BUREAU DE RECHERCHES GÉOLOGIQUES ET MINIÈRES

SERVICE GÉOLOGIQUE NATIONAL
B.P. 6009 - 45060 Orléans Cedex - Tél.: (38) 64.34.34

WATRA, programme de calcul d'équilibre dans les eaux, une version de WateqF étendue aux éléments : Ni, Co, Cu, Pb, Zn, Cd, Cr, As, Sb, Ge

Données thermodynamiques révisées et complétées

par

A. CRIAUD*, C. FOUILLAC**, P. OUSTRIÈRE***

**SGN/MGA - **SGN/IRG - ***SGN/GMX*

Département Minéralogie, Géochimie, Analyses
B.P. 6009 - 45060 Orléans Cedex - Tél.: (38) 64.34.34

Rapport du B.R.G.M.

84 SGN 388 MGA

Décembre 1984

Réalisation : Département Applications Graphiques

RESUME

Le programme WATRA permet de calculer à partir de la composition chimique d'une eau la répartition des espèces ioniques simples et complexes à l'équilibre thermodynamique.

Les résultats de cette description du milieu aqueux servent aux calculs de saturation vis-à-vis des minéraux courants.

Cette note technique est constituée d'un listing du programme WATRA et d'un descriptif des nouveautés introduites par les auteurs. Les données thermodynamiques complètes ainsi que deux exemples d'utilisation figurent dans ce rapport.

SOMMAIRE

INTRODUCTION

Le programme WATRA est une nouvelle version Fortran de WateqF (PLUMMER et al., 1976) qui a été élargie aux éléments suivants : Ni, Co, Cu, Pb, Zn, Cd, Cr, As, Sb, Ge. Il a été mis au point sur VAX 11/780 sous VMS version 3.6 en janvier 1983 au Bureau de Recherches Géologiques et Minières. L'ensemble des données thermodynamiques initiales de WateqF ainsi que celles relatives aux 115 espèces aqueuses et aux 122 minéraux ajoutés figure dans cette notice.

Les résultats d'analyses des nouveaux éléments sont entrés par l'intermédiaire des cartes CONC déjà utilisées dans WateqF. La structure du programme initial WateqF a été conservée mais des modifications ont été introduites dans le principe du calcul de la répartition des espèces traces nouvelles. L'utilisation de descripteurs de réactions (LSPEC, CSPEC pour les espèces aqueuses, LMIN et CMIN pour les minéraux) permet d'écrire de façon homogène et systématique n'importe quelle réaction de formation de l'espèce complexe "trace" ou du minéral "trace". Le remplissage de ces matrices s'effectue de la façon suivante :

LSPEC (120,6) format 501

Colonne 1 : nombre de ligands différents nécessaires à la formation du complexe.

Colonne 2 : numéro du complexe, ou de la réaction correspondante.

Colonne 3 : numéro de l'espèce simple concernée (Cd^{2+} = 1, Zn^{2+} = 2, Pb^{2+} = 3, Co^{2+} = 4, Ni^{2+} = 5, Cr^{3+} = 6, Cu^{2+} = 7, AsO_4^{3-} = 8, $Sb(OH)_3^o$ = 9, $Ge(OH)_4^o$ = 10).

Colonnes 4 à 6 : numéros des ligands nécessaires à la formation de l'espèce aqueuse (numérotation Wateq : OH^- = 27, Cl^- = 5, SO_4^{2-} = 6, F^- = 62, CO_3^{2-} = 18, HCO_3^- = 7, HS^- = 67, H^+ = 64, H_2O = 72, e^- = 251).

CSPEC (120,6) *format 502*

Colonne 1 : numéro du complexe, ou de la réaction.

Colonne 2 : coefficient stoechiométrique de l'espèce complexe (= 1 en général, dans la réaction $M + L \rightleftharpoons ML$).

Colonne 3 : coefficient stoechiométrique de l'espèce simple dans cette réaction.

Colonnes 4 à 6 : coefficients stoechométriques des ligands (pris dans le même ordre que dans LSPEC).

LMIN (140,7) *format 503*

Colonne 1 : nombre de ligands.

Colonne 2 : numéro de l'espèce minérale, ou de la réaction (numérotation Wateq).

Colonnes 3 à 7 : numéros des espèces qui prennent part à la réaction.

CMIN (140,7) *format 504*

Colonne 1 : numéro de la réaction.

Colonne 2 : coefficient stoechiométrique du minéral (= - 1 en général dans la réaction $ML_{(s)} \rightleftharpoons M + L$).

Colonnes 3 à 7 : coefficients stoechiométriques des espèces qui prennent part à la réaction ci-dessus (pris dans le même ordre que dans LMIN).

De façon générale, la réaction de formation de l'espèce dissoute dont le numéro est I [ou encore LSPEC (I, 2)] s'écrit :

CSPEC (I, 3). LSPEC (I, 3) + CSPEC (I, 4). LSPEC (I, 4) + ...
+ CSPEC (I, 6). LSPEC (I, 6) $\rightleftharpoons$ CSPEC (I, 2). LSPEC (I, 2)

De la même façon, pour la réaction qui concerne le minéral dont le numéro est LMIN (I, 2), on aura :

CMIN (I, 2). LMIN (I, 2) $\rightleftharpoons$ CMIN (I, 3). LMIN (I, 3) + ...
+ ..... + CMIN (I, 7). LMIN (I, 7).

Les coefficients CSPEC et CMIN peuvent être dans ces conditions positifs ou négatifs.

Il est possible d'utiliser le programme WATRA sans tenir compte des éléments traces, par l'intermédiaire du signal TRACES. Si TRACES = 0, le calcul ne prendra en compte que les éléments majeurs (équivalent à WateqF). Si TRACES = 1, les éléments Cu, Pb, Zn, Cd, Co, Ni, Cr, As, Sb et Ge sont considérés.

Le test de convergence a également été modifié par rapport à WateqF, il est appliqué uniquement si TRACES = 1. Ce test porte sur l'espèce trace dont la concentration totale est minimum. A chaque itération, on compare la molalité de l'espèce complexe la plus faiblement représentée à celle obtenue au pas précédent. Le test est positif lorsque la différence est inférieure un pourcentage de la concentration totale de cette espèce fixé auparavant. Sinon la totalité des calculs (répartition des espèces majeures et traces) est reprise au cours de l'itération suivante.

Les résultats des calculs (distribution des espèces et indice de saturation) sont présentés dans deux cas :

- Une eau de mer (t = 25° C) déjà utilisée par Nordström et al (1979) pour le test de comparaison des programmes du même type.
- Une eau thermominérale (t = 59,7° C) de type bicarbonaté sodique.

