

UNITED STATES DEPARTMENT OF THE INTERIOR
GEOLOGICAL SURVEY

X-ray diffraction mineral identification charts for use
in studies of uranium, thorium, and rare-earth deposits

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Open-File Report 82-280

1982

This report is preliminary and has not
been reviewed for conformity with U.S.
Geological Survey editorial standards.

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INTRODUCTION

A great deal of exploration for uranium has been carried out in the past 30 years by both government and industry. Initial location of uranium deposits is generally done with either a geiger or a scintillation counter. Some of the deposits so discovered are those of thorium instead of uranium. Uranium and thorium concentrations occur infrequently together in the same deposit. Thorium and rare earths, on the other hand, commonly occur together, as the atomic radius of thorium is similar to that of the rare earth elements. As uranium-, thorium-, and rare-earth-bearing minerals are fine grained, their identification may be difficult, and generally can not be done by visual inspection. X-ray diffraction analysis is one of the better ways to identify many of these minerals. However, this method can not be used successfully to discriminate all these minerals as the patterns of certain ones are almost identical. For example those of autunite and torbernite or of meta-autunite and metatorbernite can not be separated from each other. The method does, however, identify the general group to which these minerals belong. The specific member of the group can then be determined by chemical means.

CHARTS AND THEIR CONSTRUCTION

Generally, the method of identifying a mineral from its X-ray diffraction pattern is to first label the peak positions according to their 2θ values, and then to compare the numbers obtained for the three highest peaks with those of various minerals. This process can be long and frustrating. Several factors make this difficult. Most reference data is published as the "d" spacing in Angstrom units. Therefore, using the appropriate X-ray tube target wave length, a conversion to 2θ values must first be calculated before comparison to the unknown phase can be made. Another factor, especially in fine-grained deposits, is that even hand-picked material may consist of several minerals. A third factor is that the principal peaks of a mineral X-rayed may not correspond well to the reference pattern listed for it in the "Index to the Powder Diffraction File" (published by the Joint Committee on Powder Diffraction Standards¹). A fourth factor is that comparing a column of numbers representing peak heights to columns of numbers representing various minerals is not very easy to do.

Peak heights represented graphically are easier for most people to use. Thus, diffraction data compiled on appropriately scaled charts can be directly matched with an X-ray pattern and the mineral identified. The charts, on the other hand, become large and cumbersome if many minerals are shown. The bulk problem was handled in this report by following these procedures: (1) strictly limiting the number of minerals, (2) dividing the patterns into three

¹The Powder Diffraction File is a set of numerical search tables which list the major peaks for most organic and inorganic compounds including a separate file for minerals. These files are designed as general source references, and do not contain a sufficient variety of patterns so that members of a solid solution series can be identified. Ion substitution, which is common in uranium, thorium, and rare-earth minerals, can cause distortion in the lattice structure and subsequent shift in the 2θ peak positions.

figures, and (3) by showing from one to five minerals on each strip, and separating them by using a separate pattern for each mineral's peak. The number of minerals shown on each strip is, in general, dependent on the number of total peaks. Thus, a mineral like abernathyite, which has many peaks, is shown on a strip by itself, but the sulphides, chalcopyrite, galena, marcasite, pyrite, and sphalerite, which have only few peaks each, are shown on the same strip. The grouping of several minerals on the same strip has the additional advantage that minerals of similar structure can be put together and their structural similarities and differences can quickly be seen.

The heights of the peaks are proportional to their relative intensities. On the scale of these charts, the 100-percent peak for any mineral would have an I value of 10 and would be shown reaching the top of its strip on the chart. Peaks with an I value of less than 2 are not shown except in a few minerals that have only a few large peaks.

Some minerals shown on the same strip have one or more peaks that occur at the same position. These overlapping peaks are shown two ways. If one peak is more intense than another, the smaller peak is placed inside the larger one. Examples of this type of overlap occur between carnotite and tyuyamunite at $27.2^{\circ} 2\theta$ (fig. 1) and ilmenite and magnetite at $35.2^{\circ} 2\theta$ (fig. 3). The other type of overlap occurs where both minerals have peaks of the same intensity. In this case the mineral peak is split longitudinally down the center and one half of the peak has the pattern of one mineral and the other half of the other mineral. Examples of this type of overlap occur between autunite and torbernite at 8.6° , 19.8° , 24.8° , 25.4° , and $40.8^{\circ} 2\theta$ (fig. 1), and between anatase and brookite at $25.2^{\circ} 2\theta$ (fig. 3).

Metamict minerals were for the most part avoided because identification of some of these minerals takes a specialized knowledge. Minerals, like thorite and zircon, which are not commonly metamict but can show metamict affects, are shown. The rarer niobotantalates--such as fergusonite, euxenite, and samarskite may form a variety of structural patterns on heating and are subsequently not included. One commonly metamict mineral that is included is uraninite. This mineral is too important in uranium studies to be deleted. The two most common uranium oxide phases derived by heating are shown on the lowest strip of figure 1. These are the UO_2 or uraninite phase, whose peaks are marked with a U in figure 1, and a U_3O_8 phase, whose peaks are marked with a K. The pattern shown would be one that is commonly obtained if the uraninite was heated for one hour at $1000^{\circ}C$ in air. If the uraninite was heated in an inert atmosphere instead of air, the U peaks are the only ones developed on the X-ray diffraction pattern (DeFaria, 1964, p. 47).

Figure 1 shows the principal peaks for 34 uranium minerals and figure 2 shows the principal peaks for 22 thorium and/or rare-earth minerals. Brannerite and davidite appear on both figures 1 and 2, as these two minerals are both uranium and thorium minerals. Brockite-rhabdophane is listed in the fourth strip from the bottom on figure 2. These two minerals are isostructural and have identical X-ray diffraction patterns. They represent end members of a series in which brockite is the thorium-rich member and rhabdophane is the rare-earth-rich member.

Figure 3 shows the principal peaks for 42 minerals that are commonly found with various types of uranium, thorium, or rare-earth deposits. This chart includes rock-forming silicates, carbonates, common sulfides, iron oxide minerals, various accessory rock minerals, and some secondary minerals.

Certain silicate groups, such as pyroxene, amphibole, mica, and potassium feldspar, are represented by only one member of each family. The identification of these mineral groups by their general X-ray diffraction pattern is not difficult. The identity of specific members, however, of these groups may take additional physical, chemical, or optical data.

The peak position and intensities shown in the three figures came from two sources: X-ray patterns made by the authors' over a period of 15 years, and from data compiled by Frondel (1958). All the patterns on figures 2 and 3, as well as those of metauranocircite, kasolite, weeksite, betauranophane, sklodowskite, brannerite, davidite, and uraninite on figure 1 were taken from the authors' files. The position of the peaks and their intensities may vary somewhat for specimens of an individual mineral collected from different localities. These differences are due mainly to variations in the elemental content of a particular mineral. For example, the common shifts in peak positions and/or peak intensities of monazite may be due to changes in the thorium content, which may vary from 0 to 31.5 weight percent (Overstreet, 1967, p. 6).

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