SOFTWARE NOTICE

MINERAL: A computerized mineralogical reference manual for personal computers

E. H. NICKEL Division of Mineral Products, CSIRO, Perth 6014, Western Australia, Australia

M. C. NICHOLS Materials Department, Sandia National Laboratories, Livermore, California 94550, U.S.A.

INTRODUCTION

The MINERAL system is a computerized mineral reference book in a PC database format containing data for more than 3700 species and unnamed minerals. MINERAL is designed to function with the DayFlo TRACKER program (Stone, 1988), which allows very rapid searching of this database using the following fields, either singly or in combination: species name, name fragment, or synonym; elemental and/or polyatomic constituents; mineral group name; related species names(s); crystal system and space group; lattice parameters; JCPDS number; and/or mineral classification. Other information available for each species includes the chemical formula, number of formula units per unit cell, two general references, and an additional reference to the origin of the name.

The database comes with an on-line user-help facility that explains the use of special function keys to conveniently utilize the MINERAL database without the need to completely understand the TRACKER database manager. Also available is the ability to include information of the user's choosing for any of the species present. Examples of possible additional information include catalogue number, locality, source, etc. Also included is the ability to print, or view on the screen, summaries or detailed reports of those minerals that meet elemental or other criteria established by the user. A user manual accompanying the computerized reference contains easily understood instructions for loading and using the system as well as a listing of the name and principal reference for all species present in the database.

DATABASE DESCRIPTION

Data for forsterite are shown in Figure 1 as an example of a MINERAL database record. As shown in Figure 1, the database structure allows multiple values for any field, and every field can be of variable length. These two features are convenient for the

Name: Forsterite

mName: Formula:	Forsterite ∇ Chrysolite ∇ Olivine ∇ Peridot Mg2 SiO4		
Elements:	$Mg \nabla Si \nabla O \nabla SiO4$		
See Also:	Fayalite ∇ Ringwoodite ∇ Wadsleyite		
CrySys:	O SG: 62	Z:	4
A:	4.752 B: 10.193	C:	5.977
Alp:	Bet:	Gam:	
Ref1:	Am. Min. 61 (1976), 1280		
Ref2:	Am. Min. 53 (1968), 807		
Name Ref:	Levy, 1824		
JCPDS:	31–0795 ▽ 33–0657 ⊽ 34–0189		
Grp Name:	Olivine		
Class:	VIIIA 03		
	Copyright, 1989 by Aleph/CSIRO		

Fig. 1. A typical species record from the MINERAL database. The field names are shown in boldface type. The ∇ characters separate multiple values for a given field. These ∇ delimited values are represented in the database as unique field values and are treated as separate values for the field in question.

user, and the fact that a fixed number of characters does not have to be reserved for each field allows a more efficient use of the available disk space. The specific fields defined for the MINERAL database are discussed below.

Name field. The Name field contains the preferred name for this mineral, either IMA approved or with historical precedence.

mName field. Multiple names are used in the mName field so that the record for a mineral like forsterite can be found using either the word forsterite itself or any of the synonyms present in the mName field. A wild card symbol can be used while searching to avoid having to enter the complete name (forst* for example could be used to retrieve forsterite). It is also possible to browse through the dictionary of mineral names if the user is not certain of the correct spelling.

Formula field. Although it is not indexed, the Formula field can be searched for any formula or formula fragment.

Elements field. The Elements field contains the elements and polyatomic groups (SiO₄ for example) that are present in the mineral. The database can be searched using a selection of different criteria that include "equal," "not equal," etc. For example, data records for the more than 100 mineral species that contain both Pb and Cu can all be retrieved from the MINERAL database in less than four seconds using the Elements field and a PC/AT clone.

See Also field. The See Also field contains names of related species that could be polymorphs, solid-solution series, etc. This field is indexed and can be used to quickly retrieve all species that are listed as related to a particular mineral.

CrySys, SG, & Z fields. These fields contain the crystal system, space group, and number of formula units in the unit cell.

A, B, C, Alp, Bet, & Gam fields. These fields contain the lattice parameters for the mineral.

Ref1, **Ref2**, & **Name Ref fields**. The Ref1 and Ref2 fields give one or more references. The Name Ref field gives a reference to the source of the origin of the mineral name when available including the year of first publication.

JCPDS field. This field contains JCPDS numbers for each species where available. Since this is an indexed field, it is possible to quickly display records for species by entering this number. It is also possible to display JCPDS data for each species, either using the new JCPDS CD-ROM product or the older JCPDS file of mineral X-ray data. The JCPDS software and other X-ray diffraction SEARCH/MATCH software can be run from within MINERAL.

Grp Name field. The Grp Name field gives information regarding the mineral group for the species, if any. This field is useful for retrieving species that belong to the same mineral group.

Class field. This field contains a series of symbols corresponding to a mineral classification originally devised by Strunz and extended by us.

HARDWARE REQUIREMENTS

The MINERAL database and its retrieval program require a hard disk and occupy approximately 4 megabytes of disk space. A minimum of 384 KB RAM is required as is IBM PC-DOS 2.0 or MS-DOS 2.02 or greater. A graphics adapter is not required for this system, which uses either a monochrome or color CGA or EGA monitor.

AVAILABILITY

We update MINERAL on a quarterly basis. The MINERAL reference including the manual and the TRACKER software is distrib-

uted by Aleph Enterprises, P.O. Box 213, Livermore, California 94550, U.S.A.; phone (415) 443–7319. Further information can be obtained from Aleph Enterprises or from us.

Reference cited

Stone, M.D. (1988) DayFlo Tracker. PC Magazine, 7, no. 21, 104-107.