LISTING du PROGRAMME WATRA

```
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      INTEGER D,E,DD,RBIT,CORALK,Z(260),PRT(4)
      INTEGER PECALC,PECK,FLAG,TRACES,CSPEC(120,6)
      REAL*8 MI(260),MNTOT,LH2O,MU,NATOT,KT
     1OT,MGTOT,LITOT,NH4TOT,KW
      REAL*8 KT(450),LOGKT(450),LOGKTO(450)
      REAL*8 NSPEC(260),NREACT(450),MIPRIM(125)
      COMMON MI,KT,LOGKT,LOGKTO,KW,D,E,DD,C,R,T,F,TEMP,A,B,NSPEC,NREA
     1CT,PE,PES,PEDO,PESATO,PECK,PECALC,PH,TENMPE,TENPH,ALFA(260),GAMMA(
     2260),AP(450),XLALFA(260),Z,CUNITS(260),ANALMI(260),GFW(260),DHA(26
     30),DH(450),AH2O,LH2O,EROR1,EROR2,EROR3,EROR4,EROR5,EHM,DENS,DOX,XL
     4MI(260),ITER,RBIT,C1SAVE,CORALK,MU,LCHEK(450),CO2TIT,ANALCO,SITOT,
     5CATOT,MGTOT,KTOT,NATOT,SO4TOT,FETOT,PTOT,ALTOT,FTOT,BTOT,LITOT,NH4
     6TOT,SRTOT,BATOT,CLTOT,MNTOT,ICK,PRT,TITL(10),EPMCAT,EPMAN,NEQU,
     7ISPEC,KSPEC(260),IMIN,KMIN(450),TDS,IDAVES,IPRT,FLAG,IGO,XLGAM(260
     8),TRACES,CITOT(10),NTRACE,LSPEC(120,6),CSPEC,LMIN(140,7),
     9CMIN(140,7),EROR6,STORE(25,25),ITMIN,MIPRIM,XPCENT(125)
      OPEN (UNIT=6, ORGANIZATION='SEQUENTIAL', RECORDTYPE='FIXED',
     1 RECL=132, STATUS='NEW')
      D=250
      E=440
      NTRACE=10
      IPRT=0
      NEQU=15
      READ (5,50), (NSPEC(I),Z(I),DHA(I),GFW(I),I=1,D)
      READ (5,60), (NREACT(I),DH(I),LOGKTO(I),I=1,E)
      READ (5,501) ((LSPEC(I,J),J=1,6),I=1,115)
      READ (5,502) ((CSPEC(I,J),J=1,6),I=1,115)
      READ (5,503) ((LMIN(I,J),J=1,7),I=1,122)
      READ (5,504) ((CMIN(I,J),J=1,7),I=1,122)
   10 CONTINUE
      READ (5,70,END=40),TITL
      ICK=0
      CALL PREP
      IF (ICK.EQ.1) GO TO 10
      CALL SET
   20 CONTINUE
      CALL MODEL
      IF (ITER.EQ.25) GO TO 30
      IF (RBIT.EQ.1) GO TO 20
      IF (ITER.LT.6) GO TO 20
      CALL PRINT
      IF (PRT(4).NE.0) GO TO 10
      CALL SAT
      GO TO 10
   30 WRITE(6,80)
   80 FORMAT (10X,'LA CONVERGENCE N'EST PAS ATTEINTE A MOINS DE 25 ITER
     1ATIONS,CALCUL TERMINE')
      GO TO 10
   40 STOP
   50 FORMAT (5X,A8,2X,I2,1X,F4.1,2X,F10.4)
   60 FORMAT (5X,A8,F10.4,2X,F10.4)
  501 FORMAT ((I2,5X,I3,5X,I2,5X,I3,2(2X,I3)))
  502 FORMAT ((I3,5(3X,I2)))
  503 FORMAT ((I2,6(3X,I3)))
  504 FORMAT ((F4.0,6(2X,F5.2)))
   70 FORMAT (10A8)
 1112 FORMAT (80X)
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1117 FORMAT (80X)
     END

          **********************
          * SOUS PROGRAMME PREP *
          **********************


      SUBROUTINE PREP
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      INTEGER D,E,DD,RBIT,CORALK,Z(260),WORD,CARD(6),FLAG,PRT(4),SIGN(2)
      INTEGER PECALC,PECK,TRACES,CSPEC(120,6)
      DIMENSION INT(5), VAL(5), INPT(32), GRAMS(260), IEQU(50), COEF(5,2
     103), V(260)
      REAL*8 MI(260),MNTOT,LH2O,MU,NATOT,KT
     1OT,MGTOT,LITOT,NH4TOT,KW
      REAL*8 KT(450),LOGKT(450),LOGKTO(450)
      REAL*8 NSPEC(260),NREACT(450),MIPRIM(125)
      COMMON MI,KT,LOGKT,LOGKTO,KW,D,E,DD,C,R,T,F,TEMP,A,B,NSPEC,NREA
     1CT,PE,PES,PEDO,PESATO,PECK,PECALC,PH,TENMPE,TENPH,ALFA(260),GAMMA(
     2260),AP(450),XLALFA(260),Z,CUNITS(260),ANALMI(260),GFW(260),DHA(26
     330),DH(450),AH2O,LH2O,EROR1,EROR2,EROR3,EROR4,EROR5,EHM,DENS,DOX,XL
     4MI(260),ITER,RBIT,C1SAVE,CORALK,MU,LCHEK(450),CO2TIT,ANALCO,SITOT,
     5CATOT,MGTOT,KTOT,NATOT,SO4TOT,FETOT,PTOT,ALTOT,FTOT,BTOT,LITOT,NH4
     6TOT,SRTOT,BATOT,CLTOT,MNTOT,ICK,PRT,TITL(10),EPMCAT,EPMAN,NEQU,
     7ISPEC,KSPEC(260),IMIN,KMIN(450),TDS,IDAVEG,IPRT,FLAG,IGO,XLGAM(260
     8),TRACES,CITOT(10),NTRACE,LSPEC(120,6),CSPEC,LMIN(140,7),
     9CMIN(140,7),EROR6,STORE(25,25),ITMIN,MIPRIM,XPCENT(125)
      DATA CARD/'CONC','EROR','DELH','TABL','LOGK','    '/,SIGN/' ','*'/
      DATA IEQU/13,14,15,25,26,27,36,69,73,74,75,78,79,90,92,35*0/
      DATA COEF/60*0.0,13.543,-0.0401,-3000.,2*0.0,6.368,-0.016346,-3405
     1.9,2*0.0,39.478,-0.065927,-12355.1,47*0.0,0.684,0.0051295,3*0.0,28
     2.6059,0.012078,1573.21,2*0.0,0.6322,-0.001225,-2835.76,42*0.,-14.8
     3435,+0.032786,+3404.71,162*0.,-6.498,+0.02379,+2902.39,17*0.0,3.10
     46,0.0,-673.6,2*0.0,0.991,0.00667,3*0.0,2.319,-.011056,0.0,2.29812E
     5-05,11*0.0,-2.95,0.0133,3*0.0,-27.393,0.05617,4114.0,52*0.0,-5.350
     66,0.0183412,557.2461,7*0.0,11.17,-0.02386,-3279.0,557*0.0/
      DATA INPT/1,2,3,4,5,6,7,35,8,45,88,62,17,18,39,51,81,85,87,90,98,1
     101,126,148,167,186,196,208,219,237,244,249/
      D=2.302585092
      F=23.0603
      R=1.98719E-03
      EROR1=.01
      EROR2=.01
      EROR3=.01
      EROR4=.01
      EROR5=.01
      EROR6=.0001
      ICK=0
      PEDO=100.0
      PESATO=100.0
      PES=100.0
      DO 10 I=1,D
      CUNITS(I)=0.0
      ALFA(I)=0.0
      MI(I)=0.0
      XLMI(I)=0.0
      IF (Z(I).EQ.0) V(I)=1.0
      IF (Z(I).EQ.0) GO TO 10
      IF (Z(I).LT.0) V(I)=-1.0*Z(I)
      IF (Z(I).GT.0) V(I)=1.0*Z(I)
   10 CONTINUE
      PECK=0
```

```
      READ (5,570), TEMP,PH,EHM,EHMC,EMFZ,TRACES,DENS,DOX,FLAG,CORALK,
     1PECALC,IGO,(PRT(I),I=1,4),IDAVES,ISPEC,IMIN
      IF(TRACES.EQ.1) GO TO 11
      D=125
      E=203
   11 CONTINUE

C  CHOIX DE L'IMPRESSION DES DONNEES THERMOCHIMIQUES
C  ************************************************

      IF (PRT(1).NE.0) GO TO 70
      DO 15 I=1,115
      WRITE(6,511),LSPEC(I,1),LSPEC(I,2),LSPEC(I,3),LSPEC(I,4)
     1,LSPEC(I,5),LSPEC(I,6)
   15 CONTINUE
      DO 16 I=1,115
      WRITE(6,512),CSPEC(I,1),CSPEC(I,2),CSPEC(I,3),CSPEC(I,4)
     1,CSPEC(I,5),CSPEC(I,6)
   16 CONTINUE
      DO 17 I=1,122
      WRITE(6,513),LMIN(I,1),LMIN(I,2),LMIN(I,3),LMIN(I,4)
     1,LMIN(I,5),LMIN(I,6),LMIN(I,7)
   17 CONTINUE
      DO 18 I=1,122
      WRITE(6,514),CMIN(I,1),CMIN(I,2),CMIN(I,3),CMIN(I,4)
     1,CMIN(I,5),CMIN(I,6),CMIN(I,7)
   18 CONTINUE
  511 FORMAT (2X,I2,3X,I3,3X,I2,3X,I3,3X,I3,3X,I3)
  512 FORMAT (2X,I3,5(3X,I2))
  513 FORMAT (2X,I2,6(3X,I3))
  514 FORMAT (2X,F4.0,6(2X,F5.2))
      WRITE(6,580)
      DO 30 I=1,D
      ISIG=SIGN(1)
      DO 20 J=1,NEQU
      IF (I.EQ.IEQU(J)) ISIG=SIGN(2)
   20 CONTINUE
      WRITE(6,590),I,NREACT(I),DH(I),LOGKTO(I),ISIG,I,NSPEC(I),
     1Z(I),DHA(I),GFW(I)
   30 CONTINUE
      DD=D+1
      DO 50 I=DD,E
      ISIG=SIGN(1)
      DO 40 J=1,NEQU
      IF (I.EQ.IEQU(J)) ISIG=SIGN(2)
   40 CONTINUE
      WRITE(6,600), I,NREACT(I),DH(I),LOGKTO(I),ISIG
   50 CONTINUE
      WRITE(6,510)
      DO 60 I=1,NEQU
      WRITE(6,520), IEQU(I),NREACT(IEQU(I)),COEF(1,IEQU(I)),COE
     1F(2,IEQU(I)),COEF(3,IEQU(I)),COEF(4,IEQU(I)),COEF(5,IEQU(
     2I))
   60 CONTINUE
   70 CONTINUE
      IPRT=1
      WRITE(6,610), TITL
      READ (5,620), (CUNITS(INPT(I)),I=1,12)
      IF (ISPEC.GT.0) READ (5,530), (KSPEC(I),I=1,ISPEC)
      IF (IMIN.GT.0) READ (5,530), (KMIN(I),I=1,IMIN)

C  ENTREE D'UNE CARTE OPTIONNELLE
C  ******************************
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```
 80 READ (5,630), WORD,(INT(I),VAL(I),I=1,5)
    IF (WORD.NE.CARD(1)) GO TO 100
    DO 90 I=1,5
    IF (INT(I).EQ.0) GO TO 90
    CUNITS(INT(I))=VAL(I)
 90 CONTINUE
    GO TO 80
100 CONTINUE
    IF (WORD.NE.CARD(2)) GO TO 110
    EROR1=VAL(1)
    EROR2=VAL(2)
    EROR3=VAL(3)
    EROR4=VAL(4)
    EROR5=VAL(5)
    READ (5,630), WORD,(INT(I),VAL(I),I=1,5)
110 IF (WORD.NE.CARD(3)) GO TO 130
    DO 120 I=1,5
    IF (INT(I).EQ.0) GO TO 120
    DH(INT(I))=VAL(I)
    WRITE(6,640), INT(I),NREACT(INT(I)),VAL(I)
120 CONTINUE
    READ (5,630), WORD,(INT(I),VAL(I),I=1,5)
    GO TO 110
130 IF (WORD.NE.CARD(4)) GO TO 150
    DO 140 I=1,5
    IF (INT(I).EQ.0) GO TO 140
    LOGKTO(INT(I))=VAL(I)
    WRITE(6,650), INT(I),NREACT(INT(I)),VAL(I)
140 CONTINUE
    READ (5,630), WORD,(INT(I),VAL(I),I=1,5)
    GO TO 130
150 CONTINUE

 EQUATION DE VAN'T HOFF
 **********************

    T=TEMP+273.16
    C1=(298.16-T)/(298.16*T*C*R)
    DO 170 I=1,E
    LOGKT(I)=LOGKTO(I)-DH(I)*C1
    LCHEK(I)=0
    IF (LOGKT(I).LT.-200.0.OR.LOGKT(I).GT.200.0) LCHEK(I)=1
    IF (LCHEK(I).EQ.1) GO TO 160
    KT(I)=10.**LOGKT(I)
160 CONTINUE
170 CONTINUE
    KW=KT(153)

 EXPRESSIONS ANALYTIQUES: INFLUENCE DE T SUR K
 *********************************************

180 IF (WORD.NE.CARD(5)) GO TO 220
    IF (INT(1).EQ.0) GO TO 210
    DO 190 I=1,5
    COEF(I,INT(1))=VAL(I)
190 CONTINUE
    IEQ=0
    DO 200 I=1,NEQU
    IF (IEQU(I).EQ.INT(1)) IEQ=1
200 CONTINUE
    IF (IEQ.EQ.0) NEQU=NEQU+1
    IF (IEQ.EQ.0) IEQU(NEQU)=INT(1)
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```
      WRITE(6,660), INT(1),NREACT(INT(1)),COEF(1,INT(1)),
     1COEF(2,INT(1)),COEF(3,INT(1)),COEF(4,INT(1)),COEF(5
     2,INT(1))
  210 CONTINUE
      READ (5,630), WORD,(INT(I),VAL(I),I=1,5)
      GO TO 180
  220 CONTINUE
      IF (WORD.EQ.CARD(6)) GO TO 230
      WRITE(6,540)
      READ (5,630), WORD,(INT(I),VAL(I),I=1,5)
      GO TO 220
  230 CONTINUE
      DO 240 I=1,NEQU
      LOGKT(IEQU(I))=COEF(1,IEQU(I))+COEF(2,IEQU(I))*T+COEF(3,IEQU(I))/T
     1+COEF(4,IEQU(I))*T*T+COEF(5,IEQU(I))/(T*T)
  240 CONTINUE
      LOGKT(26)=LOGKT(26)+DLOG10(KW)-13.2258*DLOG10(T)
      DO 250 I=1,NEQU
      KT(IEQU(I))=1E1**(LOGKT(IEQU(I)))
  250 CONTINUE


 CALCUL DES MOLALITES ANALYSEES
 ******************************

      IF (FLAG.NE.1) GO TO 270
      DO 260 I=1,D
      CUNITS(I)=CUNITS(I)*GFW(I)/V(I)
  260 CONTINUE
      FLAG=2
  270 CONTINUE
      IF (FLAG.NE.2) GO TO 290
      DO 280 I=1,D
      CUNITS(I)=CUNITS(I)/DENS
  280 CONTINUE
      FLAG=3
  290 CONTINUE
      IF (FLAG.NE.3) GO TO 320
      C1=0.0
      DO 300 I=1,D
      C1=C1+CUNITS(I)
  300 CONTINUE
      DO 310 I=1,D
      C1SAVE=C1
      MI(I)=(CUNITS(I)/(1.0E+03*GFW(I)))*(1.0/(1.0-1.0E-06*C1))
      IF (MI(I).GT.0.0) XLMI(I)=DLOG10(MI(I))
      GRAMS(I)=CUNITS(I)*DENS
  310 CONTINUE
      GO TO 350
  320 CONTINUE
      C1=0.0
      IF (FLAG.NE.4) GO TO 480
      DO 330 I=1,D
      MI(I)=CUNITS(I)
      C1=C1+MI(I)*GFW(I)*1000./DENS
      IF (MI(I).GT.0.0) XLMI(I)=DLOG10(MI(I))
  330 CONTINUE
      C1SAVE=C1
      DO 340 I=1,D
      GRAMS(I)=MI(I)*1000.*GFW(I)*DENS*(1.0-1.0E-06*C1SAVE)
  340 CONTINUE
  350 CONTINUE
      TDS=0.0
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      DO 360 I=1,D
      ANALMI(I)=MI(I)
      TDS=TDS+GRAMS(I)
  360 CONTINUE

 CALCUL DE LA BALANCE CATION-ANION
 *********************************

      EPMCAT=0.0
      EPMAN=0.0
      DO 380 I=1,D
      IF (Z(I).GT.0) GO TO 370
      EPMAN=EPMAN-Z(I)*MI(I)
      GO TO 380
  370 EPMCAT=EPMCAT+Z(I)*MI(I)
  380 CONTINUE
      EPMCAT=EPMCAT*1000.
      EPMAN=EPMAN*1000.

 CALCUL DU EH A PARTIR DES DONNEES DE TERRAIN
 ********************************************

      IF (EHM.LT.9.0) GO TO 420
      IF (EMFZ.GT.9.0) GO TO 390
      C1=0.429+2.4E-03*(25.0-TEMP)-EFMZ
      GO TO 400
  390 C1=0.244+8.6E-04*(25.0-TEMP)
  400 CONTINUE
      IF (EHMC.LT.9.0) GO TO 410
      GO TO 420
  410 EHM=EHMC+C1
  420 CONTINUE
      PEEH=EHM/(C*R*T/F)
      IF (PECALC.EQ.0) PE=100.
      IF (EHM.GE.9.0) PEEH=100.
      WRITE(6,670)
      WRITE(6,671)
      WRITE(6,672)
      WRITE(6,680), TEMP,PH,EPMCAT,EPMAN
      WRITE(6,690), DOX,EHMC,EMFZ,EHM,PEEH
      IF (PECALC.EQ.1) PE=PEEH
      WRITE(6,700)
      DO 430 I=1,32
      IF (MI(INPT(I)).GT.0.0) GO TO 429
      WRITE(6,709),NSPEC(INPT(I)),Z(INPT(I))
      GO TO 430
  429 WRITE(6,710), NSPEC(INPT(I)),Z(INPT(I)),MI(INPT(I)),XLMI(INP
     1T(I)),GRAMS(INPT(I))
  430 CONTINUE
       IF (PRT(2).NE.0) GO TO 440
       WRITE(6,560)
       WRITE(6,720)
  440 CONTINUE
      IF (IGO.EQ.1) GO TO 450
      IF (PH.LT.3.0.OR.PH.GT.11.0) GO TO 490
      DUM=((EPMCAT-EPMAN)/(1.+EPMCAT+EPMAN))*100.
      IF (DABS(DUM).GT.30.0) GO TO 490
      IF (TRACES.EQ.0) GO TO 449
      ALFA(251)=10.**(-PE)
  449 CONTINUE
  450 CONTINUE

 INFLUENCE DE LA TEMPERATURE SUR LES CONSTANTES DE DEBYE-HUCKEL
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**********************************************************

      S1=374.11-TEMP
      S2=S1**(.333333
      S3=DSQRT((1.0+0.1342489*S2-3.946263E-03*S1)/(3.1975E0-.3151548E0*S
     12-1.203374E-3*S1+7.48908E-13*S1**4))
      IF (T.LT.373.16) GO TO 460
      C1=5321E0/T+233.76E0-T*(T*(8.292E-7*T-1.417E-3)+.9297E0)
      GO TO 470
460   C1=87.74E0-TEMP*(TEMP*(1.41E-6*TEMP-9.398E-4)+.4008E0)
470   CONTINUE
      C1=DSQRT(C1*T)
      A=18246.0E02*S3/C1**3
      B=50.29*S3/C1
      GO TO 500
480   WRITE(6,730)
      ICK=1
      GO TO 500
490   WRITE(6,550)
      ICK=1
500   CONTINUE
      RETURN

 FORMATS
 *******


510 FORMAT  (15X,'*' NOTER QU'UNE EXPRESSION ANALYTIQUE A ETE UTIL
     1ISEE POUR KT',/,20X,'RESUME DES EXPRESSIONS ANALYTIQUES DE LA F
     2ORME : LOG K = A+B*T+C/T+D*T**2+E/T**2',/,23X,'I    NREACT
     3   A          B          C          D          E')
520 FORMAT (22X,I3,2X,A8,3(1X,F11.4),2(1X,1PE11.4))
530 FORMAT (16I5)
540 FORMAT (10X,'VOUS AVEZ OUBLIE DE TAPER LA CARTE VIDE')
550 FORMAT (10X,'WARNING--- VERIFIER LA VALEUR DU PH  ET/OU LA BALAN
     1CE CATION/ANION ---CALCUL TERMINE')
570 FORMAT (5(F6.2,1X),13X,I1,2F5.2,1X,9I1,2I3)
580 FORMAT (1H ,64X,'**********',/,65X,'* DONNEES *',/,65X,'*********
     1**',/,18X,'I',2X,'NREACT',8X,'DH',8X,'LOGKTO',36X,'I',2X,'NSPEC'
     2,6X,'Z',2X,'DHA',6X,'GFW')
590 FORMAT (1H ,15X,I3,2X,A8,1X,F9.4,2X,F10.4,A1,33X,I3,2X,A8,2X,I2,1X
     1,F4.1,2X,F10.4)
600 FORMAT (1H ,15X,I3,2X,A8,1X,F9.4,2X,F10.4,A1)
610 FORMAT (12X,10A8)
611 FORMAT (1H ,57X,'**********************',/,57X,'* ANALYSE D'U
     1NE EAU *',/,57X,'**********************')
620 FORMAT (6(E12.5),8X)
630 FORMAT (A4,5(I3,E12.5))
640 FORMAT (5X,'NOUVELLE DONNEE *** DELTA H DE LA REACTION ',I3,1X,A8,
     1' A ETE CHANGE EN : ',F9.4)
650 FORMAT (5X,'NOUVELLE DONNEE *** LOGKTO DE LA REACTION ',I3,1X,A8,'
     1 A ETE CHANGE EN : ',F9.4)
660 FORMAT (5X,'NOUVELLE DONNEE *** LOGKT DE LA REACTION ',I3,1X,A8,'
     1 = ',1PE11.4,'+',E11.4,'*T+',E11.4,'/T+',E11.4,'*T**2+',E11.4,'*T*
     2*2')
670 FORMAT (1H ,56X,'**********************')
671 FORMAT (1H ,56X,'* SOLUTION INITIALE *')
672 FORMAT (1H ,56X,'**********************')
680 FORMAT (26X,'TEMPERATURE = ',F6.2,'DEGRES C   PH = ',F6.2,'  SOMME
     1 DES CATIONS ANALYSES  = ',F8.3,/,70X,'SOMME DES ANIONS  ANALYSES
     2 = ',F8.3)
690 FORMAT (5X,'***** OXYDATION-REDUCTION *****',/,11X,'OXYGENE DISSOU
     1S = ',F5.2,' MG/L',/,11X,'EH MESURE CALOMEL =',F7.4,'VOLTS',/,11X,
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     2'EH MEASURED OF ZOBELL SOLUTION = ',F7.4,'VOLTS',/,11X,'EH CORRIGE
     3= ',F7.4,'VOLTS',/,11X,'PE COMPUTED FROM CORRECTED EH = ',F7.3)
700  FORMAT (1H ,42X,'*** CONCENTRATION TOTALE DES ESPECES ANALYS
     1EES ***',/,51X,'MOLALITE',10X,'LOG MOLALITE',6X,'CONCENTRATION',
     2/,34X,'ESPECES',11X,'TOTALE',14X,'TOTALE',12X,'EN MG/L')
708  FORMAT(34X,A8,I3)
710  FORMAT (34X,A8,I3,3X,1PE13.6,8X,0PF9.4,8X,1PE13.6)
720  FORMAT (1H ,50X,'*** CONVERGENCE DES ITERATIONS ***',/,23X,
     1'ITERATION',4X,'S1-CO3ANAL',6X,'S2-SO4TOT',8X,'S3-FTOT',9X,'S4-PTO
     2T',9X,'S5-CLTOT')
730  FORMAT (10X,'ERREUR INTRODUITE - LES UNITES DE CONCENTRATION NE SO
     1NT PAS CONNUES')
      END


            **********************
            * SOUS PROGRAMME SET *
            **********************


      SUBROUTINE SET
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      INTEGER D,E,DD,RBIT,CORALK,Z(260),WORD,CARD(6),FLAG,PRT(4),SIGN(2)
      INTEGER PECALC,PECK,TRACES,CSPEC(120,6)
      DIMENSION INT(5), VAL(5), INPT(32), GRAMS(260), IEQU(50), COEF(5,2
     103)
      REAL*8 MI(260),MNTOT,LH2O,MU,NATOT,KT
     1OT,MGTOT,LITOT,NH4TOT,KW
      REAL*8 KT(450),LOGKT(450),LOGKTO(450)
      REAL*8 NSPEC(260),NREACT(450),MIPRIM(125)
      COMMON MI,KT,LOGKT,LOGKTO,KW,D,E,DD,C,R,T,F,TEMP,A,B,NSPEC,NREA
     1CT,PE,PES,PEDO,PESATO,PECK,PECALC,PH,TENMPE,TENPH,ALFA(260),GAMMA(
     2260),AP(450),XLALFA(260),Z,CUNITS(260),ANALMI(260),GFW(260),DHA(26
     30),DH(450),AH2O,LH2O,EROR1,EROR2,EROR3,EROR4,EROR5,EHM,DENS,DOX,XL
     4MI(260),ITER,RBIT,C1SAVE,CORALK,MU,LCHEK(450),CO2TIT,ANALCO,SITOT,
     5CATOT,MGTOT,KTOT,NATOT,SO4TOT,FETOT,PTOT,ALTOT,FTOT,BTOT,LITOT,NH4
     6TOT,SRTOT,BATOT,CLTOT,MNTOT,ICK,PRT,TITL(10),EPMCAT,EPMAN,NEQU,
     7ISPEC,KSPEC(260),IMIN,KMIN(450),TDS,IDAVES,IPRT,FLAG,IGO,XLGAM(260
     8),TRACES,CITOT(10),NTRACE,LSPEC(120,6),CSPEC,LMIN(140,7),
     9CMIN(140,7),EROR6,STORE(25,25),ITMIN,MIPRIM,XPCENT(125)

INITIALISATION DES VALEURS DE DEPART POUR LE PROCESSUS ITERATIF
***************************************************************

      AH2O=1.0
      ALFA(72)=AH2O
      DO 10 I=1,D
      GAMMA(I)=1.0
10    CONTINUE
      CO2TIT=MI(7)+2.0*MI(18)
      ANALCO=CO2TIT
      IF (CORALK.EQ.2) CO2TIT=MI(7)+MI(18)+MI(86)
      SITOT=MI(35)
      CATOT=MI(1)
      MGTOT=MI(2)
      NATOT=MI(3)
      KTOT=MI(4)
      SO4TOT=MI(6)
      FETOT=MI(8)
      PTOT=MI(45)
      ALTOT=MI(51)
      FTOT=MI(62)
      BTOT=MI(87)
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```
      CLTOT=MI(81)
      PHSTOT=MI(39)
      SRTOT=MI(88)
      BATOT=MI(90)
      CLTOT=MI(5)
      ANTOT=MI(101)
      MI(35)=0.0
      MI(87)=0.0
      TENPH=10.**PH
      ALFA(64)=10.**(-PH)
      IF(TRACES.EQ.0) GO TO 14
      CITOT(1)=MI(126)
      CITOT(2)=MI(148)
      CITOT(3)=MI(167)
      CITOT(4)=MI(186)
      CITOT(5)=MI(196)
      CITOT(6)=MI(208)
      CITOT(7)=MI(219)
      CITOT(8)=MI(237)
      CITOT(9)=MI(244)
      CITOT(10)=MI(249)
      DO 11 I=1,NTRACE
      IF (CITOT(I).EQ.0) GO TO 11
      CIMIN=CITOT(I)
      IIMIN=I
      GO TO 12
   11 CONTINUE
   12 CONTINUE
      DO 13 J=I+1,NTRACE
      IF (CITOT(J).EQ.0) GO TO 13
      IF (CITOT(J).GT.CIMIN) GO TO 13
      CIMIN=CITOT(J)
      IIMIN=J
   13 CONTINUE
   14 CONTINUE

CALCUL DES ACTIVITES DES ANIONS SAUF POUR CO2 ET PO4
***************************************************

      ALFA(5)=MI(5)*GAMMA(5)
      ALFA(6)=MI(6)*GAMMA(6)
      ALFA(62)=MI(62)*GAMMA(62)
      ALFA(85)=MI(85)*GAMMA(85)
      ALFA(98)=MI(98)*GAMMA(98)
      ALFA(27)=AH2O*KW*TENPH
      MI(27)=ALFA(27)/GAMMA(27)
      MI(64)=1E0/(TENPH*GAMMA(64))
      ALFA(63)=ALFA(6)*KT(90)/TENPH
      MI(63)=ALFA(63)/GAMMA(63)

ESPECES CO2
***********

      IF (CORALK.EQ.2) GO TO 20
      C1=2.0*TENPH/(GAMMA(18)*KT(69))
      MI(7)=CO2TIT/(1.+GAMMA(7)*C1)
      C2=KT(36)/(TENPH*GAMMA(86))
      ALFA(7)=MI(7)*GAMMA(7)
      MI(18)=C1*ALFA(7)/2.
      MI(86)=C2*ALFA(7)
      ALFA(18)=MI(18)*GAMMA(18)
      ALFA(86)=MI(86)*GAMMA(86)
      GO TO 30
```

```
20 CONTINUE
   MI(7)=CO2TIT/(1.0+GAMMA(7)*((KT(36)/(TENPH*GAMMA(86)))+TENPH/(KT(6
  19)*GAMMA(18))))
   MI(18)=MI(7)*GAMMA(7)*TENPH/(GAMMA(18)*KT(69))
   MI(86)=MI(7)*GAMMA(7)*KT(36)/(TENPH*GAMMA(86))
   ALFA(7)=MI(7)*GAMMA(7)
   ALFA(18)=MI(18)*GAMMA(18)
   ALFA(86)=MI(86)*GAMMA(86)
30 CONTINUE

FSPECES P04
**********

   MI(45)=PTOT/(1.+(KT(17)*GAMMA(45)/(GAMMA(48)*TENPH**2))+(KT(16)*GA
  1MMA(45)/(TENPH*GAMMA(47))))
   ALFA(45)=MI(45)*GAMMA(45)
   ALFA(47)=KT(16)*ALFA(45)/TENPH
   MI(47)=ALFA(47)/GAMMA(47)
   ALFA(48)=KT(17)*ALFA(45)/(TENPH**2)
   MI(48)=ALFA(48)/GAMMA(48)
   ITER=0
   RETURN
   END


        ************************
        * SOUS PROGRAMME MODEL *
        ************************


   SUBROUTINE MODEL
   IMPLICIT DOUBLE PRECISION (A-H,O-Z)
   INTEGER D,E,DD,Z(260),LIST(8),LIST1(6),LIST2(26),LIST3(6),PRT(4),P
  1ECALC,PECK,RBIT,FLAG,CORALK,TRACES,CSPEC(120,6),D1,E1
   REAL*8 MI(260),MNTOT,LH2O,MU,NATOT
  1,KTOT,MGTOT,LITOT,NH4TOT,KW,MUHALF,L1ALK(12)
   REAL*8 KT(450),LOGKT(450),LOGKTO(450)
   REAL*8 NSPEC(260),NREACT(450),MIPRIM(125)
   DIMENSION NPAIR(5), L1M(12), L1K(12), L1C(12), L1A(12), L2M(
  114), L2K(14), L2C(14), L3M(11), L3K(11), L3C(11), L4M(14), L4K(14)
  2,L4C(14), L4A(14), L5M(9), L5K(9), L5C(9),NCOMP(10),BETA(125),
  3B1(115),S(125),DIFF(25),DELTA(125)
   COMMON MI,KT,LOGKT,LOGKTO,KW,D,E,DD,C,R,T,F,TEMP,A,B,NSPEC,NREA
  1CT,PE,PES,PEDO,PESATO,PECK,PECALC,PH,TENMPE,TENPH,ALFA(260),GAMMA(
  2260),AP(450),XLALFA(260),Z,CUNITS(260),ANALMI(260),GFW(260),DHA(26
  30),DH(450),AH2O,LH2O,EROR1,EROR2,EROR3,EROR4,EROR5,EHM,DENS,DOX,XL
  4MI(260),ITER,RBIT,C1SAVE,CORALK,MU,LCHEK(450),CO2TIT,ANALCO,SITOT,
  5CATOT,MGTOT,KTOT,NATOT,SO4TOT,FETOT,PTOT,ALTOT,FTOT,BTOT,LITOT,NH4
  6TOT,SRTOT,BATOT,CLTOT,MNTOT,ICK,PRT,TITL(10),EPMCAT,EPMAN,NEQU,
  7ISPEC,KSPEC(260),IMIN,KMIN(450),TDS,IDAVES,IPRT,FLAG,IGO,XLGAM(260
  8),TRACES,CITOT(10),NTRACE,LSPEC(120,6),CSPEC,LMIN(140,7),
  9CMIN(140,7),EROR6,STORE(25,25),ITMIN,MIPRIM,XPCENT(125)
   DATA LIST/17,35,66,70,71,72,84,87/
   DATA LIST1/42,43,44,50,94,125/
   DATA LIST2/8,9,10,11,12,13,15,16,28,33,34,65,77,78,79,80,100,99,11
  17,118,119,120,121,122,123,124/
   DATA LIST3/82,83,88,89,90,91/
   DATA L1M/7,21,22,30,31,42,43,86,111,116,123,124/
   DATA L1K/69,74,75,78,79,70,71,36,167,194,201,202/
   DATA L1C/64,2,2,1,1,3,3,64,101,101,8,8/
   DATA L1A/18,18,7,7,18,18,7,7,7,18,18,7/
   DATA L1ALK/1.0,2.0,1.0,1.0,2.0,2.0,1.0,0.0,1.0,2.0,2.0,1.0/
   DATA L2M/15,23,32,34,44,46,59,60,63,83,92,96,109,119/
```

```
      DATA L2K/5,76,24,9,72,73,88,89,90,127,[illegible],135,197/
      DATA L2C/8,2,1,8,3,4,51,51,64,81,39,64,[illegible],8/
      DATA L3M/20,55,56,57,58,108,49,120,121,122,125/
      DATA L3K/23,84,85,86,87,164,80,198,199,200,203/
      DATA L3C/2,51,51,51,51,101,1,8,8,8,3/
      DATA L4M/13,40,41,47,48,50,61,65,73,74,75,76,99,100/
      DATA L4K/140,124,125,16,17,31,33,121,34,35,122,123,157,139/
      DATA L4C/8,2,2,64,64,3,4,8,2,1,1,1,8,8/
      DATA L4A/47,45,48,45,45,47,47,48,47,47,45,48,48,47/
      DATA L5M/16,28,33,93,94,95,103,104,105/
      DATA L5K/6,7,8,133,134,135,159,160,161/
      DATA L5C/8,8,8,64,3,4,101,101,101/
      DATA NMAIR/12,14,11,14,9/
      DATA NCOMP/21,18,18,9,11,10,17,6,4,1/

      ITER=ITER+1

CALCUL DE AH2O ET DE LA MOLALITE TOTALE
***************************************

      J=1
      C1=0.0
      DO 20 I=1,D
      IF (I.EQ.LIST(J)) GO TO 10
      C1=C1+MI(I)
      GO TO 20
10    J=J+1
20    CONTINUE
      AH2O=1.0-0.017*C1
      LH2O=DLOG10(AH2O)
      IF (DOX.GT.0.0) PEDO=-(DLOG10(KT(152))+PH+0.5*LH2O-0.25*DLOG10(DOX
     1/32E3))
      IF (DOX.GT.0.0) PESATO=-(DLOG10(KT(137))+PH+0.5*LH2O-0.25*DLOG10(D
     1OX/32E3))
      IF (PECALC.EQ.2) PE=PEDO
      IF (PECALC.EQ.3) PE=PESATO

CALCUL DES COEFFICIENTS D'ACTIVITE
**********************************

      MU=0.0
      DO 40 I=1,D
      MU=MU+0.5*MI(I)*Z(I)*Z(I)
40    CONTINUE
      MUHALF=DSQRT(MU)
      C1=-A*4.0*MUHALF
      GAMMA(1)=10.**(C1/(1.0+B*5.0*MUHALF)+0.165*MU)
      GAMMA(2)=10.**(C1/(1.0+B*5.5*MUHALF)+0.2*MU)
      GAMMA(3)=10.**(-A*MUHALF/(1.0+B*4.0*MUHALF)+0.075*MU)
      GAMMA(4)=10.**(-A*MUHALF/(1.0+B*3.5*MUHALF)+0.015*MU)
      GAMMA(5)=GAMMA(4)
      GAMMA(6)=10.**(C1/(1.0+B*5.0*MUHALF)-0.04*MU)
      DO 60 I=8,D
      IF (Z(I).EQ.0) GO TO 50
      IF (IDAVES.EQ.1) GAMMA(I)=10.**(-A*Z(I)**2.*(MUHALF/(1.0+MUHALF)-0
     1.3*MU))
      IF (IDAVES.EQ.1) GO TO 60
      GAMMA(I)=10.**(-A*MUHALF*Z(I)**2.0/(1.0+DHA(I)*B*MUHALF))
      GO TO 60
50    GAMMA(I)=10.**(0.1*MU)
60    CONTINUE
      GAMMA(7)=10.**(-A*MUHALF*Z(7)**2./(1.0+DHA(7)*B*MUHALF))
      GAMMA(18)=10.**(-A*MUHALF*Z(18)**2./(1.0+DHA(18)*B*MUHALF))
```

```
      GAMMA(86)=10.**(MU*(170.01/T-.8798+.0013935*T)+MU*MU*(28.81/T-.210
     18+.0003641*T))
 ESPECES SULFUREES ET CALCUL DE PE POUR S
 ****************************************
      C1=KT(92)*TENPH/GAMMA(67)
      C2=KT(92)*KT(93)*TENPH**2/GAMMA(68)
      MI(14)=MI(17)/(1E0+GAMMA(14)*(C1+C2))
      ALFA(14)=MI(14)*GAMMA(14)
      ALFA(17)=MI(17)*GAMMA(17)
      MI(67)=ALFA(14)*C1
      MI(68)=ALFA(14)*C2
      ALFA(67)=MI(67)*GAMMA(67)
      ALFA(68)=MI(68)*GAMMA(68)
      C1=ALFA(6)*ALFA(14)
      IF (C1.GT.0.0) GO TO 70
      GO TO 80
  70  PES=0.125*DLOG10(KT(91))+0.125*DLOG10(ALFA(6))-1.25*PH-0.125*DLOG1
     10(ALFA(14))-0.5*LH2O
      IF (PECALC.EQ.4) PE=PES
  80  CONTINUE
      IF (PECALC.EQ.0.OR.PE.GE.100.0) GO TO 90
      TENMPE=10.**(-PE)
      GO TO 100
  90  TENMPE=10.**(-30)
 100  CONTINUE
      IF (TRACES.EQ.0) GO TO 101
      ALFA(251)=TENMPE
 101  CONTINUE

 ESPECES SILICEUSES
 ******************

      C1=KT(14)*TENPH/GAMMA(25)
      C2=KT(15)*TENPH**2/GAMMA(26)
      MI(24)=SITOT/(1.0+GAMMA(24)*(C1+C2))
      ALFA(24)=MI(24)*GAMMA(24)
      MI(25)=ALFA(24)*C1
      MI(26)=ALFA(24)*C2
      ALFA(25)=MI(25)*GAMMA(25)
      ALFA(26)=MI(26)*GAMMA(26)

 ESPECES DU BROME
 ****************

      C1=GAMMA(36)*KT(26)*TENPH/GAMMA(37)
      MI(36)=BTOT/(1.0+C1)
      MI(37)=C1*MI(36)
      ALFA(36)=MI(36)*GAMMA(36)
      ALFA(37)=MI(37)*GAMMA(37)

 ESPECES NITRATEES
 *****************

      C1=TENPH*KT(27)/GAMMA(38)
      C2=ALFA(6)*KT(132)/GAMMA(92)
      MI(39)=NH4TOT/(1E0+GAMMA(39)*(C1+C2))
