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CNWRA INFORMATION PROCESSING STANDARD SOFTWARE SUMMARY

01. Summary Date	02. Summary prepared by (Name and phone)	03. Summary action
Yr. 92 Mo. 07 Day 08	William Murphy 512-522-5263	New ☐ Replacement ☐ Deletion ☐
04. Software Date: Yr. Mo. Day	03. Software title: EQ3/6 Software Package 1990	Previous Internal Software ID
06. Short title: EQ3/6-90		07. Internal Software ID

08. Software type	09. Processing Mode	10. APPLICATION AREA General		Specific
[X] Automated Data System	☐ Interactive	☐ Computer Systems Support/Utility	☐ Management/Business	Geochemistry
[X] Computer Program	[X] Batch	[X] Scientific/Engineering	☐ Process Control	
[X] Subroutine/Module	☐ Combination	☐ Bibliographic/Textual	☐ Other	

11. Submitting organization and address: LLNL

12. Technical contact(s) and phone:

13. Narrative

The EQ3/6 software package comprises the items on the attached list. The primary codes EQ3NR, EQ6, and EQPT do equilibrium aqueous species distributions, reaction, path mass transfer, and data base manipulation, respectively.

14. Keywords

Geochemistry, aqueous speciation, mass transfer

15. Computer manufacturer and model	16. Computer operating system	17. Programming language(s)	18. Number of source program statements
		Fortran	
19. Computer memory requirements	**20. Tape drives**	**21. Disk/Drum units**	**22. Terminals**

23. Other operational requirements

24. Software availability			25. Documentation availability		
Available	Limited	In-house only	Available	Inadequate	In-house only
[X]	☐	☐	[X]	☐	☐

26. FOR SUBMITTING ORGANIZATION USE

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CNWRA INFORMATION PROCESSING STANDARD SOFTWARE SUMMARY

01. Summary Date	02. Summary prepared by (Name and phone)	03. Summary action
Yr. 92 Mo. 07 Day 08	William Murphy	New [ ] Replacement [ ] Deletion [ ]
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[X]	[ ]	[ ]	[X]	[ ]	[ ]
X Active	Inactive				

26. FOR SUBMITTING ORGANIZATION USE

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EQ3/6, A Software Package for Geochemical Modeling
Version 3245.1090

This software package consists of the following files. Their sizes in lines, words, and bytes are given before their names. The number of words or bytes in a file as recipients may have received them may not exactly match the values given here. The file names may also have been changed to facilitate transmission by ftp. If so, any file name extensions beyond the first will be deleted, stage numbers will be deleted (e.g., con3ifR06.fsc becomes con3if.fsc), and the remaining root names will be truncated if necessary to a maximum of eight characters. If truncation would cause a non-uniqueness problem, one or more of the first eight characters in a root name will be deleted as necessary.

