The major portion of these calculations was made using IBM facilities. However, it was found that after certain preliminary computations, it would have been feasible to have found the signs (at the rate of about 100–150 per day) without the use of automatic computing machinery. The detailed procedures for the calculations of the signs were worked out by Karle, Hauptman & Christ and will be published separately at a later date.

For the preliminary structure analysis 944 observed F_{hkl}'s, together with their signs, were used to calculate electron-density sections over the xz plane at intervals of 1/60 for $y = 0$ to $y = 1/4$. The 944 terms used are those contained within a sphere of radius equal to $\sin\theta/\lambda = 0{\cdot}66$ Å^{-1}. In order to minimize termination-of-series effects, an artificial temperature factor $\exp[-B(\sin\theta/\lambda)^2]$, with $B = 2{\cdot}5$ Å^2, was multiplied into the observed F_{hkl}'s.

Colemanite is monoclinic $P2_1/a$,

$a = 8{\cdot}743 \pm 0{\cdot}004$, $b = 11{\cdot}264 \pm 0{\cdot}002$, $c = 6{\cdot}102 \pm 0{\cdot}003$ Å, $\beta = 110°\ 7'$,

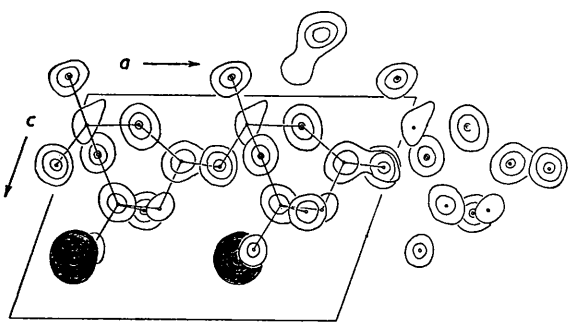

Fig. 1. Composite projection on (010) of the electron-density sections for colemanite. Only a portion sufficient to show the essential features of the structure is given. The small black circles indicate the boron positions, the small open circles the oxygen positions.

$Z = 4$; the calculated density is 2·419 g.cm.$^{-3}$, the observed density 2·42 g.cm.$^{-3}$ (Christ, 1953).

A composite projection on (010) of the electron-density sections is shown in Fig. 1. This shows clearly that there are infinite boron–oxygen chains running parallel to the a axis, the chain element being made up of a BO_3 triangle and two BO_4 tetrahedra forming a ring. The chain element has the composition $[B_3O_4(OH)_3]^{-2}$. Each Ca^{++} is roughly octahedrally coordinated by 5 oxygens and 1 water molecule. The formula for colemanite may thus be written $CaB_3O_4(OH)_3 \cdot H_2O$. The average B–O bond length in the tetrahedra is $1{\cdot}4_3$ Å, and in the triangles is $1{\cdot}3_7$ Å. Ca^{++} has as nearest neighbors 5 oxygens and 1 water molecule at an average distance of $2{\cdot}4_4$ Å. The discrepancy factor R for the $hk0$ zone is 25%.

This work was made possible only through the wholehearted cooperation of a number of people. G. J. Mowitt and Mrs Violet Rice made available the facilities of the U.S. Geological Survey IBM Section; Vincent Latorre of this Section was mainly responsible for the calculation of the electron-density sections. Mr Peter O'Hara of the Computation Laboratory of the National Bureau of Standards carried out most of the IBM calculations of the signs. As mentioned above, Drs Karle and Hauptman of the Naval Research Laboratory worked intensively with one of us (C.L.C) on the procedures for sign calculations. We are greatly indebted to all of these persons.