      ALFA(39)=MI(39)*GAMMA(39)
      MI(38)=ALFA(39)*C1
      ALFA(38)=MI(38)*GAMMA(38)
      MI(92)=ALFA(39)*C2
      ALFA(92)=MI(92)*GAMMA(92)
```

```
 ESPECES MAGNESIENNES
 ********************

    MI(19)=ALFA(27)*KT(25)/GAMMA(19)
    MI(20)=ALFA(62)*KT(23)/GAMMA(20)
    MI(21)=ALFA(18)*KT(74)/GAMMA(21)
    MI(22)=ALFA(7)*KT(75)/GAMMA(22)
    MI(23)=ALFA(6)*KT(76)/GAMMA(23)
    MI(40)=ALFA(45)*KT(124)/GAMMA(40)
    MI(41)=ALFA(48)*KT(125)/GAMMA(41)
    MI(73)=ALFA(47)*KT(34)/GAMMA(73)
    MI(2)=MGTOT/(1.0+GAMMA(2)*(MI(19)+MI(20)+MI(21)+MI(22)+MI(23)+MI(4
   10)+MI(41)+MI(73)))
    ALFA(2)=MI(2)*GAMMA(2)
    C1=ALFA(2)
    DO 110 I=19,23
    MI(I)=C1*MI(I)
    ALFA(I)=MI(I)*GAMMA(I)
110 CONTINUE
    MI(40)=C1*MI(40)
    ALFA(40)=MI(40)*GAMMA(40)
    MI(41)=C1*MI(41)
    ALFA(41)=MI(41)*GAMMA(41)
    MI(73)=C1*MI(73)
    ALFA(73)=MI(73)*GAMMA(73)

 ESPECES CALCIQUES
 *****************

    MI(29)=ALFA(27)*KT(77)/GAMMA(29)
    MI(30)=ALFA(7)*KT(78)/GAMMA(30)
    MI(31)=ALFA(18)*KT(79)/GAMMA(31)
    MI(32)=ALFA(6)*KT(24)/GAMMA(32)
    MI(74)=ALFA(47)*KT(35)/GAMMA(74)
    MI(76)=ALFA(48)*KT(123)/GAMMA(76)
    MI(75)=ALFA(45)*KT(122)/GAMMA(75)
    MI(49)=ALFA(62)*KT(80)/GAMMA(49)
    MI(1)=CATOT/(1.0+GAMMA(1)*(MI(29)+MI(30)+MI(31)+MI(32)+MI(74)+MI(7
   15)+MI(76)+MI(49)))
    C1=MI(1)*GAMMA(1)
    ALFA(1)=C1
    DO 120 I=29,32
    MI(I)=C1*MI(I)
    ALFA(I)=MI(I)*GAMMA(I)
120 CONTINUE
    MI(74)=C1*MI(74)
    ALFA(74)=MI(74)*GAMMA(74)
    MI(75)=C1*MI(75)
    ALFA(75)=MI(75)*GAMMA(75)
    MI(76)=C1*MI(76)
    ALFA(76)=MI(76)*GAMMA(76)
    MI(49)=C1*MI(49)
    ALFA(49)=MI(49)*GAMMA(49)

 ESPECES SODIQUES
 ****************

    MI(42)=ALFA(18)*KT(70)/GAMMA(42)
    MI(43)=ALFA(7)*KT(71)/GAMMA(43)
    MI(44)=ALFA(6)*KT(72)/GAMMA(44)
    MI(50)=ALFA(47)*KT(31)/GAMMA(50)
    MI(94)=ALFA(5)*KT(134)/GAMMA(94)
```

```
      MI(125)=ALFA(62)*KT(203)/GAMMA(125)
      MI(3)=NATOT/(1.0+GAMMA(3)*(MI(42)+MI(43)+MI(44)+MI(50)+MI(94)
     1+MI(125)))
      ALFA(3)=MI(3)*GAMMA(3)
      C1=ALFA(3)
      DO 130 J=1,6
      MI(LIST1(J))=C1*MI(LIST1(J))
      ALFA(LIST1(J))=MI(LIST1(J))*GAMMA(LIST1(J))
  130 CONTINUE

 ESPECES POTASSIQUES
 *******************

      MI(46)=ALFA(6)*KT(73)/GAMMA(46)
      MI(61)=ALFA(47)*KT(33)/GAMMA(61)
      MI(95)=ALFA(5)*KT(135)/GAMMA(95)
      MI(4)=KTOT/(1.0+GAMMA(4)*(MI(46)+MI(61)+MI(95)))
      ALFA(4)=MI(4)*GAMMA(4)
      C1=ALFA(4)
      MI(46)=C1*MI(46)
      ALFA(46)=MI(46)*GAMMA(46)
      MI(61)=C1*MI(61)
      ALFA(61)=MI(61)*GAMMA(61)
      MI(95)=C1*MI(95)
      ALFA(95)=MI(95)*GAMMA(95)

 ESPECES ALUMINEUSES
 *******************

      MI(52)=ALFA(27)*KT(81)/GAMMA(52)
      MI(53)=ALFA(27)**2*KT(82)/GAMMA(53)
      MI(54)=ALFA(27)**4*KT(83)/GAMMA(54)
      MI(55)=ALFA(62)*KT(84)/GAMMA(55)
      MI(56)=ALFA(62)**2*KT(85)/GAMMA(56)
      MI(57)=ALFA(62)**3*KT(86)/GAMMA(57)
      MI(58)=ALFA(62)**4*KT(87)/GAMMA(58)
      MI(59)=ALFA(6)*KT(88)/GAMMA(59)
      MI(60)=ALFA(6)**2*KT(89)/GAMMA(60)
      MI(51)=ALTOT/(1.0+GAMMA(51)*(MI(52)+MI(53)+MI(54)+MI(55)+MI(56)+MI
     1(57)+MI(58)+MI(59)+MI(60)))
      ALFA(51)=MI(51)*GAMMA(51)
      C1=ALFA(51)
      DO 140 I=52,60
      MI(I)=C1*MI(I)
      ALFA(I)=MI(I)*GAMMA(I)
  140 CONTINUE

 ESPECES DU FER
 **************

      IF (DABS(PE).LT.20.0.AND.FETOT.GT.0.0) GO TO 150
      GO TO 170
  150 MI(9)=KT(1)/(TENMPE*GAMMA(9))
      MI(10)=KT(2)*AH2O*TENPH/(TENMPE*GAMMA(10))
      MI(11)=KT(3)*AH2O*TENPH/GAMMA(11)
      MI(12)=KT(4)*AH2O**3*TENPH**3/GAMMA(12)
      MI(13)=KT(140)*ALFA(47)/(GAMMA(13)*TENMPE)
      MI(15)=KT(5)*ALFA(6)/(TENMPE*GAMMA(15))
      MI(16)=KT(6)*ALFA(5)/(TENMPE*GAMMA(16))
      MI(28)=KT(7)*ALFA(5)**2/(TENMPE*GAMMA(28))
      MI(33)=KT(8)*ALFA(5)**3/(TENMPE*GAMMA(33))
      MI(34)=KT(9)*ALFA(6)/GAMMA(34)
      MI(65)=KT(121)*ALFA(48)/GAMMA(65)
```

```
      MI(77)=KT(103)*(AH2O*TENPH)**2/(TENMPE*GAMMA(77))
      MI(78)=KT(104)*(AH2O*TENPH)**3/(TENMPE*GAMMA(78))
      MI(79)=KT(105)*(AH2O*TENPH)**4/(TENMPE*GAMMA(79))
      MI(80)=KT(106)*(AH2O*TENPH)**2/GAMMA(80)
      MI(99)=KT(157)*ALFA(48)/(TENMPE*GAMMA(99))
      MI(100)=KT(139)*ALFA(47)/GAMMA(100)
      MI(117)=KT(195)*ALFA(67)**2/GAMMA(117)
      MI(118)=KT(196)*ALFA(67)**3/GAMMA(118)
      MI(119)=KT(197)*KT(1)*ALFA(6)**2/GAMMA(119)/TENMPE
      MI(120)=KT(198)*KT(1)*ALFA(62)/GAMMA(120)/TENMPE
      MI(121)=KT(199)*KT(1)*ALFA(62)**2/GAMMA(121)/TENMPE
      MI(122)=KT(200)*KT(1)*ALFA(62)**3/GAMMA(122)/TENMPE
      MI(123)=KT(201)*ALFA(18)/GAMMA(123)
      MI(124)=KT(202)*ALFA(7)/GAMMA(124)
      MI(8)=FETOT/(1.0+GAMMA(8)*(MI(9)+MI(10)+MI(11)+MI(12)+MI(13)+MI(15
     1)+MI(16)+MI(28)+MI(33)+MI(34)+MI(65)+MI(77)+MI(78)+MI(79)+MI(80)+M
     2I(100)+MI(99)+MI(117)+MI(118)+MI(119)+MI(120)+MI(121)+MI(122)+MI(1
     323)+MI(124)))
      ALFA(8)=MI(8)*GAMMA(8)
      C1=ALFA(8)
      DO 160 J=2,26
      MI(LIST2(J))=C1*MI(LIST2(J))
      ALFA(LIST2(J))=MI(LIST2(J))*GAMMA(LIST2(J))
160   CONTINUE
      GO TO 190
170   CONTINUE
      DO 180 J=2,26
      MI(LIST2(J))=0.0
180   CONTINUE
      ALFA(8)=MI(8)*GAMMA(8)
190   CONTINUE

 ESPECES DU MANGANESE
 ********************

      IF (DABS(PE).LT.20.0.AND.MNTOT.GT.0.0) GO TO 200
      GO TO 240
200   MI(102)=KT(158)/(GAMMA(102)*TENMPE)
      MI(103)=KT(159)*MI(5)*GAMMA(5)/GAMMA(103)
      MI(104)=KT(160)*MI(5)**2*GAMMA(5)**2/GAMMA(104)
      MI(105)=KT(161)*MI(5)**3*GAMMA(5)**3/GAMMA(105)
      MI(106)=KT(162)*MI(27)*GAMMA(27)/GAMMA(106)
      MI(107)=KT(163)*MI(27)**3*GAMMA(27)**3/GAMMA(107)
      MI(108)=KT(164)*MI(62)*GAMMA(62)/GAMMA(108)
      MI(109)=KT(165)*MI(6)*GAMMA(6)/GAMMA(109)
      MI(110)=KT(166)*MI(85)**2*GAMMA(85)**2/GAMMA(110)
      MI(111)=KT(167)*MI(7)*GAMMA(7)/GAMMA(111)
      XMI112=LOGKT(168)+4*LH2O-(DLOG10(GAMMA(112))-8*PH-5*PE)
      IF (XMI112.LT.-50.) MI(112)=0.0
      IF (XMI112.GE.-50.) MI(112)=0.0
      IF (XMI112.LT.-50.) GO TO 210
      MI(112)=10.**XMI112
210   CONTINUE
      XMI113=LOGKT(169)+4*LH2O-(DLOG10(GAMMA(113))-8*PH-4*PE)
      IF (XMI113.LT.-50.) MI(113)=0.0
      IF (XMI113.GE.-50.) MI(113)=0.0
      IF (XMI113.LT.-50.0) GO TO 220
      MI(113)=10.**XMI113
220   CONTINUE
      MI(115)=KT(171)*AH2O**2/(GAMMA(115)*ALFA(64)**3)
      MI(116)=KT(194)*MI(18)/GAMMA(116)
      MI(101)=MNTOT/(1.0+GAMMA(101)*(MI(102)+MI(103)+MI(104)+MI(105)+MI(
     1106)+MI(107)+MI(108)+MI(109)+MI(110)+MI(111)+MI(112)+MI(113)+MI(11
```

```
   25)+MI(116)))
    ALFA(101)=MI(101)*GAMMA(101)
    C1=ALFA(101)
    DO 230 I=102,113
    MI(I)=C1*MI(I)
    ALFA(I)=MI(I)*GAMMA(I)
230 CONTINUE
    MI(115)=C1*MI(115)
    ALFA(115)=MI(115)*GAMMA(115)
    MI(116)=C1*MI(116)
    ALFA(116)=MI(116)*GAMMA(116)
    GO TO 260
240 DO 250 I=101,113
    MI(I)=0.0
250 CONTINUE
    MI(115)=0.0
    MI(116)=0.0
260 CONTINUE

 CALCUL DE PO2 ET PCH4
 *********************

    IF (DABS(PE).LT.19.0) GO TO 270
    GO TO 280
270 C1=DLOG10(KT(94))+PH+PE+0.5*LH2O
    ALFA(70)=10.**(4.0*C1)
280 CONTINUE
    IF (DABS(PE).LT.19.0.AND.ALFA(7).GT.0.0) GO TO 290
    GO TO 300
290 XLALFA(71)=(DLOG10(KT(95))-8.0*PE-9.0*PH-3.0*LH2O+DLOG10(ALFA(7)))
    IF (XLALFA(71).LT.-300.) GO TO 300
    ALFA(71)=10.**XLALFA(71)
300 CONTINUE

 ESPECES LITHIUM,STRONTIUM,BARIUM
 ********************************

    C1=KT(126)*ALFA(27)/GAMMA(82)
    C2=KT(127)*ALFA(6)/GAMMA(83)
    MI(81)=LITOT/(1.0+GAMMA(81)*(C1+C2))
    ALFA(81)=MI(81)*GAMMA(81)
    MI(82)=C1*ALFA(81)
    MI(83)=C2*ALFA(81)
    C1=KT(130)*ALFA(27)/GAMMA(89)
    MI(88)=SRTOT/(1.0+GAMMA(88)*C1)
    MI(89)=GAMMA(88)*MI(88)*C1
    C1=KT(131)*ALFA(27)/GAMMA(91)
    MI(90)=BATOT/(1.0+GAMMA(90)*C1)
    MI(91)=GAMMA(90)*MI(90)*C1
    DO 310 J=1,6
    ALFA(LIST3(J))=MI(LIST3(J))*GAMMA(LIST3(J))
310 CONTINUE

    REPARTITION DES ESPECES MINEURES
    ********************************

    IF (TRACES.NE.1) GO TO 1430
    D1=125
    E1=203
    M=0
    K=0
    DO 1300 J=1,125
    DELTA(J)=GAMMA(D1+J)
```

```
1300 CONTINUE
     DO 1400 I=1,NTRACE
     IF (I.NE.1) GO TO 1310
     L=1
     GO TO 1330
1310 L=I
     DO 1320 IJ=1,I-1
     L=L+NCOMP(IJ)
1320 CONTINUE
1330 CONTINUE
     S(L)=1/DELTA(L)
     DO 1360 J=1,NCOMP(I)
     K=K+1
     AA=KT(K+E1)/DELTA(K+I)
     B1(K)=KT(K+E1)
     DO 1340 N=4,LSPEC(K,1)+3
     X=DFLOTJ(CSPEC(K,N))
     IF (ALFA(LSPEC(K,N)).EQ.0) GO TO 1350
     PR=ALFA(LSPEC(K,N))**-X
     AA=AA*PR
     B1(K)=B1(K)*PR
1340 CONTINUE
     S(L)=S(L)+AA
     GO TO 1360
1350 B1(K)=0
1360 CONTINUE
     IF (CITOT(I).NE.0) GO TO 1370
     DELTA(L)=0.0
     GO TO 1380
1370 BETA(L)=CITOT(I)/S(L)
     XPCENT(L)=BETA(L)*100./CITOT(I)/DELTA(L)
1380 ALFA(D1+L)=BETA(L)
     IO=M+1
     IFIN=IO+NCOMP(I)-1
     M=IFIN
     II=1
     DO 1390 N=IO,IFIN
     BETA(N+I)=B1(N)*BETA(L)
     ALFA(D1+N+I)=BETA(N+I)
     IF (I.NE.ITMIN) GO TO 1390
     STORE(1,ITER)=BETA(L)
     II=II+1
     STORE(II,ITER)=BETA(N+I)
1390 CONTINUE
1400 CONTINUE
     DO 1410 J=1,125
     MIPRIM(J)=BETA(J)/DELTA(J)
     MI(D1+J)=MIPRIM(J)
1410 CONTINUE
     DO 1420 J=1,115
     K=J+LSPEC(J,3)
     IF(CITOT(LSPEC(J,3)).EQ.0.) GO TO 1420
     XPCENT(K)=MIPRIM(K)*100./CITOT(LSPEC(J,3))
1420 CONTINUE
1430 CONTINUE



  BALANCE DE MASSE SUR LES CARBONATES
  ***********************************

     S1=0.0
```

```
      S2=0.0
      S3=0.0
      S4=0.0
      S5=0.0
      ANALCO=CO2TIT
      IF (CO2TIT.LE.0.0) GO TO 370
      ACT=KT(69)*ALFA(64)
      SUM=0.0
      SUM1=0.0
      N=NPAIR(1)
      DO 320 J=1,N
      MI(L1M(J))=KT(L1K(J))*ALFA(L1C(J))/GAMMA(L1M(J))
      IF (L1A(J).EQ.7) MI(L1M(J))=MI(L1M(J))*ACT
      SUM=SUM+MI(L1M(J))
      SUM1=SUM1+L1ALK(J)*MI(L1M(J))
  320 CONTINUE
      IF (CORALK.NE.2) GO TO 340
      MI(18)=ANALCO/(1.0+GAMMA(18)*SUM)
      ALFA(18)=MI(18)*GAMMA(18)
      DO 330 J=1,N
      MI(L1M(J))=MI(L1M(J))*ALFA(18)
      ALFA(L1M(J))=MI(L1M(J))*GAMMA(L1M(J))
      S1=S1+MI(L1M(J))
  330 CONTINUE
      S1=S1+MI(18)
      GO TO 370
  340 CONTINUE
      IF (CORALK.EQ.1) GO TO 350
      ANALCO=CO2TIT-MI(25)-2.0*MI(26)-MI(27)-MI(37)-2.0*MI(45)-MI(47)-MI
     1(54)-MI(67)-2.0*MI(68)-MI(82)
  350 CONTINUE
      MI(18)=ANALCO/(2.0+GAMMA(18)*SUM1)
      ALFA(18)=MI(18)*GAMMA(18)
      DO 360 J=1,N
      MI(L1M(J))=MI(L1M(J))*ALFA(18)
      ALFA(L1M(J))=MI(L1M(J))*GAMMA(L1M(J))
      S1=S1+L1ALK(J)*MI(L1M(J))
  360 CONTINUE
      S1=S1+2.0*MI(18)
  370 CONTINUE
      IF (TRACES.EQ.0) GO TO 372
      S1PRIM=0
      DO 371 J=1,115
      X=DFLOTJ(CSPEC(J,4))
      IF (LSPEC(J,4).NE.18.AND.LSPEC(J,4).NE.7) GO TO 371
      S1PRIM=S1PRIM+MIPRIM(J)*(-X)
  371 CONTINUE
      S1=S1+S1PRIM
  372 CONTINUE

 BALANCE DE MASSE SUR LES SULFATES
 *********************************

      IF (SO4TOT.LE.0.0) GO TO 410
      N=NPAIR(2)
      DO 380 J=1,N-1
      MI(L2M(J))=KT(L2K(J))*ALFA(L2C(J))/GAMMA(L2M(J))
      MI(119)=KT(197)*ALFA(8)*KT(1)/GAMMA(119)/TENMPE
  380 CONTINUE
      MI(15)=MI(15)/TENMPE
      MI(60)=MI(60)*ALFA(6)
      MI(96)=MI(96)*ALFA(64)
```

```
      SUM=MI(60)
      DO 390 J=1,N
      SUM=SUM+MI(L2M(J))
  390 CONTINUE
      MI(6)=SO4TOT/(1.0+GAMMA(6)*SUM)
      ALFA(6)=MI(6)*GAMMA(6)
      DO 400 J=1,N
      MI(L2M(J))=MI(L2M(J))*ALFA(6)
      ALFA(L2M(J))=MI(L2M(J))*GAMMA(L2M(J))
      S2=S2+MI(L2M(J))
  400 CONTINUE
      S2=S2+MI(6)+MI(60)+MI(119)
  410 CONTINUE
      IF (TRACES.EQ.0) GO TO 412
      S2PRIM=0
      DO 411 J=1,115
      X=DFLOTJ(CSPEC(J,4))
      IF (LSPEC(J,4).NE.6) GO TO 411
      S2PRIM=S2PRIM+MIPRIM(J)*(-X)
  411 CONTINUE
      S2=S2+S2PRIM
  412 CONTINUE

 BALANCE DE MASSE SUR LES FLUORURES
 **********************************

      IF (FTOT.LE.0.0) GO TO 450
      N=NPAIR(3)
      DO 420 J=1,N
      MI(L3M(J))=KT(L3K(J))*ALFA(L3C(J))/GAMMA(L3M(J))
  420 CONTINUE
      MI(56)=MI(56)*ALFA(62)
      MI(57)=MI(57)*ALFA(62)*ALFA(62)
      MI(58)=MI(58)*ALFA(62)*ALFA(62)*ALFA(62)
      MI(120)=MI(120)*KT(1)/TENMPE
      MI(121)=MI(121)*KT(1)*ALFA(62)/TENMPE
      MI(122)=MI(122)*KT(1)*ALFA(62)**2/TENMPE
      SUM=MI(56)+2.0*MI(57)+3.0*MI(58)+MI(121)+2.0*MI(122)
      DO 430 J=1,N
      SUM=SUM+MI(L3M(J))
  430 CONTINUE
      MI(62)=FTOT/(1.0+GAMMA(62)*SUM)
      ALFA(62)=MI(62)*GAMMA(62)
      DO 440 J=1,N
      MI(L3M(J))=MI(L3M(J))*ALFA(62)
      ALFA(L3M(J))=MI(L3M(J))*GAMMA(L3M(J))
      S3=S3+MI(L3M(J))
  440 CONTINUE
      S3=S3+MI(62)+MI(56)+2.0*MI(57)+3.0*MI(58)+MI(121)+2.0*
     1MI(122)
  450 CONTINUE
      IF (TRACES.EQ.0) GO TO 452
      S3PRIM=0
      DO 451 J=1,115
      X=DFLOTJ(CSPEC(J,4))
      IF (LSPEC(J,4).NE.62) GO TO 451
      S3PRIM=S3PRIM+MIPRIM(J)*(-X)
  451 CONTINUE
      S3=S3+S3PRIM
  452 CONTINUE

 BALANCE DE MASSE SUR LES PHOSPHATES
 ***********************************
```

```
      IF (PTOT.LE.0.0) GO TO 490
      N=NPAIR(4)
      C1=KT(16)*ALFA(64)
      C2=KT(17)*ALFA(64)*ALFA(64)
      DO 460 J=1,N
      MI(L4M(J))=KT(L4K(J))*ALFA(L4C(J))/GAMMA(L4M(J))
      IF (L4A(J).EQ.47) MI(L4M(J))=MI(L4M(J))*C1
      IF (L4A(J).EQ.48) MI(L4M(J))=MI(L4M(J))*C2
  460 CONTINUE
      MI(13)=MI(13)/TENMPE
      MI(48)=MI(48)*ALFA(64)
      MI(99)=MI(99)/TENMPE
      SUM=0.0
      DO 470 J=1,N
      SUM=SUM+MI(L4M(J))
  470 CONTINUE
      MI(45)=PTOT/(1.0+GAMMA(45)*SUM)
      ALFA(45)=MI(45)*GAMMA(45)
      DO 480 J=1,N
      MI(L4M(J))=MI(L4M(J))*ALFA(45)
      ALFA(L4M(J))=MI(L4M(J))*GAMMA(L4M(J))
      S4=S4+MI(L4M(J))
  480 CONTINUE
      S4=S4+MI(45)
  490 CONTINUE

 BALANCE DE MASSE SUR LES CHLORURES
 **********************************

      IF (CLTOT.LE.0.0) GO TO 530
      N=NPAIR(5)
      DO 500 J=1,N
      MI(L5M(J))=KT(L5K(J))*ALFA(L5C(J))/GAMMA(L5M(J))
  500 CONTINUE
      MI(16)=MI(16)/TENMPE
      MI(28)=MI(28)*ALFA(5)/TENMPE
      MI(33)=MI(33)*ALFA(5)*ALFA(5)/TENMPE
      MI(104)=MI(104)*ALFA(5)
      MI(105)=MI(105)*ALFA(5)*ALFA(5)
      SUM=MI(28)+2.0*MI(33)+MI(104)+2.0*MI(105)
      DO 510 J=1,N
      SUM=SUM+MI(L5M(J))
  510 CONTINUE
      MI(5)=CLTOT/(1.0+GAMMA(5)*SUM)
      ALFA(5)=MI(5)*GAMMA(5)
      DO 520 J=1,N
      MI(L5M(J))=MI(L5M(J))*ALFA(5)
      ALFA(L5M(J))=MI(L5M(J))*GAMMA(L5M(J))
      S5=S5+MI(L5M(J))
  520 CONTINUE
      S5=S5+MI(5)+MI(28)+2.0*MI(33)+MI(104)+2.0*MI(105)
  530 CONTINUE
      IF (TRACES.EQ.0) GO TO 533
      S5PRIM=0
      DO 532 J=1,115
      X=DFLOTJ(CSPEC(J,4))
      IF (LSPEC(J,4).NE.5) GO TO 531
      S5PRIM=S5PRIM+MIPRIM(J)*(-X)
      GO TO 532
  531 IF(LSPEC(J,5).NE.5) GO TO 532
      XX=DFLOTJ(CSPEC(J,5))
      S5PRIM=S5PRIM+MIPRIM(J)*(-XX)
```

```
532 CONTINUE
    S5=S5+S5PRIM
533 CONTINUE

 TESTS DE CONVERGENCE
 ********************

    ALFA(85)=MI(85)*GAMMA(85)
    ALFA(98)=MI(98)*GAMMA(98)
    ALFA(27)=AH2O*KW*TENPH
    MI(27)=ALFA(27)/GAMMA(27)
    MI(64)=1E0/(TENPH*GAMMA(64))
    TEST1=S1-ANALCO
    TEST2=S2-SO4TOT
    TEST3=S3-FTOT
    TEST4=S4-PTOT
    TEST5=S5-CLTOT
    RBIT=0
    IF(TRACES.EQ.1) GO TO 600
    IF (S1.EQ.0.0.OR.ANALCO.LE.0.0) GO TO 540
    IF (DABS(TEST1).GT.EROR1*ANALCO) RBIT=1
    GO TO 550
540 ANALCO=0.0
550 CONTINUE
    IF (S2.EQ.0.0) GO TO 560
    IF (DABS(TEST2).GT.EROR2*SO4TOT) RBIT=1
560 CONTINUE
    IF (S3.EQ.0.0) GO TO 570
    IF (DABS(TEST3).GT.EROR3*FTOT) RBIT=1
570 CONTINUE
    IF (S4.EQ.0.0) GO TO 580
    IF (DABS(TEST4).GT.EROR4*PTOT) RBIT=1
580 CONTINUE
    IF (S5.EQ.0.0) GO TO 590
    IF (DABS(TEST5).GT.EROR5*CLTOT) RBIT=1
590 CONTINUE
     IF (PRT(2).NE.0) GO TO 600
     WRITE(6,610), ITER,TEST1,TEST2,TEST3,TEST4,TEST5
 610 FORMAT (1H ,24X,I3,6X,5(1PE13.6,3X))
600 CONTINUE
    IF (TRACES.EQ.0) GO TO 604
    IF(ITER.EQ.1) GO TO 604
    DO 601 II=1,NCOMP(ITMIN)+1
    DIFF(II)=STORE(II,ITER)-STORE(II,ITER-1)
601 CONTINUE
    XMAX=DIFF(1)
    IMAX=1
    DO 602 I=1,NCOMP(ITMIN)+1
    IF (DIFF(I+1).LE.XMAX) GO TO 602
    XMAX=DIFF(I+1)
    IMAX=I+1
602 CONTINUE
    IF(DABS(XMAX).GT.(EROR6*CITOT(ITMIN))) RBIT=1
     WRITE(6,603),ITER,ITMIN,XMAX,IMAX
 603 FORMAT (2X,'ITER',I2,3X,'ITMIN',I3,3X,'XMAX',E12.5,
    13X,'IMAX',I2)
604 CONTINUE
    RETURN
    END
```

```
      ************************
      * SOUS PROGRAMME PRINT *
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```
      SUBROUTINE PRINT
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      INTEGER D,E,DD,RBIT,CORALK,Z(260),LIST4(114),LIST5(8),PRT(4)
      INTEGER PECALC,PECK,FLAG,TRACES,CSPEC(120,6),DI
      REAL*8 MI(260),MNTOT,LH2O,MU,NATOT,KT
     1OT,MGTOT,LITOT,NH4TOT,KW,RATIO1(10),RATIO2(10),RATIO3(8)
      REAL*8 KT(450),LOGKT(450),LOGKTO(450)
      REAL*8 NSPEC(260),NREACT(450),MIPRIM(125)
      DIMENSION RAPFER(12),RAPSUM(12),NOM(11)
      COMMON MI,KT,LOGKT,LOGKTO,KW,D,E,DD,C,R,T,F,TEMP,A,B,NSPEC,NREA
     1CT,PE,PES,PEDO,PESATO,PECK,PECALC,PH,TENMPE,TENPH,ALFA(260),GAMMA(
     2260),AP(450),XLALFA(260),Z,CUNITS(260),ANALMI(260),GFW(260),DHA(26
     30),DH(450),AH2O,LH2O,EROR1,EROR2,EROR3,EROR4,EROR5,EHM,DENS,DOX,XL
     4MI(260),ITER,RBIT,C1SAVE,CORALK,MU,LCHEK(450),CO2TIT,ANALCO,SITOT,
     5CATOT,MGTOT,KTOT,NATOT,SO4TOT,FETOT,PTOT,ALTOT,FTOT,BTOT,LITOT,NH4
     6TOT,SRTOT,BATOT,CLTOT,MNTOT,ICK,PRT,TITL(10),EPMCAT,EPMAN,NEQU,ISP
     7EC,KSPEC(260),IMIN,KMIN(450),TDS,IDAVES,IPRT,FLAG,IGO,XLGAM(260)
     8,TRACES,CITOT(10),NTRACE,LSPEC(120,6),CSPEC,LMIN(140,7),
     9CMIN(140,7),EROR6,STORE(25,25),ITMIN,MIPRIM,XPCENT(125)
      DATA LIST4/1,2,3,4,64,5,6,7,18,86,27,62,98,19,23,22,21,20,29,32,30
     1,31,49,44,43,42,94,125,46,95,63,96,93,24,25,26,14,67,68,8,9,10,11,
     212,77,78,79,80,13,100,65,99,15,16,28,33,34,117,118,119,120,121,122
     3,123,124,101,102,106,107,111,109,110,103,104,105,108,112,113,115,1
     416,51,52,53,54,55,56,57,58,59,60,45,47,48,40,73,41,75,74,76,61,50,
     536,37,85,38,39,92,81,82,83,88,89,90,91/
      DATA LIST5/1,2,3,4,51,8,6,7/
      DATA NOM/'CD','ZN','PB','CO','NI','CR','CU','AS','SB','GE','MN'/
      D1=125
      CEPMAN=0.0
      CEPMCT=0.0
      DO 20 I=1,D
      IF(MI(I).EQ.0.0) GO TO 20
      IF (Z(I).GT.0) GO TO 10
      CEPMAN=CEPMAN-Z(I)*MI(I)
      GO TO 20
10    CEPMCT=CEPMCT+Z(I)*MI(I)
20    CONTINUE
      CEPMAN=CEPMAN*1000.
      CEPMCT=CEPMCT*1000.
      S1=MI(7)+MI(18)+MI(21)+MI(22)+MI(30)+MI(31)+MI(42)+MI(49)+MI(86)+M
     1I(111)+MI(43)
      PCO2=0.0
      IF (ALFA(86).GT.0.0) GO TO 30
      GO TO 40
30    PCO2=10.**(DLOG10(ALFA(86))-2385.73/T-1.5264E-2*T+14.0184)
      XLPCO2=DLOG10(PCO2)
40    CONTINUE
      EHPE=PE*C*R*T/F
      WRITE(6,120), AH2O,EPMCAT,CEPMCT,PH,PCO2,EPMAN,CEPMAN,XLPCO2,ALFA
     1(70),EHM,PE,TEMP,ALFA(71),PES,S1,PEDO,DENS,PESATO,MU,TDS
      ELECT=(CEPMCT-CEPMAN)/1000.
      WRITE(6,121) ELECT
      WRITE(6,130), PE,EHPE
      WRITE(6,140)
      WRITE(6,141)
      WRITE(6,142)
      WRITE(6,143)
      WRITE(6,144)
      DUM=10.**(-70.)
      DO 50 I=1,D
```

```
      CUNITS(I)=0.0
      IF (MI(I).LT.DUM) GO TO 50
      CUNITS(I)=MI(I)*1000.*GFW(I)*(1.0-1.0E-06*C1SAVE)
      IF (MI(I).LE.0.0.OR.ALFA(I).LE.0.0.OR.GAMMA(I).LE.0.0) GO TO 50
      XLMI(I)=DLOG10(MI(I))
      XLALFA(I)=DLOG10(ALFA(I))
      XLGAM(I)=DLOG10(GAMMA(I))
   50 CONTINUE
      DO 80 I=1,114
      IF(MI(LIST4(I)).NE.0.0) GO TO 59
      WRITE(6,152),LIST4(I),NSPEC(LIST4(I)),Z(LIST4(I))
      GO TO 80
   59 IF (ISPEC.EQ.0) GO TO 70
      DO 60 J=1,ISPEC
      IF (LIST4(I).EQ.KSPEC(J)) GO TO 70
   60 CONTINUE
      GO TO 80
   70 CONTINUE
      WRITE(6,150), LIST4(I),NSPEC(LIST4(I)),Z(LIST4(I)),CUNITS(LIST4(I
     1)),MI(LIST4(I)),XLMI(LIST4(I)),ALFA(LIST4(I)),XLALFA(LIST4(I)),GA
     2MMA(LIST4(I)),XLGAM(LIST4(I))
   80 CONTINUE
      IF(TRACES.EQ.0) GO TO 84
      WRITE(6,163)
      WRITE(6,167)
      DO 83 I=D1+1,D
      IF(MI(I).NE.0.0) GO TO 82
      WRITE(6,152),I,NSPEC(I),Z(I)
      GO TO 83
   82 WRITE(6,151),I,NSPEC(I),Z(I),CUNITS(I),MI(I),XLMI(I),ALFA(I),
     1XLALFA(I),GAMMA(I),XPCENT(I-D1)
   83 CONTINUE
   84 CONTINUE
      IF (PRT(3).NE.0) GO TO 100

CALCUL DES RAPPORTS MOLAIRES ET DES RAPPORTS DES LOG D'ACTIVITES
****************************************************************

      DO 90 I=1,8
      IF (ANALMI(LIST5(I)).LT.1.E-70) ANALMI(LIST5(I))=1.E-70
      IF (MI(LIST5(I)).LT.1.E-70) MI(LIST5(I))=1.E-70
      IF (MI(LIST5(I)).LT.1.E-70) XLALFA(LIST5(I))=-70.
      RATIO1(I)=ANALMI(5)/ANALMI(LIST5(I))
      RATIO2(I)=MI(5)/MI(LIST5(I))
   90 CONTINUE
      RATIO1(9)=ANALMI(1)/ANALMI(2)
      RATIO1(10)=ANALMI(3)/ANALMI(4)
      RATIO2(9)=MI(1)/MI(2)
      RATIO2(10)=MI(3)/MI(4)
      RATIO3(1)=XLALFA(1)+PH*2.
      RATIO3(2)=XLALFA(2)+PH*2.
      RATIO3(3)=XLALFA(3)+PH
      RATIO3(4)=XLALFA(4)+PH
      RATIO3(5)=XLALFA(51)+PH*3.
      RATIO3(6)=XLALFA(8)+PH*2.
      RATIO3(7)=XLALFA(1)-XLALFA(2)
      RATIO3(8)=XLALFA(3)-XLALFA(4)
      WRITE(6,160)
      WRITE(6,161)
      WRITE(6,162), (RATIO1(I),RATIO2(I),RATIO3(I),I=1,8),(RATIO1(I),
     1RATIO2(I),I=9,10)
      IF(LITOT.NE.0.) GO TO 99
      WRITE(6,168)
```

```
      GO TO 100
   99 XNALI=NATOT/LITOT
      YNALI=MI(3)/MI(81)
      WRITE(6,164),XNALI,YNALI
  100 CONTINUE
      IF(TRACES.EQ.0) GO TO 103
      DO 109 N=1,NTRACE
      RAPSUM(N)=0.0
      RAPFER(N)=0.0
  109 CONTINUE
      WRITE(6,165)
      DO 102 I=1,NTRACE
      IF(CITOT(I).EQ.0.) GO TO 102
      IF(FETOT.NE.0) GO TO 104
      RAPFER(I)=1.E+70
      GO TO 105
  104 RAPFER(I)=CITOT(I)/FETOT
  105 RAPSUM(I)=CITOT(I)/TDS
  102 CONTINUE
      IF(FETOT.NE.0.) GO TO 106
      RAPFER(11)=1.E+70
      GO TO 107
  106 RAPFER(11)=MNTOT/FETOT
  107 RAPSUM(11)=MNTOT/TDS
      DO 101 I=1,11
      IF(RAPFER(I).NE.0.) GO TO 108
      WRITE(6,169),NOM(I)
      GO TO 101
  108 WRITE(6,166),NOM(I),RAPFER(I),RAPSUM(I)
  101 CONTINUE
  103 CONTINUE
      RETURN

 FORMATS
 *******

  120 FORMAT (1H ,48X,'**** DESCRIPTION DE LA SOLUTION ****',/,4
     10X,'ANALYSES',4X,'CALCULES',10X,'PH',16X,'ACTIVITE DE H2O = ',F7.4
     2,/,21X,'SOMME DES CATIONS',F9.3,3X,F9.3,9X,F6.3,14X,'PCO2 = ',1PE1
     33.6,/,21X,'SOMME DES ANIONS ',0PF9.3,3X,F9.3,29X,'LOG PCO2 = ',F8.
     44,/,66X,'TEMPERATURE',11X,'PO2 = ',1PE13.6,/,21X,'EH = ',0PF6.4,4X
     5,'PE = ',F7.3,17X,F6.2,' DEG C ',10X,'PCH4 = ',1PE13.6,/,21X,'PE C
     6ALC S    = ',E13.6,39X,'CO2 TOT = ',E13.6,/,21X,'PE CALC DOX  = ',
     7E13.6,17X,'FORCE IONIQUE',9X,'DENSITE = ',0PF8.4,/,21X,'PE SATO DO
     8X  = ',E13.6,16X,E13.6,10X,'TDS = ',0PF9.1,'MG/L')
  121 FORMAT(50X,'BALANCE ELECTRIQUE=',E13.6)
  130 FORMAT (21X,'EN CALCULANT LA DISTRIBUTION DES ESPECES: PE = ',F7.3
     1,5X,'EH EQUIVALENT = ',F7.3,'VOLTS')
  140 FORMAT (1H ,54X,'-------------------------')
  141 FORMAT (1H ,54X,'DISTRIBUTION DES ESPECES')
  142 FORMAT (1H ,54X,'-------------------------')
  143 FORMAT (1H ,7X,'I',1X,'ESPECES',11X,'PPM',11X,'MOLALITE',8X,'LOG M
     1OL',6X,'ACTIVITE',7X,'LOG ACT',5X,'COEFF. ACT.',6X,'LOG COEFF.')
  144 FORMAT (1H ,7X,'-',1X,'--------',11X,'---',11X,'---------',8X,'-----
     1--',6X,'---------',7X,'-------',5X,'-----------',6X,'----------')
  150 FORMAT (1H ,5X,I3,1X,A8,I3,2X,1PE12.5,4X,E12.5,4X,0PF9.4,4X,1PE12.
     15,4X,0PF9.4,4X,1PE12.5,5X,0PF9.4)
  151 FORMAT (1H ,5X,I3,1X,A8,I3,2X,1PE12.5,4X,E12.5,4X,0PF9.4,4X,1PE12.
     15,4X,0PF9.4,4X,1PE12.5,5X,0PF9.6)
  152 FORMAT(1H ,5X,I3,1X,A8,I3)
  160 FORMAT (1H ,6X,'RAPPORTS MOLAIRES POUR LA MOLALITE ANALYTIQUE   RA
     2PPORTS MOLAIRES POUR LA MOLALITE CALCULEE   RAPPORTS DES LOG D'ACT
     3IVITE')
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161 FORMAT (1H ,6X,'-------------------------------------------   --
   1----------------------------------------  ----------------------
   2-----')
162 FORMAT (1H ,20X,'CL/CA = ',1PE11.4,27X,'CL/CA = ',E11.4,18X,'LOG C
   1A/H2 = ',0PF9.4,/,21X,'CL/MG = ',1PE11.4,27X,'CL/MG = ',E11.4,18X,
   2'LOG MG/H2 = ',0PF9.4,/,21X,'CL/NA = ',1PE11.4,27X,'CL/NA = ',E11.
   34,18X,'LOG NA/H1 = ',0PF9.4,/,21X,'CL/K =  ',1PE11.4,27X,'CL/K =
   4',E11.4,18X,'LOG K/H1 =  ',0PF9.4,/,21X,'CL/A1 = ',1PE11.4,27X,'CL
   5/AL = ',E11.4,18X,'LOG AL/H3 = ',0PF9.4,/,21X,'CL/FE = ',1PE11.4,2
   67X,'CL/FE = ',E11.4,18X,'LOG FE/H2 = ',0PF9.4,/,21X,'CL/SO4 = ',1P
   7E11.4,26X,'CL/SO4 = ',E11.4,17X,'LOG CA/MG = ',0PF9.4,/,21X,'CL/HC
   803 = ',1PE11.4,25X,'CL/HCO3 = ',E11.4,16X,'LOG NA/K  = ',0PF9.4,/,
   921X,'CA/MG = ',1PE11.4,27X,'CA/MG = ',E11.4,/,21X,'NA/K  = ',1PE11
   8.4,27X,'NA/K = ',E11.4)
163 FORMAT(1H ,7X,'I',1X,'ESPECES',11X,'PPM',11X,'MOLALITE',8X,'LOG MO
   1L',6X,'ACTIVITE',7X,'LOG ACT',5X,'COEFF. ACT.',6X,' MOLAL %  ')
164 FORMAT(1H ,20X,'NA/LI=',1PE11.4,29X,'NA/LI=',E11.4)
165 FORMAT(1H ,10X,'ESPECE',5X,'CITOT/FETOT',10X,'CITOT/TDS')
166 FORMAT(1H ,12X,A2,7X,E11.4,11X,E11.4)
167 FORMAT(1H ,7X,'_',1X,'_______',11X,'___',11X,'________',8X,'______
   1_',6X,'________',7X,'_______',5X,'-----------',6X,'----------')
168 FORMAT(1H ,20X,'NA/LI=',40X,'NA/LI=')
169 FORMAT(1H ,12X,A2)
    END
```

