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APPENDIXES

Appendix I

Intermolecular pair potential functions

Intermolecular pair potential functions employed in the $LiCl/H_2O/NH_2OH$ systems which have been obtained from the references. The energies are given in Kcal/mol and the distances in Å.

Li^+-Li^+

$$V_{LiLi} = 332.330271/r + 0.142900576\ [\ (2.37/r)^{12} - (2.37/r)^{6}\ ]$$

Cl^--Cl^-

$$V_{ClCl} = 332.330271/r + 0.160619095\ [\ (4.86/r)^{12} - (4.86/r)^{6}\ ]$$

Li^+-Cl^-

$$V_{LiCl} = -332.330271/r + 0.073755136\ [\ (3.83/r)^{12} - (3.83/r)^{6}\ ]$$

H_2O - H_2O

$$V_{OO} = 144.629212/r + 26765.0474/r^{8.86}$$
$$- 0.250076008\{\exp[-4(r-3.4)^2]+\exp[-1.5(r-4.5)^2]\}$$

$$V_{OH} = -72.3002007/r + 6.2374949/r^{9.2}$$
$$- 9.9972782/\{1+ \exp[40(r-1.05)]\}$$
$$- 4.0046734/\{1+ \exp[5.493(r-2.2)]\}$$

$$V_{HH} = 36.1428977/r + 100.2176721/\{1+ \exp[29.9(r-1.968)]\}$$

NH_2OH -NH_2OH

V_{NN} = $77.17142964/r - 38.21393/r^3 + 22039.10274/r^9$

V_{NO} = $84.05601776/r - 275.24918/r^3 + 30223.48495/r^9$

$V_{NH(N)}$ = $-48.19211685/r - 11.16649/r^3 + 1049.88991/r^9$

$V_{NH(O)}$ = $-64.8432137r + 9.50863/r^3 + 107.3018/r^9$

V_{OO} = $91.55479113/r + 1.36358/r^2 + 13130.35297/r^9$

$V_{OH(N)}$ = $-52.49141358/r + 48.86516/r^3 + 134.28470/r^9$

$V_{OH(O)}$ = $-70.62798173/r + 23.68087/r^3 + 121.38345/r^9$

$V_{H(N)H(N)}$ = $30.09507712/r + 28.57197/r^3 + 4.07493/r^9$

$V_{H(N)H(O)}$ = $40.49337619/r + 27.20365/r^3 + 1.51723/r^9$

$V_{H(O)H(O)}$ = $54.48444305/r + 6.15294/r^3 + 42.20302/r^9$

NH_2OH - H_2O

V_{NO} = $105.638401/r + 271.7194129352669/r^3$

$+ 637.6833268766926/r^6 + 2281.781055361015/r^{12}$

$+ 958.1899785253236\exp(-2.289576175038605r)$

V_{NH} = $-52.81920049/r - 175.6928506252253/r^3$

$+ 511.7899350962408/r^6 + 153.9287366486491/r^{12}$

$+ 3.435687893124913\exp(-0.179033579680110r)$

V_{OO} = $115.0625737/r - 669.9111986997827/r^3$

$+ 4671.42094925515/r^6 + 27.65235453608738/r^{12}$

$+ 139.636123171862\exp(-0.6733788519395670r)$

V_{OH} = $-57.53128684/r - 88.5951818324213/r^3$
$+ 318.249044936195/r^6 + 4.68595232196771/r^{12}$
$+ 34.65534699660206\exp(-0.7678584659676180r)$

$V_{H(N)O}$ = $-65.96920892/r - 147.1486538024156/r^3$
$+ 588.3075763079961/r^6 + 107.661737127527/r^{12}$
$- 90626.01829234084\exp(-5.61329889206091r)$

$V_{H(N)H}$ = $32.98460446/r + 12.36691679413945/r^3$
$+ 17.49344995871357/r^6 + 2.814228190014940/r^{12}$
$+ 78.99888768298514\exp(-1.600584320424739r)$