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Divisors for converting $\sin^2\theta$ for a standard wavelength.*

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In determining precision lattice parameters by X-ray diffraction (e.g. Cohen's method) it is common to use the $\sin^2\theta$ form of the Bragg equation. It then becomes convenient to convert values of $\sin^2\theta$ for several wavelengths to a value representing one standard wavelength for the purpose of calculation. We have found that a table listing divisors for converting $\sin^2\theta(\lambda')$ to $\sin^2\theta(\lambda)$, where λ is a desired standard wavelength, is very helpful in speeding computations by calculating machine. Such a table is based on the wavelengths in Ångström units (Table 1) given by Lonsdale (1950), although of course the divisors apply also to calculations based on kX. units. Conversion divisors for these wavelengths, the ratio

Table 1. *Wavelengths of emission lines of certain elements*

Element	$K\alpha_1$	$K\alpha_2$	$K\beta_1$
Cr	2·28962 Å	2·29351 Å	2·08480 Å
Mn	2·10175	2·10569	1·91015
Fe	1·93597	1·93991	1·75653
Co	1·78892	1·79278	1·62075
Ni	1·65784	1·66169	1·50010
Cu	1·54051	1·54433	1·39217
Zn	1·43511	1·43894	1·29522
Ga	1·34003	1·34394	1·20784
Ge	1·25401	1·25797	1·12890
Mo	0·70926	0·71354	0·63225
Ag	0·55936	0·56378	0·49701

$(\lambda'/\lambda)^2$, are listed in Table 2, and also, for convenience, the values of $\lambda^2/3$ and $\lambda^2/4$.

Reference

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Table 2. *Divisors for converting* $\sin^2\theta(\lambda')$ to $\sin^2\theta(\lambda)$: *the ratio* $(\lambda'/\lambda)^2$