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      **********************
      * SOUS PROGRAMME SAT *
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```
    SUBROUTINE SAT
    IMPLICIT DOUBLE PRECISION (A-H,O-Z)
    INTEGER D,E,DD,RBIT,CORALK,Z(260),LIST6(24),PRT(4)
    INTEGER PECALC,PECK,FLAG,TRACES,CSPEC(120,6),E2
    DIMENSION LIST7(101), LIST8(15),PACT(450)
    REAL*8 MI(260),MNTOT,LH2O,MU,NATOT,KT
   1OT,MGTOT,LITOT,NH4TOT,KW
    REAL*8 KT(450),LOGKT(450),LOGKTO(450)
    REAL*8 NSPEC(260),NREACT(450),MIPRIM(125)
    COMMON MI,KT,LOGKT,LOGKTO,KW,D,E,DD,C,R,T,F,TEMP,A,B,NSPEC,NREA
   1CT,PE,PES,PEHQ,PESATQ,PECK,PECALC,PH,TENMPE,TENPH,ALFA(260),GAMMA(
   2260),AP(450),XLALFA(260),Z,CUNITS(260),ANALMI(260),GFW(260),DHA(26
   30),DH(450),AH2O,LH2O,EROR1,EROR2,EROR3,EROR4,EROR5,EHM,DENS,DOX,XL
   4MI(260),ITER,RBIT,C1SAVE,CORALK,MU,LCHEK(450),CO2TIT,ANALCO,SITOT,
   5CATOT,MGTOT,KTOT,NATOT,SO4TOT,FETOT,PTOT,ALTOT,FTOT,BTOT,LITOT,NH4
   6TOT,SRTOT,BATOT,CLTOT,MNTOT,ICK,PRT,TITL(10),EPMCAT,EPMAN,NEQU,
   7ISPEC,KSPEC(260),IMIN,KMIN(450),TDS,IDAYES,IPRT,FLAG,IGO,XLGAM(260
   8),TRACES,CITOT(10),NTRACE,LSPEC(120,6),CSPEC,LMIN(140,7),
   9CMIN(140,7),EROR6,STORE(25,25),ITMIN,MIPRIM,XPCENT(125)
    DATA LIST6/1,2,3,4,5,6,7,8,9,11,18,24,27,40,45,47,51,54,62,6
   17,88,90,101,102/
    DATA LIST7/40,41,141,51,43,18,114,42,22,151,145,49,53,20,13,144,98
   1,50,21,30,57,100,29,12,56,113,120,97,63,28,52,111,112,119,19,65,48
   2,109,118,39,96,46,47,44,129,148,68,99,110,11,108,64,116,117,58,67,
   359,61,150,55,45,142,115,54,102,37,10,101,147,143,38,66,62,32,60,10
   47,146,154,155,156,172,173,174,175,176,177,178,179,180,181,183,184,
   5185,186,187,188,189,190,191,192,193/
    DATA LIST8/107,108,109,110,111,112,113,114,115,119,120,173,174,175
   1,177/
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CALCUL DES PRODUITS D'ACTIVITES IONIQUES
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      DO 20 I=1,24
      IF (ALFA(LIST6(I)).LT.1.E-040) GO TO 10
      ALFA(LIST6(I))=DLOG10(ALFA(LIST6(I)))
      GO TO 20
   10 ALFA(LIST6(I))=-2E4
   20 CONTINUE
      AP(10)=ALFA(8)+ALFA(18)
      AP(11)=ALFA(2)+ALFA(18)
      AP(12)=ALFA(1)+AP(11)+ALFA(18)
      AP(13)=ALFA(1)+ALFA(18)
      AP(18)=ALFA(1)+ALFA(6)
      AP(19)=AP(18)+2E0*LH20
      AP(20)=ALFA(2)+2E0*ALFA(27)
      AP(21)=3E0*ALFA(2)+2E0*ALFA(24)+6E0*ALFA(27)-5E0*LH20
      AP(22)=AP(13)
      AP(28)=2E0*ALFA(2)+ALFA(24)+4E0*(ALFA(27)-LH20)
      AP(29)=ALFA(1)+ALFA(2)+2E0*ALFA(24)+4E0*ALFA(27)-6E0*LH20
      AP(30)=ALFA(2)+ALFA(24)+2E0*ALFA(27)-3E0*LH20
      AP(32)=2E0*ALFA(1)+5E0*ALFA(2)+8E0*ALFA(24)+14E0*ALFA(27)-22E0*LH2
     10
      AP(37)=2E0*ALFA(2)+3E0*ALFA(24)+4E0*ALFA(27)-4.5E0*LH20
      AP(38)=3E0*ALFA(2)+4E0*ALFA(24)+6E0*ALFA(27)-1E1*LH20
      AP(39)=4E0*ALFA(2)+3E0*ALFA(18)+2E0*ALFA(27)+3E0*LH20
      AP(40)=ALFA(4)+ALFA(54)+3E0*ALFA(24)-8E0*LH20
      AP(41)=AP(40)-ALFA(4)+ALFA(3)
      AP(42)=ALFA(1)+2E0*(ALFA(54)+ALFA(24))-8E0*LH20
      AP(43)=ALFA(3)+ALFA(54)+2E0*ALFA(24)-5E0*LH20
      AP(44)=ALFA(4)+3E0*(ALFA(54)+ALFA(24))-2E0*PH-12E0*LH20
      AP(45)=ALFA(4)+ALFA(54)+3E0*(ALFA(2)+ALFA(24))+6E0*ALFA(27)-1E1*LH
     120
      AP(46)=.6E0*ALFA(4)+.25E0*ALFA(2)+2.3E0*ALFA(54)+3.5E0*ALFA(24)-1.
     12E0*PH-11.2E0*LH20
      AP(47)=2E0*(ALFA(54)+ALFA(24)-PH)-7E0*LH20
      AP(48)=AP(47)
      C1=(DSQRT(MI(1)*GAMMA(1)+MI(2)*GAMMA(2)+MI(3)*GAMMA(3)))
      IF (C1.GT.0.0) C1=DLOG10(C1)
      IF (C1.LE.0.0) C1=-2E4
      AP(49)=.33E0*C1+2.33E0*ALFA(54)+3.67E0*ALFA(24)-2E0*PH-12E0*LH20
      AP(50)=5E0*ALFA(2)+2E0*ALFA(54)+3E0*ALFA(24)+8E0*ALFA(27)-1E1*LH20
      AP(51)=ALFA(4)+3E0*ALFA(51)+6E0*ALFA(27)+2E0*ALFA(6)
      AP(52)=ALFA(51)+3E0*ALFA(27)
      AP(53)=AP(52)-LH20
      AP(54)=2E0*ALFA(54)+4E0*ALFA(24)-2E0*PH-12.0*LH20
      AP(55)=.5E0*(ALFA(3)+ALFA(4))+ALFA(54)+3E0*ALFA(24)-7E0*LH20
      AP(56)=ALFA(3)+ALFA(54)+3.5E0*ALFA(24)-6E0*LH20
      C2=(MI(3)*GAMMA(3)+MI(4)*GAMMA(4))
      IF (C2.GT.0.0) C2=DLOG10(C2)
      IF (C2.LE.0.0) C1=-2E4
      AP(57)=.5E0*C2+ALFA(54)+5E0*ALFA(24)-8.5E0*LH20
      AP(58)=.5E0*C2+ALFA(54)+4.5E0*ALFA(24)-8E0*LH20
      AP(59)=ALFA(3)+ALFA(7)
      AP(60)=3E0*ALFA(3)+ALFA(7)+ALFA(18)+2E0*LH20
      AP(62)=2E0*ALFA(3)+ALFA(18)+LH20
      AP(61)=AP(62)+9E0*LH20
      AP(63)=ALFA(1)+2E0*ALFA(62)
      AP(64)=.167E0*ALFA(1)+2.33E0*ALFA(54)+3.67E0*ALFA(24)-2E0*PH-12E0*
     1LH20
      AP(65)=ALFA(3)+ALFA(5)
      AP(66)=2E0*ALFA(3)+ALFA(6)
      AP(67)=AP(66)+1E1*LH20
      AP(68)=ALFA(8)+ALFA(67)+PH
      AP(96)=5E0*ALFA(1)+3E0*(ALFA(47)-LH20)+4E0*ALFA(27)
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      AP(97)=5E0*ALFA(1)+3E0*(ALFA(47)-LH20)+3E0*ALFA(27)+ALFA(62)
      AP(98)=ALFA(24)-2E0*LH20
      AP(99)=ALFA(4)+7E0*ALFA(24)+PH-9E0*LH20
      AP(100)=AP(98)
      AP(101)=AP(98)
      AP(102)=AP(98)
      IF (DABS(PE).LT.20.0) GO TO 30
      GO TO 40
   30 CONTINUE
      AP(107)=3E0*ALFA(8)+2E0*ALFA(45)+8E0*LH20
      AP(108)=3E0*ALFA(9)-2E0*PE+4E0*LH20+8E0*PH
      AP(109)=2E0*ALFA(9)+3E0*LH20+6E0*PH
      AP(110)=AP(109)
      AP(111)=ALFA(9)+3E0*ALFA(27)-LH20
      AP(112)=3E0*ALFA(8)+2E0*ALFA(24)+6E0*ALFA(27)-5E0*LH20
      AP(113)=ALFA(9)+3E0*(LH20+PH)
      AP(114)=AP(45)+3E0*(ALFA(8)-ALFA(2))
      AP(115)=ALFA(8)+2E0*(ALFA(67)+PE+PH)
      AP(119)=3E0*ALFA(8)+4E0*ALFA(67)+2E0*PE+4E0*PH
      AP(120)=AP(68)
      AP(173)=ALFA(102)+2*LH20+4*PH+PE
      AP(174)=AP(173)
      AP(175)=AP(173)
      AP(177)=3*ALFA(101)+4*LH20+8*PH+2*PE
      GO TO 60
   40 CONTINUE
      DO 50 I=1,15
      JK=LIST8(I)
      AP(JK)=-6000.
   50 CONTINUE
      PECK=1
   60 CONTINUE
      AP(116)=.29*ALFA(2)+.23*ALFA(9)+1.58*ALFA(54)+3.93*ALFA(24)-10.*LH
     120
      AP(117)=.45*ALFA(2)+.34*ALFA(9)+1.47*ALFA(54)+3.82*ALFA(24)-9.2*LH
     120+.76*PH
      AP(118)=3E0*ALFA(2)+ALFA(1)+4E0*ALFA(18)
      AP(129)=ALFA(1)+2E0*ALFA(54)+4E0*ALFA(24)-8E0*LH20
      AP(141)=AP(52)
      AP(142)=2E0*(ALFA(1)+ALFA(54)+PH)+3E0*ALFA(24)-8E0*LH20
      AP(143)=ALFA(88)+ALFA(18)
      AP(144)=ALFA(88)+ALFA(6)
      AP(145)=ALFA(90)+ALFA(6)
      AP(146)=ALFA(90)+ALFA(18)
      AP(147)=ALFA(9)+ALFA(45)+2E0*LH20
      AP(148)=2E0*ALFA(1)+4E0*ALFA(54)+8E0*ALFA(24)-17E0*LH20
      AP(150)=ALFA(2)+ALFA(18)+3E0*LH20
      AP(151)=2E0*ALFA(1)+ALFA(18)+2E0*ALFA(27)+3E0*LH20
      AP(172)=ALFA(101)+LH20+2*PH
      AP(176)=2*ALFA(102)+3*LH20+6*PH
      AP(178)=ALFA(101)+2*ALFA(27)
      AP(179)=ALFA(102)+3*ALFA(27)
      AP(180)=ALFA(102)+2*LH20+3*PH
      AP(181)=ALFA(101)+ALFA(18)
      AP(183)=ALFA(101)+2*ALFA(5)
      AP(184)=AP(183)+LH20
      AP(185)=AP(183)+2*LH20
      AP(186)=AP(183)+4*LH20
      AP(187)=2*ALFA(101)+ALFA(24)+4*PH
      AP(188)=2*ALFA(101)+ALFA(24)+2*PH-LH20
      AP(189)=ALFA(101)+ALFA(67)+PH
      AP(190)=ALFA(101)+ALFA(6)
      AP(191)=2*ALFA(102)+3*ALFA(6)
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      AP(192)=3*ALFA(101)+2*ALFA(45)
      AP(193)=ALFA(101)+ALFA(47)
      AP(154)=AP(37)
      AP(155)=AP(52)-LH2O
      AP(156)=AP(129)-2*LH2O
      IF(TRACES.EQ.0) GO TO 2000
      DO 61 I=1,24
      ALFA(LIST6(I))=10.**ALFA(LIST6(I))
   61 CONTINUE
      E2=318
      K=0
      DO 63 N=1,E-E2
      K=K+1
      PR=1
      XLOGPR=DLOG10(PR)
      DO 62 I=3,LMIN(K,1)+2
      IF(ALFA(LMIN(K,I)).NE.0.0) GO TO 1000
      PR=0
      GO TO 1003
 1000 PR=PR*ALFA(LMIN(K,I))**CMIN(K,I)
 1003 CONTINUE
   62 CONTINUE
      PACT(E2+N)=PR
   63 CONTINUE
 2000 CONTINUE
      WRITE(6,290)
      WRITE(6,300)
      WRITE(6,310)
      WRITE(6,320)
      WRITE(6,330)
      DO 100 I=1,101
      IF (IMIN.EQ.0) GO TO 80
      K=0
      DO 70 J=1,IMIN
      IF (LIST7(I).EQ.KMIN(J)) K=1
   70 CONTINUE
      IF (K.EQ.1) GO TO 80
      GO TO 100
   80 CONTINUE
      IF (AP(LIST7(I)).LT.-300.0.OR.AP(LIST7(I)).GT.300.0) GO TO 90
      IF (LCHEK(LIST7(I)).EQ.1) GO TO 90
      DUM=AP(LIST7(I))-DLOG10(KT(LIST7(I)))
      IF (DUM.GT.75.) GO TO 90
      XIAP=10.**AP(LIST7(I))
      RAT=XIAP/KT(LIST7(I))
      XLRAT=DLOG10(RAT)
      DELGR=C*R*T*XLRAT
      WRITE(6,160), LIST7(I),NREACT(LIST7(I)),XIAP,KT(LIST7(I)),AP
     1(LIST7(I)),LOGKT(LIST7(I)),RAT,XLRAT,DELGR
      GO TO 100
   90 IF(AP(LIST7(I)).GE.-5000.0.AND.AP(LIST7(I)).LE.5000.) GO TO 91
      WRITE(6,171),LIST7(I),NREACT(LIST7(I))
      GO TO 100
   91 XLRAT=AP(LIST7(I))-LOGKT(LIST7(I))
      DELGR=C*R*T*XLRAT
      WRITE(6,170), LIST7(I),NREACT(LIST7(I)),AP(LIST7(I)),LOGKT(LIST7
     1(I)),XLRAT,DELGR
  100 CONTINUE
      IF (PECK.EQ.1.AND.PECALC.NE.0) GO TO 110
      GO TO 130
  110 WRITE(6,180)
      DO 120 I=1,15
      WRITE(6,190), NREACT(LIST8(I))
```

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120 CONTINUE
130 CONTINUE
    IF(TRACES.EQ.0) GO TO 150
    E2=318
    DO 140 I=E2+1,E
    IF(PACT(I).NE.0.) GO TO 131
    WRITE(6,171),I,NREACT(I)
    GO TO 140
131 AP(I)=DLOG10(PACT(I))
    RAT=PACT(I)/KT(I)
    XLRAT=DLOG10(RAT)
    DELGR=C*R*T*XLRAT
    WRITE(6,160),I,NREACT(I),PACT(I),KT(I),AP(I),LOGKT(I)
   1,RAT,XLRAT,DELGR
140 CONTINUE
150 CONTINUE
    RETURN

 FORMATS
 *******

290 FORMAT (1H ,54X,'************************')
300 FORMAT (1H ,54X,'* SATURATION MINERALE *')
310 FORMAT (1H ,54X,'************************')
320 FORMAT (16X,'PHASE',9X,'IAP',11X,'KT',8X,'LOG IAP',4X,'LOG KT',
   16X,'IAP/KT',5X,'LOG IAP/KT',2X,'DEG DE SATURATION')
330 FORMAT (1H ,15X,'-----',9X,'---',11X,'--',8X,'-------',4X,'------'
   1,6X,'------',5X,'----------',2X,'----------------')
160 FORMAT (1H ,11X,I3,1X,A8,2(2X,1PE11.4),2(2X,0PF9.4),2X,1PE11.4,2X,
   10PF10.5,5X,0PF10.5)
530 FORMAT (1H ,19X,'*',2X,'I',2X,'*',1X,'REACTION',1X,'*',2X,'P.D'ACT
   1.',2X,'*',3X,'KT(I)',3X,'*',1X,'LOG  PA',1X,'*',2X,'LOGKT',2X,'*',
   22X,'P.A./KT',2X,'*',1X,'LOG PA/KT',1X,'*',1X,'D.DE SAT.',1X,'*')
170 FORMAT (1H ,9X,'*',1X,I3,1X,'*',1X,A8,1X,'*',12X,'*',E10.3,1X,'*'
   1,F8.3,1X,'*',F8.3,1X,'*',11X,'*',F10.5,1X,'*',F10.5,1X,'*')
171 FORMAT(1H ,11X,I3,1X,A8)
180 FORMAT (20X,'PE EST PLUS GRAND QUE 20 OU PLUS PETIT QUE -20',/
   1,20X,'AND THE FOLLOWING MINERAL REACTIONS HAVE BEEN DISREGARDED')
190 FORMAT (1H ,20X,A8)
    END
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RECAPITULATIF des DONNEES THERMODYNAMIQUES

			a_o	m				a_o	m
1	CA	2	6.0	40.0800					
2	MG	2	6.5	24.3120	65	FEH2PO4	1	5.4	152.8340
3	NA	1	4.0	22.9898	66	H2S CALC	0	0.0	34.0799
4	K	1	3.0	39.1020	67	HS	-1	3.5	33.0720
5	CL	-1	3.0	35.4530	68	S	-2	5.0	32.0640
6	SO4	-2	4.0	96.0616	69	BLANK	0	0.0	1.0000
7	HCO3	-1	5.4	61.0173	70	PO2	0	0.0	31.9988
8	FE	2	6.0	55.8470	71	PCH4	0	0.0	16.0430
9	FE	3	9.0	55.8470	72	AH2O	0	0.0	18.0153
10	FEOH	2	5.0	72.8544	73	MGHPO4	0	0.0	120.2914
11	FEOH	1	5.0	72.8549	74	CAHPO4	0	0.0	136.0594
12	FE(OH)3	-1	5.0	106.8690	75	CAPO4	-1	5.4	135.0514
13	FEHPO4	1	5.4	151.8200	76	CAH2PO4	1	5.4	137.0673
14	H2S AQ	0	0.0	34.0799	77	FE(OH)2	1	5.4	89.8616
15	FESO4	1	5.0	151.9086	78	FE(OH)3	0	0.0	106.8689
16	FECL	2	5.0	91.3000	79	FE(OH)4	-1	5.4	123.8762
17	ANAL H2S	0	0.0	34.0799	80	FE(OH)2	0	0.0	89.8616
18	CO3	-2	5.4	60.0094	81	LI	1	6.0	6.9390
19	MGOH	1	6.5	41.3194	82	LIOH	0	0.0	23.9464
20	MGF	1	4.5	43.3104	83	LISO4	-1	5.0	103.0006
21	MGCO3 AQ	0	0.0	84.3214	84	NH4CALC	1	2.5	18.0386
22	MGHCO3	1	4.0	85.3293	85	NO3	-1	3.0	62.0049
23	MGSO4 AQ	0	0.0	120.3736	86	H2CO3	0	0.0	62.0253
24	H4SIO4AQ	0	0.0	96.1155	87	B TOT	0	0.0	10.8100
25	H3SIO4	-1	4.0	95.1075	88	SR	2	5.0	87.6200
26	H2SIO4	-2	5.4	94.0995	89	SROH	1	5.0	104.6274
27	OH	-1	3.5	17.0074	90	BA	2	5.0	137.3400
28	FECL2	1	5.0	126.7530	91	BAOH	1	5.0	154.3474
29	CAOH	1	6.0	57.0874	92	NH4SO4	-1	5.0	114.1002
30	CAHCO3	1	6.0	101.0973	93	HCL	0	0.0	36.4610
31	CACO3 AQ	0	0.0	100.0890	94	NACL	0	0.0	58.4428
32	CASO4 AQ	0	0.0	136.1416	95	KCL	0	0.0	74.5550
33	FECL3	0	0.0	162.2060	96	H2SO4	0	0.0	98.0775
34	FESO4	0	0.0	151.9086	97	BLANK	0	0.0	1.0000
35	SIO2 TOT	0	0.0	60.0848	98	BR	-1	4.0	79.9090
36	H3BO3 AQ	0	0.0	61.8331	99	FEH2PO4	2	5.4	152.8340
37	H2BO3	-1	2.5	60.8251	100	FEHPO4	0	0.0	151.8200
38	NH3 AQ	0	0.0	17.0306	101	MN	2	6.0	54.9400
39	NH4	1	2.5	18.0386	102	MN	3	9.0	54.9400
40	MGPO4	-1	5.4	119.2834	103	MNCL	1	5.0	90.3970
41	MGH2PO4	1	5.4	121.2993	104	MNCL2	0	0.0	125.8540
42	NACO3	-1	5.4	82.9992	105	MNCL3	-1	5.0	161.3110
43	NAHCO3	0	0.0	83.9909	106	MNOH	1	5.0	71.8480
44	NASO4	-1	5.4	119.0514	107	MN(OH)3	-1	5.0	105.9640
45	PO4	-3	5.0	94.9714	108	MNF	1	5.0	73.9400
46	KSO4	-1	5.4	135.1636	109	MNSO4	0	0.0	151.0060
47	HPO4	-2	5.0	95.9794	110	MN(NO3)2	0	0.0	178.9560
48	H2PO4	-1	5.4	96.9873	111	MNHCO3	1	5.0	115.9590
49	CAF+	1	5.0	59.0784	112	MNO4	-1	3.0	118.9400
50	NAHPO4	-1	5.4	118.9692	113	MNO4	-2	5.0	118.9400
51	AL	3	9.0	26.9815	114	BLANK	0	0.0	1.0000
52	ALOH	2	5.4	43.9889	115	HMNO2	-1	5.0	87.9480
53	AL(OH)2	1	5.4	60.9962	116	MNCO3	0	0.0	114.951
54	AL(OH)4	-1	4.5	95.0110	117	FE(HS)2	0	0.0	121.991
55	ALF	2	5.4	45.9799	118	FE(HS)3-	-1	4.0	155.063
56	ALF2	1	5.4	64.9783	119	FE(SO4)2	-1	4.0	247.970
57	ALF3	0	0.0	83.9767	120	FEF+2	+2	5.0	74.845
58	ALF4	-1	4.5	102.9751	121	FEF2+	+1	4.0	93.843
59	ALSO4	1	4.5	123.0431	122	FEF3	0	0.0	112.841
60	AL(SO4)2	-1	4.5	219.1047	123	FECO3	0	0.0	115.8560
61	KHPO4	-1	5.4	135.0814	124	FEHCO3+	+1	4.0	116.864
62	F	-1	3.5	18.9984	125	NAF	0	0.0	41.9882
63	HSO4	-1	4.5	97.0696	126	CD+2	+2	6.0	112.400
64	H	1	9.0	1.0080	127	CDOH+	+1	4.0	129.41

			a_o		m
128	CD(OH)2	0	0.0	146.42
129	CD(OH)3-	-1	4.0	163.43
130	CD(OH)4	-2	5.0	180.44
131	CDCL+	+1	4.0	147.85
132	CDCL2	0	0.0	183.30
133	CDCL3-	-1	4.0	218.75
134	CDCL4-2	-2	5.0	254.20
135	CDSO4	0	0.0	208.46
136	CD(SO4)2	-2	5.0	304.52
137	CD(SO4)3	-4	9.0	400.58
138	CDF+	+1	4.0	131.4
139	CDF2	0	0.0	150.4
140	CDOHCL	0	0.0	164.86
141	CDCO3	0	0.0	172.41
142	CD(CO3)3	-4	9.0	292.43
143	CDHCO3+	+1	4.0	173.42
144	CDHS+	+1	4.0	145.47
145	CD(HS)2	0	0.0	178.54
146	CD(HS)3-	-1	4.0	211.61
147	CD(HS)4	-2	5.0	244.68
148	ZN+2	+2	6.0	65.38
149	ZNOH+	+1	4.0	82.39
150	ZN(OH)2	0	0.0	99.40
151	ZN(OH)3-	-1	4.0	116.41
152	ZN(OH)4	-2	5.0	133.42
153	ZNCL+	+1	4.0	100.83
154	ZNCL2	0	0.0	136.28
155	ZNCL3-	-1	4.0	171.73
156	ZNCL4-2	-2	5.0	207.18
157	ZNSO4	0	0.0	161.44
158	ZN(SO4)2	-2	5.0	257.50
159	ZN(SO4)3	-4	9.0	353.56
160	ZN(SO4)4	-6	9.0	449.62
161	ZNF+	+1	4.0	84.38
162	ZNOHCL	0	0.0	117.84
163	ZNCO3	0	0.0	125.39
164	ZNHCO3+	+1	4.0	126.40
165	ZN(HS)2	0	0.0	178.54
166	ZN(HS)3-	-1	4.0	164.59
167	PB+2	+2	4.5	207.20
168	PBOH+	+1	4.0	224.21
169	PB(OH)2	0	0.0	241.22
170	PB(OH)3-	-1	4.0	258.23
171	PBCL+	+1	4.0	242.65
172	PBCL2	0	0.0	278.10
173	PBCL3-	-1	4.0	313.55
174	PBCL4-2	-2	5.0	349.00
175	PBSO4	0	0.0	303.26
176	PB(SO4)2	-2	5.0	399.32
177	PBF+	+1	4.0	226.20
178	PBF2	0	0.0	245.20
179	PBF3-	-1	4.0	264.2
180	PBF4-2	-2	5.0	283.20
181	PBCO3	0	0.0	267.21
182	PB(CO3)2	-2	5.0	327.22
183	PBHCO3+	+1	4.0	268.22
184	PB(HS)2	0	0.0	274.40
185	PB(HS)3-	-1	4.0	307.47
186	CO+2	+2	6.0	58.93
187	COOH+	+1	4.0	75.94
188	CO(OH)2	0	0.0	92.95
189	CO(OH)3-	-1	4.0	109.96
190	CO(OH)4	-2	5.0	126.97
191	COCL+	+1	4.0	94.38
192	COSO4	0	0.0	154.99
193	COF+	+1	4.0	77.93
194	COCO3	0	0.0	118.94
195	COHCO3+	+1	4.0	119.95
196	NI+2	+2	6.0	58.70
197	NIOH+	+1	4.0	75.71
198	NI(OH)2	0	0.0	92.72
199	NI(OH)3-	-1	4.0	109.73
200	NI(OH)4	-2	5.0	126.74
201	NICL+	+1	4.0	94.15
202	NICL2	0	0.0	129.60
203	NISO4	0	0.0	154.76
204	NI(SO4)2	-2	5.0	250.82
205	NIF+	+1	4.0	77.70
206	NICO3	0	0.0	118.71
207	NIHCO3+	+1	4.0	119.72
208	CR+3	+3	9.0	52.00
209	CROH+2	+2	5.0	69.01
210	CR(OH)2+	+1	4.0	86.02
211	CR(OH)3	0	0.0	103.03
212	CR(OH)4-	-1	4.0	120.04
213	CRCL+2	+2	5.0	87.45
214	CRCL2+	+1	4.0	122.90
215	CRSO4+	+1	4.0	148.06
216	CRF+2	+2	5.0	71.00
217	CRF2+	+1	4.0	90.00
218	CRF3	0	0.0	109.00
219	CU+2	+2	6.0	63.55
220	CUOH+	+1	4.0	80.56
221	CU(OH)2	0	0.0	97.57
222	CU(OH)3-	-1	4.0	114.58
223	CU(OH)4	-2	5.0	131.59
224	CUCL+	+1	4.0	99.00
225	CUCL2	0	0.0	134.45
226	CUCL3-	-1	4.0	169.90
227	CUCL4-2	-2	5.0	205.35
228	CUSO4	0	0.0	159.61
229	CUF+	+1	4.0	82.55
230	CUCO3	0	0.0	123.56
231	CU(CO3)2	-2	5.0	183.57
232	CUHCO3+	+1	4.0	124.57
233	CU+	+1	4.0	63.55
234	CUCL2-	-1	4.0	134.45
235	CUCL3-2	-2	5.0	169.90
236	CU(HS)3-	-1	4.0	96.62
237	ASO4-3	-3	9.0	138.92
238	H3ASO4	0	0.0	141.95
239	H2ASO4	-1	4.0	140.94
240	HASO4	-2	5.0	139.93
241	ASO3-3	-3	9.0	122.92
242	AS(OH)4-	-1	4.0	142.96
243	AS(OH)3	0	0.0	125.95
244	SB(OH)3	0	0.0	172.78
245	SBOH+2	+2	5.0	155.77
246	SB(OH)4-	-1	4.0	189.79
247	SB(OH)5	0	0.0	206.80
248	SB(OH)6-	-1	4.0	223.81
249	GE(OH)4	0	0.0	140.63
250	GEO(OH)3	-1	4.0	139.62

		ΔH	logK
1	KFE+3	9.7000	-13.0130
2	KFEH+2	20.1150	-15.4730
3	KFEOH+	13.2180	-9.3190
4	KFE2OH	32.9950	-29.4580
5	KFESO4	15.9200	-8.8860
6	KFECL	18.1520	-11.6000
7	KFECL2	0.0	-10.9190
8	KFECL3	0.0	-11.9250
9	KFE3O	0.5600	2.2000
10	SIDERITE	-5.3280	-10.5500
11	MAGNESIT	-6.1690	-8.4100
12	DOLOMITE	-8.2900	-17.0200
13	CALCITE	-3.1900	-8.4100*
14	KH3SIO4	8.9350	-9.9290*
15	KH2SIO4	29.7170	-21.6170*
16	KHPO4	-3.5300	12.3460
17	KH2PO4	-4.5200	19.5530
18	ANHYDRIT	-3.7690	-4.5480
19	GYPSE	0.2610	-4.7590
20	BRUCITE	0.8500	-11.4100
21	CHRYSOTL	27.5850	-51.8000
22	ARAGONIT	-2.9590	-8.2150
23	KMGF	4.6740	1.8200
24	KCASO4	1.5000	2.3090
25	KMGOH	2.0900	2.2100*
26	KH3BO3	3.2240	-9.2400*
27	KNH3	12.4770	-9.2440*
28	FORSTRIT	4.8700	-28.1100
29	DIOPSIDE	21.1000	-36.2200
30	CLENSTIT	6.6750	-16.8700
31	KNAHPO	0.0	0.2900
32	TREMOLIT	90.2150	-140.3000
33	KKHPO4	0.0	0.2900
34	KMGHPO4	3.3000	2.8700
35	KCAHPO4	3.3000	2.7390
36	KH2CO3	-2.2430	6.5310*
37	SEPIOLIT	26.5320	-40.1000
38	TALC	45.0650	-62.2900
39	HYDMAG	-25.5200	-37.8200
40	ADULAIRE	30.8200	-20.5700
41	ALBITE	25.8960	-18.0000
42	ANORTHIT	17.5300	-19.3300
43	ANALCIME	18.2060	-12.7000
44	KMICA	67.8600	-49.0900
45	PHLOGOPI	0.0	-63.5300
46	ILLITE	54.6840	-40.3100
47	KAOLINIT	49.1500	-36.9100
48	HALLOYSI	44.6800	-32.8200
49	BEIDEL	60.3550	-45.2600
50	CHLORITE	54.7600	-90.6100
51	ALUNITE	29.8200	-85.3200
52	GIBCRS	14.4700	-32.7700
53	BOEHMITE	11.9050	-33.4100
54	PYROPHYL	0.0	-42.4300
55	PHILIST	0.0	-19.8600
56	ERIONITE	0.0	0.0
57	CLINOP	0.0	0.0
58	MORDENIT	0.0	0.0
59	NAHCOLIT	3.7200	-0.5180
60	TRONA	-18.0000	-0.7950
61	NATRON	15.7450	-1.3110
62	THRNAT	-2.8020	0.1250
63	FLUORITE	1.5300	-10.5000
64	MONTCA	58.3730	-45.0000
65	HALITE	0.9180	1.5820
66	THENARDI	-0.5720	-0.1790
67	MIRABILI	18.9870	-1.1130
68	MACKIT	0.0	-4.6310
69	KHCO3	-3.6040	10.3300*
70	KNACO3	8.9110	1.2680
71	KNAHCO3	0.0	-0.2500
72	KNASO4	1.1000	0.7200
73	KKSO4	3.0820	0.8470*
74	KMGCO3	2.7100	2.9800*
75	KMGHCO3	1.0770	1.0660*
76	KMGSO4	1.2700	2.2380
77	KCAOH	1.1900	1.4000
78	KCAHCO3	5.4100	1.0150*
79	KCACO3	4.0230	3.1530*
80	KCAF+	4.1200	0.9400
81	KALOH	1.9900	8.9980
82	KALOH2	0.0	18.2350
83	KALOH4	-9.3200	33.9380
84	KALF	0.0	7.0100
85	KALF2	20.0000	12.7500
86	KALF3	2.5000	17.0200
87	KALF4	0.0	19.7200
88	KALSO4	2.2900	3.2000
89	KAS042	3.0700	5.1000
90	KHSO4	4.8190	2.0540*
91	KH2SO	-45.4400	40.6440
92	KH2S	5.2990	-6.9420*
93	KHS	12.1000	-12.9180
94	KOXY	34.1570	-20.7300
95	KOH4	-57.4350	30.7410
96	HYXAPT	17.2250	-59.3500
97	FLUAPT	19.6950	-66.7900
98	CALCEDON	4.6150	-3.5230
99	MAGADITE	0.0	-14.3000
100	CRISTOBA	5.5000	-3.5860
101	SILGEL	4.4400	-3.0170
102	QUARTZ	6.2200	-4.0050
103	KFEOH2	0.0	-20.1730
104	KFEOH3	0.0	-26.5710
105	KFEOH4	0.0	-34.8940
106	KFEOH2	28.5650	-20.5700
107	VIVIANIT	0.0	-36.0000
108	MAGNETIT	-40.6600	-9.5650
109	HEMATITE	-30.8450	-4.0070
110	MAGHEMIT	0.0	6.3700
111	GOETHITE	25.5550	-41.2000
112	GREENALI	0.0	-63.1900
113	FEOH3A	0.0	4.8850
114	ANNITE	62.4800	-84.2400
115	PYRITE	11.3000	-18.4800
116	MONTBF	0.0	-34.9700
117	MONTAB	0.0	-29.7800
118	HUNTITE	-25.7600	-30.5100
119	GREGITE	0.0	-17.9700
120	FESPPT	0.0	-3.9100
121	KFEH2P	0.0	2.7000
122	KCAPO4	3.1000	6.4590
123	KCAH2P	3.4000	1.4080
124	KMGPO4	3.1000	6.5890
125	KMGH2P	3.4000	1.5130
126	KLIOH	4.8320	0.2000
127	KLISO4	0.0	0.6400
128	KNH4R	-187.0550	119.0770
129	LAUMONTI	39.6100	-31.9600

		ΔH	logK
130	KSROH	1.1500	0.8200
131	KBAOH	1.7500	0.6400
132	KNH4SO	0.0	1.1100
133	KHCL	18.6300	-8.1000
134	KNACL	0.0	-1.6020
135	KKCL	0.0	-1.5850
136	KH2SO4	0.0	-1.0000
137	KO2 GATO	0.0	-11.3850
138	KCO2	-5.0000	-1.4520
139	KFEHPO	0.0	3.6000
140	KFEHP+	0.0	-7.6130
141	ALOH3A	12.9900	-31.6100
142	PREHNITE	10.3900	-11.5200
143	STRONTIA	2.3610	-11.4100
144	CELESTIT	-1.0540	-5.9740
145	BARITE	6.1410	-9.7560
146	WITHERIT	6.9500	-13.3200
147	STRENGIT	-2.0300	-26.4000
148	LEONHARD	90.0700	-69.5700
149	BLANK	0.0	0.0
150	NESQUHO	-4.5510	-5.2110
151	ARTINITE	0.4980	-18.4000
152	KO2 AQ	33.4570	-21.4950
153	KW	13.3450	-13.9980
154	SEP FT	0.0	-37.2120
155	DIASPORE	-15.4050	-35.0600
156	WAIRAKIT	26.1400	-26.6200
157	KFEH2	0.0	-7.5830
158	KMN3+	25.7600	-25.5070
159	KMNCL+	0.0	0.6070
160	KMNCL2	0.0	0.0410
161	KMNCL3-	0.0	-0.3050
162	KMNOH+	0.0	3.4490
163	KMN(OH)3	0.0	7.7820
164	KMNF+	0.0	0.8500
165	KMNSO4	3.7000	1.7080
166	KMNNO3,2	-0.3960	0.0590
167	KMNHCO3+	0.0	1.7160
168	KMNO4-	176.6200	-127.8240
169	KMNO4--	150.0200	-118.4400
170	BLANK	0.0	0.0
171	KHMNO2--	0.0	-34.4400
172	MANGANO	-24.0250	17.9380
173	PYROLUST	-29.1800	15.8610
174	BIRNESIT	0.0	18.0910
175	NUSTITE	0.0	17.5040
176	BIXBYITE	-15.2450	-0.6110
177	HAUSMANI	-80.1400	61.5400
178	MNOH2	4.1000	-12.9120
179	MNOH3	20.0900	-35.6440
180	MANGANIT	0.0	-0.2380
181	RHODOCHR	-2.0790	-10.5390
182	BLANK	0.0	0.0
183	MNCL2	-17.6220	8.7600
184	MNCL2,1W	-7.1750	5.5220
185	MNCL2,2W	1.7100	3.9740
186	MNCL2,4W	17.3800	2.7100
187	TEPHRITE	-40.0600	23.1220
188	RHODONIT	-21.8850	9.5220
189	MNS GRN	-5.7900	3.8000
190	MNSO4	-15.4800	2.6690
191	MN2SO4,3	-39.0600	-5.7110
192	MN3PO4,2	2.1200	-23.8270
193	MNHPO4	0.0	-12.9470
194	KMNCO3	0.45	4.32
195	KFE(HS)2	0.0	8.95
196	KFE(HS)3	0.0	10.99
197	KFESO4,2	4.60	5.42
198	KFEF+2	2.7	6.2
199	KFEF2+	4.8	10.8
200	KFEF3	5.4	14.0
201	KFECO3	1.68	3.47
202	KFEHCO3	1.04	2.17
203	KNAF	0.0	-0.95
204	KCDOH+	-0.25	3.92
205	KCD(OH)2	-1.19	7.65
206	KCD(OH)3	-2.18	8.70
207	KCD(OH)4	-5.31	8.65
208	KCDCL+	0.59	1.98
209	KCDCL2	1.24	2.60
210	KCDCL3	3.90	2.40
211	KCDCL4	9.00	1.47
212	KCDSO4	1.08	2.45
213	KCDSO4,2	0.00	3.44
214	KCDSO4,3	0.00	3.09
215	KCDF+	1.20	1.08
216	KCDF2	0.50	1.41
217	KCDOHCL	4.35	6.60
218	KCDCO3	0.13	4.35
219	KCDCO3,3	0.00	6.22
220	KCDHCO3	1.01	2.00
221	KCDHS+	0.00	10.17
222	KCD(HS)2	0.00	16.53
223	KCD(HS)3	0.00	18.71
224	KCD(HS)4	0.00	20.90
225	KZNOH+	-0.5	5.04
226	KZN(OH)2	-5.8	11.1
227	KZN(OH)3	-10.6	13.6
228	KZN(OH)4	-12.5	14.8
229	KZNCL+	7.79	0.49
230	KZNCL2	8.5	0.62
231	KZNCL3	9.56	0.51
232	KZNCL4	10.96	0.2
233	KZNSO4	1.36	2.36
234	KZNSO4,2	0.00	3.63
235	KZNSO4,3	0.00	2.70
236	KZNSO4,4	0.00	-0.82
237	KZNF+	3.80	1.15
238	KZNOHCL	0.00	6.52
239	KZNCO3	-0.09	4.80
240	KZNHCO3	1.03	2.20
241	KZN(HS)2	0.00	14.94
242	KZN(HS)3	0.00	16.10
243	KPBOH+	-2.60	6.29
244	KPB(OH)2	-8.50	10.88
245	KPB(OH)3	-12.7	13.94
246	KPBCL+	4.38	1.58
247	KPBCL2	1.08	1.82
248	KPBCL3	2.17	1.71
249	KPBCL4	3.53	1.40
250	KPBSO4	0.26	2.75
251	KPBSO4,2	0.00	4.51
252	KPBF+	0.84	2.06
253	KPBF2	0.00	3.42
254	KPBF3	0.00	3.42
255	KPBF4	0.00	3.10

		ΔH	logK			ΔH	logK
256	KPBCO3	-4.1	7.20	319	OTAVITE	-0.58	-13.74
257	KPBCO3,2	0.00	10.64	320	CDCL2	-4.47	-0.68
258	KPBHCO3	0.87	1.90	321	CDCL2,W	-1.82	-1.71
259	KPB(HS)2	0.00	15.27	322	CDCL25/2	1.71	-1.94
260	KPB(HS)3	0.00	16.57	323	CDF2	-9.72	-2.98
261	KCOOH	0.10	4.35	324	CD(OH)2A	-20.77	13.73
262	KCO(OH)2	-2.00	9.20	325	CD(OH)2C	0.00	13.65
263	KCO(OH)3	-3.33	10.50	326	CDOHCL	-7.407	3.52
264	KCO(OH)4	-5.44	9.70	327	CD3OH4SO	0.00	22.56
265	KCOCL	0.52	0.57	328	CD3OH2SO	0.00	6.71
266	KCOSO4	0.50	2.36	329	CD3OH6SO	0.00	28.40
267	KCOF+	4.14	1.02	330	MONTEPON	-24.76	15.12
