

PACKAGE ID - 001146C760000 MINEQL-EIR

KWIC TITLE - Chemical Equilibrium Composition of Aqueous
Systems

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LIMITATION CODE -UNL **AUDIENCE CODE** - UNL

COMPLETION DATE - 01/01/1996 **PUBLICATION DATE** - 11/21/1986

DESCRIPTION - MINEQL is a subroutine package to calculate equilibrium composition of an aqueous system, accounting for mass transfer. MINEQL-EIR contains an additional base on enthalpy and heat capacity data and has the option to do calculations at temperatures different from 25 degrees C.

PACKAGE CONTENTS - Media Directory; Software Abstract; User's Guide; Information File (2 pages); Installation Instructions (1 page); Media Includes Test Case Input and Output; Data Library;

SOURCE CODE INCLUDED? - No

MEDIA QUANTITY - 1 3.5 Diskette

METHOD OF SOLUTION - In MINEQL-EIR the iteration scheme to solve the system of equations has been improved to make the probability of divergence very small.

COMPUTER - CDC7600

OPERATING SYSTEMS - Machine Dependent

PROGRAMMING LANGUAGES - FORTRAN-77

SOURCE CODE AVAILABLE (Y/N) - N

OTHER PROG/OPER SYS INFO - In MINEQL-EIR, new output routines have been added for more convenient presentation of the results.

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OTHER PROG/OPER SYS INFO - (CONT)

REFERENCES - M. Schweingruber, Revision 1 of User's Guide for Extended
MINEQL (EIR-version) Standard Subroutine Data Library Package,
November 21, 1986.

ABSTRACT STATUS - Released tested 2/6/97

SUBJECT CLASS CODE - RU

KEYWORDS -

COMPUTER PROGRAM DOCUMENTATION
M CODES
AQUEOUS SOLUTIONS
MASS TRANSFER
ENTHALPY
SPECIFIC HEAT
FREE ENTHALPY
MASS BALANCE
ITERATIVE METHODS
THERMODYNAMIC PROPERTIES
COMPUTER CALCULATIONS
FORTRAN
CHEMICAL EFFLUENTS
GEOCHEMISTRY
GROUND WATER
CHEMICAL REACTIONS
CHEMICAL ANALYSIS

EDB SUBJECT CATEGORIES -

990200 540230 400201 661300

SPONSOR - NEA

PACKAGE TYPE - TESTED