$V_{H(O)O}$ = $-88.76255684/r - 90.50806853680839/r^3$
$+ 0.08717270238281494/r^6 + 8.147607592682787/r^{12}$
$+ 3132.775919194144\exp(-3.233407216555994r)$

$V_{H(O)H}$ = $44.38127842/r + 11.48670529661016/r^3$
$+ 0.3559967592193338/r^6 + 2.157735693481683/r^{12}$
$+ 110.2035327686086\exp(-2.207773316328812r)$

Li^+ - H_2O

V_{LiO} = $-219.248666/r - 116.8125777/r^2 + 21593.5447\exp(-3.93r)$

V_{LiH} = $109.60999277/r + 56.6704502/r^2 + 275.14123\exp(-5.87r)$

8. Cl^- - H_2O

V_{ClO} = $219.248666/r - 0.26073593/r^2 + 8974.5019\exp(-3.28r)$

V_{ClH} = $-109.60999277/r - 4.033484/r^2 + 2620.32407\exp(-3.314r)$

$Li^+ - NH_2OH$

V_{LiO} = $-174.3790781/r + 438.151/r^4 - 7202.369/r^7 + 553645.735\exp(-4.829r)$

V_{LiN} = $-160.0966013/r - 2490.941/r^4 + 4743.527/r^7 + 6580.365\exp(-2.145r)$

$V_{LiH(N)}$ = $99.97733813/r - 294.882/r^4 + 499.368/r^7 + 377.458\exp(-1.266r)$

$V_{LiH(O)}$ = $134.5210031/r - 659.565/r^4 - 1160.711/r^7 + 690.983\exp(-1.472r)$

$Cl^- - NH_2OH$

V_{ClO} = $174.3790781/r - 2142.729/r^4 + 6523.416/r^5 + 0.73468\exp(0.3070$

V_{ClN} = $160.0966013/$ $.103/r^4 + 8625.442/r^5 + 137.11$ $10214r)$

$V_{ClH(N)}$ = -99.97 $13/r - 1421.366/r^4 + 1826.340/r^5 + 1281.625\exp(2.01397r)$

$V_{ClH(O)}$ = $-134.5210031/r - 898.081/r^4 + 1569.6686/r^5 - 0.4327\exp(0.02244r)$

Appendix II

Explanations to input-variables for MC92I programme

USED MC92-PARAMETER SETTING (DEFINES SIZE OF ARRAYS) : MNS = 5
MNSS = 5
MNPB = 1414

PART 1 : SYS

TITLE ... NAME OF MC-SIMULATION -> FOR DOCUMENTATION ONLY.
MAX.: 70 CHARACTERS
DEFAULT = "

TK ... TEMPERATURE OF SYSTEM IN KELVIN.
IST DIE TEMPERATUR DES SYSTEMS IN KELVIN.
DEFAULT = 298.15

DEN ... DENSITY OF YOUR SYSTEM IN G/CM**3 (ACC. TO TK).
IST DIE DICHTE DES SYSTEMS IN G/CM**3.
DEFAULT = 0.0

ELB ... ELEMENTARY LENGTH OF THE EDGE OF THE BOX IN ANGSTROEM
(ACC. TO DEN).
IST DIE KANTENLAENGE DER ELEMENTARZELLE IN ANGSTROEM.
DEFAULT = 0.0

YOU HAVE TO SPECIFY EITHER DEN OR ELB .GT. 0.0 !!!

RCS ... CUTOFF-RADIUS FOR SHORT-RANGE POTENTIAL-TERMS IN ANGSTROEM.
SHOULD NOT BE SET LOWER THAN 7.0 ANGSTROEM !
GIBT AN, AB WELCHEM ABSTAND (IN ANGSTROEM) "NAHKAMPF"-
POTENTIAL-TERME VERNACHLAESSIGT WERDEN KOENNEN.
DEFAULT = ELB/2.0

DMC ... MINIMAL DISTANCE OF 2 MOLECULAR CENTERS IN ANGSTROEM.
3-TIMES MINIMAL DISTANCE OF 2 MOLECULAR SITES.
IF YOU SPECIFY 0.0, THE DEFAULT-VALUE IS USED !
GIBT AN, AB WELCHEM ABSTAND IN ANGSTROEM SICH
ZWEI MOLEKUEL-ZENTREN SO NAHE SIND, DASS DIE KONFIGURATION
VERWORFEN WERDEN KANN.
DEFAULT = ELB/((NPSX(NPT)**(1/3))*SQRT(3))
(NPSX(NPT) = TOTAL NUMBER OF PARTICLES IN THE BOX)
(SQRT(3) = ARBITRARY FACTOR > 1.0 !)