268	KCOCO3	-0.22	4.90	331	CDSIO3	-16.63	9.06
269	KCOHCO3	1.03	2.20	332	CDSO4	-14.74	-0.10
270	KNIOH	0.40	4.14	333	CDSO4,W	-7.52	-1.66
271	KNI(OH)2	-4.20	9.00	334	CDSO48/3	-4.30	-1.87
272	KNI(OH)3	-15.10	12.00	335	ZDCL2	-17.48	7.03
273	KNI(OH)4	-28.20	12.00	336	SMITHSON	-4.36	-10.00
274	KNICL	0.00	0.72	337	ZNCO3,W	0.00	-10.26
275	KNICL2	0.00	0.96	338	ZN(OH)2A	0.00	12.45
276	KNISO4	1.52	2.29	339	ZN(OH)2C	0.00	12.2
277	KNISO4,2	0.00	3.20	340	ZN(OH)2B	0.00	11.75
278	KNIF	4.06	1.12	341	ZN(OH)2G	0.00	11.71
279	KNICO3	-0.77	5.37	342	ZN(OH)2E	0.00	11.50
280	KNIHCO3	1.10	2.20	343	ZN2OH3CL	0.00	15.20
281	KCROH	-3.65	10.00	344	ZN5OH8CL	0.00	38.50
282	KCR(OH)2	-7.17	18.30	345	ZN2OH2SO	0.00	7.50
283	KCR(OH)3	-10.84	24.00	346	ZN4OH6SO	0.00	28.40
284	KCR(OH)4	-15.84	28.60	347	ZNNO326W	5.51	3.44
285	KCRCL	0.00	0.60	348	ZNO ACT	0.00	11.31
286	KCRCL2	0.00	0.11	349	ZNO CRYS	-21.86	11.14
287	KCRSO4	2.66	4.61	350	ZN3OSO42	-62.00	19.02
288	KCRF+2	1.41	5.21	351	ZNS AM	3.67	-9.052
289	KCRF2+	0.00	9.31	352	SPHALERI	8.25	-11.618
290	KCRF3	0.00	11.91	353	WURTZITE	5.06	-9.682
291	KCUOH	-1.35	6.00	354	ZNSIO3	-18.27	2.93
292	KCU(OH)2	-3.60	10.70	355	WILLEMIT	-33.37	15.33
293	KCU(OH)3	-7.92	14.20	356	ZINCOSIT	-19.20	3.01
294	KCU(OH)4	-14.11	16.40	357	ZNSO4,W	-10.64	-0.57
295	KCUCL+	8.65	0.02	358	BIANCHIT	-0.16	-1.765
296	KCUCL2	10.56	-0.71	359	GOSLARIT	3.30	-1.96
297	KCUCL3-	13.69	-2.29	360	COTUNNIT	5.60	-4.77
298	KCUCL4	17.78	-4.59	361	MATLOCKI	7.95	-9.43
299	KCUSO4	1.22	2.31	362	PHOSGENI	0.00	-19.81
300	KCUF+	1.62	1.52	363	CERRUSIT	4.86	-13.13
301	KCUCO3	-2.70	6.75	364	PBF2	-0.70	-7.44
302	KCUCO3,2	0.00	10.69	365	MASSICOT	-16.78	12.91
303	KCUHCO3	1.06	2.20	366	LITHARGE	-16.38	12.72
304	KCU+	1.65	2.72	367	PBO,W/3	0.00	12.98
305	KCUCL2-	1.23	8.22	368	PB2OCO3	-11.46	-0.50
306	KCUCL3-2	1.91	8.42	369	LARNAKIT	-6.44	-0.28
307	KCU(HS)3	0.00	25.90	370	PB3O2SO4	-20.75	10.40
308	KH3ASO4	-3.43	20.68	371	PB4O3SO4	-35.07	22.10
309	KH2ASO4	-5.12	18.44	372	PBHPO4	7.04	-11.46
310	KHASO4	-4.35	11.50	373	PB3O2CO3	-26.43	11.02
311	KASO3	-13.19	5.4	374	PBSIO3	-9.26	7.32
312	KAS(OH)4	-28.865	30.90	375	PB2SIO4	-26.00	19.76
313	KAS(OH)3	-33.445	40.15	376	ANGLESIT	2.15	-7.79
314	KSB(OH)2	-5.1	1.42	377	GALENE	19.4	-15.132
315	KSB(OH)4	15.90	-11.82	378	PLATTNER	-70.73	49.30
316	KSB(OH)5	0.00	-28.58	379	PB2O3	0.00	61.04
317	KSB(OH)6	0.00	-31.30	380	PB(OH)2	-13.99	8.15
318	KGEOOH,4	0.00	-9.31	381	LAURIONI	0.00	0.623

		ΔH	logK
382	PB2OH3CL	0.00	8.79
383	HYDCERRU	0.00	-17.46
384	PB2OOH2	0.00	26.20
385	PB4OH4SO	0.00	21.1
386	MELANOTH	-12.32	3.73
387	CUCO3	0.00	-9.63
388	CUF2	-13.32	0.65
389	CUF2,2W	-3.65	-4.55
390	CU(OH)2	-15.25	8.64
391	MALACHIT	-19.76	5.15
392	AZURITE	-30.87	3.75
393	ATACAMIT	-18.69	7.34
394	ANTLERIT	0.00	8.29
395	CU2OH3NO	-17.35	9.24
396	BROCHANT	0.00	15.34
397	LANGITE	-39.61	16.79
398	TENORITE	-15.24	7.62
399	CU2OSO4	-35.37	11.53
400	CUSO4	-18.14	3.01
401	CHALCAN	1.44	-2.64
402	CUPRIFER	-38.69	5.88
403	NICO3	-9.94	-6.84
404	NI(OH)2	-20.20	10.80
405	NI4OH4SO	0.00	32.00
406	BUNSENIT	-23.92	12.45
407	RETGERSI	1.10	-2.04
408	MORENOSI	2.94	-2.38
409	NI2SIO4	-33.36	14.54
410	NISO4	-21.48	4.48
411	COO	-25.21	13.64
412	COOH2PIN	-21.20	13.12
413	COOH2TRA	0.00	12.35
414	JAIPURIT	1.60	7.05
415	COSO4	-18.76	2.83
416	COSO4,W	-12.65	-1.01
417	COSO4,6W	0.16	-2.16
418	BIEBERIT	70.93	-43.67
419	COCO3	-4.69	-9.79
420	CO3ARS8W	0.00	-28.02
421	AS2O5	-5.40	6.70
422	CU3ARS6W	0.00	-35.12
423	NI3ARS8W	0.00	-25.51
424	PB3ARS2	0.00	-35.4
425	ZN3ARS2	0.00	-27.55
426	ARSENOLI	14.33	-2.80
427	CLAUDETI	13.29	-3.06
428	ORPIMENT	82.89	-60.97
429	REALGAR	30.54	-19.75
430	SENARMON	7.32	-10.11
431	VALENTIN	4.54	-8.51
432	SB2O5	0.00	-7.40
433	SB(OH)3	7.20	-4.38
434	STIBNITE	65.19	-1.21
435	CR(OH)3	-22.34	11.96
436	ALASO4W2	0.00	-15.84
437	CA3ASO42	0.00	-18.90
438	FEASO4W2	0.00	-20.25
439	MN3ASO42	0.00	-28.71
440	HYDROZIN	0.00	-73.20

LSPEC

1	1	1	27	0	0	1	68	5	27	0	0
1	2	1	27	0	0	1	69	5	27	0	0
1	3	1	27	0	0	1	70	5	27	0	0
1	4	1	27	0	0	1	71	5	5	0	0
1	5	1	5	0	0	1	72	5	5	0	0
1	6	1	5	0	0	1	73	5	6	0	0
1	7	1	5	0	0	1	74	5	6	0	0
1	8	1	5	0	0	1	75	5	62	0	0
1	9	1	6	0	0	1	76	5	18	0	0
1	10	1	6	0	0	1	77	5	7	0	0
1	11	1	6	0	0	1	78	6	27	0	0
1	12	1	62	0	0	1	79	6	27	0	0
1	13	1	62	0	0	1	80	6	27	0	0
2	14	1	27	5	0	1	81	6	27	0	0
1	15	1	18	0	0	1	82	6	5	0	0
1	16	1	18	0	0	1	83	6	5	0	0
1	17	1	7	0	0	1	84	6	6	0	0
1	18	1	67	0	0	1	85	6	62	0	0
1	19	1	67	0	0	1	86	6	62	0	0
1	20	1	67	0	0	1	87	6	62	0	0
1	21	1	67	0	0	1	88	7	27	0	0
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1	24	2	27	0	0	1	91	7	27	0	0
1	25	2	27	0	0	1	92	7	5	0	0
1	26	2	5	0	0	1	93	7	5	0	0
1	27	2	5	0	0	1	94	7	5	0	0
1	28	2	5	0	0	1	95	7	5	0	0
1	29	2	5	0	0	1	96	7	6	0	0
1	30	2	6	0	0	1	97	7	62	0	0
1	31	2	6	0	0	1	98	7	18	0	0
1	32	2	6	0	0	1	99	7	18	0	0
1	33	2	6	0	0	1	100	7	7	0	0
1	34	2	62	0	0	1	101	7	251	0	0
2	35	2	27	5	0	2	102	7	251	5	0
1	36	2	18	0	0	2	103	7	251	5	0
1	37	2	7	0	0	1	104	7	67	0	0
1	38	2	67	0	0	1	105	8	64	0	0
1	39	2	67	0	0	1	106	8	64	0	0
1	40	3	27	0	0	1	107	8	64	0	0
1	41	3	27	0	0	3	108	8	64	251	72
1	42	3	27	0	0	2	109	8	64	251	0
1	43	3	5	0	0	3	110	8	64	251	72
1	44	3	5	0	0	2	111	9	64	72	0
1	45	3	5	0	0	2	112	9	72	64	0
1	46	3	5	0	0	3	113	9	72	251	64
1	47	3	6	0	0	3	114	9	72	251	64
1	48	3	6	0	0	1	115	10	64	0	0
1	49	3	62	0	0						
1	50	3	62	0	0						
1	51	3	62	0	0						
1	52	3	62	0	0						
1	53	3	18	0	0						
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1	55	3	7	0	0						
1	56	3	67	0	0						
1	57	3	67	0	0						
1	58	4	27	0	0						
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1	62	4	5	0	0						
1	63	4	6	0	0						
1	64	4	62	0	0						
1	65	4	18	0	0						
1	66	4	7	0	0						
1	67	5	27	0	0						

CSPEC

1	+1	-1	-1	0	0
2	+1	-1	-2	0	0
3	+1	-1	-3	0	0
4	+1	-1	-4	0	0
5	+1	-1	-1	0	0
6	+1	-1	-2	0	0
7	+1	-1	-3	0	0
8	+1	-1	-4	0	0
9	1	-1	-1	0	0
10	1	-1	-2	0	0
11	1	-1	-3	0	0
12	1	-1	-1	0	0
13	1	-1	-2	0	0
14	1	-1	-1	-1	0
15	1	-1	-1	0	0
16	1	-1	-3	0	0
17	1	-1	-1	0	0
18	1	-1	-1	0	0
19	1	-1	-2	0	0
20	1	-1	-3	0	0
21	1	-1	-4	0	0
22	1	-1	-1	0	0
23	1	-1	-2	0	0
24	1	-1	-3	0	0
25	1	-1	-4	0	0
26	1	-1	-1	0	0
27	1	-1	-2	0	0
28	1	-1	-3	0	0
29	1	-1	-4	0	0
30	1	-1	-1	0	0
31	1	-1	-2	0	0
32	1	-1	-3	0	0
33	1	-1	-4	0	0
34	1	-1	-1	0	0
35	1	-1	-1	-1	0
36	1	-1	-1	0	0
37	1	-1	-1	0	0
38	1	-1	-2	0	0
39	1	-1	-3	0	0
40	1	-1	-1	0	0
41	1	-1	-2	0	0
42	1	-1	-3	0	0
43	1	-1	-1	0	0
44	1	-1	-2	0	0
45	1	-1	-3	0	0
46	1	-1	-4	0	0
47	1	-1	-1	0	0
48	1	-1	-1	0	0
49	1	-1	-1	0	0
50	1	-1	-2	0	0
51	1	-1	-3	0	0
52	1	-1	-4	0	0
53	1	-1	-1	0	0
54	1	-1	-2	0	0
55	1	-1	-1	0	0
56	1	-1	-2	0	0
57	1	-1	-3	0	0
58	1	-1	-1	0	0
59	1	-1	-2	0	0
60	1	-1	-3	0	0
61	1	-1	-4	0	0
62	1	-1	-1	0	0
63	1	-1	-1	0	0
64	1	-1	-1	0	0
65	1	-1	-1	0	0
66	1	-1	-1	0	0
67	1	-1	-1	0	0
68	1	-1	-2	0	0
69	1	-1	-3	0	0
70	1	-1	-4	0	0
71	1	-1	-1	0	0
72	1	-1	-2	0	0
73	1	-1	-1	0	0
74	1	-1	-2	0	0
75	1	-1	-1	0	0
76	1	-1	-1	0	0
77	1	-1	-1	0	0
78	1	-1	-1	0	0
79	1	-1	-2	0	0
80	1	-1	-3	0	0
81	1	-1	-4	0	0
82	1	-1	-1	0	0
83	1	-1	-2	0	0
84	1	-1	-1	0	0
85	1	-1	-1	0	0
86	1	-1	-2	0	0
87	1	-1	-3	0	0
88	1	-1	-1	0	0
89	1	-1	-2	0	0
90	1	-1	-3	0	0
91	1	-1	-4	0	0
92	1	-1	-1	0	0
93	1	-1	-2	0	0
94	1	-1	-3	0	0
95	1	-1	-4	0	0
96	1	-1	-1	0	0
97	1	-1	-1	0	0
98	1	-1	-1	0	0
99	1	-1	-2	0	0
100	1	-1	-1	0	0
101	1	-1	-1	0	0
102	1	-1	-1	-2	0
103	1	-1	-1	-3	0
104	1	-1	-3	0	0
105	1	-1	-3	0	0
106	1	-1	-2	0	0
107	1	-1	-1	0	0
108	1	-1	-2	-2	1
109	1	-1	-4	-2	0
110	1	-1	-5	-2	1
111	1	-1	-1	+1	0
112	1	-1	-1	1	0
113	1	-1	-2	2	2
114	1	-1	-3	2	3
115	1	-1	1	0	0

LMIN

2	319	126	18	0	0	0
2	320	126	5	0	0	0
3	321	126	5	72	0	0
3	322	126	5	72	0	0
2	323	126	62	0	0	0
3	324	64	126	72	0	0
3	325	64	126	72	0	0
4	326	64	126	72	5	0
4	327	64	126	72	6	0
4	328	64	126	72	6	0
4	329	64	126	72	6	0
3	330	64	126	72	0	0
4	331	72	64	126	24	0
2	332	126	6	0	0	0
3	333	126	6	72	0	0
3	334	126	6	72	0	0
2	335	148	5	0	0	0
2	336	148	18	0	0	0
3	337	148	18	72	0	0
3	338	64	148	72	0	0
3	339	64	148	72	0	0
3	340	64	148	72	0	0
3	341	64	148	72	0	0
3	342	64	148	72	0	0
4	343	64	148	72	5	0
4	344	64	148	72	5	0
4	345	64	148	72	6	0
4	346	64	148	72	6	0
3	347	148	85	72	0	0
3	348	64	148	72	0	0
3	349	64	148	72	0	0
4	350	64	148	6	72	0
3	351	64	148	67	0	0
3	352	64	148	67	0	0
3	353	64	148	67	0	0
4	354	64	72	148	24	0
3	355	64	148	24	0	0
2	356	148	6	0	0	0
3	357	148	6	72	0	0
3	358	148	6	72	0	0
3	359	148	6	72	0	0
2	360	167	5	0	0	0
3	361	167	5	62	0	0
3	362	167	5	18	0	0
2	363	167	18	0	0	0
2	364	167	62	0	0	0
3	365	64	167	72	0	0
3	366	64	167	72	0	0
3	367	64	167	72	0	0
4	368	64	167	18	72	0
4	369	64	167	6	72	0
4	370	64	167	6	72	0
4	371	64	167	6	72	0
2	372	167	47	0	0	0
4	373	64	167	18	72	0
4	374	72	64	167	24	0
3	375	64	167	24	0	0
2	376	167	6	0	0	0
3	377	64	167	67	0	0
4	378	64	251	167	72	0
4	379	64	251	167	72	0
3	380	64	167	72	0	0
4	381	64	167	5	72	0
4	382	64	167	72	5	0
4	383	64	167	18	72	0
3	384	64	167	72	0	0
4	385	64	167	6	72	0
2	386	219	5	0	0	0
2	387	219	18	0	0	0
2	388	219	62	0	0	0
3	389	219	62	72	0	0
3	390	64	219	72	0	0
4	391	64	219	72	7	0
4	392	64	219	72	7	0
4	393	64	219	72	5	0
4	394	64	219	72	6	0
4	395	64	219	72	85	0
4	396	64	219	72	6	0
4	397	64	219	72	6	0
3	398	64	219	72	0	0
4	399	64	219	72	6	0
2	400	219	6	0	0	0
3	401	219	6	72	0	0
4	402	64	219	9	72	0
2	403	196	18	0	0	0
3	404	64	196	72	0	0
4	405	64	196	6	72	0
3	406	64	196	72	0	0
3	407	196	6	72	0	0
3	408	196	6	72	0	0
3	409	64	196	24	0	0
2	410	196	6	0	0	0
3	411	64	186	72	0	0
3	412	64	186	72	0	0
3	413	64	186	72	0	0
3	414	64	186	67	0	0
2	415	186	6	0	0	0
3	416	186	6	72	0	0
3	417	186	6	72	0	0
3	418	186	6	72	0	0
2	419	186	18	0	0	0
3	420	186	237	72	0	0
2	421	72	238	0	0	0
3	422	219	237	72	0	0
3	423	196	237	72	0	0
2	424	167	237	0	0	0
3	425	148	237	72	0	0
2	426	72	243	0	0	0
2	427	72	243	0	0	0
4	428	72	243	67	64	0
5	429	72	243	67	64	251
2	430	72	244	0	0	0
2	431	72	244	0	0	0
2	432	72	247	0	0	0
1	433	244	0	0	0	0
4	434	72	244	67	64	0
3	435	64	208	72	0	0
3	436	51	237	72	0	0
3	437	1	237	72	0	0
3	438	9	237	72	0	0
3	439	101	237	72	0	0
3	440	148	27	18	0	0

CMIN

319.	-1.0	+1.0	+1.0	0.0	0.0	0.0
320.	-1.0	+1.0	+1.0	0.0	0.0	0.0
321.	-1.0	+1.0	+2.0	+1.0	0.0	0.0
322.	-1.0	+1.0	+2.0	+2.5	0.0	0.0
323.	-1.0	+1.0	+2.0	0.0	0.0	0.0
324.	-1.0	-2.0	+1.0	+2.0	0.0	0.0
325.	-1.0	-2.0	+1.0	+2.0	0.0	0.0
326.	-1.0	-1.0	+1.0	+1.0	+1.0	0.0
327.	-1.0	-4.0	+3.0	+4.0	+1.0	0.0
328.	-1.0	-2.0	+3.0	+2.0	+2.0	0.0
329.	-1.0	-6.0	+4.0	+6.0	+1.0	0.0
330.	-1.0	-2.0	+1.0	+1.0	0.0	0.0
331.	-1.0	-1.0	-2.0	+1.0	+1.0	0.0
332.	-1.0	+1.0	+1.0	0.0	0.0	0.0
333.	-1.0	-1.0	+1.0	+1.0	+1.0	0.0
334.	-1.0	+1.0	+1.0	+2.67	0.0	0.0
335.	-1.0	+1.0	+2.00	0.0	0.0	0.0
336.	-1.0	+1.0	+1.0	0.0	0.0	0.0
337.	-1.0	+1.0	+1.0	+1.0	0.0	0.0
338.	-1.0	-2.0	+1.0	+2.0	0.0	0.0
339.	-1.0	-2.0	+1.0	+2.0	0.0	0.0
340.	-1.0	-2.0	+1.0	+2.0	0.0	0.0
341.	-1.0	-2.0	+1.0	+2.0	0.0	0.0
342.	-1.0	-2.0	+1.0	+2.0	0.0	0.0
343.	-1.0	-3.0	+2.0	+3.0	+1.0	0.0
344.	-1.0	-8.0	+5.0	+8.0	+2.0	0.0
345.	-1.0	-2.0	+2.0	+2.0	+1.0	0.0
346.	-1.0	-6.0	+4.0	+6.0	+1.0	0.0
347.	-1.0	+1.0	+2.0	+6.0	0.0	0.0
348.	-1.0	-2.0	+1.0	+1.0	0.0	0.0
349.	-1.0	-2.0	+1.0	+1.0	0.0	0.0
350.	-1.0	-2.0	+3.0	+2.0	+1.0	0.0
351.	-1.0	-1.0	+1.0	+1.0	0.0	0.0
352.	-1.0	-1.0	+1.0	+1.0	0.0	0.0
353.	-1.0	-1.0	+1.0	+1.0	0.0	0.0
354.	-1.0	-2.0	-1.0	+1.0	+1.0	0.0
355.	-1.0	-4.0	+2.0	+1.0	0.0	0.0
356.	-1.0	+1.0	+1.0	0.0	0.0	0.0
357.	-1.0	+1.0	+1.0	+1.0	0.0	0.0
358.	-1.0	+1.0	+1.0	+6.0	0.0	0.0
359.	-1.0	+1.0	+1.0	+7.0	0.0	0.0
360.	-1.0	+1.0	+2.0	0.0	0.0	0.0
361.	-1.0	+1.0	+1.0	+1.0	0.0	0.0
362.	-1.0	+2.0	+2.0	+1.0	0.0	0.0
363.	-1.0	+1.0	+1.0	0.0	0.0	0.0
364.	-1.0	+1.0	+2.0	0.0	0.0	0.0
365.	-1.0	-2.0	+1.0	+1.0	0.0	0.0
366.	-1.0	-2.0	+1.0	+1.0	0.0	0.0
367.	-1.0	-2.0	+1.0	+1.33	0.0	0.0
368.	-1.0	-2.0	+2.0	+1.0	+1.0	0.0
369.	-1.0	-2.0	+2.0	+1.0	+1.0	0.0
370.	-1.0	-4.0	+3.0	+1.0	+2.0	0.0
371.	-1.0	-6.0	+4.0	+1.0	+3.0	0.0
372.	-1.0	+1.0	+1.0	0.0	0.0	0.0
373.	-1.0	-4.0	+3.0	+1.0	+2.0	0.0
374.	-1.0	-1.0	-2.0	+1.0	+1.0	0.0
375.	-1.0	-4.0	+2.0	+1.0	0.0	0.0
376.	-1.0	+1.0	+1.0	0.0	0.0	0.0
377.	-1.0	-1.0	+1.0	+1.0	0.0	0.0
378.	-1.0	-4.0	-2.0	+1.0	+2.0	0.0
379.	-1.0	-6.0	-2.0	+2.0	+3.0	0.0

CMIN (suite)

380.	-1.0	-2.0	+1.0	+2.0	0.0	0.0
381.	-1.0	-1.0	+1.0	+1.0	+1.0	0.0
382.	-1.0	-3.0	+2.0	+3.0	+1.0	0.0
383.	-1.0	-2.0	+3.0	+2.0	+2.0	0.0
384.	-1.0	-4.0	+2.0	+3.0	0.0	0.0
385.	-1.0	-6.0	+4.0	+1.0	+6.0	0.0
386.	-1.0	+1.0	+2.0	0.0	0.0	0.0
387.	-1.0	+1.0	+1.0	0.0	0.0	0.0
388.	-1.0	+1.0	+2.0	0.0	0.0	0.0
389.	-1.0	+1.0	+2.0	+2.0	0.0	0.0
390.	-1.0	-2.0	+1.0	+2.0	0.0	0.0
391.	-1.0	-3.0	+2.0	+2.0	+1.0	0.0
392.	-1.0	-4.0	+3.0	+2.0	+2.0	0.0
393.	-1.0	-3.0	+2.0	+3.0	+1.0	0.0
394.	-1.0	-4.0	+3.0	+4.0	+1.0	0.0
395.	-1.0	-3.0	+2.0	+3.0	+1.0	0.0
396.	-1.0	-6.0	+4.0	+6.0	+1.0	0.0
397.	-1.0	-6.0	+4.0	+7.0	+1.0	0.0
398.	-1.0	-2.0	+1.0	+1.0	0.0	0.0
399.	-1.0	-2.0	+1.0	+1.0	+1.0	0.0
400.	-1.0	+1.0	+1.0	0.0	0.0	0.0
401.	-1.0	+1.0	+1.0	+5.0	0.0	0.0
402.	-1.0	-8.0	+1.0	+2.0	+4.0	0.0
403.	-1.0	+1.0	+1.0	0.0	0.0	0.0
404.	-1.0	-2.0	+1.0	+2.0	0.0	0.0
405.	-1.0	-6.0	+4.0	+1.0	+6.0	0.0
406.	-1.0	-2.0	+1.0	+1.0	0.0	0.0
407.	-1.0	+1.0	+1.0	+6.0	0.0	0.0
408.	-1.0	+1.0	+1.0	+7.0	0.0	0.0
409.	-1.0	-4.0	+2.0	+1.0	0.0	0.0
410.	-1.0	+1.0	+1.0	0.0	0.0	0.0
411.	-1.0	-2.0	+1.0	+1.0	0.0	0.0
412.	-1.0	-2.0	+1.0	+2.0	0.0	0.0
413.	-1.0	-2.0	+1.0	+2.0	0.0	0.0
414.	-1.0	-1.0	+1.0	+1.0	0.0	0.0
415.	-1.0	+1.0	+1.0	0.0	0.0	0.0
416.	-1.0	+1.0	+1.0	+1.0	0.0	0.0
417.	-1.0	+1.0	+1.0	+6.0	0.0	0.0
418.	-1.0	+1.0	+1.0	+7.0	0.0	0.0
419.	-1.0	+1.0	+1.0	0.0	0.0	0.0
420.	-1.0	+3.0	+2.0	+8.0	0.0	0.0
421.	-1.0	-3.0	+2.0	0.0	0.0	0.0
422.	-1.0	+3.0	+2.0	+6.0	0.0	0.0
423.	-1.0	+3.0	+2.0	+8.0	0.0	0.0
424.	-1.0	+3.0	+2.0	0.0	0.0	0.0
425.	-1.0	+3.0	+2.0	+2.50	0.0	0.0
426.	-1.0	-6.0	+4.0	0.0	0.0	0.0
427.	-1.0	-6.0	+4.0	0.0	0.0	0.0
428.	-1.0	-6.0	+2.0	+3.0	+3.0	0.0
429.	-1.0	-3.0	+1.0	+1.0	+2.0	+1.0
430.	-1.0	-3.0	+2.0	0.0	0.0	0.0
431.	-1.0	-3.0	+2.0	0.0	0.0	0.0
432.	-1.0	-5.0	+2.0	0.0	0.0	0.0
433.	-1.0	-1.0	0.0	0.0	0.0	0.0
434.	-1.0	-6.0	+2.0	+3.0	+3.0	0.0
435.	-1.0	-3.0	+1.0	+3.0	0.0	0.0
436.	-1.0	+1.0	+1.0	+2.0	0.0	0.0
437.	-1.0	+3.0	+2.0	+4.0	0.0	0.0
438.	-1.0	+1.0	+1.0	+2.0	0.0	0.0
439.	-1.0	+3.0	+2.0	+8.0	0.0	0.0
440	-1.0	+5.0	+6.0	+2.0	0.0	0.0

SELECTION des DONNEES (logK, ΔH)

pour les ELEMENTS NOUVEAUX

REACTION	kcal $\Delta H°$ 298 K	REFERENCE ΔH	log k à 25° C	REFERENCE log k
$Cd^{2+} + OH^- = CdOH^+$	- 0.25	Baes et Mesmer (1981)	3.92	Baes et Mesmer (1976)
$Cd^{2+} + 2\ OH^- = Cd(OH)_2$	- 1.19	Baes et Mesmer (1981)	7.65	Baes et Mesmer (1976)
$Cd^{2+} + 3\ OH^- = Cd(OH)_3^-$	- 2.18	Baes et Mesmer (1981)	8.70	Baes et Mesmer (1976)
$Cd^{2+} + 4\ OH^- = Cd(OH)_4^{2-}$	- 5.31	Baes et Mesmer (1981)	8.65	Baes et Mesmer (1976)
$Cd^{2+} + Cl^- = CdCl^+$	0.59	NBS (1968-71)	1.98	Smith et Martell (1976)
$Cd^{2+} + 2\ Cl^- = CdCl_2$	1.24	NBS (1968-71)	2.6	Smith et Martell (1976)
$Cd^{2+} + 3\ Cl^- = CdCl_3^-$	3.90	NBS (1968-71)	2.4	Smith et Martell (1976)
$Cd^{2+} + 4\ Cl^- = CdCl_4^{2-}$	9.00	Criaud (1983)	1.47	Smith et Martell (1976)
$Cd^{2+} + SO_4^{2-} = CdSO_4$	1.08	Nordström (1977)	2.45	Smith et Martell (1976)
$Cd^{2+} + 2\ SO_4^{2-} = Cd(SO_4)_2^{2-}$			3.44	Smith et Martell (1976)
$Cd^{2+} + 3\ SO_4^{2-} = Cd(SO_4)_3^{4-}$			3.09	Smith et Martell (1976)
$Cd^{2+} + F^- = CdF^+$	1.2	Smith et Martell (1976)	1.08	Smith et Martell (1976)
$Cd^{2+} + 2\ F^- = CdF_2$	0.5	Smith et Martell (1976)	1.41	Smith et Martell (1976)
$Cd^{2+} + OH^- + Cl^- = CdOHCl$	4.35	NBS (1968-71)	6.6	NBS (1968-71)
$Cd^{2+} + CO_3^{2-} = CdCO_3$	0.13	Fouillac et Criaud 1984)	4.35	Bilinski et al. (1976)
$Cd^{2+} + 3\ CO_3^{2-} = Cd(CO_3)_3^{4-}$			6.22	Naumov et al. (1974)

REACTION	kcal Δ H° 298 K	REFERENCE Δ H	log k à 25° C	REFERENCE log k
$Cd^{2+} + HCO_3^- = CdHCO_3^+$	1.01	Fouillac et Criaud (1984)	2.0	modèle électrostatique
$Cd^{2+} + HS^- = CdHS^+$			10.17	Naumov et al.(1974)
$Cd^{2+} + 2\ HS^- = Cd(HS)_2$			16.53	Naumov et al.(1974)
$Cd^{2+} + 3\ HS^- = Cd(HS)_3^-$			18.71	Naumov et al.(1974)
$Cd^{2+} + 4\ HS^- = Cd(HS)_4^{2-}$			20.90	Naumov et al.(1974)
$Zn^{2+} + OH^- = Zn(OH)^+$	- 0.5	Baes et Mesmer (1981)	5.04	Baes et Mesmer (1976)
$Zn^{2+} + 2\ OH^- = Zn(OH)_2$	- 5.8	Baes et Mesmer (1981)	11.1	Baes et Mesmer (1976)
$Zn^{2+} + 3\ OH^- = Zn(OH)_3^-$	- 10.6	Baes et Mesmer (1981)	13.6	Baes et Mesmer (1976)
$Zn^{2+} + 4\ OH^- = Zn(OH)_4^{2-}$	- 12.5	Baes et Mesmer (1981)	14.8	Baes et Mesmer (1976)
$Zn^{2+} + Cl^- = ZnCl^+$	7.79	Helgeson (1969)	0.49	Smith et Martell (1976)
$Zn^{2+} + 2\ Cl^- = ZnCl_2$	8.50	Helgeson (1969)	0.62	Smith et Martell (1976)
$Zn^{2+} + 3\ Cl^- = ZnCl_3^-$	9.56	Helgeson (1969)	0.51	Smith et Martell (1976)
$Zn^{2+} + 4\ Cl^- = ZnCl_4^{2-}$	10.96	Helgeson (1969)	0.2	Smith et Martell (1976)
$Zn^{2+} + SO_4^{2-} = ZnSO_4$	1.36	Christensen et al. (1975)	2.36	Helgeson (1969)
$Zn^{2+} + 2\ SO_4^{2-} = Zn(SO_4)_2^{2-}$			3.63	Smith et Martell (1976)
$Zn^{2+} + 3\ SO_4^{2-} = Zn(SO_4)_3^{4-}$			2.70	Smith et Martell (1976)
$Zn^{2+} + 4\ SO_4^{2-} = Zn(SO_4)_4^{6-}$			- 0.82	Smith et Martell (1976)

REACTION	kcal Δ H° 298 K	REFERENCE Δ H	log k à 25° C	REFERENCE log k
$Zn^{2+} + F^- = ZnF^+$	3.8	Smith et Martell (1976)	1.15	Smith et Martell (1976)
$Zn^{2+} + OH^- + Cl^- = ZnOHCl$			6.52	NBS (1968-71)
$Zn^{2+} + CO_3^{2-} = ZnCO_3$	- 0.09	Fouillac et Criaud (1984)	4.80	Bilinski et al. (1976)
$Zn^{2+} + HCO_3^- = ZnHCO_3^+$	1.03	Fouillac et Criaud (1984)	2.2	Fouillac et Criaud (1984)
$Zn^{2+} + 2\ HS^- = Zn(HS)_2$			14.94	Naumov et al. (1974)
$Zn^{2+} + 3\ HS^- = Zn(HS)_3^-$			16.10	Naumov et al. (1974)
$Pb^{2+} + OH^- = PbOH^+$	- 2.6	Baes et Mesmer (1981)	6.29	Baes et Mesmer (1976)
$Pb^{2+} + 2\ OH^- = Pb(OH)_2$	- 8.5	Baes et Mesmer (1981)	10.88	Baes et Mesmer (1976)
$Pb^{2+} + 3\ OH^- = Pb(OH)_3^-$	- 12.7	Baes et Mesmer (1981)	13.94	Baes et Mesmer (1976)
$Pb^{2+} + Cl^- = PbCl^+$	4.38	Christensen et al. (1975)	1.58	Smith et Martell (1976)
$Pb^{2+} + 2\ Cl^- = PbCl_2$	1.08	Helgeson (1969)	1.82	Smith et Martell (1976)
$Pb^{2+} + 3\ Cl^- = PbCl_3^-$	2.17	Helgeson (1969)	1.71	Smith et Martell (1976)
$Pb^{2+} + 4\ Cl^- = PbCl_4^{2-}$	3.53	Helgeson (1969)	1.40	Smith et Martell (1976)
$Pb^{2+} + SO_4^{2-} = PbSO_4$	0.26	Criaud (1983)	2.75	Smith et Martell (1976)
$Pb^{2+} + 2\ SO_4^{2-} = Pb(SO_4)_2^{2-}$			4.51	Smith et Martell (1976)
$Pb^{2+} + F^- = PbF^+$	0.84	Criaud (1983)	2.06	Smith et Martell (1976)

REACTION	kcal Δ H° 298 K	REFERENCE Δ H	log k à 25° C	REFERENCE log k
$Pb^{2+} + 2\ F^- = PbF_2$			3.42	Smith et Martell (1976)
$Pb^{2+} + 3\ F^- = PbF_3^-$			3.42	Smith et Martell (1964)
$Pb^{2+} + 4\ F^- = PbF_4^{2-}$			3.10	Smith et Martell (1964)
$Pb^{2+} + CO_3^{2-} = PbCO_3$	- 4.1	Fouillac et Criaud (1984)	7.20	Hem (1976)
$Pb^{2+} + 2\ CO_3^{2-} = Pb(CO_3)_2^{2-}$			10.64	Hem (1976)
$Pb^{2+} + HCO_3^- = PbHCO_3^+$	0.87	Fouillac et Criaud (1984)	1.9	Fouillac et Criaud (1984)
$Pb^{2+} + 2\ HS^- = Pb(HS)_2$			15.27	Naumov et al. (1974)
$Pb^{2+} + 3\ HS^- = Pb(HS)_3^-$			16.57	Naumov et al. (1974)
$Co^{2+} + OH^- = CoOH^+$	0.10	Baes et Mesmer (1981)	4.35	Baes et Mesmer (1976)
$Co^{2+} + 2\ OH^- = Co(OH)_2$	- 2.0	Baes et Mesmer (1981)	9.20	Baes et Mesmer (1976)
$Co^{2+} + 3\ OH^- = Co(OH)_3^-$	- 3.33	Baes et Mesmer (1981)	10.50	Baes et Mesmer (1976)
$Co^{2+} + 4\ OH^- = Co(OH)_4^{2-}$	- 5.44	Baes et Mesmer (1981)	9.70	Baes et Mesmer (1976)
$Co^{2+} + Cl^- = CoCl^+$	0.52	Naumov et al. (1974)	0.57	Smith et Martell (1976)
$Co^{2+} + SO_4^{2-} = CoSO_4$	0.50	Naumov et al. (1974)	2.36	Smith et Martell (1976)
$Co^{2+} + F^- = CoF^+$	4.14	Criaud (1983)	1.02	Smith et Martell (1976)
$Co^{2+} + CO_3^{2-} = CoCO_3$	- 0.22	Fouillac et Criaud (1984)	4.90	Fouillac et Criaud (1984)
$Co^{2+} + HCO_3^- = CoHCO_3^+$	1.03	Fouillac et Criaud (1984)	2.2	Fouillac et Criaud (1984)

REACTION	kcal Δ H° 298 K	REFERENCE Δ H	log k à 25° C	REFERENCE log k
$Ni^{2+} + OH^- = NiOH^+$	0.4	Baes et Mesmer (1981)	4.14	Baes et Mesmer (1976)
$Ni^{2+} + 2\ OH^- = Ni(OH)_2$	- 4.2	Baes et Mesmer (1981)	9.00	Baes et Mesmer (1976)
$Ni^{2+} + 3\ OH^- = Ni(OH)_3^-$	- 15.1	Baes et Mesmer (1981)	12.00	Baes et Mesmer (1976)
$Ni^{2+} + 4\ OH^- = Ni(OH)_4^{2-}$	- 28.2	Baes et Mesmer (1981)	12.00	Baes et Mesmer (1976)
$Ni^{2+} + Cl^- = NiCl^+$	0.5	Smith et Martell (1976)	0.72	Smith et Martell (1976)
$Ni^{2+} + 2\ Cl^- = NiCl_2^\circ$			0.96	Mattigod et Sposito (1977)
$Ni^{2+} + SO_4^{2-} = NiSO_4$	1.52	Christensen (1975)	2.29	Smith et Martell (1976)
$Ni^{2+} + 2\ SO_4^{2-} = Ni(SO_4)_2^{2-}$			3.20	Smith et Martell (1976)
$Ni^{2+} + F^- = NiF^+$	4.06	Criaud (1983)	1.12	Smith et Martell (1976)
$Ni^{2+} + CO_3^{2-} = NiCO_3$	- 0.77	Fouillac et Criaud (1984)	5.37	Fouillac et Criaud (1984)
$Ni^{2+} + HCO_3^- = NiHCO_3^+$	1.10	Fouillac et Criaud (1984)	2.2	Fouillac et Criaud (1984)
$Cr^{3+} + OH^- = CrOH^{2+}$	- 3.65	Baes et Mesmer (1981)	10.00	Baes et Mesmer (1976)
$Cr^{3+} + 2\ OH^- = Cr(OH)_2^+$	- 7.17	Baes et Mesmer (1981)	18.30	Baes et Mesmer (1976)
$Cr^{3+} + 3\ OH^- = Cr(OH)_3^\circ$	- 10.84	Baes et Mesmer (1981)	24.00	Baes et Mesmer (1976)
$Cr^{3+} + 4\ OH^- = Cr(OH)_4^-$	- 15.84	Baes et Mesmer (1981)	28.60	Baes et Mesmer (1976)
$Cr^{3+} + Cl^- = CrCl^{2+}$			0.62	Naumov et al.(1974)
$Cr^{3+} + 2\ Cl^- = CrCl_2^+$	0.0	Naumov et al.(1974)	0.11	Naumov et al. (1974)

REACTION	kcal Δ H° 298 K	REFERENCE Δ H	log k à 25° C	REFERENCE log k
$Cr^{3+} + SO_4^{2-} = CrSO_4^+$	2.66	Criaud (1983)	4.61	Smith et Martell (1976)
$Cr^{3+} + F^- = CrF^{2+}$	1.41	Criaud (1983)	5.21	Smith et Martell (1976)
$Cr^{3+} + 2\ F^- = CrF^{2+}$			9.31	Smith et Martell (1976)
$Cr^{3+} + 3\ F^- = CrF_3$			11.91	Smith et Martell (1976)
$Cu^{2+} + OH^- = CuOH^+$	- 1.35	Baes et Mesmer (1981)	6.0	Baes et Mesmer (1976)
$Cu^{2+} + 2\ OH^- = Cu(OH)_2$	- 3.60	Baes et Mesmer (1981)	10.7	Baes et Mesmer (1976)
$Cu^{2+} + 3\ OH^- = Cu(OH)_3^-$	- 7.92	Baes et Mesmer (1981)	14.2	Baes et Mesmer (1976)
$Cu^{2+} + 4\ OH^- = Cu(OH)_4^{2-}$	- 14.11	Baes et Mesmer (1981)	16.4	Baes et Mesmer (1976)
$Cu^{2+} + Cl^- = CuCl^+$	8.65	Helgeson (1969)	0.02	Helgeson (1969)
$Cu^{2+} + 2\ Cl^- = CuCl_2$	10.56	Helgeson (1969)	- 0.71	Helgeson (1969)
$Cu^{2+} + 3\ Cl^- = CuCl_3^-$	13.69	Helgeson (1969)	- 2.29	Helgeson (1969)
$Cu^{2+} + 4\ Cl^- = CuCl_4^{2-}$	17.78	Helgeson (1969)	- 4.59	Helgeson (1969)
$Cu^{2+} + SO_4^{2-} = CuSO_4$	1.22	Nordström (1977)	2.31	Nordström (1977)
$Cu^{2+} + F^- = CuF^+$	1.62	NBS (1968-71)	1.52	Smith et Martell (1976)
$Cu^{2+} + CO_3^{2-} = CuCO_3$	- 2.70	Fouillac et Criaud (1984)	6.75	Schindler et al. (1968)
$Cu^{2+} + 2\ CO_3^{2-} = Cu(CO_3)_2^{2-}$			10.69	Smith et Martell (1976)

REACTION	kcal ΔH° 298 K	REFERENCE Δ H	log k à 25° C	REFERENCE log k
$Cu^{2+} + HCO_3^- = CuHCO_3^+$	1.06	Fouillac et Criaud (1984)	2.2	Fouillac et Criaud (1984)
$Cu^{2+} + e^- = Cu^+$	1.65	NBS (1968-71)	2.72	NBS (1968-71)
$Cu^{2+} + 2\ Cl^- + e^- = CuCl_2^-$	1.23	NBS (1968-71)	8.22	Smith et Martell (1976)
$Cu^{2+} + 3\ Cl^- + e^- = CuCl_3^{2-}$	1.91	NBS (1968-71)	8.42	Smith et Martell (1976)
$Cu^{2+} + 3\ HS^- = Cu(HS)_3^-$			25.9	
$AsO_4^{3-} + 3\ H^+ = AsO(OH)_3^\circ$	- 3.43	NBS (1968-71)	20.68	Baes et Mesmer (1976)
$AsO_4^{3-} + 2\ H^+ = AsO_2(OH)_2^-$	- 5.12	NBS (1968-71)	18.44	Baes et Mesmer (1976)
$AsO_4^{3-} + 3\ H^+ = AsO_3(OH)^{2-}$	- 4.35	NBS (1968-71)	11.5	Baes et Mesmer (1976)
$AsO_4^{3-} + 2\ H^+ + 2e^- = AsO_3^{3-} + H_2O$	- 13.19	NBS (1968-71) Naumov et al.(1974)	5.4	NBS (1968-71)
$AsO_4^{3-} + 4\ H^+ + 2e^- = As(OH)_4^-$	- 28.86	Baes et Mesmer (1976) NBS (1968-71)	30.9	Baes et Mesmer (1976)
$AsO_4^{3-} + 5\ H^+ + 2e^- = As(OH)_3^\circ + H_2O$	- 33.44	NBS (1968-71) Naumov et al. (1974)	40.15	Baes et Mesmer (1976)