λ'	λ Cr $K\alpha_1$	λ Mn $K\alpha_1$	λ Fe $K\alpha_1$	λ Co $K\alpha_1$	λ Ni $K\alpha_1$	λ Cu $K\alpha_1$	λ Zn $K\alpha_1$	λ Ga $K\alpha_1$	λ Ge $K\alpha_1$	λ Mo $K\alpha_1$	λ Ag $K\alpha_1$
Cr $K\alpha_1$	1	$1{\cdot}18676_5$	$1{\cdot}39871_6$	$1{\cdot}63811_7$	$1{\cdot}90739_9$	$2{\cdot}20901_0$	$2{\cdot}54540_2$	$2{\cdot}91942_8$	$3{\cdot}33368_7$	$10{\cdot}421_2$	$16{\cdot}755_0$
α_2	$1{\cdot}00340_1$	$1{\cdot}19080_1$	$1{\cdot}40347_3$	$1{\cdot}64368_8$	$1{\cdot}91388_6$	$2{\cdot}21652_3$	$2{\cdot}55405_9$	$2{\cdot}92935_7$	$3{\cdot}34502_4$	$10{\cdot}456_6$	$16{\cdot}812_0$
β_1	$0{\cdot}829090_6$	$0{\cdot}983935_6$	$1{\cdot}15966_2$	$1{\cdot}35814_8$	$1{\cdot}58140_7$	$1{\cdot}83147_0$	$2{\cdot}11036_9$	$2{\cdot}42047_0$	$2{\cdot}76392_8$	$8{\cdot}6400_8$	$13{\cdot}891_4$
Mn $K\alpha_1$	$0{\cdot}842626_8$	1	$1{\cdot}17859_6$	$1{\cdot}38032_2$	$1{\cdot}60722_6$	$1{\cdot}86137_2$	$2{\cdot}14482_4$	$2{\cdot}45998_8$	$2{\cdot}80905_4$	$8{\cdot}7811_5$	$14{\cdot}118_2$
α_2	$0{\cdot}845789_0$	$1{\cdot}00375_3$	$1{\cdot}18301_9$	$1{\cdot}38550_2$	$1{\cdot}61325_7$	$1{\cdot}86835_7$	$2{\cdot}15287_3$	$2{\cdot}46922_0$	$2{\cdot}81959_6$	$8{\cdot}8141_0$	$14{\cdot}171_2$
β_1	$0{\cdot}695998_2$	$0{\cdot}825986_3$	$0{\cdot}973503_9$	$1{\cdot}14012_7$	$1{\cdot}32754_6$	$1{\cdot}53746_7$	$1{\cdot}77159_5$	$2{\cdot}03191_7$	$2{\cdot}32024_0$	$7{\cdot}2531_1$	$11{\cdot}661_4$
Fe $K\alpha_1$	$0{\cdot}714941_4$	$0{\cdot}848467_3$	1	$1{\cdot}17115_8$	$1{\cdot}36367_9$	$1{\cdot}57931_3$	$1{\cdot}81981_3$	$2{\cdot}08722_0$	$2{\cdot}38339_1$	$7{\cdot}4505_2$	$11{\cdot}978_8$
α_2	$0{\cdot}717854_4$	$0{\cdot}851924_4$	$1{\cdot}00407_4$	$1{\cdot}17593_0$	$1{\cdot}36923_5$	$1{\cdot}58574_8$	$1{\cdot}82722_8$	$2{\cdot}09572_4$	$2{\cdot}39310_2$	$7{\cdot}4808_7$	$12{\cdot}027_6$
β_1	$0{\cdot}588551_3$	$0{\cdot}698472_0$	$0{\cdot}823216_2$	$0{\cdot}964116_0$	$1{\cdot}12260_2$	$1{\cdot}30011_6$	$1{\cdot}49810_0$	$1{\cdot}71823_3$	$1{\cdot}96204_6$	$6{\cdot}1333_8$	$9{\cdot}8611_7$
Co $K\alpha_1$	$0{\cdot}610456_9$	$0{\cdot}724468_9$	$0{\cdot}853855_9$	1	$1{\cdot}16438_5$	$1{\cdot}34850_6$	$1{\cdot}55385_8$	$1{\cdot}78218_5$	$2{\cdot}03507_2$	$6{\cdot}3616_7$	$10{\cdot}228_2$
α_2	$0{\cdot}613094_2$	$0{\cdot}727598_6$	$0{\cdot}857544_7$	$1{\cdot}00432_0$	$1{\cdot}16941_5$	$1{\cdot}35433_1$	$1{\cdot}56057_1$	$1{\cdot}78988_4$	$2{\cdot}04386_4$	$6{\cdot}3891_5$	$10{\cdot}272_4$