EWALD ... 0 : CALCULATION OF ALL 1/R INTERACTIONS WITHOUT EWALD-SUM
BUT INCLUDING SUMMATION OVER IMAGINARY-BOXES.
ALLE 1/R WW WERDEN OHNE EWALD-SUMME ABER MIT AUFSUMMIEREN
UEBER IMAGINAERE BOXEN BERECHNET.
1 : CALCULATION OF 1/R INTERACTIONS WITH
EWALD-SUMMATION FOR ION-ION ENERGIES.
BERECHNUNG DER EWALD-SUMME FUER 1/R ION-ION ENERGIEN.
2 : CALCULATION OF 1/R INTERACTIONS WITH
EWALD-SUMMATION FOR ION-ION AND ION-DIPOLE ENERGIES.
BERECHNUNG DER EWALD-SUMME FUER 1/R
ION-ION UND ION-DIPOL ENERGIEN.
3 : CALCULATION OF ALL 1/R INTERACTIONS WITH EWALD-SUM.
ALLE 1/R WW WERDEN MIT EWALD-SUMME BERECHNET.
!!! IF POSSIBLE, USE ONLY "EWALD=0" OR "EWALD=3",
OTHERWISE YOU CALCULATE AN ARBITRARY DIPOLEMOMENT-CONTRIBUTION !!!
!!! EWALD > 0 ONLY FOR ELECTRICALLY NEUTRAL SYSTEMS !!!
!!! DIESE VARIABLE DARF NUR FUER ELEKTROSTATISCH NEUTRALE BOXEN
ALS SIMULATIONSSYSTEME > 0 GESETZT WERDEN !!!
DEFAULT = 3

NIBD ... MAXIMUM NUMBER OF IMAGINARY-BOXES IN ONE AXIS DIRECTION(+/-)
FOR SUMMATION OF 1/R INTERACTIONS AND EWALD=0.
SUMMATION FROM OUTSIDE TO INSIDE (SMALLER TERMS FIRST !).
NIBD=0 CORRESPONDS TO A TOTAL OF 1 BOX (NO IMAGINARY-BOXES)
NIBD=1 CORRESPONDS TO A TOTAL OF 7 BOXES (6 IMAGINARY-BOXES)
NIBD=2 CORRESPONDS TO A TOTAL OF 33 BOXES

(32 IMAGINARY-BOXES).
NIBD=3 CORRESPONDS TO A TOTAL OF 123 BOXES.
NIBD=4 CORRESPONDS TO A TOTAL OF 257 BOXES.
NIBD=5 CORRESPONDS TO A TOTAL OF 515 BOXES.
NIBD=6 CORRESPONDS TO A TOTAL OF 925 BOXES.
NIBD=7 CORRESPONDS TO A TOTAL OF 1419 BOXES.
NIBD=8 CORRESPONDS TO A TOTAL OF 2109 BOXES.
NIBD=9 CORRESPONDS TO A TOTAL OF 3071 BOXES.
NIBD=10 CORRESPONDS TO A TOTAL OF 4169 BOXES.
MAX. VALUE : 10 !!!
IST DIE MAXIMALE ANZAHL VON ZUSAETZLICHEN BOXEN IN EINER ACHSENRICHTUNG(+/-) FUER DIE AUFSUMMIERUNG VON 1/R WW OHNE EWALD. DIE AUFSUMMIERUNG DER WW UEBER DIE BOXEN ERFOLGT IN KUGELNAHER FORM VON AUSSEN NACH INNEN.
!!! NIBD > 0 ONLY FOR ELECTRICALLY NEUTRAL SYSTEMS !!!
!!! DIESE VARIABLE DARF NUR FUER ELEKTROSTATISCH NEUTRALE BOXEN ALS SIMULATIONSSYSTEME > 0 GESETZT WERDEN !!!
DEFAULT = 0