$Sb(OH)_3^\circ + H^+ = Sb(OH)_2^+ + H_2O$	- 5.1	Baes et Mesmer (1981)	1.42	Baes et Mesmer (1976)
$Sb(OH)_3 + H_2O = Sb(OH)_4^- + H^+$	15.9	Baes et Mesmer (1981)	- 11.82	Baes et Mesmer (1976)
$Sb(OH)_3 + 2\ H_2O = Sb(OH)_5 + 2e^- + 2\ H^+$			- 28.58	Naumov et al.(1974) Baes et Mesmer (1976)

REACTION	kcal ΔH° 298 K	REFERENCE Δ H	log k à 25° C	REFERENCE log k
$Sb(OH)_3 + 3\ H_2O = Sb(OH)_6^- + 2e^- + 3\ H^+$			- 31.3	Baes et Mesmer (1976)
$Ge(OH)_4 = H^+ + GeO(OH)_3^-$			- 9.31	Baes et Mesmer (1976)
$Fe^{2+} + 2\ HS^- = Fe(HS)_2$			8.95	Naumov et al. (1974)
$Fe^{2+} + 3\ HS^- = Fe(HS)_3^-$			10.99	Naumov et al. (1974)
$Fe^{2+} + 2\ SO_4^{2-} = Fe(SO_4)_2^-$	4.60	Nordström (1977)	5.42	Nordström (1977)
$Fe^{2+} + 2\ F^- = FeF_2^+$	4.80	Nordström et Jenne (1977)	10.80	Nordström et Jenne (1977)
$Fe^{2+} + 3\ F^- = FeF_3$	5.4	Nordström et Jenne (1977)	14.0	Nordström et Jenne (1977)
$Fe^{3+} + F^- = FeF^{2+}$	2.7	Nordström et Jenne (1977)	6.2	Nordström et Jenne (1977)
$Fe^{2+} + CO_3^{2-} = FeCO_3$	- 0,07	Fouillac et Criaud (1984)	4.73	Fouillac et Criaud (1984)
$Fe^{2+} + HCO_3^- = FeHCO_3^+$	1.04	Fouillac et Criaud (1984)	2.17	Fouillac et Criaud (1984)
$Mn^{2+} + CO_3^{2-} = MnCO_3$	0.45	Fouillac et Criaud (1984)	4.32	Fouillac et Criaud (1984)
$Na^+ + F^- = NaF$			- 0.95	Richardson (1979)

	REACTION	ΔH en kcal	log K 25° C	
OTAVITE	$CdCO_3 = Cd^{2+} + CO_3^{2-}$	- 0.58	- 13.74	
$CdCl_2$	$CdCl_2 = Cd^{2+} + 2\ Cl^-$	- 4.47	- 0.68	
$CdCl_2 . H_2O$	$CdCl_2 . H_2O = Cd^{2+} + 2\ Cl^- + H_2O$	- 1.82	- 1.71	
$CdCl_2 . \frac{5}{2} H_2O$	$CdCl_2 . \frac{5}{2} H_2O = Cd^{2+} + 2\ Cl^- + \frac{5}{2} H_2O$	1.71	- 1.94	
CdF_2	$CdF_2 = Cd^{2+} + 2\ F^-$	- 9.72	- 2.98	
$Cd(OH)_2$ A	$Cd(OH)_2 am + 2\ H^+ = Cd^{2+} + 2\ H_2O$	- 20.77	13.73	
$Cd(OH)_2$ C	$Cd(OH)_2 cryst + 2\ H^+ = Cd^{2+} + 2\ H_2O$		13.65	
CdOHCl	$CdOHCl + H^+ = Cd^{2+} + H_2O + Cl^-$	- 7.407	3.52	
$Cd_3(OH)_4SO_4$	$Cd_3(OH)_4SO_4 + 4\ H^+ = 3\ Cd^{2+} + 4\ H_2O + SO_4^{2-}$		22.56	
$Cd_3(OH)_2(SO_4)_2$	$Cd_3(OH)_2(SO_4)_2 + 2\ H^+ = 3\ Cd^{2+} + 2\ H_2O + 2\ SO_4^{2-}$		6.71	
$Cd_4(OH)_6SO_4$	$Cd_4(OH)_6(SO_4) + 6\ H^+ = 4\ Cd^{2+} + 6\ H_2O + SO_4^{2-}$		28.4	
MONTEPONITE	$CdO + 2\ H^+ = Cd^{2+} + H_2O$	- 24.76	15.12	
$CdSiO_3$	$CdSiO_3 + H_2O + 2\ H^+ = Cd^{2+} + H_4SiO_4$	- 16.63	9.06	
$CdSO_4$	$CdSO_4 = Cd^{2+} + SO_4^{2-}$	- 14.74	- 0.10	

	REACTION	ΔH en kcal	log k 25° C	
$CdSO_4 \cdot H_2O$	$CdSO_4 \cdot H_2O = Cd^{2+} + SO_4^{2-} + H_2O$	- 7.52	- 1.66	
$CdSO_4 \cdot \frac{8}{3} H_2O$	$CdSO_4 \cdot \frac{8}{3} H_2O = Cd^{2+} + SO_4^{2-} + \frac{8}{3} H_2O$	- 4.30	- 1.87	
$ZnCl_2$	$ZnCl_2 = Zn^{2+} + 2\,Cl^-$	- 17.48	7.03	
SMITHSONITE	$ZnCO_3 = Zn^{2+} + CO_3^{2-}$	- 4.36	- 10.00	
$ZnCO_3 \cdot H_2O$	$ZnCO_3 \cdot H_2O = Zn^{2+} + CO_3^{2-} + H_2O$		- 10.26	
$Zn(OH)_2$ A	$Zn(OH)_2 am + 2\,H^+ = Zn^{2+} + 2\,H_2O$		12.45	
$Zn(OH)_2$ C	$Zn(OH)_2 cryst + 2\,H^+ = Zn^{2+} + 2\,H_2O$		12.20	
$Zn(OH)_2$ β	$Zn(OH)_2 \beta + 2\,H^+ = Zn^{2+} + 2\,H_2O$		11.75	
$Zn(OH)_2$ γ	$Zn(OH)_2 \gamma + 2\,H^+ = Zn^{2+} + 2\,H_2O$		11.71	
$Zn(OH)_2$ ε	$Zn(OH)_2 \varepsilon + 2\,H^+ = Zn^{2+} + 2\,H_2O$		11.50	
$Zn_2(OH)_3Cl$	$Zn_2(OH)_3Cl + 3\,H^+ = 2\,Zn^{2+} + 3\,H_2O + Cl^-$		15.2	
$Zn_5(OH)_8Cl_2$	$Zn_5(OH)_8Cl_2 + 8\,H^+ = 5\,Zn^{2+} + 8\,H_2O + 2\,Cl^-$		38.5	
$Zn_2(OH)_2SO_4$	$Zn_2(OH)_2SO_4 + 2\,H^+ = 2\,Zn^{2+} + 2\,H_2O + SO_4^{2-}$		7.5	
$Zn_4(OH)_6SO_4$	$Zn_4(OH)_6SO_4 + 6\,H^+ = 4\,Zn^{2+} + 6\,H_2O + SO_4^{2-}$		28.4	

	REACTION	ΔH en kcal	log k 25° C	
$Zn(NO_3)_2\ 6\ H_2O$	$Zn(NO_3)_2 . 6\ H_2O = Zn^{2+} + 2\ NO_3^- + 6\ H_2O$	5.51	3.44	
ZnO active	$ZnO + 2\ H^+ = Zn^{2+} + H_2O$		11.31	
ZnO cryst	$ZnO + 2\ H^+ = Zn^{2+} + H_2O$	- 21.86	11.14	
$Zn_3O(SO_4)_2$	$ZnO . 2\ ZnSO_4 + 2\ H^+ = 3\ Zn^{2+} + 2SO_4^{2-} + H_2O$	- 62.0	19.02	
ZnS A	ZnS amorphe $+ H^+ = Zn^{2+} + HS^-$	3.67	- 9.052	
SPHALERITE	$ZnS + H^+ = Zn^{2+} + HS^-$	8.25	- 11.618	
WURTZITE	$ZnS + H^+ = Zn^{2+} + HS^-$	5.06	- 9.682	
$ZnSiO_3$	$ZnSiO_3 + 2\ H^+ + H_2O = Zn^{2+} + H_4SiO_4$	- 18.27	2.93	
WILLEMITE	$Zn_2SiO_4 + 4\ H^+ = 2\ Zn^{2+} + H_4SiO_4$	- 33.37	15.33	
ZINCOSITE	$ZnSO_4 = Zn^{2+} + SO_4^{2-}$	- 19.2	3.01	
$ZnSO^\circ_4 . H_2O$	$ZnSO_4 . H_2O = Zn^{2+} + SO_4^{2-} + H_2O$	- 10.64	- 0.57	
BIANCHITE	$ZnSO_4 . 6\ H_2O = Zn^{2+} + SO_4^{2-} + 6\ H_2O$	- 0.16	- 1.765	
GOSLARITE	$ZnSO_4 . 7\ H_2O = Zn^{2+} + SO_4^{2-} + 7\ H_2O$	3.3	- 1.96	
HYDROZINCITE	$Zn_5(OH)_6(CO_3)_2 = 5\ Zn^{2+} + 6\ OH^- + 2\ CO_3^{2-}$		- 73.2	

	REACTION	ΔH en kcal	log k 25° C	
COTUNNITE	$PbCl_2 = Pb^{2+} + 2\,Cl^-$	5.6	- 4.77	
MATLOCKITE	$PbClF = Pb^{2+} + Cl^- + F^-$	7.95	- 9.43	
PHOSGENITE	$PbCl_2 \cdot PbCO_3 = 2\,Pb^{2+} + 2\,Cl^- + CO_3^{2-}$		- 19.81	
CERRUSITE	$PbCO_3 = Pb^{2+} + CO_3^{2-}$	4.86	- 13.13	
PbF_2	$PbF_2 = Pb^{2+} + 2\,F^-$	- 0.7	- 7.44	
MASSICOT	$PbO + 2\,H^+ = Pb^{2+} + H_2O$	- 16.78	12.91	
LITHARGE	$PbO + 2\,H^+ = Pb^{2+} + H_2O$	- 16.38	12.72	
$PbO \cdot \frac{1}{3} H_2O$	$PbO \cdot \frac{1}{3} H_2O + 2\,H^+ = Pb^{2+} + \frac{4}{3} H_2O$		12.98	
Pb_2OCO_3	$PbO \cdot PbCO_3 + 2\,H^+ = 2\,Pb^{2+} + CO_3^{2-} + H_2O$	- 11.46	- 0.5	
LARNAKITE	$PbO \cdot PbSO_4 + 2\,H^+ = 2\,Pb^{2+} + SO_4^{2-} + H_2O$	- 6.44	- 0.28	
$Pb_3O_2SO_4$	$2\,PbO \cdot PbSO_4 + 4\,H^+ = 3\,Pb^{2+} + SO_4^{2-} + 2\,H_2O$	- 20.75	10.4	
$Pb_4O_3SO_4$	$3\,PbO \cdot PbSO_4 + 6\,H^+ = 4\,Pb^{2+} + SO_4^{2-} + 3\,H_2O$	- 35.07	22.1	
$PbHPO_4$	$PbHPO_4 = Pb^{2+} + HPO_4^{2-}$	7.04	- 11.46	
$Pb_3O_2CO_3$	$2\,PbO \cdot PbCO_3 + 4\,H^+ = 3\,Pb^{2+} + CO_3^{2-} + 2\,H_2O$	- 26.43	11.02	

	REACTION	ΔH en kcal	log k 25° C	
$PbSiO_3$	$PbSiO_3 + H_2O + 2H^+ = Pb^{2+} + H_4SiO_4$	- 9.26	7.32	
Pb_2SiO_4	$Pb_2SiO_4 + 4H^+ = 2Pb^{2+} + H_4SiO_4$	- 26.0	19.76	
ANGLESITE	$PbSO_4 = Pb^{2+} + SO_4^{2-}$	2.15	- 7.79	
GALENE	$PbS + H^+ = Pb^{2+} + HS^-$	19.4	- 15.132	
PLATTNERITE	$PbO_2 + 4H^+ + 2e^- = Pb^{2+} + 2H_2O$	- 70.73	49.3	
Pb_2O_3	$Pb_2O_3 + 6H^+ + 2e^- = 2Pb^{2+} + 3H_2O$		61.04	
$Pb(HO)_2$	$Pb(OH)_2 + 2H^+ = Pb^{2+} + 2H_2O$	- 13.99	8.15	
LAURIONITE	$PbOHCl + H^+ = Pb^{2+} + Cl^- + H_2O$		0.623	
$Pb_2(OH)_3Cl$	$Pb_2(OH)_3Cl + 3H^+ = 2Pb^{2+} + 3H_2O + Cl^-$		8.79	
HYDROCERRUSITE	$2PbCO_3 . Pb(OH)_2 + 2H^+ = 3Pb^{2+} + 2CO_3^{2-} + 2H_2O$		- 17.46	
$Pb_2O . (OH)_2$	$PbO . Pb(OH)_2 + 4H^+ = 2Pb^{2+} + 3H_2O$		26.2	
$Pb_4(OH)_6SO_4$	$Pb_4(OH)_6SO_4 + 6H^+ = 4Pb^{2+} + SO_4^{2-} + 6H_2O$		21.1	
MELANOTHALLITE	$CuCl_2 = Cu^{2+} + 2Cl$	- 12.32	3.73	
$CuCO_3$	$CuCO_3 = Cu^{2+} + CO_3^{2-}$		- 9.63	
CuF_2	$CuF_2 = Cu^{2+} + 2F^-$	- 13.32	- 0.62	

	REACTION	ΔH en kcal	log k 25° C	
$CuF_2 . 2 H_2O$	$CuF_2 . 2 H_2O = Cu^{2+} + 2 F^- + 2 H_2O$	- 3.65	- 4.55	
$Cu(OH)_2$	$Cu(OH)_2 + 2 H^+ = Cu^{2+} + 2 H_2O$	- 15.25	8.64	
MALACHITE	$Cu_2(OH)_2CO_3 + 3 H^+ = 2 Cu^{2+} + 2 H_2O + HCO_3^-$	- 19.76	5.15	
AZURITE	$Cu_3(OH)_2(CO_3)_2 + 4 H^+ = 3 Cu^{2+} + 2 H_2O + 2 HCO_3^-$	- 30.87	3.75	
ATACAMITE	$Cu_2(OH)_3Cl + 3 H^+ = 2 Cu^{2+} + 3 H_2O + Cl^-$	- 18.69	7.34	
ANTLERITE	$Cu_3(OH)_4SO_4 + 4 H^+ = 3 Cu^{2+} + 4 H_2O + SO_4^{2-}$	-	8.29	
$Cu_2(OH)_3NO_3$	$Cu_2(OH)_3NO_3 + 3 H^+ = 2 Cu^{2+} + 3 H_2O + NO_3^-$	- 17.35	9.24	
BROCHANTITE	$Cu_4(OH)_6SO_4 + 6 H^+ = 4 Cu^{2+} + 6 H_2O + SO_4^{2-}$		15.34	
LANGETITE	$Cu_4(OH)_6SO_4 . H_2O + 6 H^+ = 4 Cu^{2+} + 7 H_2O + SO_4^{2-}$	- 39.61	16.79	
TENDRITE	$CuO + 2 H^+ = Cu^{2+} + H_2O$	- 15.24	7.62	
Cu_2OSO_4	$CuO . CuSO_4 + 2 H^+ = Cu^{2+} + H_2O + SO_4^{2-}$	- 35.57	11.53	
$CuSO_4$	$CuSO_4 = Cu^{2+} + SO_4^{2-}$	- 18.14	3.01	
CHALCANTHITE	$CuSO_4 . 5 H_2O = Cu^{2+} + SO_4^{2-} + 5 H_2O$	1.44	- 4.64	
CUPRIC FERRITE	$CuFe_2O_4 + 8 H^+ = Cu^{2+} + 2 Fe^{3+} + 4 H_2O$	- 38.69	5.88	

	REACTION	ΔH en kcal	log k 25° C	
$NiCO_3$	$NiCO_3 = Ni^{2+} + CO_3^{2-}$	- 9.94	- 6.84	*
$Ni(OH)_2$	$Ni(OH)_2 + 2\,H^+ = Ni^{2+} + 2\,H_2O$	- 20.2	10.8	
$Ni_4(OH)_6SO_4$	$Ni_4(OH)_6SO_4 + 6\,H^+ = 4\,Ni^{2+} + SO_4^{2-} + 6\,H_2O$		32	
BUNSENITE	$NiO + 2\,H^+ = Ni^{2+} + H_2O$	- 23.92	12.45	
RETGERSITE	$NiSO_4 . 6\,H_2O = Ni^{2+} + SO_4^{2-} + 6\,H_2O$	1.1	- 2.04	
MORENOSITE	$NiSO_4 . 7\,H_2O = Ni^{2+} + SO_4^{2-} + 7\,H_2O$	2.94	- 2.36	
Ni_2SiO_4	$Ni_2SiO_4 + 4\,H^+ = 2\,Ni^{2+} + H_4SiO_4$	- 33.36	14.54	
$NiSO_4$	$NiSO_4 = Ni^{2+} + SO_4^{2-}$	- 21.48	4.48	*
CoO	$CoO + 2\,H^+ = Co^{2+} + H_2O$	- 25.21	13.64	*
$Co(OH)_2$	$Co(OH)_2 + 2\,H^+ = Co^{2+} + 2\,H_2O$	- 21.2	13.12	*
TRANSVAALITE	$Co(OH)_2 + 2\,H^+ = Co^{2+} + 2\,H_2O$		12.35	*
JAIPURITE	$CoS\,\beta + H^+ = Co^{2+} + HS^-$	1.6	7.05	*
$CoSO_4$	$CoSO_4 = Co^{2+} + SO_4^{2-}$	- 18.76	2.83	*
$CoSO_4 . H_2O$	$CoSO_4 . H_2O = Co^{2+} + SO_4^{2-} + H_2O$	- 12.65	- 1.01	*

	REACTION	ΔH en kcal	log k 25° C	
$CoSO_4 . 6 H_2O$	$CoSO_4 . 6 H_2O = CO^{2+} + SO_4^{2-} + 6 H_2O$	0.16	- 2.16	*
BIEBERITE	$CoSO_4 . 7 H_2O = CO^{2+} + SO_4^{2-} + 7 H_2O$	70.93	- 43.67	*
$CoCO_3$	$CoCO_3 = Co^{2+} + CO_3^{2-}$	- 4.69	- 9.79	*
$Co_3(AsO_4)_2 . 8 H_2O$	$Co_3(AsO_4)_2 . 8 H_2O = 3 Co^{2+} + 2 AsO_4^{3-} + 8 H_2O$		- 28.02	*
As_2O_5	$As_2O_5 + 3 H_2O = 2 H_3AsO_4°$	- 5.4	6.70	
$Al(AsO_4) . 2H_2O$	$Al(AsO_4) . 2 H_2O = Al^{3+} + AsO_4^{3-} + 2 H_2O$		- 15.84	*
$Ca_3(AsO_4)_2 . 4 H_2O$	$Ca_3(AsO_4)_2 . 4 H_2O = 3 Ca^{2+} + 2 AsO_4^{3-} + 4 H_2O$		- 18.90	*
$Cu_3(AsO_4)_2 . 6 H_2O$	$Cu_3(AsO_4)_2 . 6 H_2O = 3 Cu^{2+} + 2 AsO_4^{3-} + 6 H_2O$		- 35.12	*
$FeAsO_4 . 2 H_2O$	$FeAsO_4 . 2 H_2O = Fe^{3+} + AsO_4^{3-} + 2 H_2O$		- 20.25	*
$Mn_3(AsO_4)_2 . 8 H_2O$	$Mn_3(AsO_4)_2 . 8 H_2O = 3 Mn^{2+} + 2 AsO_4^{3-} + 8 H_2O$		- 28.71	*
ANNABERGITE	$Ni_3(AsO_4)_2 . 8 H_2O = 3 Ni^{2+} + 2 AsO_4^{3-} + 8 H_2O$		- 25.51	*
$Pb_3(AsO_4)_2$	$Pb_3(AsO_4)_2 = 3 Pb^{2+} + 2 AsO_4^{3-}$		- 35.40	*
LEGRANDITE	$Zn_3(AsO_4)_2 . \frac{5}{2} H_2O = 3 Zn^{2+} + 2 AsO_4^{3-} + \frac{5}{2} H_2O$		- 27.55	*
ARSENOLITE	$As_4O_6 + 6 H_2O = 4 H_3AsO_3°$	14.33	- 2.80	

	REACTION	ΔH en kcal	log k 25° C	
CLAUDETITE	$As_4O_6 + 6\ H_2O = 4\ H_3AsO_3^\circ$	13.29	- 3.06	
ORPIMENT	$As_2S_3 + 6\ H_2O = 2\ H_3AsO_3^\circ + 3\ HS^- + 3\ H^+$	82.29	- 60.97	
REALGAR	$AsS + 3\ H_2O = H_3AsO_3^\circ + HS^- + 2\ H^+ + e^-$	30.54	- 19.75	
$Cr(OH)_3$	$Cr(OH)_3 + 3\ H^+ = Cr^{3+} + 3\ H_2O$	- 22.34	11.96	**
SENARMONTITE	$Sb_2O_3 + 3\ H_2O = 2\ Sb(OH)_3^\circ$	7.32	- 10.11	*
VALENTINITE	$Sb_2O_3 + 3\ H_2O = 2\ Sb(OH)_3^\circ$	4.54	- 8.51	**
Sb_2O_5	$Sb_2O_5 + 5\ H_2O = 2\ Sb(OH)_5^\circ$		- 7.4	**
$Sb(OH)_3$	$Sb(OH)_3 = Sb(OH)_3$	7.2	- 4.38	*
STIBNITE	$Sb_2S_3 + 6\ H_2O = 2\ Sb(OH)_3^\circ + 3\ HS^- + 3\ H^+$	65.19	- 1.21	**

Les références sont celles de Wateq 2 (1980) sauf indiqué :

* Naumov et al.(1974)

** Robie et al.(1978)

EXEMPLE 1 :

EAU de MER

Test eau de mer d'apres Nordstrom et al(1979)

****
* SOLUTION INITIALE *
****

TEMPERATURE = 25.00DEGRES C PH = 8.22 SOMME DES CATIONS ANALYSES = 629.856
SOMME DES ANIONS ANALYSES = 629.796

***** OXYDATION-REDUCTION *****
OXYGENE DISSOUS = 6.60 MG/L
EH MESURE CALOMEL = 9.9000VOLTS
EH MEASURED OF ZOBELL SOLUTION = 9.9000VOLTS
EH CORRIGE = 0.5000VOLTS
PE COMPUTED FROM CORRECTED EH = 8.451

*** CONCENTRATION TOTALE DES ESPECES ANALYSEES ***

ESPECES		MOLALITE TOTALE	LOG MOLALITE TOTALE	CONCENTRATION EN MG/L
CA	2	1.069821E-02	-1.9707	4.219300E+02
MG	2	5.525980E-02	-1.2576	1.322000E+03
NA	1	4.871301E-01	-0.3124	1.102000E+04
K	1	1.061467E-02	-1.9741	4.084200E+02
CL	-1	5.677020E-01	-0.2459	1.980500E+04
SO4	-2	2.936018E-02	-1.5322	2.775300E+03
HCO3	-1	2.414814E-03	-2.6171	1.449900E+02
SIO2 TOT	0	7.408120E-05	-4.1303	4.380000E+00
FE	2	3.730376E-08	-7.4282	2.050000E-03
PO4	-3	6.570132E-07	-6.1824	6.140000E-02
SR	2	9.661637E-05	-4.0149	8.330200E+00
F	-1	7.609109E-05	-4.1187	1.422500E+00
ANAL H2S	0			
CO3	-2			
NH4	1	1.729554E-06	-5.7621	3.070000E-02
AL	3	7.721227E-08	-7.1123	2.050000E-03
LI	1			
NO3	-1	4.864480E-06	-5.3130	2.968000E-01
B TOT	0	4.281201E-04	-3.3684	4.554000E+00
BA	2			
BR	-1	8.758819E-04	-3.0576	6.887200E+01
MN	2	3.791960E-09	-8.4211	2.050000E-04
CD+2	2	9.222155E-10	-9.0352	1.020000E-04
ZN+2	2	7.793597E-08	-7.1083	5.014000E-03
PB+2	2	2.511185E-10	-9.6001	5.120000E-05
CO+2	2	8.829418E-10	-9.0541	5.120000E-05
NI+2	2	3.012380E-08	-7.5211	1.740000E-03
CR+3	3	5.999756E-09	-8.2219	3.070000E-04
CU+2	2	1.144975E-08	-7.9412	7.160000E-04
AS04-3	-3	2.991969E-09	-8.5240	4.090000E-04
SB(OH)3	0	1.986260E-09	-8.7020	3.377000E-04
GE(OH)4	0			

**** DESCRIPTION DE LA SOLUTION ****

	ANALYSES	CALCULES
SOMME DES CATIONS	629.856	605.649
SOMME DES ANIONS	629.796	605.595

PH 8.220
TEMPERATURE 25.00 DEG C
FORCE IONIQUE 0.679798E+00

ACTIVITE DE H2O = 0.9805
PCO2 = 4.000204E-04
LOG PCO2 = -3.3979
PO2 = 3.536984E-17
PCH4 = 1.515103-114
CO2 TOT = 2.150060E-03
DENSITE = 1.0200
TDS = 35985.6MG/L

EH = 0.5000 PE = 8.451
PE CALC S = 1.000000E+02
PE CALC DOX = 1.235788E+01
PE SATO DOX = 0.224788E+01

BALANCE ELECTRIQUE= 0.549287E-04
EN CALCULANT LA DISTRIBUTION DES ESPECES; PE = 8.451 EH EQUIVALENT = 0.500VOLTS

DISTRIBUTION DES ESPECES

I	ESPECES		PPM	MOLALITE	LOG MOL	ACTIVITE	LOG ACT	COEFF. ACT.	LOG COEFF.
1	CA	2	3.66759E+02	9.48531E-03	-2.0229	2.36472E-03	-2.6262	2.49303E-01	-0.6033

2	MG	2	1.15022E+03	4.90407E-02	-1.3094	1.41254E-02	-1.8500	2.88034E-01	-0.5406
3	NA	1	1.05950E+04	4.77711E-01	-0.3208	3.37313E-01	-0.4720	7.06103E-01	-0.1511
4	K	1	3.92061E+02	1.03933E-02	-1.9832	6.46814E-03	-2.1892	6.22337E-01	-0.2060
64	H	1	7.84389E-06	8.06622E-09	-8.0933	6.02560E-09	-8.2200	7.47016E-01	-0.1267
5	CL	-1	1.93282E+04	5.65115E-01	-0.2479	3.51692E-01	-0.4530	6.22337E-01	-0.2060
6	SO4	-2	1.43806E+03	1.55177E-02	-1.8092	2.80671E-03	-2.5518	1.80871E-01	-0.7426
7	HCO3	-1	8.83294E+01	1.50055E-03	-2.8237	1.01219E-03	-2.9947	6.74544E-01	-0.1710
18	CO3	-2	2.19926E+00	3.79888E-05	-4.4203	7.86499E-06	-5.1043	2.07034E-01	-0.6840
86	H2CO3	0	6.98057E-01	1.16660E-05	-4.9331	1.36869E-05	-4.8637	1.17323E+00	0.0694
27	OH	-1	3.59049E-02	2.18834E-06	-5.6599	1.63473E-06	-5.7866	7.47016E-01	-0.1267
62	F	-1	7.05050E-01	3.84682E-05	-4.4149	2.87363E-05	-4.5416	7.47016E-01	-0.1267
98	BR	-1	6.75216E+01	8.75882E-04	-3.0576	6.54298E-04	-3.1842	7.47016E-01	-0.1267
19	MGOH	1	2.01411E-01	5.05275E-06	-5.2965	3.77448E-06	-5.4231	7.47016E-01	-0.1267
23	MGSO4 AQ	0	6.81005E+02	5.86432E-03	-2.2318	6.85800E-03	-2.1638	1.16944E+00	0.0680
22	MGHCO3	1	1.83227E+01	2.22582E-04	-3.6525	1.66272E-04	-3.7792	7.47016E-01	-0.1267
21	MGCO3 AQ	0	7.37539E+00	9.06664E-05	-4.0426	1.06029E-04	-3.9746	1.16944E+00	0.0680
20	MGF	1	1.50002E+00	3.59006E-05	-4.4449	2.68184E-05	-4.5716	7.47016E-01	-0.1267
29	CAOH	1	7.15873E-03	1.29785E-07	-6.8861	9.71012E-08	-7.0128	7.47016E-01	-0.1267
32	CASO4 AQ	0	1.51841E+02	1.15610E-03	-2.9370	1.35200E-03	-2.8690	1.16944E+00	0.0680
30	CAHCO3	1	3.23877E+00	3.32077E-05	-4.4788	2.48067E-05	-4.6054	7.47016E-01	-0.1267
31	CACO3 AQ	0	2.18219E+00	2.25999E-05	-4.6459	2.64293E-05	-4.5779	1.16944E+00	0.0680
49	CAF+	1	4.51555E-02	7.92284E-07	-6.1011	5.91849E-07	-6.2278	7.47016E-01	-0.1267
44	NASO4	-1	7.63899E+02	6.65120E-03	-2.1771	4.96856E-03	-2.3038	7.47016E-01	-0.1267
43	NAHCO3	0	1.33030E+01	1.64178E-04	-3.7847	1.91997E-04	-3.7167	1.16944E+00	0.0680
42	NACO3	-1	5.27080E+00	6.58266E-05	-4.1816	1.91735E-05	-4.3083	7.47016E-01	-0.1267
94	NACL	0	1.43004E+02	2.53639E-03	-2.5958	2.96617E-03	-2.5278	1.16944E+00	0.0680
125	NAF	0	3.76716E-02	9.30005E-07	-6.0315	1.08759E-06	-5.9635	1.16944E+00	0.0680
46	KSO4	-1	2.22698E+01	1.70788E-04	-3.7675	1.27581E-04	-3.8942	7.47016E-01	-0.1267
95	KCL	0	3.63781E+00	5.05780E-05	-4.2960	5.91482E-05	-4.2281	1.16944E+00	0.0680
63	HSO4	-1	2.05785E-04	2.19750E-09	-8.6581	1.64157E-09	-8.7847	7.47016E-01	-0.1267
96	H2SO4	0	8.24494E-16	8.71399E-21	-20.0598	1.01905E-20	-19.9918	1.16944E+00	0.0680
93	HCL	0	5.06305E-11	1.43940E-15	-14.8418	1.68330E-15	-14.7738	1.16944E+00	0.0680
24	H4SIO4AQ	0	6.66496E+00	7.18792E-05	-4.1434	8.40587E-05	-4.0754	1.16944E+00	0.0680
25	H3SIO4	-1	2.01876E-01	2.20023E-06	-5.6575	1.64361E-06	-5.7842	7.47016E-01	-0.1267
26	H2SIO4	-2	1.63169E-04	1.79742E-09	-8.7454	5.59719E-10	-9.2520	3.11401E-01	-0.5067
14	H2S AQ	0							
67	HS	-1							
68	S	-2							
8	FE	2	1.03223E-09	1.91591E-14	-13.7176	5.96618E-15	-14.2243	3.11401E-01	-0.5067
9	FE	3	1.21776E-13	2.26028E-18	-17.6158	1.63732E-19	-18.7859	7.24387E-02	-1.1400
10	FEOH	2	2.08504E-08	2.96659E-13	-12.5277	9.23798E-14	-13.0344	3.11401E-01	-0.5067
11	FEOH	1	4.38199E-11	6.23464E-16	-15.2052	1.65738E-16	-15.3319	7.47016E-01	-0.1267
12	FE(OH)3	-1	1.23582E-14	1.19867E-19	-18.9213	8.95430E-20	-19.0480	7.47016E-01	-0.1267
77	FE(OH)2	1	3.48071E-05	4.01506E-10	-9.3963	2.99932E-10	-9.5230	7.47016E-01	-0.1267
78	FE(OH)3	0	1.72084E-03	1.66912E-08	-7.7775	1.95194E-08	-7.7095	1.16944E+00	0.0680
79	FE(OH)4	-1	2.41530E-03	2.02107E-08	-7.6944	1.50977E-08	-7.8211	7.47016E-01	-0.1267
80	FE(OH)2	0	3.15197E-14	3.63586E-19	-18.4394	4.25193E-19	-18.3714	1.16944E+00	0.0680
13	FEHPO4	1	2.57899E-16	1.76084E-21	-20.7543	1.31537E-21	-20.8810	7.47016E-01	-0.1267
100	FEHPO4	0	9.51401E-14	6.49581E-19	-18.1874	7.59649E-19	-18.1194	1.16944E+00	0.0680
65	FEH2PO4	1	1.83191E-15	1.24246E-20	-19.9057	9.28139E-21	-20.0324	7.47016E-01	-0.1267
99	FEH2PO4	2	6.47664E-17	4.39267E-22	-21.3573	1.36788E-22	-21.8640	3.11401E-01	-0.5067
15	FESO4	1	1.20777E-12	8.24136E-18	-17.0840	6.15643E-18	-17.2107	7.47016E-01	-0.1267
16	FECL	2	4.21547E-13	4.78602E-18	-17.3200	1.49037E-18	-17.8267	3.11401E-01	-0.5067
28	FECL2	1	4.11612E-13	3.36611E-18	-17.4729	2.51454E-18	-17.5995	7.47016E-01	-0.1267
33	FECL3	0	1.16711E-14	7.45836E-20	-19.1274	8.72214E-20	-19.0594	1.16944E+00	0.0680
34	FESO4	0	3.32581E-10	2.26941E-15	-14.6441	2.65395E-15	-14.5761	1.16944E+00	0.0680
117	FE(HS)2	0							
118	FE(HS)3-	-1							
119	FE(SO4)2	-1	3.87079E-11	1.61808E-16	-15.7910	1.20873E-16	-15.9177	7.47016E-01	-0.1267
120	FEF+2	2	1.72905E-12	2.39166E-17	-16.6208	7.45699E-18	-17.1274	3.11401E-01	-0.5067
121	FEF2+	1	1.03388E-12	1.14200E-17	-16.9423	8.53094E-18	-17.0690	7.47016E-01	-0.1267
122	FEF3	0	3.61675E-14	3.32239E-19	-18.4785	3.88535E-19	-18.4106	1.16944E+00	0.0680
123	FECO3	0	1.32353E-11	1.18417E-16	-15.9266	1.38482E-16	-15.8586	1.16944E+00	0.0680

124	FEHCO3+	1	1.34806E-10	1.19572E-15	-14.9224	8.93219E-16	-15.0490	7.47016E-01	-0.1267
101	MN	2	1.05129E-04	1.98350E-09	-8.7026	6.17663E-10	-9.2092	3.11401E-01	-0.5067
102	MN	3	3.97655E-21	7.50269E-26	-25.1248	5.43485E-27	-26.2648	7.24387E-02	-1.1400
106	MNOH	1	2.63442E-07	3.80074E-12	-11.4201	2.83922E-12	-11.5468	7.47016E-01	-0.1267
107	MN(OH)3	-1	2.23523E-14	2.18657E-19	-18.6602	1.63340E-19	-18.7869	7.47016E-01	-0.1267
111	MNHCO3	1	4.86843E-06	4.35195E-11	-10.3613	3.25097E-11	-10.4880	7.47016E-01	-0.1267
109	MNSO4	0	1.10246E-05	7.56779E-11	-10.1210	8.85011E-11	-10.0531	1.16944E+00	0.0680
110	MN(NO3)2	0	1.37928E-15	7.98923E-21	-20.0975	9.34297E-21	-20.0295	1.16944E+00	0.0680
103	MNCL	1	1.02598E-04	1.17618E-09	-8.9294	8.78849E-10	-9.0561	7.47016E-01	-0.1267
104	MNCL2	0	8.71700E-06	7.17958E-11	-10.1439	8.39612E-11	-10.0759	1.16944E+00	0.0680
105	MNCL3	-1	2.77318E-06	1.78202E-11	-10.7491	1.33120E-11	-10.8758	7.47016E-01	-0.1267
108	MNF	1	1.19987E-08	1.68211E-13	-12.7741	1.25656E-13	-12.9008	7.47016E-01	-0.1267
112	MNO4	-1							
113	MNO4	-2							
115	HMNO2	-1	1.11928E-14	1.31920E-19	-18.8797	9.85467E-20	-19.0064	7.47016E-01	-0.1267
116	MNCO3	0	9.62463E-06	8.67901E-11	-10.0615	1.01495E-10	-9.9936	1.16944E+00	0.0680
51	AL	3	3.34734E-13	1.28598E-17	-16.8908	9.31544E-19	-18.0308	7.24387E-02	-1.1400
52	ALOH	2	2.06573E-10	4.86775E-15	-14.3127	1.51582E-15	-14.8194	3.11401E-01	-0.5067
53	AL(OH)2	1	3.36874E-07	5.72485E-12	-11.2422	4.27655E-12	-11.3689	7.47016E-01	-0.1267
54	AL(OH)4	-1	7.07667E-03	7.72065E-08	-7.1123	5.76715E-08	-7.2390	7.47016E-01	-0.1267
55	ALF	2	3.90197E-11	8.79660E-16	-15.0557	2.73927E-16	-15.5624	3.11401E-01	-0.5067
56	ALF2	1	3.63001E-10	5.79079E-15	-14.2373	4.32582E-15	-14.3639	7.47016E-01	-0.1267
57	ALF3	0	1.60355E-10	1.97934E-15	-14.7035	2.31473E-15	-14.6355	1.16944E+00	0.0680
58	ALF4	-1	1.43341E-12	1.46277E-17	-16.3504	3.33376E-17	-16.4771	7.47016E-01	-0.1267
59	ALSO4	1	6.58459E-13	5.54715E-18	-17.2559	4.14381E-18	-17.3826	7.47016E-01	-0.1267
60	AL(SO4)2	-1	2.61412E-13	1.23672E-18	-17.9077	9.23851E-19	-18.0344	7.47016E-01	-0.1267
45	PO4	-3	3.02650E-06	3.30328E-11	-10.4811	2.39286E-12	-11.6211	7.24387E-02	-1.1400
47	HPO4	-2	9.50990E-03	1.02706E-07	-6.9884	3.19828E-08	-7.4951	3.11401E-01	-0.5067
48	H2PO4	-1	3.88779E-04	4.15515E-09	-8.3814	3.10396E-09	-8.5081	7.47016E-01	-0.1267
40	MGPO4	-1	2.02101E-02	1.75625E-07	-6.7554	1.31195E-07	-6.8821	7.47016E-01	-0.1267
73	MGHPO4	0	3.32333E-02	2.86377E-07	-6.5431	3.34902E-07	-6.4751	1.16944E+00	0.0680
41	MGH2PO4	1	2.23793E-04	1.91244E-09	-8.7184	1.42862E-09	-8.8451	7.47016E-01	-0.1267
75	CAPO4	-1	2.83966E-03	2.17955E-08	-7.6616	1.62816E-08	-7.7883	7.47016E-01	-0.1267
74	CAHPO4	0	4.65121E-03	3.54582E-08	-7.4503	4.14664E-08	-7.3823	1.16944E+00	0.0680
76	CAH2PO4	1	3.32431E-05	2.51401E-10	-9.5996	1.87800E-10	-9.7263	7.47016E-01	-0.1267
61	KHPO4	-1	7.03660E-05	5.39965E-10	-9.2676	4.03363E-10	-9.3943	7.47016E-01	-0.1267
50	NAHPO4	-1	3.23189E-03	2.81592E-08	-7.5504	2.10354E-08	-7.6770	7.47016E-01	-0.1267
36	H3BO3 AQ	0	2.22239E+01	3.72562E-04	-3.4288	4.35691E-04	-3.3608	1.16944E+00	0.0680
37	H2BO3	-1	3.26011E+00	5.55581E-05	-4.2553	4.15028E-05	-4.3819	7.47016E-01	-0.1267
85	NO3	-1	2.90980E-01	4.86448E-06	-5.3130	3.63385E-06	-5.4396	7.47016E-01	-0.1267
38	NH3 AQ	0	1.56657E-03	9.53494E-08	-7.0207	1.11506E-07	-6.9527	1.16944E+00	0.0680
39	NH4	1	2.74464E-02	1.57718E-06	-5.8021	1.17818E-06	-5.9288	7.47016E-01	-0.1267
92	NH4SO4	-1	6.27719E-03	5.70266E-08	-7.2439	4.25998E-08	-7.3706	7.47016E-01	-0.1267
81	LI	1							
82	LIOH	0							
83	LISO4	-1							
88	SR	2	8.16683E+00	9.66159E-05	-4.0150	3.00863E-05	-4.5216	3.11401E-01	-0.5067
89	SROH	1	4.39067E-05	4.34995E-10	-9.3615	3.24948E-10	-9.4882	7.47016E-01	-0.1267
90	BA	2							
91	BAOH	1							

I	ESPECES		PPM	MOLALITE	LOG MOL	ACTIVITE	LOG ACT	COEFF. ACT.	MOLAL %
126	CD+2	2	2.93626E-06	2.70786E-11	-10.5674	8.43232E-12	-11.0741	3.11401E-01	2.936260
127	CDOH+	1	1.91616E-08	1.53184E-13	-12.8139	1.14655E-13	-12.9406	7.47016E-01	0.016643
128	CD(OH)2	0	1.21579E-10	8.60712E-16	-15.0651	1.00655E-15	-14.9972	1.16944E+00	0.000093
129	CD(OH)3-	-1	3.89660E-15	2.47145E-20	-19.6070	1.84622E-20	-19.7337	7.47016E-01	0.000000
130	CD(OH)4	-2	1.50363E-20	8.63789E-26	-25.0636	2.68985E-26	-25.5703	3.11401E-01	0.000000
131	CDCL+	1	5.40759E-05	3.79124E-10	-9.4212	2.83212E-10	-9.5479	7.47016E-01	41.110144
132	CDCL2	0	6.27856E-05	3.55055E-10	-9.4497	4.15218E-10	-9.3817	1.16944E+00	38.500253
133	CDCL3-	-1	2.60291E-05	1.23342E-10	-9.9089	9.21383E-11	-10.0356	7.47016E-01	13.374501
134	CDCL4-2	-2	2.99820E-06	1.22260E-11	-10.9127	3.80719E-12	-11.4194	3.11401E-01	1.325719
135	CDSO4	0	1.14708E-06	5.70386E-12	-11.2438	6.67035E-12	-11.1759	1.16944E+00	0.618496
136	CD(SO4)2	-2	1.72603E-07	5.87530E-13	-12.2310	1.82958E-13	-12.7376	3.11401E-01	0.063709

137	CD(SO4)3	-4	9.42673E-09	2.43933E-14	-13.6127	2.29378E-16	-15.6394	9.40332E-03	0.002645
138	CDF+	1	4.94364E-10	3.89787E-15	-14.4089	2.91327E-15	-14.5356	7.47016E-01	0.000423
139	CDF2	0	2.22066E-14	1.53050E-19	-18.8152	1.78984E-19	-18.7472	1.16944E+00	0.000000
140	CDOHCL	0	2.62478E-06	1.65035E-11	-10.7824	1.93000E-11	-10.7144	1.16944E+00	1.789552
141	CDCO3	0	2.11169E-07	1.26960E-12	-11.8963	1.48473E-12	-11.8284	1.16944E+00	0.137669
142	CD(CO3)3	-4	2.04262E-13	7.24045E-19	-18.1402	6.80842E-21	-20.1670	9.40332E-03	0.000000