β_1	$0{\cdot}501077_9$	$0{\cdot}594661_7$	$0{\cdot}700865_7$	$0{\cdot}820824_3$	$0{\cdot}955755_6$	$1{\cdot}10688_6$	$1{\cdot}27544_5$	$1{\cdot}46286_1$	$1{\cdot}67043_7$	$5{\cdot}2218_1$	$8{\cdot}3955_5$
Ni $K\alpha_1$	$0{\cdot}524274_1$	$0{\cdot}622190_1$	$0{\cdot}733310_6$	$0{\cdot}858822_5$	1	$1{\cdot}15812_7$	$1{\cdot}33448_9$	$1{\cdot}53058_0$	$1{\cdot}74776_6$	$5{\cdot}4635_4$	$8{\cdot}7842_0$
α_2	$0{\cdot}526712_0$	$0{\cdot}625083_3$	$0{\cdot}736720_5$	$0{\cdot}862816_0$	$1{\cdot}00465_0$	$1{\cdot}16351_2$	$1{\cdot}34069_4$	$1{\cdot}53769_8$	$1{\cdot}75589_3$	$5{\cdot}4889_5$	$8{\cdot}8250_5$
β_1	$0{\cdot}429253_3$	$0{\cdot}509422_7$	$0{\cdot}600403_4$	$0{\cdot}703167_2$	$0{\cdot}818757_3$	$0{\cdot}948224_9$	$1{\cdot}09262_2$	$1{\cdot}25317_4$	$1{\cdot}43099_6$	$4{\cdot}4733_1$	$7{\cdot}1921_3$
Cu $K\alpha_1$	$0{\cdot}452691_4$	$0{\cdot}537238_3$	$0{\cdot}633186_7$	$0{\cdot}741561_6$	$0{\cdot}863463_2$	1	$1{\cdot}15228_2$	$1{\cdot}32160_0$	$1{\cdot}50913_1$	$4{\cdot}7175_7$	$7{\cdot}5848_4$
α_2	$0{\cdot}454939_2$	$0{\cdot}539905_9$	$0{\cdot}636330_8$	$0{\cdot}745243_8$	$0{\cdot}867750_7$	$1{\cdot}00496_6$	$1{\cdot}15800_3$	$1{\cdot}32816_2$	$1{\cdot}51662_5$	$4{\cdot}7409_9$	$7{\cdot}6225_0$
β_1	$0{\cdot}369707_0$	$0{\cdot}438755_4$	$0{\cdot}517115_2$	$0{\cdot}605623_5$	$0{\cdot}705178_9$	$0{\cdot}816686_7$	$0{\cdot}941053_2$	$1{\cdot}07933_3$	$1{\cdot}23248_8$	$3{\cdot}8527_7$	$6{\cdot}1944_4$
Zn $K\alpha_1$	$0{\cdot}392865_2$	$0{\cdot}466238_6$	$0{\cdot}549506_9$	$0{\cdot}643559_3$	$0{\cdot}749350_8$	$0{\cdot}867843_3$	1	$1{\cdot}14694_2$	$1{\cdot}30969_0$	$4{\cdot}0941_1$	$6{\cdot}5824_5$
α_2	$0{\cdot}394964_9$	$0{\cdot}468730_5$	$0{\cdot}552443_8$	$0{\cdot}646998_9$	$0{\cdot}753355_8$	$0{\cdot}872481_7$	$1{\cdot}00534_5$	$1{\cdot}15307_2$	$1{\cdot}31668_9$	$4{\cdot}1159_9$	$6{\cdot}6176_3$
β_1	$0{\cdot}320007_6$	$0{\cdot}379773_8$	$0{\cdot}447599_8$	$0{\cdot}524209_9$	$0{\cdot}610382_2$	$0{\cdot}706900_1$	$0{\cdot}814548_0$	$0{\cdot}934239_1$	$1{\cdot}06680_5$	$3{\cdot}3348_5$	$5{\cdot}3617_2$
Ga $K\alpha_1$	$0{\cdot}342532_3$	$0{\cdot}406506_0$	$0{\cdot}479106_2$	$0{\cdot}561109_0$	$0{\cdot}653346_9$	$0{\cdot}756658_6$	$0{\cdot}871883_9$	1	$1{\cdot}14189_7$	$3{\cdot}5695_9$	$5{\cdot}7391_3$
α_2	$0{\cdot}344534_7$	$0{\cdot}408881_7$	$0{\cdot}481906_2$	$0{\cdot}564388_2$	$0{\cdot}657165_2$	$0{\cdot}761080_7$	$0{\cdot}876979_4$	$1{\cdot}00584_4$	$1{\cdot}14857_1$	$3{\cdot}5904_5$	$5{\cdot}7726_7$