EPSC ... DIELECTRIC-CONSTANT (EPSILON) OUTSIDE YOUR BOX(ES) FOR ENERGY-CORRECTION ACCORDING TO SURFACE-TERM.
THIS FEATURE IS ACTIVE ONLY FOR EWALD=3 OR EWALD=0 AND NIBD >= 7 !
EPSC < 0.0 : NO CORRECTION WILL BE CALCULATED.
0.0 <= EPSC < 1.0 : EPSILON = INFINITE : METALLIC SURROUNDING.
1.0 <= EPSC : EPSILON = EPSC (EPSILON = 1.0 : VACUUM SURROUNDING).
IST DIE DIELEKRTIZITAETSKONSTANTE (EPSILON) AUSSERHALB DER BOX(EN).
!!! EPSC >= 0.0 ONLY FOR ELECTRICALLY NEUTRAL SYSTEMS !!!
!!! DIESE VARIABLE DARF NUR FUER ELEKTROSTATISCH NEUTRALE BOXEN ALS SIMULATIONSSYSTEME >= 0.0 GESETZT WERDEN !!!
DEFAULT = 0.0

MCY ... USE OF CF2-POTENTIAL (MCY=0) OR MCY-POTENTIAL (MCY=1) FOR WATER-WATER-INTERACTIONS.
DEFAULT = 0

RDVRES ... RESOLUTION OF RADIAL-DENSITY-VECTORS IN ANGSTROEM.
AUFLOESUNG DER RADIAL-DICHTE-VEKTOREN IN ANGSTROEM.
DEFAULT = 0.05

NRDVS ... NUMBER OF STEPS FOR COLLECTION OF RDV'S
AND CALCULATION OF RDF'S.
BESTIMMT DIE ANZAHL DER PUNKTE FUER DIE AUFSUMMIERUNG DER
RDV'S UND DIE BERECHNUNG DER RDF'S.
NRDVS = 0 : CALCULATED BY RDVRES -> ALL DISTANCES INCLUDED !
NRDVS = 1 : CALCULATED BY RDVRES -> DISTANCES UP TO ELB/2 INCLUDED !
NRDVS = 2 - 499 : THIS VALUE WILL BE USED !
DEFAULT = 0

TSF ... MAXIMUM TRANSLATIONAL SHIFT FOR A PARTICLE-MOVE IN ANGSTROEM.
IF YOU SPECIFY 0.0, THE DEFAULT-VALUE IS USED !
GIBT DIE MAXIMALE VERSCHIEBUNG IN EINER RICHTUNG (+/-)
IN ANGSTROEM AN.
DEFAULT = DMC/12

ASF ... MAXIMUM ANGULAR SHIFT FOR A PARTICLE-MOVE IN RAD.
IF YOU SPECIFY 0.0, THE DEFAULT-VALUE IS USED !
GIBT DIE MAXIMALE DREHUNG UM EINEN EULERSCHEN WINKEL (+/-)
IN RAD AN.
DEFAULT = 2*PI/SQRT(3)/12

TSF AND ASF INFLUENCE THE RATIO OF ACCEPTED TO REJECTED CONFIGURATIONS
(METROPOLIS-METHOD). FOR AUTOMATIC ADAPTION BY VARIABLE RRARC
THEY ARE JUST START-VALUES.
DURCH DIESE 2 VARIABLEN (TSF, ASF) KANN DAS VERHAELTNIS
VON AUFGENOMMENEN ZU VERWORFENEN KONFIGURATIONEN VERAENDERT
WERDEN.
DIE ANPASSUNG DIESER WERTE DURCH RRARC AN DIE AKTUELLE SITUATION
KANN AUTOMATISCH ERFOLGEN -> DANN SIND DIES NUR STARTWERTE !