143	CDHCO3+	1	1.91153E-07	1.14256E-12	-11.9421	8.53514E-13	-12.0688	7.47016E-01	0.123893
144	CDHS+	1							
145	CD(HS)2	0							
146	CD(HS)3-	-1							
147	CD(HS)4	-2							
148	ZN+2	2	1.78820E-03	2.83510E-08	-7.5474	8.82854E-09	-8.0541	3.11401E-01	36.377332
149	ZNOH+	1	1.68376E-04	2.11838E-09	-8.6740	1.58247E-09	-8.8007	7.47016E-01	2.718105
150	ZN(OH)2	0	2.43550E-04	2.53980E-09	-8.5952	2.97016E-09	-8.5272	1.16944E+00	3.258830
151	ZN(OH)3-	-1	2.30827E-07	2.05539E-12	-11.6871	1.53541E-12	-11.8138	7.47016E-01	0.002637
152	ZN(OH)4	-2	1.64426E-11	1.27747E-16	-15.8937	3.97805E-17	-16.4003	3.11401E-01	0.000000
153	ZNCL+	1	1.24944E-03	1.28447E-08	-7.8913	9.59519E-09	-8.0179	7.47016E-01	16.481069
154	ZNCL2	0	5.11766E-04	3.89258E-09	-8.4098	4.55216E-09	-8.3418	1.16944E+00	4.994592
155	ZNCL3-	-1	2.75613E-04	1.66361E-09	-8.7789	1.24274E-09	-8.9056	7.47016E-01	2.134588
156	ZNCL4-2	-2	1.37396E-04	6.87426E-10	-9.1628	2.14065E-10	-9.6695	3.11401E-01	0.882039
157	ZNSO4	0	7.56003E-04	4.85113E-09	-8.3139	5.67663E-09	-8.2459	1.16944E+00	6.228350
158	ZN(SO4)2	-2	2.36674E-04	9.52735E-10	-9.0210	2.96683E-10	-9.5277	3.11401E-01	1.222458
159	ZN(SO4)3	-4	3.54876E-06	1.01043E-11	-10.9828	9.78349E-14	-13.0095	9.40332E-03	0.013350
160	ZN(SO4)4	-6	1.30635E-09	3.01171E-15	-14.5212	8.29269E-20	-19.0813	2.75349E-05	0.000004
161	ZNF+	1	3.90511E-07	4.79725E-12	-11.3190	3.58362E-12	-11.4457	7.47016E-01	0.006155
162	ZNOHCL	0	1.63385E-03	1.43721E-08	-7.8425	1.68073E-08	-7.7745	1.16944E+00	18.440846
163	ZNCO3	0	4.53183E-04	3.74636E-09	-8.4264	4.38116E-09	-8.3584	1.16944E+00	4.806968
164	ZNHCO3+	1	2.31191E-04	1.89593E-09	-8.7222	1.41629E-09	-8.8488	7.47016E-01	2.432678
165	ZN(HS)2	0							
166	ZN(HS)3-	-1							
167	PB+2	2	3.62115E-07	1.81157E-12	-11.7419	5.64126E-13	-12.2486	3.11401E-01	0.721401
168	PBOH+	1	5.20651E-07	2.10708E-12	-11.6185	1.79813E-12	-11.7452	7.47016E-01	0.958544
169	PB(OH)2	0	2.27563E-08	9.77882E-14	-13.0097	1.14358E-13	-12.9417	1.16944E+00	0.038941
170	PB(OH)3-	-1	7.15796E-11	2.87330E-16	-15.5416	2.14640E-16	-15.6683	7.47016E-01	0.000114
171	PBCL+	1	2.36370E-06	1.00974E-11	-10.9958	7.54293E-12	-11.1225	7.47016E-01	4.020974
172	PBCL2	0	1.05761E-06	3.94207E-12	-11.1043	4.61004E-12	-11.3363	1.16944E+00	1.569805
173	PBCL3-	-1	5.09620E-07	1.68476E-12	-11.7735	1.25854E-12	-11.9001	7.47016E-01	0.670903
174	PBCL4-2	-2	2.34390E-07	6.96166E-13	-12.1573	2.16787E-13	-12.6640	3.11401E-01	0.277226
175	PBSO4	0	2.22748E-07	7.61373E-13	-12.1184	8.90384E-13	-12.0504	1.16944E+00	0.303193
176	PB(SO4)2	-2	6.33840E-05	1.64535E-10	-9.7837	5.12363E-11	-10.2904	3.11401E-01	65.520664
177	PBF+	1	5.43717E-10	2.49160E-15	-14.6035	1.86127E-15	-14.7302	7.47016E-01	0.000992
178	PBF2	0	2.47847E-13	1.04776E-18	-17.9797	1.22530E-18	-17.9118	1.16944E+00	0.000000
179	PBF3-	-1	1.20138E-17	4.71352E-23	-22.3267	3.52107E-23	-22.4533	7.47016E-01	0.000000
180	PBF4-2	-2	4.24896E-22	1.55521E-27	-26.8082	4.84293E-28	-27.3149	3.11401E-01	0.000000
181	PBCO3	0	1.55006E-05	6.01306E-11	-10.2209	7.03195E-11	-10.1529	1.16944E+00	23.945120
182	PB(CO3)2	-2	1.54417E-06	4.89165E-12	-11.3105	1.52326E-12	-11.8172	3.11401E-01	1.947943
183	PBHCO3+	1	1.57109E-08	6.07168E-14	-13.2167	4.53565E-14	-13.3434	7.47016E-01	0.024179
184	PB(HS)2	0							
185	PB(HS)3-	-1							
186	CO+2	2	2.55366E-05	4.49185E-10	-9.3476	1.39877E-10	-9.8543	3.11401E-01	50.873735
187	COOH+	1	5.02034E-07	6.85269E-12	-11.1641	5.11907E-12	-11.2908	7.47016E-01	0.776120
188	CO(OH)2	0	4.54263E-08	5.06590E-13	-12.2953	5.92429E-13	-12.2274	1.16944E+00	0.057375
189	CO(OH)3-	-1	2.74402E-12	2.58673E-17	-16.5872	1.93233E-17	-16.7139	7.47016E-01	0.000003
190	CO(OH)4	-2	1.96929E-18	1.60770E-23	-22.7938	5.00641E-24	-23.3005	3.11401E-01	0.000000
191	COCL+	1	2.22772E-05	2.44670E-10	-9.6114	1.82772E-10	-9.7381	7.47016E-01	27.710742
192	COSO4	0	1.14993E-05	7.69073E-11	-10.1140	8.99389E-11	-10.0461	1.16944E+00	8.710353
193	COF+	1	4.23599E-09	5.63442E-14	-13.2492	4.20900E-14	-13.3758	7.47016E-01	0.006381
194	COCO3	0	8.57423E-06	7.47250E-11	-10.1265	8.73868E-11	-10.0586	1.16944E+00	8.463188
195	COHCO3+	1	3.47601E-06	3.00386E-11	-10.5223	2.24393E-11	-10.6490	7.47016E-01	3.402102
196	NI+2	2	6.10093E-04	1.07735E-08	-7.9676	3.35488E-09	-8.4743	3.11401E-01	35.764088
197	NIOH+	1	7.40196E-06	1.01343E-10	-9.9942	7.57046E-11	-10.1209	7.47016E-01	0.336421
198	NI(OH)2	0	6.85745E-07	7.66633E-12	-11.1154	8.96535E-12	-11.0474	1.16944E+00	0.025449
199	NI(OH)3-	-1	2.07687E-09	1.96193E-14	-13.7073	1.46559E-14	-13.8340	7.47016E-01	0.000065

200 NI(OH)4	-2	2.40703E-15	7.69374E-20	-19.1139	2.79504E-20	-19.6205	3.11401E-01	0.000000
201 NICL+	1	7.52893E-04	8.28919E-09	-8.0815	6.19215E-09	-8.2082	7.47016E-01	27.517037
202 NICL2	0	4.04604E-04	3.23613E-09	-8.4900	3.78448E-09	-8.4220	1.16944E+00	10.742770
203 NISO4	0	2.34401E-04	1.57000E-09	-8.8041	1.83603E-09	-8.7361	1.16944E+00	5.211819
204 NI(SO4)2	-2	3.25479E-05	1.34512E-10	-9.8712	4.18971E-11	-10.3779	3.11401E-01	0.446530
205 NI++	1	1.27527E-07	1.70130E-12	-11.7692	1.27070E-12	-11.8959	7.47016E-01	0.005648
206 NICO3	0	6.05739E-04	5.28929E-09	-8.2766	6.18553E-09	-8.2086	1.16944E+00	17.558504
207 NIHCO3+	1	8.32106E-05	7.20461E-10	-9.1424	5.38196E-10	-9.2691	7.47016E-01	2.391668
208 CR+3	3	3.67483E-10	7.32542E-15	-14.1352	5.30644E-16	-15.2752	7.24387E-02	0.000122
209 CROH+2	2	1.85456E-06	2.70566E-11	-10.5551	8.67458E-12	-11.0618	3.11401E-01	0.464295
210 CR(OH)2+	1	3.14314E-04	3.78759E-09	-8.4216	2.82939E-09	-8.5483	7.47016E-01	63.129118
211 CR(OH)3	0	1.77026E-04	1.98225E-09	-8.7028	2.31313E-09	-8.6349	1.16944E+00	33.038869
212 CR(OH)4-	-1	2.33873E-05	2.01955E-10	-9.6947	1.50863E-10	-9.8214	7.47016E-01	3.366046
213 CRCL+2	2	2.10770E-10	2.49831E-15	-14.6024	7.77978E-16	-15.1090	3.11401E-01	0.000042
214 CRCL2+	1	1.34201E-11	1.13188E-16	-15.9462	8.45535E-17	-16.0729	7.47016E-01	0.000002
215 CRSO4+	1	1.16015E-08	8.12222E-14	-13.0903	6.06743E-14	-13.2170	7.47016E-01	0.001354
216 CRF+2	2	5.43971E-10	7.94174E-15	-14.1001	2.47307E-15	-14.6068	3.11401E-01	0.000132
217 CRF2+	1	1.03788E-10	1.19768E-15	-14.9217	8.94683E-16	-15.0483	7.47016E-01	0.000020
218 CRF3	0	9.20344E-13	8.75231E-18	-17.0579	1.02353E-17	-16.9899	1.16944E+00	0.000000
219 CUI2	2	4.13529E-05	6.71511E-10	-9.1710	2.10044E-10	-9.6777	3.11401E-01	5.891057
220 CUOH+	1	3.57228E-05	4.59647E-10	-9.3376	3.43364E-10	-9.4642	7.47016E-01	4.014474
221 CU(OH)2	0	2.26432E-06	2.40558E-11	-10.6188	2.81320E-11	-10.5508	1.16944E+00	0.210099
222 CU(OH)3-	-1	2.15191E-08	1.94677E-13	-12.7107	1.45427E-13	-12.8374	7.47016E-01	0.001700
223 CU(OH)4	-2	1.53601E-11	1.20996E-16	-15.9172	3.76782E-17	-16.4239	3.11401E-01	0.000001
224 CUCL+	1	9.88964E-06	1.03549E-10	-9.9849	7.73524E-11	-10.1115	7.47016E-01	0.904373
225 CUCL2	0	5.61850E-07	4.33170E-12	-11.3633	5.06569E-12	-11.2954	1.16944E+00	0.037832
226 CUCL3-	-1	1.02818E-08	6.27296E-14	-13.2025	4.68600E-14	-13.3292	7.47016E-01	0.000548
227 CUCL4-2	-2	5.25463E-11	2.65245E-16	-15.5764	8.25975E-17	-16.0830	3.11401E-01	0.000002
228 CUSO4	0	1.58487E-05	1.02928E-10	-9.9875	1.20368E-10	-9.9195	1.16944E+00	0.898950
229 CUF+	1	2.13074E-08	2.67555E-13	-12.5726	1.99868E-13	-12.6993	7.47016E-01	0.002337
230 CUCO3	0	9.46910E-04	7.94382E-09	-8.1000	9.28987E-09	-8.0320	1.16944E+00	69.379891
231 CU(CO3)2	-2	3.61903E-04	2.04357E-09	-8.6896	6.36369E-10	-9.1963	3.11401E-01	17.848137
232 CUHCO3+	1	5.42073E-06	4.51069E-11	-10.3458	3.36956E-11	-10.4724	7.47016E-01	0.393955
233 CU+	1	3.19934E-11	5.21848E-16	-15.2825	3.89829E-16	-15.4091	7.47016E-01	0.000005
234 CUCL2-	-1	2.64749E-06	2.04114E-11	-10.6901	1.52476E-11	-10.8168	7.47016E-01	0.178269
235 CUCL3-2	-2	4.47343E-06	2.72927E-11	-10.5640	8.49898E-12	-11.0706	3.11401E-01	0.238369
236 CU(HS)3-	-1							
237 AS04-3	-3	8.83316E-07	6.58098E-12	-11.1810	4.77442E-13	-12.3211	7.24387E-02	0.220289
238 H3AS04	0	5.85434E-12	4.27505E-17	-16.3691	1.99941E-17	-16.3011	1.16944E+00	0.000001
239 H2AS04	-1	8.69013E-06	6.39132E-11	-10.1944	4.77442E-11	-10.3211	7.47016E-01	2.136160
240 HAS04	-2	3.94378E-04	2.92146E-09	-8.5344	9.09748E-10	-9.0411	3.11401E-01	97.643549
241 AS03-3	-3	8.91461E-35	7.51759E-40	-39.1239	5.44565E-41	-40.2640	7.24387E-02	0.000000
242 AS(OH)4-	-1	1.15434E-26	8.36988E-32	-31.0773	6.25244E-32	-31.2040	7.47016E-01	0.000000
243 AS(OH)3	0	6.96096E-26	5.72088E-31	-30.2419	6.69961E-31	-30.1740	1.16944E+00	0.000000
244 SB(OH)3	0	1.15454E-14	6.92650E-20	-19.1595	8.10016E-20	-19.0915	1.16944E+00	0.000000
245 SBOH+2	2	6.19525E-21	4.12262E-26	-25.3848	1.28379E-26	-25.8915	3.11401E-01	0.000000
246 SB(OH)4-	-1	4.98699E-18	2.72373E-23	-22.5648	2.03467E-23	-22.6915	7.47016E-01	0.000000
247 SB(OH)5	0	8.00456E-10	4.01223E-15	-14.3966	4.69208E-15	-14.3286	1.16944E+00	0.000202
248 SB(OH)6-	-1	4.28860E-04	1.98626E-09	-8.7020	1.48377E-09	-8.8286	7.47016E-01	99.999798
249 GE(OH)4	0							
250 GEO(OH)3	-1							

RAPPORTS MOLAIRES POUR LA MOLALITE ANALYTIQUE

CL/CA	5.3065E+01
CL/MG	1.0273E+01
CL/NA	1.1654E+00
CL/K	5.3183E+01
CL/AL	7.3525E+06
CL/FE	1.5218E+07
CL/SO4	1.9336E+01
CL/HCO3	2.3509E+02
CA/MG	1.9360E-01
NA/K	4.5892E+01

RAPPORTS MOLAIRES POUR LA MOLALITE CALCULEE

CL/CA	5.9578E+01
CL/MG	1.1523E+01
CL/NA	1.1830E+00
CL/K	5.4373E+01
CL/AL	4.3944E+16
CL/FE	2.9496E+13
CL/SO4	3.6417E+01
CL/HCO3	3.7660E+02
CA/MG	1.9342E-01
NA/K	4.5963E+01

RAPPORTS DES LOG D'ACTIVITE

LOG CA/H2	13.8138
LOG MG/H2	14.5900
LOG NA/H1	7.7490
LOG K/H1	6.0308
LOG AL/H3	6.6292
LOG FE/H2	2.2157
LOG CA/MG	-0.7762
LOG NA/K	1.7173

NA/LI=

ESPECE	CITOT/FETOT	CITOT/TDS
CD	0.2472E-01	0.2563E-13
ZN	0.2089E+01	0.2166E-11
PB	0.6732E-02	0.6978E-14
CO	0.2367E-01	0.2454E-13
NI	0.8075E+00	0.8371E-12
CR	0.1608E+00	0.1667E-12
CU	0.3069E+00	0.3182E-12
AS	0.8021E-01	0.8314E-13
SB	0.5325E-01	0.5520E-13
GE		
MN	0.1017E+00	0.1054E-12

NA/LI=

*** SATURATION MINERALE ***

	PHASE	IAP	KT	LOG IAP	LOG KT	IAP/KT	LOG IAP/KT	DEG DE SATURATION
40	ADULAIRE	2.5939E-22	2.6915E-21	-21.5860	-20.5700	9.6372E-02	-1.01605	-1.38618
41	ALBITE	1.3527E-20	1.0000E-18	-19.8688	-18.0000	1.3527E-02	-1.86879	-2.54956
141	ALOH3A	4.0695E-36	2.4547E-32	-35.3905	-31.6100	1.6578E-04	-3.78046	-5.15762
51	ALUNITE	7.8606E-97	4.7863E-86	-96.1045	-85.3200	1.6423E-11	-10.78455	-14.71317
43	ANALCIME	1.5167E-16	1.9953E-13	-15.8190	-12.7000	7.6025E-04	-3.11904	-4.25526
18	ANHYDRIT	6.6371E-06	2.8314E-05	-5.1780	-4.5480	2.3441E-01	-0.63002	-0.85953
114	ANNITE	1.0935E-99	5.7541E-85	-98.9612	-84.2400	1.9003E-15	-14.72118	-20.08385
42	ANORTHIT	6.5066E-26	4.6774E-20	-25.1866	-19.3300	1.3911E-06	-5.85665	-7.99012
22	ARAGONIT	1.8598E-08	6.0954E-09	-7.7305	-8.2150	3.0512E+00	0.48448	0.66096
151	ARTINITE	1.1079E-22	3.9811E-19	-21.9555	-18.4000	2.7828E-04	-3.55552	-4.85073
145	BARITE							
49	BEIDEL							
53	BOEHMITE	4.1504E-36	3.8905E-34	-35.3819	-33.4100	1.0668E-02	-1.97191	-2.69024
20	BRUCITE	3.7748E-14	3.8905E-12	-13.4231	-11.4100	9.7027E-03	-2.01311	-2.74645
13	CALCITE	1.8598E-08	3.3502E-09	-7.7305	-8.4749	5.5514E+00	0.74441	1.01558
144	CELESTIT	8.4443E-08	1.0617E-06	-7.0731	-5.9740	7.9536E-02	-1.09943	-1.49994
98	CALCEDON	8.7437E-05	2.9992E-04	-4.0583	-3.5230	2.9154E-01	-0.53531	-0.73031
50	CHLORITE	6.8997E-83	2.4547E-91	-82.1612	-90.6100	2.8108E+08	8.44883	11.52660
21	CHRYSOTL	4.1939E-49	1.5849E-52	-48.3774	-51.8000	2.6461E+03	3.42261	4.66941
30	CLENSTIT	3.3662E-18	1.3490E-17	-17.4729	-16.8700	2.4954E-01	-0.60286	-0.82247
57	CLINOP	1.6779E-28	1.0000E+00	-27.7752	0.0000	1.6779E-28	-27.77524	-37.89329
100	CRISTOBA	8.7437E-05	2.5942E-04	-4.0583	-3.5860	3.3705E-01	-0.47231	-0.64436
29	DIOPSIDE	1.8970E-36	6.0256E-37	-35.7219	-36.2200	3.1482E+00	0.49806	0.67949
12	DOLOMITE	2.0662E-15	9.5499E-18	-14.6848	-17.0200	2.1636E+02	2.33518	3.18584
56	ERIONITE	1.1923E-22	1.0000E+00	-21.9236	0.0000	1.1923E-22	-21.92361	-29.91001
113	FEOH3A	7.0545E+05	7.6736E+04	5.8485	4.8850	9.1932E+00	0.96347	1.31444
120	FESPPT							
97	FLUAPT	3.2217E-58	1.6218E-67	-57.4919	-66.7900	1.9865E+09	9.29808	12.68521
63	FLUORITE	1.9527E-12	3.1623E-11	-11.7094	-10.5000	6.1751E-02	-1.20936	-1.64991
28	FORSTRIT	1.2959E-31	7.7625E-29	-30.8874	-28.1100	1.6695E-03	-2.77742	-3.78918
52	GIBCRS	4.0695E-36	1.6982E-33	-35.3905	-32.7700	2.3963E-03	-2.62046	-3.57505
111	GOETHITE	7.2949E-37	6.3096E-42	-36.1370	-41.2000	1.1562E+05	5.06302	6.90740
112	GREENALI	3.1601E-86	6.4565E-64	-85.5003	-63.1900	4.8944E-23	-22.31030	-30.43756
119	GREGITE							
19	GYPSE	6.3807E-06	1.7418E-05	-5.1951	-4.7590	3.6632E-01	-0.43613	-0.59501
65	HALITE	1.1863E-01	3.8194E+01	-0.9258	1.5820	3.1060E-03	-2.50780	-3.42135
48	HALLOYSI	9.7953E-40	1.5136E-33	-39.0090	-32.8200	6.4717E-07	-6.18898	-8.44352
109	HEMATITE	5.2796E+11	9.8101E-05	11.7226	-4.0070	5.3654E+15	15.72960	21.45962
118	HUNTITE	2.5502E-29	3.0903E-31	-28.5934	-30.5100	8.2523E+01	1.91657	2.61475
39	HYDMAG	4.8789E-35	1.5136E-38	-34.3117	-37.8200	3.2235E+03	3.50832	4.78634
96	HYXAPT	1.8327E-59	4.4668E-60	-58.7369	-59.3500	4.1029E+00	0.61309	0.83643
46	ILLITE	3.4841E-43	4.8978E-41	-42.4579	-40.3100	7.1136E-03	-2.14791	-2.93036
47	KAOLINIT	9.7953E-40	1.2303E-37	-39.0090	-36.9100	7.9619E-03	-2.09898	-2.86360
44	KMICA	3.3895E-53	8.1283E-50	-52.4699	-49.0900	4.1700E-04	-3.37986	-4.61108
129	LAUMONTI	4.5975E-34	1.0965E-32	-33.3375	-31.9600	4.1929E-02	-1.37748	-1.87927

148	LEONHARD	2.1557E-67	2.6915E-70	-66.6664	-69.5700	8.0093E+02	2.90359	3.96132
68	MACKIT							
99	MAGADITE	3.8006E-23	5.0119E-15	-22.4201	-14.3000	7.5832E-09	-8.12015	-11.07818
110	MAGHEMIT	5.2796E+11	2.3442E+06	11.7226	6.3700	2.2522E+05	5.35260	7.30246
11	MAGNESIT	1.1110E-07	3.8905E-09	-6.9543	-8.4100	2.8556E+01	1.45570	1.98599
108	MAGNETIT	2.9195E-08	2.7227E-10	-7.5347	-9.5650	1.0723E+02	2.03031	2.76991
64	MONTCA	2.5142E-49	1.0000E-45	-48.5996	-45.0000	2.5142E-04	-3.59961	-4.91088
116	MONTBF	5.9466E-33	1.0715E-35	-32.2257	-34.9700	5.5497E+02	2.74427	3.74396
117	MONTAB	7.8843E-28	1.6596E-30	-27.1032	-29.7800	4.7508E+02	2.67676	3.65186
58	MORDENIT	1.8121E-26	1.0000E+00	-25.7418	0.0000	1.8121E-26	-25.74181	-35.11912
67	MIRABILI	2.6225E-04	7.7090E-02	-3.5813	-1.1130	3.4018E-03	-2.46829	-3.36744
59	NAHCOLIT	3.4142E-04	3.0339E-01	-3.4667	-0.5180	1.1254E-03	-2.94870	-4.02287
61	NATRON	7.3488E-07	4.8865E-02	-6.1338	-1.3110	1.5039E-05	-4.82279	-6.57964
150	NESQUHO	1.0472E-07	6.1518E-06	-6.9800	-5.2110	1.7023E-02	-1.76897	-2.41337
55	PHTLIST	1.8366E-21	1.3804E-20	-20.7360	-19.8600	1.3305E-01	-0.87598	-1.19508
45	PHLOGOPI	1.4512E-62	2.9512E-64	-61.8383	-63.5300	4.9174E+01	1.69173	2.30800
142	PREHNITE	3.5622E-16	3.0200E-12	-15.4483	-11.5200	1.1795E-04	-3.92828	-5.35929
115	PYRITE							
54	PYROPHYL	7.6377E-48	3.7154E-43	-47.1170	-42.4300	2.0557E-05	-4.68704	-6.39445
102	QUARTZ	8.7437E-05	9.8855E-05	-4.0583	-4.0050	8.8449E-01	-0.05331	-0.07273
37	SEPIOLIT	9.2476E-40	7.9433E-41	-39.0340	-40.1000	1.1642E+01	1.06603	1.45436
10	SIDERITE	4.6924E-20	2.8184E-11	-19.3286	-10.5500	1.6649E-09	-8.77861	-11.97650
101	SILGEL	8.7437E-05	9.6161E-04	-4.0583	-3.0170	9.0927E-02	-1.04131	-1.42064
147	STRENGIT	3.7665E-31	3.9811E-27	-30.4241	-26.4000	9.4610E-05	-4.02406	-5.48996
143	STRONTIA	2.3663E-10	3.8905E-12	-9.6259	-11.4100	6.0823E+01	1.78407	2.43397
38	TALC	3.2700E-57	5.1286E-63	-56.4854	-62.2900	6.3761E+05	5.80455	7.91905
66	THENARDI	3.1935E-04	6.6222E-01	-3.4957	-0.1790	4.8224E+04	-3.31674	-4.52497
62	THRNAT	8.7742E-07	1.3335E+00	-6.0568	0.1250	6.5798E+07	-6.18179	-8.43371
32	TREMOLIT	1.1767-128	5.0119-141	-127.9293	-140.3000	2.3478E+12	12.37067	16.87709
60	TRONA	2.9373E-10	1.6032E-01	-9.5320	-0.7950	1.8321E-09	-8.73705	-11.91981
107	VIVIANIT	1.0387E-66	1.0000E-36	-65.9835	-36.0000	1.0387E-30	-29.98352	-40.90600
146	WITHERIT							
154	SEP FT	9.2476E-40	6.1376E-38	-39.0340	-37.2120	1.5067E-02	-1.82197	-2.48569
155	DIASPORE	4.1504E-36	8.7096E-36	-35.3819	-35.0600	4.7653E-01	-0.32191	-0.43917
156	WAIRAKIT	4.7822E-34	2.3988E-27	-33.3204	-26.6200	1.9936E-07	-6.70037	-9.14120
172	MANGANO	1.6680E+07	8.6696E+17	7.2222	17.9380	1.9240E-11	-10.71580	-14.61939
173	PYROLUST	1.1208E+15	7.2611E+15	15.0495	15.8610	1.5435E-01	-0.81149	-1.10710
174	BIRNESIT	1.1208E+15	1.2331E+18	15.0495	18.0910	9.0889E-04	-3.04149	-4.14945
175	NUSTITE	1.1208E+15	3.1915E+17	15.0495	17.5040	3.5117E-03	-2.45449	-3.34861
176	BIXBYITE	5.8172E-04	2.4491E-01	-3.2353	-0.6110	2.3753E-03	-2.62429	-3.58027
177	HAUSMANI	1.0021E+55	3.4674E+61	55.0009	61.5400	2.8901E-07	-6.53909	-8.92117
178	MNOH2	1.6506E-21	1.2246E-13	-20.7824	-12.9120	1.3479E-08	-7.87036	-10.73740
179	MNOH3	2.3742E-44	2.2699E-36	-43.6245	-35.6440	1.0460E-08	-7.98048	-10.88763
180	MANGANIT	2.3882E-02	5.7810E-01	-1.6219	-0.2380	4.1312E-02	-1.38392	-1.88806
181	RHODOCHR	4.8579E-15	2.8907E-11	-14.3136	-10.5390	1.6805E-04	-3.77455	-5.14955
183	MNCL2	7.6397E-11	5.7544E+08	-10.1169	8.7600	1.3276E-19	-18.87692	-25.75347
184	MNCL2,1W	7.4907E-11	3.3266E+05	-10.1255	5.5220	2.2518E-16	-15.64748	-21.34759
185	MNCL2,2W	7.3446E-11	9.4189E+03	-10.1340	3.9740	7.7977E-15	-14.10803	-19.24735
186	MNCL2,4W	7.0608E-11	5.1286E+02	-10.1511	2.7100	1.3768E-13	-12.86114	-17.54624
187	TEPHRITE	2.4327E+10	1.3213E+23	10.3861	23.1220	1.8369E-13	-12.73591	-17.37539
188	RHODONIT	9.0083E-07	3.3266E+09	-6.0454	9.5220	2.7080E-16	-15.56736	-21.23828
189	MNS GRN							
190	MNSO4	1.7336E-12	4.6666E+02	-11.7611	2.6690	3.7149E-15	-14.43005	-19.68667
191	MN2SO4,3	6.5308E-61	1.9454E-06	-60.1850	-5.7110	3.3571E-55	-54.47403	-74.31800
192	MN3PO4,2	1.3492E-51	1.4894E-24	-50.8699	-23.8270	9.0592E-28	-27.04291	-36.89418
193	MNHPO4	1.9755E-17	1.1298E-13	-16.7043	-12.9470	1.7485E-04	-3.75733	-5.12606
319	OTAVITE	6.6320E-17	1.8197E-14	-16.1784	-13.7400	3.6446E-03	-2.43835	-3.32661
320	CDCL2	2.9656E-12	2.0893E-01	-11.5279	-0.6800	1.4194E-11	-10.84789	-14.79959
321	CDCL2,W	1.0430E-12	1.9498E-02	-11.9817	-1.7100	5.3490E-11	-10.27173	-14.01354
322	CDCL25/2	1.0430E-12	1.1482E-02	-11.9817	-1.9400	9.0839E-11	-10.04173	-13.69976
323	CDF2	6.9632E-21	1.0471E-03	-20.1572	-2.9800	6.6498E-18	-17.17719	-23.43455
324	CD(OH)2A	2.3225E+05	5.3703E+13	5.3659	13.7300	4.3246E-09	-8.36405	-11.41093
325	CD(OH)2C	2.3225E+05	4.4668E+13	5.3659	13.6500	5.1993E-09	-8.28405	-11.30179

326	CDOHCL	4.9216E-04	3.3113E+03	-3.3079	3.5200	1.4863E-07	-6.82789	-9.31517
327	CD3OH4SO	1.2766E-03	3.6308E+22	-2.8940	22.5600	3.5159E-26	-25.45396	-34.72641
328	CD3OH2SO	1.3009E-22	5.1286E+06	-21.8858	6.7100	2.5365E-27	-28.59576	-39.01272
329	CD3OH6SO	2.9647E+02	2.5119E+28	2.4720	28.4000	1.1803E-26	-25.92801	-35.37315
330	MONTEPON	2.3225E+05	1.3183E+15	5.3659	15.1200	1.7618E-10	-9.75405	-13.30729
331	CDSIO3	1.9522E+01	1.1482E+09	1.2905	9.0600	1.7003E-08	-7.76947	-10.59976
332	CDSO4	2.3667E-14	7.9133E-01	-13.6259	-0.1000	2.9795E-14	-13.52586	-18.45310
333	CDSO4,W	3.3285E+08	2.1878E-02	8.5222	-1.6600	1.5214E+10	10.18225	13.89147
334	CDSO48/3	2.3667E-14	1.3490E-02	-13.6259	-1.8700	1.7545E-12	-11.75586	-16.03831
335	ZDCL2	1.0920E-09	1.0715E+07	-8.9618	7.0300	1.0191E-16	-15.99179	-21.81732
336	SMITHSON	6.9436E-14	1.0000E-10	-13.1584	-10.0000	6.9436E-04	-3.15841	-4.30897
337	ZNCO3,W	6.9436E-14	5.4954E-11	-13.1584	-10.2600	1.2635E-03	-2.89841	-3.95426
338	ZN(OH)2A	2.4316E+08	2.8181E+12	8.3859	12.4500	8.6276E-05	-4.06411	-5.54460
339	ZN(OH)2C	2.4316E+08	1.5849E+12	8.3859	12.2000	1.5342E-04	-3.81411	-5.20353
340	ZN(OH)2B	2.4316E+08	5.6234E+11	8.3859	11.7500	4.3240E-04	-3.36411	-4.58960
341	ZN(OH)2G	2.4316E+08	5.1286E+11	8.3859	11.7100	4.7412E-04	-3.32411	-4.53503
342	ZN(OH)2E	2.4316E+08	3.1623E+11	8.3859	11.5000	7.6893E-04	-3.11411	-4.24853
343	ZN2OH3CL	1.2530E+08	1.5849E+15	8.0979	15.2000	7.9057E-08	-7.10206	-9.68922
344	ZN5OH8CL	3.8174E+24	3.1623E+38	24.5818	38.5000	1.2072E-14	-13.91823	-18.98840
345	ZN2OH2SO	6.0252E-03	3.1623E+07	-2.2200	7.5000	1.9054E-10	-9.72002	-13.26086
346	ZN4OH6SO	3.5625E+14	2.5119E+28	14.5518	28.4000	1.4183E-14	-13.84825	-18.89293
347	ZNNO326W	1.1658E-19	2.7542E+03	-18.9334	3.4400	4.2327E-23	-22.37338	-30.52362
348	ZNO ACT	2.4316E+08	2.0417E+11	8.3859	11.3100	1.1909E-03	-2.92411	-3.98931
349	ZNO CRYS	2.4316E+08	1.3804E+11	8.3859	11.1400	1.7615E-03	-2.75411	-3.75739
350	ZN3OSO42	1.4930E-13	1.0471E+19	-12.8259	19.0200	1.4258E-32	-31.84594	-43.44687
351	ZNS AM							
352	SPHALERI							
353	WURTZITE							
354	ZNSIO3	2.0440E+04	8.5114E+02	4.3105	2.9300	2.4014E+01	1.38047	1.88335
355	WILLEMIT	4.9701E+12	2.1380E+15	12.6964	15.3300	2.3247E-03	-2.63364	-3.59303
356	ZINCOSIT	2.4779E-11	1.0233E+03	-10.6059	3.0100	2.4215E-14	-13.61591	-18.57596
357	ZNSO4,W	2.4779E-11	2.6915E-01	-10.6059	-0.5700	9.2063E-11	-10.03591	-13.69183
358	BIANCHIT	2.4779E-11	1.7179E-02	-10.6059	-1.7650	1.4424E-09	-8.84091	-12.06151
359	GOSLARIT	2.4779E-11	1.0965E-02	-10.6059	-1.9600	2.2599E-09	-8.64591	-11.79547
360	COTUNNIT	6.9775E-14	1.6982E-05	-13.1563	-4.7700	4.1087E-09	-8.38630	-11.44129
361	MATLOCKI	5.7012E-18	3.7154E-10	-17.2440	-9.4300	1.5345E-08	-7.81403	-10.66055
362	PHOSGENI	3.0958E-31	1.5488E-20	-30.5092	-19.8100	1.9988E-11	-10.69923	-14.59677
363	CERRUSIT	4.4360E-18	7.4131E-14	-17.3529	-13.1300	5.9851E-05	-4.22293	-5.76127
364	PBF2	4.6594E-22	3.6308E-08	-21.3318	-7.4400	1.2830E-14	-13.89176	-18.95229
365	MASSICOT	1.5537E+04	8.1283E+12	4.1914	12.9100	1.9115E-09	-8.71862	-11.89467
366	LITHARGE	1.5537E+04	5.2481E+12	4.1914	12.7200	2.9606E-09	-8.52862	-11.63546
367	PBO,W/3	1.5537E+04	9.5499E+12	4.1914	12.9800	1.6270E-09	-8.78862	-11.99017
368	PB2OCO3	6.8937E-14	3.1623E-01	-13.1616	-0.5000	2.1800E-13	-12.66155	-17.27394
369	LARNAKIT	2.4601E-11	5.2481E-01	-10.6091	-0.2800	4.6876E-11	-10.32905	-14.09175
370	PB3O2SO4	3.8223E-07	2.5119E+10	-6.4177	10.4000	1.5217E-17	-16.81768	-22.94407
371	PB4O3SO4	5.9388E-03	1.2589E+22	-2.2263	22.1000	4.7174E-25	-24.32630	-33.18796
372	PBHFO4	1.8042E-20	3.4674E-12	-19.7437	-11.4600	5.2035E-09	-8.28371	-11.30132
373	PB3O2CO3	1.0711E-09	1.0471E+11	-8.9702	11.0200	1.0229E-20	-19.99017	-27.27226
374	PBSIO3	1.3060E+00	2.0893E+07	0.1160	7.3200	6.2511E-08	-7.20404	-9.82835
375	PB2SIO4	2.0292E+04	5.7544E+19	4.3073	19.7600	3.5264E-16	-15.45267	-21.08181
376	ANGLESIT	1.5833E-15	1.6218E-08	-14.8004	-7.7900	9.7628E-08	-7.01043	-9.56421
377	GALENE							
378	PLATTNER	3.4217E+37	1.9953E+49	37.5342	49.3000	1.7149E-12	-11.76575	-16.05182
379	PB2O3	5.3165E+41	1.0965E+61	41.7256	61.0400	4.8487E-20	-19.31438	-26.35028
380	PB(OH)2	1.5537E+04	1.4125E+08	4.1914	8.1500	1.1000E-04	-3.95862	-5.40068
381	LAURIONI	3.2926E-05	4.1976E+00	-4.4825	0.6230	7.8440E-06	-5.10546	-6.96529
382	PB2OH3CL	5.1158E-01	6.1660E+08	-0.2911	8.7900	8.2969E-10	-9.08109	-12.38917
383	HYDCERRU	3.0586E-31	3.4674E-18	-30.5145	-17.4600	8.8211E-14	-13.05448	-17.81000
384	PB2OOH2	2.4141E+08	1.5849E+26	8.3828	26.2000	1.5232E-18	-17.81725	-24.30777
385	PB4OH4SO	5.9388E-03	1.2589E+21	-2.2263	21.1000	4.7174E-24	-23.32630	-31.82367
386	MELANOTH	2.5980E-11	5.3703E+03	-10.5854	3.7300	4.8376E-15	-14.31537	-19.53021
387	CUCO3	1.6520E-15	2.3412E-10	-14.7820	-9.6300	7.0471E-06	-5.15199	-7.02878
388	CUF2	1.7345E-19	4.4668E+00	-18.7608	0.6500	3.8830E-20	-19.41083	-26.48186

389	CUF2,2W	1.7345E-19	2.8184E-05	-18.7608	-4.5500	6.1542E-15	-14.21083	-19.38759
390	CU(OH)2	5.7851E+06	4.3652E+08	6.7623	8.6400	1.3253E-02	-1.87769	-2.56170
391	MALACHIT	2.0412E+02	1.4125E+05	2.3099	5.1500	1.4150E-03	-2.84012	-3.87473
392	AZURITE	7.2020E-03	5.6234E+03	-2.1425	3.7500	1.2807E-06	-5.89255	-8.03910
393	ATACAMIT	7.0922E+04	2.1878E+07	4.8508	7.3100	3.2418E-03	-2.48922	-3.39600