90	90	1036	ALIST.txt
90	90	948	ALISTA.txt
78	514	3820	BUGS.txt
140	724	5712	CONTENTS.txt
57	335	2712	DOCS.txt
10	41	327	FIXES1.txt
104	638	4523	FORMATS.txt
283	2297	14615	INSTALL.txt
123	804	5819	README.txt
235	1709	11936	WHATSNEW.txt
107	566	3888	boratebufs.3i
164	1025	10875	calhalite.6i
2473	10232	105129	calhalite.6o
80	515	3383	calnacl.3i
121	738	5277	canshbrine.3i
54	296	2066	caso4nacl.3i
79	389	2749	co3aqui.3i
2654	11953	210208	con3ifR06.fsc
2576	11734	203831	con3nfR03.fsc
4974	21003	398727	con6ifR06.fsc
4880	20886	390715	con6nfR03.fsc
147	798	8350	crisqtz.6i
61	315	2315	cristobalite.3i
39693	175825	2106657	data0.com.R7
3909	13912	152102	data0.hmw.R7
8785	38558	462345	data0.nea.R7
14229	60684	697914	data0.pit.R7
9821	43142	508679	data0.sup.R7
77	420	2789	deadseabr.3i
149	779	8857	dedolo.6i
1894	8221	89112	dedolo.6o
172	750	22188	dedolo.6t
11806	44535	956286	eq3nrR124.fsc
31248	116855	2531088	eq6R119.fsc
13999	54211	1133919	eqlibR153.fsc
5366	19531	434646	eqptR80.fsc
144	764	8527	evswgyphal.6i
68	330	2329	fo2mineq.3i
187	1171	12163	fwbrmix.6i
1302	5871	59111	fwbrmix.6o
146	838	9231	gypnacl.6i
131	738	8136	gypsum.6i
133	686	8264	heatqf.6i
1393	6837	78177	heatqf.6o
113	528	14577	heatqf.6t
152	739	8277	heatsw.6i
118	603	4037	j13ww.3i
141	658	4487	j13wwsf.3i
192	855	10631	j13wwsf.6i

```
   258    1246   14490 j13v tuff.6i
   153     752    8963 meti ne.6i
  5179   21213  247856 methane.6o
   299    1545   38571 methane.6t
   143     772    8231 microhcl.6i
   327    2172   24040 microhcl.6iN
  2710   11076  114875 microhcl.6o
   228    1024   29412 microhcl.6t
  2064    4785   67247 out.com.R7
   190     614    6012 out.hmw.R7
   568    1483   18213 out.nea.R7
   649    1747   21001 out.pit.R7
   640    1828   20776 out.sup.R7
    71     338    2447 oxcalhem.3i
   163     952    9390 pcalciteA.6i
    71     385    2733 ph4hcl.3i
   168    1024   10094 pquartz.6i
   174    1075   10582 pquartzA.6i
    80     407    2787 quenchfl.3i
   156     730    5027 rwtst.3i
  1784    9004  104305 rwtst.3o
    82     472    3292 sio2.3i
  1071    3457   59705 slist.com.R7
    91     252    3425 slist.hmw.R7
   288     940   14692 slist.nea.R7
   341    1176   17367 slist.pit.R7
   343    1268   17171 slist.sup.R7
    87     444    3148 swbasw.3i
    63     318    2238 swcaarag.3i
    63     324    2262 swco2.3i
    61     312    2205 swmaj.3i
    64     342    2405 swmajd.3i
    72     394    2762 swmajp.3i
   681    2915   29959 swmajp.3o
    73     397    2739 swphcl.3i
   684    2932   30184 swphcl.3o
   135     804    9858 swphclA.3iN
   733    3314   35939 swphclA.3o
    82     426    2870 swrdxcp.3i
   161     725    5025 swtst.3i
  1928    9606  112365 swtst.3o

188126  780723 11860153 total
```

Note that there are 90 files, and that the total size of the export package is just under 12 megabytes.

The ".txt" files contain text describing the software package and should be read by the recipient before installing it. The ".fsc" files are FORTRAN source files. The "data0." files are supporting thermodynamic data files. The "out." and "slist." files are output and "species list" files, respectively, obtained by running the EQPT data file preprocessor code on the data files. The ".3i" and ".3iN" files are EQ3NR input files in old and new format, respectively. Most of these are in the old format. They can be converted to the new format by running the utility code CON3NF. The ".3o" files are EQ3NR output files. the The ".6i" and ".6iN" files are EQ6 input files in old and new format, respectively. Most of these are in the old format. They can be converted to the new format by running the utility code CON6NF. The ".6o" and ".6t" files are EQ6 output and tab files, respectively.

ALIST.txt is a file containing the names of the files, one name per line. It may be useful in assigning names to files read from an ASCII tape. ALISTA.txt is a parallel file which contains shortened versions of the file names which are required for some non-UNIX systems.

---

end of the CONTENTS.txt file

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SOFTWARE PROBLEM/CHANGE REPORT

CNWRA

SPCR Number:	3704-SPCR-001

Project Title:	Project Number:
Geochemistry	20-3704-012

SPCR Title: Implementation of EQ3/6 source codes at SwRI CTC VAX

AFFECTED SOFTWARE AND/OR DOCUMENTATION

Among the EQ3/6 package affected software is: EQ3NR, EQ6, EQLIB, EQPT source codes from EQ3/6 92 package.
LLNL versions 3245R-x.