RRARC ... REQUESTED RATIO OF ACCEPTED TO REJECTED CONFIGURATIONS.
USED FOR AUTOMATIC ADAPTION OF TSF AND ASF.

BESTIMMT DAS GEWUENSCHTE VERHAELTNIS VON
AUFGENOMMENEN ZU VERWORFENEN KONFIGURATIONEN.
DURCH DIESE VARIABLE KOENNEN TSF UND ASF
AUTOMATISCH NACHGESTELLT WERDEN !

RRARC <= 0.0 : NO AUTOMATIC ADAPTION OF TSF AND ASF.
OPTION AUSGESCHALTET, KEINE AUTOMATISCHE ANPASSUNG
VON TSF UND ASF, STARTWERTE WERDEN VERWENDET !

RRARC = 3.0 : 75% OF ALL CONFIGURATIONS SHOULD BE ACCEPTED.

RRARC = 1.0 : 50% OF ALL CONFIGURATIONS SHOULD BE ACCEPTED.

RRARC = 0.5 : 33% OF ALL CONFIGURATIONS SHOULD BE ACCEPTED.

RRARC = 0.3 : 23% OF ALL CONFIGURATIONS SHOULD BE ACCEPTED.

RRARC = 0.1 : 9% OF ALL CONFIGURATIONS SHOULD BE ACCEPTED.

%(ACCEPTED CONFIGURATIONS) = 100*RRARC/(1+RRARC) !

DEFAULT = 0.5

```
$SYS
TITLE='LITHIUM CHLORIDE & H2O/NH2OH 32 deg. C  2/195/5  PARTICLES  ',
TK=305.2,DEN=1.00688,ELB=0.0,RCS=0.0,DMC=2.2,EWALD=3,NIBD=0,EPSC=75.91,MCY=0,
RDVRES=0.025,NRDVS=1,TSF=0.0,ASF=0.0,RRARC=0.5,
$END
```

PART 2 : PAR - NO DEFAULT VALUES !

NPS(X) (X=1,5) ... NUMBER OF PARTICLES OF TYPE X.
GIBT DIE ANZAHL DER TEILCHEN VOM TYP X AN.

X=1 : WATER
X=2 : COPPER OR ZINC (2 PROGRAM-VERSIONS !)
X=3 : LITHIUM
X=4 : AMMONIA
X=5 : CHLORIDE
X=6 : HYDROXYLAMINE

```
$PAR
NPS(1)=195,
NPS(2)=0,
NPS(3)=2,
NPS(4)=0,
```

NPS(5)=2,
NPS(6)=5,
$END

PART 3 : RUN

RSC ... DETERMINES, HOW STARTING CONFIGURATION IS OBTAINED.
BESTIMMT, WIE DIE STARTKONFIGURATION
DEM PROGRAMM ZUGAENGLICH GEMACHT WIRD.
1 : READ START-CONFIGURATION FROM FILE MC92SC.
STARTKONFIGURATION WIRD VOM FILE MC92SC EINGELESEN.
0 : START-CONFIGURATION GENERATED RANDOMLY.
STARTKONFIGURATION WIRD UEBER EINEN ZUFALLSZAHLENGENERATOR
BERECHNET.
DEFAULT = 0

USC ... DETERMINES CONTENTS OF FILE MC92SC.
BESTIMMT, WELCHE DATEN DER FILE MC92SC ENTHAELT.
1 : MC92SC WILL BE PERIODICALLY UPDATED. THIS NEW COORDINATES
CAN BE USED LATER ON AS IMPROOVED START-COORDINATES.
DER FILE MC92SC ENTHAELT DIE VERAENDERTEN KOORDINATEN
DES SYSTEMS, ER WIRD REGELMAESSIG NEU BESCHRIEBEN.
DIESE KOORDINATEN KOENNEN SPAETER WIEDER ALS NEUE,
VERBESSERTE STARTKONFIGURATION EINGELESEN WERDEN.
0 : MC92SC RETAINS ORIGINAL FORM.
DER FILE MC92SC ENTHAELT DIE KOORDINATEN DES SYSTEMS
IN UNVERAENDERTER ORIGINALVERSION, DIE
TATSAECHLICHE STARTKONFIGURATION BLEIBT ERHALTEN.
DEFAULT = 1

WCON ... DETERMINES WHETHER FILE MCCON WILL BE WRITTEN OR NOT.
BESTIMMT, OB DER FILE MCCON BESCHRIEBEN WIRD ODER NICHT.
1 : MCCON WILL BE EXPANDED EVERY MACRO-STEP.
DER FILE MCCON WIRD PRO MACRO-STEP ERWEITERT.
0 : MCCON WILL NOT BE WRITTEN.
DER FILE MCCON WIRD NICHT BESCHRIEBEN.