β_1	$0{\cdot}278286_4$	$0{\cdot}330260_6$	$0{\cdot}389243_7$	$0{\cdot}455865_8$	$0{\cdot}530803_3$	$0{\cdot}614737_6$	$0{\cdot}708350_9$	$0{\cdot}812437_1$	$0{\cdot}927719_8$	$2{\cdot}9000_7$	$4{\cdot}6626_8$
Ge $K\alpha_1$	$0{\cdot}299968_2$	$0{\cdot}355991_7$	$0{\cdot}419570_3$	$0{\cdot}491383_0$	$0{\cdot}572159_0$	$0{\cdot}662632_8$	$0{\cdot}763539_7$	$0{\cdot}875735_5$	1	$3{\cdot}1260_1$	$5{\cdot}0259_6$
α_2	$0{\cdot}301865_7$	$0{\cdot}358243_6$	$0{\cdot}422224_4$	$0{\cdot}494491_4$	$0{\cdot}575778_4$	$0{\cdot}666824_5$	$0{\cdot}768369_6$	$0{\cdot}881275_1$	$1{\cdot}00632_6$	$3{\cdot}1457_9$	$5{\cdot}0577_5$
β_1	$0{\cdot}243099_5$	$0{\cdot}288502_0$	$0{\cdot}340027_2$	$0{\cdot}398225_5$	$0{\cdot}463687_9$	$0{\cdot}537009_4$	$0{\cdot}618786_1$	$0{\cdot}709711_6$	$0{\cdot}810417_8$	$2{\cdot}5333_8$	$4{\cdot}0731_3$
Mo $K\alpha_1$	$0{\cdot}095958_6$	$0{\cdot}11388_0$	$0{\cdot}13421_9$	$0{\cdot}15719_2$	$0{\cdot}18303_1$	$0{\cdot}21197_4$	$0{\cdot}24425_3$	$0{\cdot}28014_4$	$0{\cdot}31989_6$	1	$1{\cdot}6077_9$
α_2	$0{\cdot}097120_3$	$0{\cdot}11525_9$	$0{\cdot}13584_4$	$0{\cdot}15909_4$	$0{\cdot}18524_7$	$0{\cdot}21454_0$	$0{\cdot}24721_0$	$0{\cdot}28353_6$	$0{\cdot}32376_9$	$1{\cdot}0121_1$	$1{\cdot}6272_5$
β_1	$0{\cdot}076251_9$	$0{\cdot}090493_1$	$0{\cdot}10665_5$	$0{\cdot}12491_0$	$0{\cdot}14544_3$	$0{\cdot}16844_1$	$0{\cdot}19409_2$	$0{\cdot}22261_2$	$0{\cdot}25420_0$	$0{\cdot}79463_3$	$1{\cdot}2776_0$
Ag $K\alpha_1$	$0{\cdot}059683_7$	$0{\cdot}070830_6$	$0{\cdot}083480_6$	$0{\cdot}097769_0$	$0{\cdot}11384_1$	$0{\cdot}13184_2$	$0{\cdot}15191_9$	$0{\cdot}17424_2$	$0{\cdot}19896_7$	$0{\cdot}62197_3$	1
α_2	$0{\cdot}060630_7$	$0{\cdot}071954_4$	$0{\cdot}084805_1$	$0{\cdot}099320_2$	$0{\cdot}11564_7$	$0{\cdot}13393_4$	$0{\cdot}15432_9$	$0{\cdot}17700_7$	$0{\cdot}20212_4$	$0{\cdot}63184_2$	$1{\cdot}0158_7$
β_1	$0{\cdot}047119_8$	$0{\cdot}055920_1$	$0{\cdot}065907_2$	$0{\cdot}077187_8$	$0{\cdot}089876_3$	$0{\cdot}10408_8$	$0{\cdot}11993_9$	$0{\cdot}13756_3$	$0{\cdot}15708_3$	$0{\cdot}49104_3$	$0{\cdot}78949_1$
$\lambda^2/3$*	$1{\cdot}74745_3$	$1{\cdot}47245_1$	$1{\cdot}24932_7$	$1{\cdot}06674_5$	$0{\cdot}916144_5$	$0{\cdot}791057_0$	$0{\cdot}686513_6$	$0{\cdot}598560_1$	$0{\cdot}524180_4$	$0{\cdot}16768_3$	$0{\cdot}10429_5$
$\lambda^2/4$*	$1{\cdot}31059_0$	$1{\cdot}10433_8$	$0{\cdot}936995_0$	$0{\cdot}800058_7$	$0{\cdot}687108_4$	$0{\cdot}593292_8$	$0{\cdot}514885_2$	$0{\cdot}448920_1$	$0{\cdot}393135_3$	$0{\cdot}12576_2$	$0{\cdot}078220_9$

* In 10^{-16} cm.^{2} units, calculated from wavelengths given by Lonsdale (1950).