WM 6/3/92

DESCRIPTION OF PROBLEM/CHANGE

Comment out LLNL system dependent clock routines; implement SwRI VAX routines. Implement read only restriction on data base file open statement in EQLIB to permit multiple users at CNWRA.

WM 6/3/92

PROBLEM SOLUTION/NEED FOR CHANGE

Minor code changes.

Originator:	Title:	Date:
W. Murphy	Senior Research Scientist	06/03/92

PROJECT

Need By Date:	06/03/92	Approved	✓	Disapproved	

Element Manager: John Kimball	Date: 6/3/92
CCB/Quality Assurance Engineer: Richard Burt no CCB action req'd	Date: 6/3/92

IMPLEMENTED SOLUTION

Required changes made: SwRI clock calls implement in source codes. Read only limitation implemented in EQLIB data base open. New versions designated as:

EQ3NR.3245R124xWM WM 6/3/92 WM 6/3/92 EQPT.3245xR80xMUR WM 6/3/92
EQ6.3245R119xWMM EQLIB.3245xR153xMUR WM 6/3/92

Reference controlled notebook 037 (Murphy).

Implemented By:	Date:
W. Murphy WM 6/3/92	06/03/92

BEM
RDB
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Memorandum

To: EQ3/6 Users at CNWRA
cc: J.L. Russell, B. Sagar, W.C. Patrick, B.E. Mabrito, J.E. Latz

From: W. M. Murphy 5/29/92

Date: May 29, 1992

Re: Controlled use of EQ3/6 (Version EQ3/6-92) RDB 5/31/92

Controlled versions of the EQ3/6 software exist on the CTCVAX in the directory user3:[wmm.eq36control]. All CNWRA users may access these files. If users have no requirement to make modifications to these versions, then they need not retain copies of the codes and data bases in their individual accounts. Command files can be constructed to access the executable versions of the programs and the data files directly from the controlled account. A sample command file is attached to this memorandum. Files in the eq36control directory are:

DATA0.DAT	(=DATA0.COM.R12)
DATA0.HMW	(=DATA0.HMW.R12)
DATA0.PIT	(=DATA0.PIT.R12)
DATA1.COMP	(=DATA1 version of DATA0.DAT)
DATA1.HMW	(=DATA1version of DATA0.HMW)
DATA1.PIT	(=DATA1version of DATA0.PIT)
EQ3NR.FSC	(=EQ3NR version 3245R124xWM)
EQ3NR.OBJ	(=object version of EQ3NR.FSC)
EQ3NR.EXE	(=executable version of EQ3NR.FSC)
EQ6.FSC	(=EQ6 version 3245R119xWMM)
EQ6.OBJ	(=object version of EQ6.FSC)
EQ6.EXE	(=executable version of EQ6.FSC)
EQLIB.FSC	(=EQLIB version 3245R153xMUR)
EQLIB.OBJ	(=object version of EQLIB.FSC)
EQPT.FSC	(=EQPT version 3245R80xMUR)
EQPT.OBJ	(=object version of EQPT.FSC)
EQPT.EXE	(=executable version of EQPT.FSC)

Documentation in support of these files is in CNWRA controlled notebook 037 in my possession. Please contact me with any questions.

```
$!
$!              EQ6
$!
$  set def [user.directory]
$!
$  assign       [user.directory]EQ6.OUT                  OUTPUT
$  assign       user3:[wmm.eq36control]DATA1.comp        DATA1
$  assign       [user.directory]PICKUP.DAT               PICKUP
$  assign       [user.directory]TAB.DAT                  TAB
$  assign       [user.directory]TABS.DAT                 TABS
$  assign       [user.directory]TABX.DAT                 TABX
$  assign       [user.directory]INPUT.DAT                INPUT
$  assign       [user.directory]INPUTS.DAT               INPUTS
$!
$   run user3:[wmm.eq36control]eq6
$!
$  deassign     OUTPUT
$  deassign     DATA1
$  deassign     PICKUP
$  deassign     TAB
$  deassign     TABS
$  deassign     TABX
$  deassign     INPUT
$  deassign     INPUTS
$  exit
```