DEFAULT = 1

RNGO ... RANDOM-NUMBER-GENERATOR OPTION (CHOICE OF TYPE OF RNG).
WAEHLT DEN ZUFALLSZAHLENGENERATOR (RNG).
1 : INTERNAL RNG OF THIS PROGRAM (NORMAL CASE).
INTERNER RNG, IM PROGRAMM EINGEBAUT.
2 : CYBER 840 (NOS/VE) RNG.
CYBER 840 (NOS/VE) RNG.
DER WERTEBEREICH KANN ERWEITERT WERDEN, WENN AUCH DIE
FUNCTION RNG() UND DIE SUBROUTINES RNGS UND RNGG
MODIFIZIERT WERDEN !
DEFAULT = 1

IJC, KLC ... THIS ARE THE SEED-VALUES FOR THE RANDOM-NUMBER-GENERATOR :
0 <= IJC <= 31328 , 0 <= KLC <= 30081
DEFAULT = 10443, 20054

EXPM ... LARGEST X FOR EXP(X) AND
SMALLEST -X FOR EXP(-X) FOR YOUR COMPUTER.
CHECK THIS VARIABLE-SETTING ON YOUR MACHINE (TEST PROGRAM)
FOR CYBER 840 : 2839.823
FOR 32-BIT MACHINES NORMALLY 88. IS O.K.
DEFAULT = 88.

MAXCON ... TOTAL NUMBER OF CONFIGURATIONS FOR THIS SIMULATION.
GIBT DIE GESAMTDAUER DER RECHNUNG IN SCHRITTEN
(KONFIGURATIONEN) AN.
UEBER DIESE VARIABLE KOENNEN AUCH KURZE TESTLAEUFE DES
PROGRAMMS GESTEUERT WERDEN.
DEFAULT = 1000*NPSX(NPT)
(NPSX(NPT) = TOTAL NUMBER OF PARTICLES IN THE BOX)

NUPDAT ... NUMBER OF STEPS (CONFIGURATIONS / MACRO-STEP) FOR UPDATING
OF STATISTICAL DATA; ALSO THESE FILES WILL BE ACTUALIZED :
FILE MC92SC (FOR USC=1)
FILE MC92CV (FOR UCV=1)

FILE MCENE
FILE MCCON (FOR WCON=1)
FILE SRNG
FILE MC92IS (RESTART-INFORMATION)
GIBT AN, NACH JEWEILS WIEVIELEN SCHRITTEN DIE STATISTISCHEN
MITTELWERTE ERNEUERT WERDEN SOLLEN; AUSSERDEM :
DER FILE MC92SC WIRD AKTUALISIERT (WENN USC=1).
DER FILE MC92CV WIRD AKTUALISIERT (WENN UCV=1).
DER FILE MCENE WIRD AKTUALISIERT.
DER FILE MCCON WIRD AKTUALISIERT (WENN WCON=1).
DER FILE SRNG WIRD ERNEUERT.
DER FILE MC92IS WIRD ERNEUERT.
DIE ERNEUERUNG DER FILES SRNG UND MC92IS
IST WICHTIG, UM DIE RESTART-INFORMATIONEN ABZUSPEICHERN !
DEFAULT = 2*NPSX(NPT)
(NPSX(NPT) = TOTAL NUMBER OF PARTICLES IN THE BOX)

