	1.43$_6$	1.07$_6$	Manganbabingtonite	$Ca_2(Mn,Fe)FeSi_5O_{14}OH$	26- 313
	2.93$_x$	3.09$_x$	3.18$_8$	1.79$_6$	3.37$_5$	2.57$_5$	2.29$_5$	2.14$_5$	Wolfeite	$(Fe,Mn)_2(PO_4)(OH)$	5- 612
i	2.92$_8$	3.09$_x$	2.65$_7$	8.81$_6$	3.03$_6$	2.68$_6$	4.49$_6$	2.69$_6$	Penikisite	$Ba(Mg,Fe)_2Al_2(PO_4)_3(OH)_3$	29-. 169
	2.94$_8$	3.08$_x$	2.79$_8$	3.44$_8$	3.26$_5$	2.24$_5$	2.08$_5$	1.88$_4$	Kalborsite	$K_6BAl_4Si_6O_{20}(OH)_4Cl$	33- 999
	2.91$_8$	3.08$_x$	1.64$_8$	4.69$_7$	4.81$_6$	2.36$_6$	4.20$_5$	4.27$_4$	Canasite	$(Na,K)_6Ca_5Si_{12}O_{30}(OH,F)_4$	13- 553
i	2.90$_x$	3.08$_4$	1.76$_3$	3.06$_2$	3.31$_2$	3.27$_2$	2.16$_2$	2.73$_1$	Pectolite	$NaCa_2HSi_3O_9$	33-1223
o	2.92$_x$	3.07$_x$	2.59$_4$	1.84$_3$	1.50$_4$	3.68$_3$	1.90$_3$	11.0$_2$	Samarskite, heated	$(Y,U,Fe)(Nb,Ta,Ti)_2O_6$	4- 617
i	2.94$_x$	3.06$_8$	1.89$_6$	3.96$_4$	2.63$_4$	2.48$_4$	1.82$_4$	2.20$_3$	Rosenbuschite	$(Na,Ca)_3(Fe,Ti,Zr)(SiO_4)_2F$	14- 447
	2.92$_x$	3.06$_8$	4.21$_8$	3.52$_6$	3.24$_6$	6.15$_4$	6.51$_7$	2.18$_2$	Kasolite	$Pb(UO_2)SiO_4 \cdot H_2O$	29- 788
o	2.93$_8$	3.04$_x$	2.99$_x$	3.32$_7$	2.08$_7$	1.56$_7$	1.52$_7$	1.97$_6$	Mimetite, phosphatian	$Pb_5Cl((As,P)O_4)_3$	13- 124
i	2.92$_x$	3.04$_x$	3.35$_x$	2.78$_8$	2.91$_8$	3.83$_8$	1.91$_8$	2.56$_7$	Reinhardbraunsite	$Ca_5(SiO_4)_2(OH)_2$	29- 380
i	2.89$_x$	3.03$_x$	3.19$_8$	2.52$_7$	1.91$_7$	1.75$_7$	2.75$_6$	2.63$_5$	Rustumite	$Ca_{10}(Si_2O_7)_2SiO_4Cl_2(OH)_2$	18- 305
o	2.95$_x$	3.02$_x$	3.09$_3$	5.50$_2$	2.97$_2$	2.66$_2$	4.43$_2$	2.80$_2$	Yttropyrochlore	$(Y,Ce,Nd,Th)(Nb,Ti,Ta)_2O_6$	18- 765
i	2.91$_8$	3.02$_x$	2.90$_x$	3.21$_8$	2.58$_6$	1.63$_6$	1.49$_6$	1.39$_6$	Pigeonite	$(Fe,Mg,Ca)SiO_3$	13- 421
i	2.90$_x$	3.02$_x$	3.21$_8$	2.91$_8$	2.58$_6$	1.63$_6$	1.49$_6$	1.39$_6$	Pigeonite	$(Fe,Mg,Ca)SiO_3$	13- 421
	2.94$_x$	3.01$_x$	2.81$_x$	1.75$_8$	2.25$_7$	1.98$_7$	1.66$_7$	1.63$_7$	Sahlinite	$Pb_{14}(AsO_4)_2O_9Cl_4$	22- 664
	2.89$_x$	3.01$_x$	5.75$_8$	3.20$_8$	3.93$_7$	3.08$_7$	2.82$_6$	5.01$_4$	Realgar, high, syn	β-AsS	25- 57
i	2.95$_x$	3.00$_x$	4.84$_7$	3.78$_6$	3.70$_6$	2.50$_6$	2.88$_5$	1.73$_5$	Huebnerite, syn	$MnWO_4$	13- 434
	2.94$_x$	3.00$_8$	3.06$_8$	3.20$_7$	2.88$_7$	2.53$_7$	2.20$_7$	2.11$_7$	Roeblingite	$Ca_7Pb_2(SO_4)_2Si_6O_{14}(OH)_{10}$	18- 292
	2.94$_x$	3.00$_x$	1.58$_7$	2.65$_x$	1.70$_x$	1.86$_x$	3.71$_3$	2.21$_3$	Tantalaeschynite-(Y), heated	$(Y,Ce,Ca)(Ta,Ti,Nb)_2O_6$	26- 1
*	2.90$_x$	3.00$_8$	2.89$_x$	4.18$_3$	2.42$_3$	2.09$_3$	2.08$_3$	4.16$_2$	Arcanite, syn	K_2SO_4	5- 613
i	2.91$_x$	2.99$_8$	3.07$_3$	1.57$_3$	1.51$_3$	2.59$_2$	1.85$_2$	2.77$_2$	Aeschynite-(Y), syn	$YTiNbO_6$	20-1401
i	2.89$_x$	2.99$_x$	2.29$_8$	1.93$_7$	4.96$_6$	1.50$_4$	5.77$_3$	1.90$_3$	Alunite	$(K,Na)Al_3(SO_4)_2(OH)_6$	14- 136
o	2.91$_8$	2.98$_x$	2.52$_7$	2.49$_8$	2.20$_5$	2.02$_5$	1.41$_5$	2.54$_4$	Diopside, manganoan	$(Ca,Mn)(Mg,Fe,Mn)Si_2O_6$	22- 534
i	2.95$_8$	2.97$_x$	4.78$_8$	3.76$_8$	3.67$_8$	2.49$_5$	2.86$_3$	2.39$_3$	Wolframite, syn	$FeMn(WO_4)_2$	12- 727
i	2.94$_x$	2.97$_x$	3.11$_x$	2.93$_x$	1.78$_x$	4.35$_x$	1.98$_4$	2.68$_3$	Okanoganite	$(Na,Ca)_3Ln_{12}Si_6B_2O_{27}F_{14}$	35- 483
	2.93$_x$	2.97$_x$	1.83$_x$	11.7$_8$	6.00$_8$	3.13$_8$	4.21$_7$	4.06$_6$	Fedorite	$(K,Na)_{2.5}(Ca,Na)_3Si_{16}O_{38}(OH,F)_2 \cdot H_2O$	19- 466
	2.89$_x$	2.94$_x$	4.43$_x$	3.29$_x$	2.61$_x$	1.39$_x$	1.87$_5$	3.05$_4$	Joaquinite	$Ba_2NaCe_2FeTiSi_8O_{26}(OH)$	26-1034
*	2.91$_x$	2.93$_x$	3.73$_x$	4.69$_x$	3.62$_x$	2.47$_x$	2.46$_x$	2.86$_3$	Sanmartinite, syn	$ZnWO_4$	15- 774
*	2.90$_x$	2.92$_x$	4.37$_3$	3.79$_3$	2.73$_3$	2.51$_3$	4.66$_3$	2.45$_3$	Pumpellyite	$Ca_2MgAl_2(Si_2O_{11})(OH)_2 \cdot H_2O$	25- 156
*	2.93$_x$	2.91$_x$	3.73$_4$	4.69$_x$	3.62$_x$	2.47$_x$	2.46$_x$	2.86$_3$	Sanmartinite, syn	$ZnWO_4$	15- 774
c	2.89$_x$	2.91$_x$	3.24$_x$	3.02$_x$	3.44$_3$	2.25$_3$	3.73$_3$	2.14$_2$	Bustamite, ferroan	$(Ca,Mn)_3Si_3O_9$	33- 292
c	2.91$_x$	2.89$_x$	3.24$_x$	3.02$_x$	3.44$_3$	2.25$_3$	3.73$_3$	2.14$_2$	Bustamite, ferroan	$(Ca,Mn)_3Si_3O_9$	33- 292
i	2.95$_8$	2.88$_x$	2.78$_4$	3.02$_4$	2.84$_4$	2.71$_3$	4.54$_3$	3.30$_3$	Ilmeriite	$Y_2(SiO_4)(CO_3)$	35- 640
i	2.89$_x$	2.87$_7$	5.90$_7$	6.60$_x$	4.41$_6$	4.72$_5$	4.37$_5$	2.94$_5$	Mesolite	$Na_2Ca_2Al_6Si_9O_{30} \cdot 9H_2O$	24-1064