NCONB ... NUMBER OF STEPS (CONFIGURATIONS) UNTIL THE SIMULATION BREAKS.
USE THIS FEATURE FOR SUBMITTING NUMEROUS SHORT JOBS RATHER
THAN ONE LONG JOB. NORMALLY, SET NCONB=+INTEGER*NUPDAT
(ACCORDING TO THE RESOURCES ON YOUR MACHINE) - TEST !
THE SUBMISSION OF SHORT JOBS IN A CHAIN CAN BE MANAGED
AUTOMATICALLY VIA A SHELL-SCRIPT OR PROCEDURE ETC..
GIBT AN, NACH JEWEILS WIEVIELEN SCHRITTEN DIE SIMULATION
UNTERBROCHEN WERDEN SOLL. DAS IST VOR ALLEM FUER MASCHINEN
MIT LIMITIERTER JOB-ZEIT WICHTIG !
DEFAULT = 0 (ONLY ONE BREAK AFTER INITIALIZING (STEP 0 : START-RUN))

UCV ... DETERMINES WHETHER RADIAL-DENSITY-VECTORS AND
RADIAL-DENSITY-FUNCTIONS (INCLUDING INTEGRATIONS
-> COORDINATION-NUMBERS) ARE EVALUATED OR NOT.
BESTIMMT, OB DIE RADIAL-DICHTE-VEKTOREN BERECHNET
WERDEN ODER NICHT.
1 : CONTINUOUS EVALUATION AND SUMMATION OF RDV'S.
RDV'S STORED IN FILE MC92CV.
FORTLAUFENDE BERECHNUNG UND AUFSUMMIERUNG

DER RADIAL-DICHTE-VEKTOREN.
0 : NO RDV-EVALUATION.
KEINE BERECHNUNG DER RADIAL-DICHTE-VEKTOREN.
DEFAULT = 1

NCF ... SPEFIFIES HOW OFTEN RADIAL-DENSITY-FUNCTIONS ARE EVALUATED AND UPDATED ON FILES MC92CFxxxx (ONLY ACTIVE FOR UCV=1).
BESTIMMT, WIE OFT DIE RADIAL-DICHTE-FUNKTIONEN BERECHNET UND DIE FILES MC92CFxxxx ERNEUERT WERDEN (NUR WENN UCV=1).
NCF = 1 : EVERY MACRO-STEP
NCF = 10 : EVERY 10th MACRO-STEP
NCF = 100 : EVERY 100th MACRO-STEP
DEFAULT = MAXCON/NUPDAT

MWCF ... MODE (FORMAT) FOR WRITING TO FILES MC92CFxxxx.
BESTIMMT, IN WELCHEM FORMAT DIE FILES MC92CFxxxx BESCHRIEBEN WERDEN.
0 : PARALLEL (4 COLUMNS)
1 : SERIAL (3-TIMES 2 COLUMNS)
DEFAULT = 0

UNIT9: MC92I: THIS FILE (FORMATTED).
DIESER FILE (FORMATIERT).
DEFAULT = 'MC92I' --- STANDARD-FILE-NAME
! THIS NAME MAY BE CHANGED IN THE PROGRAM ONLY !

UNIT10: MC92IS: RESTART-INFORMATION FILE (UNFORMATTED).
FILE BEINHALTET RESTARTINFORMATION (UNFORMATIERT).
DEFAULT = 'MC92IS' --- STANDARD-FILE-NAME
! THIS NAME MAY BE CHANGED IN THE PROGRAM ONLY !

UNIT11: MC92SC: START-COORDINATES OF THE PARTICLES IN THE BOX (FORMATTED).
FILE BEINHALTET STARTKOORDINATEN DER TEILCHEN IN DER BOX (FORMATIERT).
DEFAULT = 'MC92SC'

UNIT12: MC92CV: RADIAL-DENSITY-VECTORS (FORMATTED).
FILE BEINHALTET RADIAL-DICHTE-VEKTOREN (FORMATIERT).
DEFAULT = 'MC92CV'

UNIT13: MCOUT: STANDARD-INFORMATION, STATISTICS, ERROR-MESSAGES ETC.
(FORMATTED, APPEND-MODE).
FILE BEINHALTET STANDARDINFORMATIONEN, FEHLERMELDUNGEN
ETC. (FORMATIERT).
DEFAULT = 'MCOUT'