	2.95$_x$	2.86$_x$	1.76$_8$	1.14$_8$	3.31$_6$	2.77$_6$	2.42$_6$	1.55$_5$	Nordite-(La)	$Na_2LnSrMnSi_6O_{17}$	27- 672
o	2.93$_x$	2.86$_x$	2.14$_x$	1.85$_x$	2.06$_8$	2.80$_7$	3.23$_6$	1.99$_6$	Tyretskite-1Tc	$Ca_2B_2O_5(OH)_2$	26- 2
	2.91$_x$	2.86$_x$	2.61$_8$	1.72$_8$	1.19$_8$	2.64$_7$	1.86$_7$	1.14$_7$	Vysotskite	$((Pd,Ni)S)$	15- 151
	2.90$_x$	2.86$_x$	2.74$_x$	3.71$_8$	3.51$_8$	3.24$_8$	2.84$_8$	5.56$_7$	Kentrolite, ferroan	$Pb_2(Mn,Fe)_2Si_2O_9$	20- 586
c	2.95$_8$	2.84$_x$	2.86$_x$	3.08$_x$	2.54$_x$	2.90$_x$	3.82$_x$	3.29$_x$	Latiumite	$(Ca,K)_4(Si,Al)_2O_{11}(SO_4,CO_3)$	25-1202
	2.91$_x$	2.84$_8$	2.82$_8$	1.87$_x$	3.99$_7$	2.67$_7$	3.43$_6$	3.21$_6$	Svabite	$Ca_5(AsO_4)_3(OH,Cl,F)$	19- 215
	2.94$_x$	2.82$_x$	3.10$_8$	4 25$_x$	4 05$_4$	3.35$_4$	3.19$_4$	2.58$_4$	Eudialyte, yttrian	$Na_3(Ca,Ln)_2ZrSi_6O_{17}(OH)_2$	25- 814
c	2.93$_x$	2.82$_x$	2.51$_x$	1 80$_x$	1.75$_x$	1.81$_x$	1.52$_x$	1.54$_x$	Zirkelite	$CaZrTi_2O_7$	34- 167
*	2.92$_x$	2.82$_4$	2.03$_x$	1 93$_x$	1.47$_x$	3.20$_7$	1.83$_7$	1.97$_7$	Strontium-apatite, syn	$Sr_5(PO_4)_3OH$	33-1348
	2.90$_x$	2.82$_7$	2.80$_7$	3 98$_x$	3 47$_x$	2.68$_x$	1.88$_x$	2.03$_4$	Johnbaumite	$Ca_5(AsO_4)_3(OH)$	33- 265
	2.89$_x$	2.82$_x$	2.78$_x$	2 14$_x$	2.05$_8$	1.99$_x$	1.84$_8$	1.83$_8$	Hilgardite-1Tc, strontian	$(Ca,Sr)_2B_5O_9(OH)_2Cl$	11- 405
	2.93$_x$	2.81$_x$	8.43$_x$	2 23$_x$	6 18$_x$	4.22$_x$	2.10$_x$	3.32$_x$	Kafehydrocyanite, syn	$K_4Fe(CN)_6 \cdot 3H_2O$	14- 695
	2.89$_x$	2.81$_x$	3.22$_x$	6 79$_x$	3.99$_x$	2.41$_x$	2.01$_x$	1.79$_x$	Lavenite	$(Na,Ca,Mn)_2Zr(Si_2O_4)_3F$	14- 586
*	2.92$_x$	2.79$_8$	4.21$_8$	6 12$_x$	4.36$_4$	3.44$_4$	3.19$_4$	2.45$_3$	Spodumene	rr-$LiAlSi_2O_6$	33- 786
*	2.92$_x$	2.79$_x$	2.02$_x$	2.06$_x$	1.48$_x$	1.44$_x$	1.21$_x$	1.66$_x$	Tin, syn	Sn	4- 673
i	2.89$_x$	2.79$_x$	2.59$_x$	2 68$_x$	2 67$_x$	2.40$_x$	2.29$_x$	2.10$_x$	Clinozoisite	$Ca_2(Al,Fe)Al_2(SiO_4)_3OH$	21- 128
i	2.89$_x$	2.78$_x$	2.66$_x$	2 17$_x$	2.32$_x$	1.87$_x$	2.54$_x$	1.67$_x$	Barentsite	$Na_7AlH_2(CO_3)_4F_4$	35- 693
i	2.95$_x$	2.75$_x$	3.52$_x$	3 46$_x$	2.33$_x$	3.86$_x$	2.63$_x$	4.13$_x$	Sartorite	$PbAs_2S_4$	11- 76