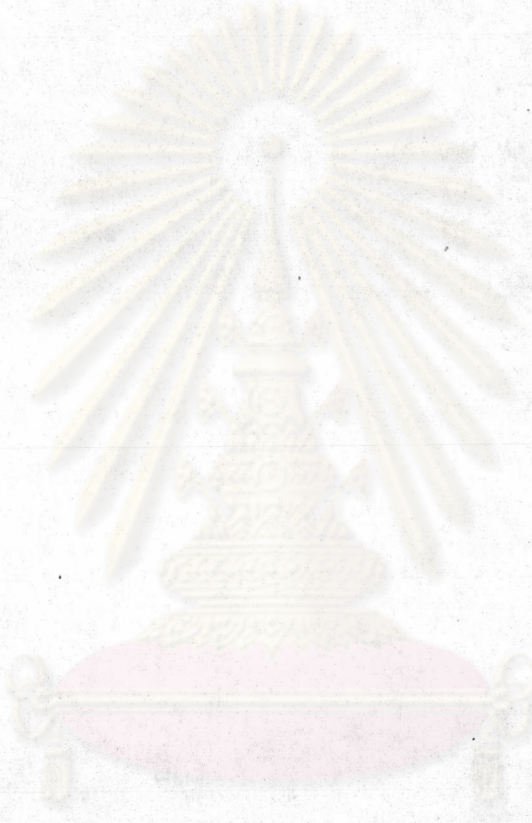
UNIT14: MCENE: NCON, NCON/NUPDAT AND ENERGY DATA FOR GRAPHICS
(FORMATTED, APPEND-MODE).
FILE BEINHALTET NCON GEGEN NCON/NUPDAT GEGEN ENERGIEN
ZUR GRAPHISCHEN DARSTELLUNG DES SIMULATIONSVERLAUFES
(FORMATIERT).
DEFAULT = 'MCENE'

UNIT15: MCCON: DOCUMENTATION OF SIMULATION-RUN
- CONFIGURATION OF THE SYSTEM (PER MACRO-STEP)
(FORMATTED, APPEND-MODE).
FILE BEINHALTET DOKUMENTATION DER SIMULATIONS-ENTWICKLUNG
- KONFIGURATION DES SYSTEMS (PRO MACRO-STEP)
(FORMATIERT).
DEFAULT = 'MCCON'

UNIT21: STES: TABLE FOR EWALD-SUM VALUES (UNFORMATTED).
FILE BEINHALTET EWALD-TABELLE (UNFORMATIERT).
DEFAULT = 'STES'

UNIT22: SRNG: RESTART-INFORMATION FOR INTERNAL RNG (UNFORMATTED).
FILE BEINHALTET RESTART-INFORMATION FUER INTERNEN RNG
(UNFORMATIERT).
DEFAULT = 'SRNG'
MNNNLC: MAXIMUM NUMBER OF NEAREST NEIGHBOUR LIGANDS CONSIDERED
DEFAULT = 20

```
$RUN
RSC=1,USC=1,WCON=0,RNGO=1,IJC=10443,KLC=20054,EXPM=88.,
MAXCON=1000000,NUPDAT=1000,NCONB=0,UCV=1,NCF=10,MWCF=0,
MC92SC='MC92SC    ',MC92CV='MC92CV    ',
MCOUT='MCOUT    ',MCENE='MCENE    ',MCCON='MCCON    ',
STES='STES    ',SRNG='SRNG    ',MNNNLC=0,
$END
```



CURRICULUM VITAE

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1970	Born October, 7th in Rayong, Thailand
	Father : Mr.Arrom Suwannachot
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1977-1983	Elementary School
1983-1989	High School (Kleang Wittayasathaworn)
1989-1993	Bachelor of Science (Chemistry),
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1993-1995	Master degree study at Department of Chemistry,
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The paper which has been submitted in international journal is :

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Suwannachot, Y., Hannongbua, S., Rode, B.M., J.Chem.Phys., in press