394	ANTLERIT	1.9730E+01	1.9498E+08	1.2951	8.2900	1.0119E-07	-6.99487	-9.54299
395	CU2OH3NO	7.3280E-01	1.7378E+09	-0.1350	9.2400	4.2168E-10	-9.37501	-12.79017
396	BROCHANT	1.1414E+08	2.1878E+15	8.0574	15.3400	5.2172E-08	-7.28256	-9.93548
397	LANGITE	1.1414E+08	6.1660E+16	8.0574	16.7900	1.8511E-09	-8.73256	-11.91369
398	TENORITE	5.7851E+06	4.1687E+07	6.7623	7.6200	1.3877E-01	-0.85769	-1.17013
399	CU2OSO4	1.6237E+04	3.3881E+11	4.2105	11.5300	4.7919E-08	-7.31949	-9.98586
400	CUSO4	5.8953E-13	1.0233E+03	-12.2295	3.0100	5.7611E-16	-15.23949	-20.79098
401	CHALCAN	5.8953E-13	2.2909E-03	-12.2295	-2.6100	2.5734E-10	-9.58949	-13.08278
402	CUPRIFER	3.2402E+18	7.5858E+05	18.5106	5.8800	4.2714E+12	12.63057	17.23168
403	NICO3	2.6386E-14	1.4454E-07	-13.5786	-6.8400	1.8255E-07	-6.73862	-9.19339
404	NI(OH)2	9.2401E+07	6.3096E+10	7.9657	10.8000	1.4645E-03	-2.83432	-3.86682
405	NI4OH4SO	7.4286E+12	1.0000E+32	12.8709	32.0000	7.4286E-20	-19.12909	-26.09750
406	BUNSENIT	9.2401E+07	2.8184E+12	7.9657	12.4500	3.2785E-05	-4.48432	-6.11789
407	RETGERSI	9.4162E-12	9.1201E-03	-11.0261	-2.0400	1.0325E-09	-8.98613	-12.25962
408	MORENOSI	9.4162E-12	4.3652E-03	-11.0261	-2.3600	2.1571E-09	-8.66613	-11.82305
409	NI2SIO4	7.1769E+11	3.4674E+14	11.8559	14.5400	2.0698E-03	-2.68406	-3.66182
410	NISO4	9.4162E-12	3.0200E+04	-11.0261	4.4800	3.1180E-16	-15.50613	-21.15474
411	COO	3.8525E+06	4.3652E+13	6.5857	13.6400	8.8256E-08	-7.05425	-9.62400
412	COOH2PIN	3.8525E+06	1.3183E+13	6.5857	13.1200	2.9224E-07	-6.53425	-8.91457
413	COOH2TRA	3.8525E+06	2.2387E+12	6.5857	12.3500	1.7209E-06	-5.76425	-7.86407
414	JAIPURIT							
415	COSO4	3.9259E-13	6.7608E+02	-12.4061	2.8300	5.8069E-16	-15.23606	-20.78629
416	COSO4,W	3.9259E-13	9.7724E-02	-12.4061	-1.0100	4.0174E-12	-11.39606	-15.54745
417	COSO4,6W	3.9259E-13	6.9183E-03	-12.4061	-2.1600	5.6747E-11	-10.24606	-13.97852
418	BIEBERIT	3.9259E-13	2.1380E-11	-12.4061	-43.6700	1.8363E+31	31.26394	42.65287
419	COCO3	1.1001E-15	1.6218E-10	-14.9586	-9.7900	6.7833E-06	-5.16856	-7.05137
420	CO3ARS8W	6.2385E-55	9.5499E-29	-54.2049	-28.0200	6.5325E-27	-26.18492	-35.72364
421	AS2O5	2.4994E-33	5.0119E+06	-32.6022	6.7000	4.9870E-40	-39.30216	-53.61927
422	CU3ARS6W	2.1124E-54	7.5858E-36	-53.6752	-35.1200	2.7847E-19	-18.55523	-25.31458
423	NI3ARS8W	8.6074E-51	3.0903E-26	-50.0651	-25.5100	2.7853E-25	-24.55513	-33.50014
424	PB3ARS2	4.0923E-62	3.9811E-36	-61.3880	-35.4000	1.0279E-26	-25.98803	-35.45503
425	ZN3ARS2	1.5686E-49	2.8184E-28	-48.8045	-27.5500	5.5656E-22	-21.25449	-28.99714
426	ARSENOLI	2.0146-121	1.5849E-03	-120.6958	-2.8000	1.2712-118	-117.89580	-160.84324
427	CLAUDETI	2.0146-121	8.7096E-04	-120.6958	-3.0600	2.3131-118	-117.63580	-160.48852
428	ORPIMENT							
429	REALGAR							
430	SENARMON	6.5613E-39	7.7625E-11	-38.1830	-10.1100	8.4525E-29	-28.07301	-38.29953
431	VALENTIN	6.5613E-39	3.0903E-09	-38.1830	-8.5100	2.1232E-30	-29.67301	-40.48239
432	SB2O5	2.2016E-29	3.9811E-08	-28.6573	-7.4000	5.5301E-22	-21.25727	-29.00093
433	SB(OH)3	1.2345E+19	4.1687E-05	19.0915	-4.3800	2.9615E+23	23.47151	32.02178
434	STIBNITE							
435	CR(OH)3	2.4255E+09	9.1201E+11	9.3848	11.9600	2.6595E-03	-2.57520	-3.51330
436	ALASO4W2	4.4476E-31	1.4454E-16	-30.3519	-15.8400	3.0770E-15	-14.51188	-19.79830
437	CA3ASO42	3.0143E-33	1.2589E-19	-32.5208	-18.9000	2.3943E-14	-13.62082	-18.58265
438	FEASO4W2	7.8172E-32	5.6234E-21	-31.1069	-20.2500	1.3901E-11	-10.85695	-14.81195
439	MN3ASO42	5.3715E-53	1.9498E-29	-52.2699	-28.7100	2.7548E-24	-23.55990	-32.14237
440	HYDROZIN	6.3316E-86	6.3096E-74	-85.1985	-73.2000	1.0035E-12	-11.99849	-16.36933

EXEMPLE 2 :

EAU THERMOMINERALE CARBOGAZEUSE

TEST WATRA:SOURCE DOME (VICHY) dome

****
* SOLUTION INITIALE *
****

TEMPERATURE = 59.70DEGRES C PH = 6.93 SOMME DES CATIONS ANALYSES = 93.121
SOMME DES ANIONS ANALYSES = 89.289

***** OXYDATION-REDUCTION *****
OXYGENE DISSOUS = 1.57 MG/L
EH MESURE CALOMEL = 9.9000VOLTS
EH MEASURED OF ZOBELL SOLUTION = 9.9000VOLTS
EH CORRIGE = -0.0300VOLTS
PE COMPUTED FROM CORRECTED EH = -0.454

*** CONCENTRATION TOTALE DES ESPECES ANALYSEES ***

ESPECES		MOLALITE TOTALE	LOG MOLALITE TOTALE	CONCENTRATION EN MG/L
CA	2	1.230000E-03	-2.9101	4.893664E+01
MG	2	4.100000E-04	-3.3872	9.894775E+00
NA	1	8.661000E-02	-1.0624	1.976535E+03
K	1	2.414000E-03	-2.6173	9.369957E+01
CL	-1	9.700000E-03	-2.0132	3.413706E+02
SO4	-2	2.020000E-03	-2.6946	1.926205E+02
HCO3	-1	7.510000E-02	-1.1244	4.548773E+03
SIO2 TOT	0	9.150000E-04	-3.0386	5.457416E+01
FE	2	4.500000E-06	-5.3468	2.494674E-01
PO4	-3			
SR	2			
F	-1	4.200000E-04	-3.3768	7.920775E+00
ANAL H2S	0			
CO3	-2			
NH4	1	5.800000E-05	-4.2366	1.038561E+00
AL	3	2.600000E-06	-5.5850	6.963712E-02
LI	1	7.400000E-04	-3.1308	5.097180E+00
NO3	-1			
B TOT	0	1.894400E-04	-3.7225	2.032819E+00
BA	2			
BR	-1			
MN	2	1.050000E-06	-5.9788	5.726369E-02
CD+2	2	2.900000E-09	-8.5376	3.235681E-04
ZN+2	2	4.900000E-08	-7.3098	3.180112E-03
PB+2	2	1.800000E-08	-7.7447	3.702232E-03
CO+2	2	2.300000E-08	-7.6383	1.345144E-03
NI+2	2	6.000000E-08	-7.2218	3.496155E-03
CR+3	3	4.700000E-09	-8.3279	2.426066E-04
CU+2	2	2.500000E-08	-7.6021	1.577092E-03
ASO4-3	-3	9.500000E-06	-5.0223	1.310056E+00
SB(OH)3	0	3.600000E-08	-7.4437	6.174437E-03
GE(OH)4	0	2.200000E-07	-6.6576	3.071157E-02

**** DESCRIPTION DE LA SOLUTION ****

	ANALYSES	CALCULES
SOMME DES CATIONS	93.121	89.648
SOMME DES ANIONS	89.289	85.812

PH 6.930
TEMPERATURE 59.70 DEG C
FORCE IONIQUE 0.903617E-01

ACTIVITE DE H2O = 0.9968
PCO2 = 7.718707E-01
LOG PCO2 = -0.1125
PO2 = 1.661023E-47
PCH4 = 2.340026E-34
CO2 TOT = 8.753832E-02
DENSITE = 1.0000
TDS = 7284.2MG/L

EH = -.0300 PE = -0.454
PE CALC S = 1.000000E+02
PE CALC DOX = 1.093186E+01
PE SATO DOX = 0.337839E+01

BALANCE ELECTRIQUE= 0.383665E-02

EN CALCULANT LA DISTRIBUTION DES ESPECES: PE = -0.454 EH EQUIVALENT = -0.030VOLTS

DISTRIBUTION DES ESPECES

I	ESPECES		PPM	MOLALITE	LOG MOL	ACTIVITE	LOG ACT	COEFF. ACT.	LOG COEFF.
1	CA	2	2.51678E+01	6.32581E-04	-3.1989	2.39819E-04	-3.6201	3.79112E-01	-0.4212

2	MG	2	6.45227E+00	2.67357E-04	-3.5729	1.05471E-04	-3.9769	3.94197E-01	-0.4040
3	NA	1	1.91708E+03	8.40045E-02	-1.0757	6.51972E-02	-1.1858	7.76115E-01	-0.1101
4	K	1	9.30326E+01	2.39682E-03	-2.6204	1.81885E-03	-2.7402	7.58859E-01	-0.1198
64	H	1	1.51861E-04	1.51769E-07	-6.8188	1.17490E-07	-6.9300	7.74134E-01	-0.1112
5	CL	-1	3.40945E+02	9.68792E-03	-2.0138	7.35176E-03	-2.1336	7.58859E-01	-0.1198
6	SO4	-2	1.55667E+02	1.63247E-03	-2.7872	5.93047E-04	-3.2269	3.63282E-01	-0.4398
7	HCO3	-1	4.33944E+03	7.16439E-02	-1.1448	5.61028E-02	-1.2510	7.83079E-01	-0.1062
18	CO3	-2	5.47635E+00	9.19329E-05	-4.0365	3.45695E-05	-4.4613	3.76030E-01	-0.4248
86	H2CO3	0	7.90871E+02	1.28151E-02	-1.8913	1.31005E-02	-1.8827	1.01986E+00	0.0085
27	OH	-1	1.94513E-02	1.15215E-06	-5.9385	8.91919E-07	-6.0497	7.74134E-01	-0.1112
62	F	-1	7.71989E+00	4.09348E-04	-3.3879	3.16890E-04	-3.4991	7.74134E-01	-0.1112
98	BR	-1							
19	MGOH	1	1.22745E-03	2.99260E-08	-7.5240	2.31668E-08	-7.6351	7.74134E-01	-0.1112
23	MGSO4 AQ	0	1.58330E+00	1.32505E-05	-4.8778	1.35291E-05	-4.8687	1.02102E+00	0.0090
22	MGHCO3	1	9.91568E+00	1.17064E-04	-3.9316	9.06231E-05	-4.0428	7.74134E-01	-0.1112
21	MGCO3 AQ	0	4.86080E-01	5.80722E-06	-5.2360	5.92931E-06	-5.2270	1.02102E+00	0.0090
20	MGF	1	2.79108E-01	6.49200E-06	-5.1876	5.02568E-06	-5.2988	7.74134E-01	-0.1112
29	CAOH	1	1.84915E-04	8.55705E-09	-8.0677	6.62430E-09	-8.1789	7.74134E-01	-0.1112
32	CASO4 AQ	0	4.99284E+00	3.69450E-05	-4.4324	3.77218E-05	-4.4234	1.02102E+00	0.0090
30	CAHCO3	1	5.23156E+01	5.21303E-04	-3.2829	4.03559E-04	-3.3941	7.74134E-01	-0.1112
31	CACO3 AQ	0	3.71557E+00	3.73971E-05	-4.4272	3.81834E-05	-4.4181	1.02102E+00	0.0090
49	CAF+	1	1.03520E-01	1.76521E-06	-5.7532	1.36651E-06	-5.8644	7.74134E-01	-0.1112
44	NASO4	-1	3.75917E+01	3.18094E-04	-3.4974	2.46248E-04	-3.6086	7.74134E-01	-0.1112
43	NAHCO3	0	1.67962E+02	2.01455E-03	-2.6958	2.05690E-03	-2.6868	1.02102E+00	0.0090
42	NACO3	-1	2.13251E+01	2.58831E-04	-3.5870	2.00370E-04	-3.6982	7.74134E-01	-0.1112
94	NACL	0	6.80952E-01	1.17377E-05	-4.9304	1.19845E-05	-4.9214	1.02102E+00	0.0090
125	NAF	0	9.46303E-02	2.27040E-06	-5.6439	2.31813E-06	-5.6349	1.02102E+00	0.0090
46	KSO4	-1	2.25973E+00	1.68421E-05	-4.7736	1.30380E-05	-4.8848	7.74134E-01	-0.1112
95	KCL	0	2.52017E-02	3.40527E-07	-6.4678	3.47686E-07	-6.4588	1.02102E+00	0.0090
63	HSO4	-1	2.32715E-03	2.41513E-08	-7.6171	1.86964E-08	-7.7282	7.74134E-01	-0.1112
96	H2SO4	0	7.80592E-14	8.01776E-19	-18.0959	8.18633E-19	-18.0869	1.02102E+00	0.0090
93	HCL	0	6.44981E-10	1.78204E-14	-13.7491	1.81950E-14	-13.7400	1.02102E+00	0.0090
24	H4SIO4AQ	0	8.68172E+01	9.09936E-04	-3.0410	9.29067E-04	-3.0320	1.02102E+00	0.0090
25	H3SIO4	-1	4.77625E-01	5.05908E-06	-5.2959	3.91641E-06	-5.4071	7.74134E-01	-0.1112
26	H2SIO4	-2	4.55724E-04	4.87880E-09	-8.3117	1.75218E-09	-8.7564	3.59141E-01	-0.4447
14	H2S AQ	0							
67	HS	-1							
68	S	-2							
8	FE	2	4.35612E-02	7.85777E-07	-6.1047	2.82205E-07	-6.5494	3.59141E-01	-0.4447
9	FE	3	2.94439E-14	5.31121E-19	-18.2748	5.30323E-20	-19.2755	9.98498E-02	-1.0007
10	FEOH	2	1.96322E-09	2.71464E-14	-13.5663	9.74941E-15	-14.0110	3.59141E-01	-0.4447
11	FEOH	1	1.09807E-03	1.51834E-08	-7.8186	1.17540E-08	-7.9298	7.74134E-01	-0.1112
12	FE(OH)3	-1	2.73171E-08	2.57503E-13	-12.5892	1.99342E-13	-12.7004	7.74134E-01	-0.1112
77	FE(OH)2	1	5.52213E-09	6.19058E-14	-13.2083	4.79234E-14	-13.3195	7.74134E-01	-0.1112
78	FE(OH)3	0	1.68953E-08	1.59263E-13	-12.7979	1.62611E-13	-12.7888	1.02102E+00	0.0090
79	FE(OH)4	-1	1.04166E-09	8.47105E-15	-14.0721	6.55773E-15	-14.1832	7.74134E-01	-0.1112
80	FE(OH)2	0	7.27492E-07	8.15554E-12	-11.0885	8.32700E-12	-11.0795	1.02102E+00	0.0090
13	FEHPO4	1							
100	FEHPO4	0							
65	FEH2PO4	1							
99	FEH2PO4	2							
15	FESO4	1	2.45178E-13	1.62592E-18	-17.7889	1.25868E-18	-17.9001	7.74134E-01	-0.1112
16	FECL	2	1.12662E-14	1.21309E-19	-18.9055	1.46446E-20	-19.3502	3.59141E-01	-0.4447
28	FECL2	1	1.04971E-17	8.34272E-23	-22.0787	6.45839E-23	-22.1899	7.74134E-01	-0.1112
33	FECL3	0	7.38495E-21	4.58648E-26	-25.3385	4.68291E-26	-25.3295	1.02102E+00	0.0090
34	FESO4	0	4.32307E-03	2.86687E-08	-7.5426	2.92715E-08	-7.5336	1.02102E+00	0.0090
117	FE(HS)2	0							
118	FE(HS)3-	-1							
119	FE(SO4)2	-1	5.90896E-12	2.40055E-17	-16.6197	1.85835E-17	-16.7309	7.74134E-01	-0.1112
120	FEF+2	2	8.86057E-12	1.19261E-16	-15.9235	4.28315E-17	-16.3682	3.59141E-01	-0.4447
121	FEF2+	1	9.40859E-11	1.01000E-15	-14.9957	7.81876E-16	-15.1069	7.74134E-01	-0.1112
122	FEF3	0	4.78769E-11	4.27423E-16	-15.3691	4.36409E-16	-15.3601	1.02102E+00	0.0090
123	FECO3	0	4.35827E-03	3.78961E-08	-7.4214	3.86928E-08	-7.4124	1.02102E+00	0.0090

124	FEHCO3+	1	4.21389E-01	3.63247E-06	-5.4398	2.81202E-06	-5.5510	7.74134E-01	-0.1112
101	MN	2	1.83470E-02	3.36414E-07	-6.4731	1.20820E-07	-6.9179	3.59141E-01	-0.4447
102	MN	3	6.70871E-26	1.23013E-30	-29.9100	1.22828E-31	-30.9107	9.98498E-02	-1.0007
106	MNOH	1	2.79168E-05	3.91426E-10	-9.4074	3.03016E-10	-9.5185	7.74134E-01	-0.1112
107	MN(OH)3	-1	7.05115E-13	6.70348E-18	-17.1737	5.18940E-18	-17.2849	7.74134E-01	-0.1112
111	MNHCO3	1	5.24100E-02	4.55311E-07	-6.3417	3.52472E-07	-6.4529	7.74134E-01	-0.1112
109	MNSO4	0	1.02971E-03	6.86940E-09	-8.1631	7.01383E-09	-8.1540	1.02102E+00	0.0090
110	MN(NO3)2	0							
103	MNCL	1	4.16553E-04	4.64211E-09	-8.3333	3.59361E-09	-8.4445	7.74134E-01	-0.1112
104	MNCL2	0	8.78123E-07	7.02889E-12	-11.1531	7.17667E-12	-11.1441	1.02102E+00	0.0090
105	MNCL3	-1	4.91998E-09	3.07254E-14	-13.5125	2.37856E-14	-13.6237	7.74134E-01	-0.1112
108	MNF	1	2.56988E-05	3.50133E-10	-9.4558	2.71050E-10	-9.5670	7.74134E-01	-0.1112
112	MNO4	-1							
113	MNO4	-2							
115	HMNO2	-1	3.03080E-16	3.47160E-21	-20.4595	2.68749E-21	-20.5707	7.74134E-01	-0.1112
116	MNCO3	0	1.05559E-02	9.25088E-08	-7.0338	9.44537E-08	-7.0248	1.02102E+00	0.0090
51	AL	3	4.95604E-10	1.85041E-14	-13.7327	1.84763E-15	-14.7334	9.98498E-02	-1.0007
52	ALOH	2	2.83061E-07	6.48239E-12	-11.1883	2.32809E-12	-11.6330	3.59141E-01	-0.4447
53	AL(OH)2	1	1.97494E-04	3.26174E-09	-8.4866	2.52502E-09	-8.5977	7.74134E-01	-0.1112
54	AL(OH)4	-1	2.39614E-01	2.54061E-06	-5.5951	1.96677E-06	-5.7062	7.74134E-01	-0.1112
55	ALF	2	7.61425E-07	1.66824E-11	-10.7777	5.99133E-12	-11.2225	3.59141E-01	-0.4447
56	ALF2	1	2.93381E-03	4.51841E-08	-7.3421	3.52110E-08	-7.4533	7.74134E-01	-0.1112
57	ALF3	0	7.80362E-04	9.36129E-09	-8.0287	9.55811E-09	-8.0196	1.02102E+00	0.0090
58	ALF4	-1	1.29112E-04	1.26309E-09	-8.8986	9.77800E-10	-9.0097	7.74134E-01	-0.1112
59	ALSO4	1	4.09949E-10	3.35638E-15	-14.4741	2.59829E-15	-14.5853	7.74134E-01	-0.1112
60	AL(SO4)2	-1	3.94472E-11	1.81369E-16	-15.7414	1.40404E-16	-15.8526	7.74134E-01	-0.1112
45	PO4	-3							
47	HPO4	-2							
48	H2PO4	-1							
40	MGPO4	-1							
73	MGHPO4	0							
41	MGH2PO4	1							
75	CAPO4	-1							
74	CAHPO4	0							
76	CAH2PO4	1							
61	KHPO4	-1							
50	NAHPO4	-1							
36	H3BO3 AQ	0	1.14940E+01	1.87262E-04	-3.7275	1.91199E-04	-3.7185	1.02102E+00	0.0090
37	H2BO3	-1	1.31484E-01	2.17766E-06	-5.6620	1.68580E-06	-5.7732	7.74134E-01	-0.1112
85	NO3	-1							
38	NH3 AQ	0	3.08407E-02	1.82428E-06	-5.7389	1.86264E-06	-5.7299	1.02102E+00	0.0090
39	NH4	1	9.98269E-01	5.57498E-05	-4.2538	4.31578E-05	-4.3649	7.74134E-01	-0.1112
92	NH4SO4	-1	4.82415E-02	4.25925E-07	-6.3707	3.29723E-07	-6.4819	7.74134E-01	-0.1112
81	LI	1	5.08401E+00	7.38087E-04	-3.1319	5.71379E-04	-3.2431	7.74134E-01	-0.1112
82	LIOH	0	4.40027E-05	1.85113E-09	-8.7326	1.89005E-09	-8.7235	1.02102E+00	0.0090
83	LISO4	-1	1.95361E-01	1.91072E-06	-5.7188	1.47915E-06	-5.8300	7.74134E-01	-0.1112
88	SR	2							
89	SROH	1							
90	BA	2							
91	BAOH	1							

I	ESPECES		PPM	MOLALITE	LOG MOL	ACTIVITE	LOG ACT	COEFF. ACT.	MOLAL %
126	CD+2	2	6.66382E-05	5.97249E-10	-9.2238	2.14497E-10	-9.6686	3.59141E-01	20.594795
127	CDOH+	1	2.52695E-07	1.96710E-12	-11.7062	1.52280E-12	-11.8174	7.74134E-01	0.067831
128	CD(OH)2	0	8.80049E-10	6.05488E-15	-14.2179	6.18218E-15	-14.2089	1.02102E+00	0.000209
129	CD(OH)3-	-1	1.08927E-14	6.71433E-20	-19.1730	5.19779E-20	-19.2842	7.74134E-01	0.000000
130	CD(OH)4	-2	1.18807E-20	6.63298E-26	-25.1783	2.38218E-26	-25.6230	3.59141E-01	0.000000
131	CDCL+	1	3.16739E-05	2.15814E-10	-9.6659	1.67069E-10	-9.7771	7.74134E-01	7.441857
132	CDCL2	0	1.02302E-06	5.62236E-12	-11.2501	5.74057E-12	-11.2410	1.02102E+00	0.193875
133	CDCL3-	-1	1.19271E-08	5.49272E-14	-13.2602	4.25210E-14	-13.3714	7.74134E-01	0.001894
134	CDCL4-2	-2	6.33008E-11	2.50861E-16	-15.6006	9.00944E-17	-16.0453	3.59141E-01	0.000009
135	CDSO4	0	8.78666E-06	4.24619E-11	-10.3720	4.33547E-11	-10.3630	1.02102E+00	1.464204
136	CD(SO4)2	-2	1.74885E-07	5.78542E-13	-12.2377	2.07778E-13	-12.6824	3.59141E-01	0.019950

137	CD(SO4)3	-4	1.31558E-09	3.30817E-15	-14.4804	5.50414E-17	-16.2593	1.66365E-02	0.000114
138	CDF+	1	1.70061E-07	1.30379E-12	-11.8848	1.00931E-12	-11.9960	7.74134E-01	0.044958
139	CDF2	0	8.84012E-11	5.92119E-16	-15.2276	6.04568E-16	-15.2186	1.02102E+00	0.000020
140	CDOHCL	0	1.92935E-06	1.17895E-11	-10.9285	1.20374E-11	-10.9195	1.02102E+00	0.406535
141	CDCO3	0	2.84692E-05	1.66346E-10	-9.7790	1.69843E-10	-9.7700	1.02102E+00	5.736062
142	CD(CO3)3	-4	2.56604E-10	8.83974E-16	-15.0536	1.47062E-17	-16.8325	1.66365E-02	0.000030
143	CDHCO3+	1	3.19644E-04	1.85680E-09	-8.7312	1.43741E-09	-8.8424	7.74134E-01	64.027658
144	CDHS+	1							
145	CD(HS)2	0							
146	CD(HS)3-	-1							
147	CD(HS)4	-2							
148	ZN+2	2	4.62908E-04	7.13260E-09	-8.1468	2.56161E-09	-8.5915	3.59141E-01	14.556331
149	ZNOH+	1	2.42378E-05	2.96358E-10	-9.5282	2.29421E-10	-9.6394	7.74134E-01	0.604812
150	ZN(OH)2	0	8.93562E-06	9.05601E-11	-10.0431	9.24641E-11	-10.0340	1.02102E+00	0.184817
151	ZN(OH)3-	-1	1.67300E-09	1.44778E-14	-13.8393	1.12078E-14	-13.9505	7.74134E-01	0.000030
152	ZN(OH)4	-2	4.18233E-14	3.15788E-19	-18.5006	1.13413E-19	-18.9453	3.59141E-01	0.000000
153	ZNCL+	1	2.96300E-05	2.96033E-10	-9.5287	2.29170E-10	-9.6398	7.74134E-01	0.604150
154	ZNCL2	0	3.41192E-07	2.52212E-12	-11.5982	2.57514E-12	-11.5892	1.02102E+00	0.005147
155	ZNCL3-	-1	3.89961E-09	2.28756E-14	-13.6406	1.77088E-14	-13.7518	7.74134E-01	0.000047
156	ZNCL4-2	-2	4.67135E-11	2.27140E-16	-15.6437	8.15753E-17	-16.0884	3.59141E-01	0.000000
157	ZNSO4	0	6.93905E-05	4.33000E-10	-9.3635	4.42103E-10	-9.3545	1.02102E+00	0.883673
158	ZN(SO4)2	-2	2.73530E-06	1.07011E-11	-10.9706	3.84320E-12	-11.4153	3.59141E-01	0.021839
159	ZN(SO4)3	-4	5.64917E-09	1.60961E-14	-13.7933	2.67782E-16	-15.5722	1.66365E-02	0.000033
160	ZN(SO4)4	-6	2.15342E-13	4.82484E-19	-18.3165	4.79592E-23	-22.3191	9.94006E-05	0.000000
161	ZNF+	1	2.42111E-06	2.89050E-11	-10.5390	2.23764E-11	-10.6502	7.74134E-01	0.058990
162	ZNOHCL	0	6.37219E-06	5.44746E-11	-10.2638	5.56199E-11	-10.2548	1.02102E+00	0.111173
163	ZNCO3	0	6.70437E-04	5.38634E-09	-8.2687	5.49958E-09	-8.2597	1.02102E+00	10.992527
164	ZNHCO3+	1	4.42522E-03	3.52685E-08	-7.4526	2.73025E-08	-7.5638	7.74134E-01	71.976433
165	ZN(HS)2	0							
166	ZN(HS)3-	-1							
167	PB+2	2	2.18572E-05	1.06268E-10	-9.9736	3.81654E-11	-10.4183	3.59141E-01	0.590380
168	PBOH+	1	1.20771E-05	5.42634E-11	-10.2655	4.20071E-11	-10.3767	7.74134E-01	0.301463
169	PB(OH)2	0	1.21058E-07	5.05568E-13	-12.2962	5.16198E-13	-12.2872	1.02102E+00	0.002809
170	PB(OH)3-	-1	8.35991E-11	3.26132E-16	-15.4866	2.52470E-16	-15.5978	7.74134E-01	0.000002
171	PBCL+	1	7.17319E-06	2.97804E-11	-10.5261	2.30540E-11	-10.6373	7.74134E-01	0.165447
172	PBCL2	0	4.45599E-08	1.61414E-13	-12.7921	1.64808E-13	-12.7830	1.02102E+00	0.000897
173	PBCL3-	-1	4.58090E-10	1.47178E-15	-14.8322	1.13935E-15	-14.9433	7.74134E-01	0.000008
174	PBCL4-2	-2	5.02727E-12	1.45113E-17	-16.8383	5.21160E-18	-17.2830	3.59141E-01	0.000000
175	PBSO4	0	3.92832E-06	1.30494E-11	-10.8844	1.33237E-11	-10.8754	1.02102E+00	0.072497
176	PB(SO4)2	-2	8.08381E-04	2.03936E-09	-8.6905	7.32418E-10	-9.1352	3.59141E-01	11.329772
177	PBF+	1	4.66920E-07	2.07945E-12	-11.6821	1.60977E-12	-11.7932	7.74134E-01	0.011553
178	PBF2	0	2.40311E-09	9.87305E-15	-14.0055	1.00806E-14	-13.9965	1.02102E+00	0.000055
179	PBF3-	-1	1.08222E-12	4.12648E-18	-17.3844	3.19445E-18	-17.4956	7.74134E-01	0.000000
180	PBF4-2	-2	3.79258E-16	1.34909E-21	-20.8700	4.84513E-22	-21.3147	3.59141E-01	0.000000
181	PBCO3	0	2.64053E-03	9.95489E-09	-8.0020	1.01642E-08	-7.9929	1.02102E+00	55.304928
182	PB(CO3)2	-2	1.80066E-03	5.54359E-09	-8.2562	1.99093E-09	-8.7009	3.59141E-01	30.797718
183	PBHCO3+	1	6.81725E-05	2.56045E-10	-9.5917	1.98213E-10	-9.7029	7.74134E-01	1.422473
184	PB(HS)2	0							
185	PB(HS)3-	-1							
186	CO+2	2	1.93509E-04	3.30798E-09	-8.4804	1.18803E-09	-8.9252	3.59141E-01	14.382517
187	COOH+	1	2.35099E-06	3.11874E-11	-10.5060	2.41432E-11	-10.6172	7.74134E-01	0.135597
188	CO(OH)2	0	9.52071E-08	1.03185E-12	-11.9864	1.05355E-12	-11.9773	1.02102E+00	0.004486
189	CO(OH)3-	-1	2.09205E-12	1.91662E-17	-16.7175	1.48372E-17	-16.8286	7.74134E-01	0.000000
190	CO(OH)4	-2	5.07790E-19	4.02886E-24	-23.3948	1.44693E-24	-23.8396	3.59141E-01	0.000000
191	COCL+	1	4.30347E-06	4.59344E-11	-10.3379	3.55594E-11	-10.4490	7.74134E-01	0.199715
192	COSO4	0	2.65578E-05	1.72619E-10	-9.7629	1.76248E-10	-9.7539	1.02102E+00	0.750516
193	COF+	1	8.16157E-07	1.05504E-11	-10.9767	8.16741E-12	-11.0879	7.74134E-01	0.045871
194	COCO3	0	3.62914E-04	3.07379E-09	-8.5123	3.13842E-09	-8.5033	1.02102E+00	13.364321
195	COHCO3+	1	1.94761E-03	1.63569E-08	-7.7863	1.26624E-08	-7.8975	7.74134E-01	71.116976
196	NI+2	2	4.07606E-04	6.99521E-09	-8.1552	2.51227E-09	-8.5999	3.59141E-01	11.658679
197	NIOH+	1	3.22177E-06	4.28687E-11	-10.3679	3.31861E-11	-10.4790	7.74134E-01	0.071448
198	NI(OH)2	0	8.60447E-08	9.34866E-13	-12.0293	9.54521E-13	-12.0202	1.02102E+00	0.001558
199	NI(OH)3-	-1	1.76006E-11	1.61585E-16	-15.7916	1.25088E-16	-15.9028	7.74134E-01	0.000000

200	NI(OH)4	-2	3.89933E-18	3.09938E-23	-22.5087	1.11312E-23	-22.9535	3.59141E-01	0.000000
201	NICL+	1	1.17021E-05	1.25211E-10	-9.9024	9.69298E-11	-10.0135	7.74134E-01	0.208684
202	NICL2	0	1.56034E-07	1.21287E-12	-11.9162	1.23837E-12	-11.9072	1.02102E+00	0.002021
203	NISO4	0	5.71118E-05	3.71763E-10	-9.4297	3.79579E-10	-9.4207	1.02102E+00	0.619605
204	NI(SO4)2	-2	9.70830E-07	3.89924E-12	-11.4090	1.40038E-12	-11.8538	3.59141E-01	0.006499
205	NIF+	1	2.13607E-06	2.76944E-11	-10.5576	2.14392E-11	-10.6688	7.74134E-01	0.046157
206	NICO3	0	2.05199E-03	1.74135E-08	-7.7591	1.77796E-08	-7.7501	1.02102E+00	29.022484
207	NIHCO3+	1	4.16156E-03	3.50177E-08	-7.4557	2.71084E-08	-7.5669	7.74134E-01	58.362864
208	CR+3	3	3.47349E-09	6.72917E-14	-13.1720	6.71906E-15	-14.1727	9.98498E-02	0.001432
209	CROH+2	2	6.01419E-06	8.77938E-11	-10.0565	3.15304E-11	-10.5013	3.59141E-01	1.867954
210	CR(OH)2+	1	3.33172E-04	3.90182E-09	-8.4087	3.02053E-09	-8.5199	7.74134E-01	83.017448
211	CR(OH)3	0	7.09096E-05	6.93330E-10	-9.1591	7.07907E-10	-9.1500	1.02102E+00	14.751695
212	CR(OH)4-	-1	1.60528E-06	1.34717E-11	-10.8706	1.04289E-11	-10.9818	7.74134E-01	0.286633
213	CRCL+2	2	4.97733E-11	5.73370E-16	-15.2416	2.05921E-16	-15.6863	3.59141E-01	0.000012
214	CRCL2+	1	7.37274E-14	6.04332E-19	-18.2187	4.67834E-19	-18.3299	7.74134E-01	0.000000
215	CRSO4+	1	4.92128E-08	3.34841E-13	-12.4752	2.59212E-13	-12.5863	7.74134E-01	0.007124
216	CRF+2	2	8.68467E-08	1.23224E-12	-11.9093	4.42547E-13	-12.3540	3.59141E-01	0.026218
217	CRF2+	1	1.58984E-07	1.77955E-12	-11.7997	1.37761E-12	-11.8609	7.74134E-01	0.037863
218	CRF3	0	1.84174E-08	1.70216E-13	-12.7690	1.73794E-13	-12.7600	1.02102E+00	0.003622
219	CU+2	2	9.76272E-08	1.54758E-12	-11.8103	5.55801E-13	-12.2551	3.59141E-01	0.006190
220	CUOH+	1	4.03825E-08	5.04978E-13	-12.2967	3.90920E-13	-12.4079	7.74134E-01	0.002020
221	CU(OH)2	0	1.11575E-09	1.15199E-14	-13.9385	1.17621E-14	-13.9295	1.02102E+00	0.000046
222	CU(OH)3-	-1	2.27932E-12	2.00398E-17	-16.6981	1.55135E-17	-16.8093	7.74134E-01	0.000000
223	CU(OH)4	-2	2.68413E-16	2.05484E-21	-20.6872	7.37979E-22	-21.1320	3.59141E-01	0.000000
224	CUCL+	1	2.48827E-09	2.53199E-14	-13.5965	1.96010E-14	-13.7077	7.74134E-01	0.000101
225	CUCL2	0	4.90843E-12	3.67774E-17	-16.4344	3.75506E-17	-16.4254	1.02102E+00	0.000000
226	CUCL3-	-1	2.74383E-15	1.62691E-20	-19.7886	1.25944E-20	-19.8998	7.74134E-01	0.000000
227	CUCL4-2	-2	5.10913E-19	2.65357E-24	-23.5762	9.53008E-25	-24.0209	3.59141E-01	0.000000
228	CUSO4	0	1.29437E-08	8.16951E-14	-13.0878	8.34127E-14	-13.0788	1.02102E+00	0.000327
229	CUF+	1	8.20953E-10	1.00184E-14	-13.9992	7.75562E-15	-14.1104	7.74134E-01	0.000040
230	CUCO3	0	8.07129E-06	6.58057E-11	-10.1817	6.71892E-11	-10.1727	1.02102E+00	0.263223
231	CU(CO3)2	-2	1.65061E-05	9.05818E-11	-10.0430	3.25317E-11	-10.4877	3.59141E-01	0.362327
232	CUHCO3+	1	9.51261E-07	7.69281E-12	-11.1139	5.95527E-12	-11.2251	7.74134E-01	0.030771
233	CU+	1	9.04323E-05	1.43353E-09	-8.8436	1.10975E-09	-8.9548	7.74134E-01	5.734121
234	CUCL2-	-1	3.03710E-03	2.27560E-08	-7.6429	1.76162E-08	-7.7541	7.74134E-01	91.024159
235	CUCL3-2	-2	1.08641E-04	6.44168E-10	-9.1910	2.31348E-10	-9.6357	3.59141E-01	2.576674
236	CU(HS)3-	-1							
237	ASO4-3	-3	1.74564E-04	1.26587E-09	-8.8976	1.26396E-10	-9.8983	9.98498E-02	0.013325
238	H3ASO4	0	7.40528E-06	5.25539E-11	-10.2794	5.36588E-11	-10.2704	1.02102E+00	0.000553
239	H2ASO4	-1	3.52796E-01	2.52167E-06	-5.5983	1.95211E-06	-5.7095	7.74134E-01	26.543852
240	HASO4	-2	8.44867E-01	6.08241E-06	-5.2159	2.18445E-06	-5.6607	3.59141E-01	64.025408
241	ASO3-3	-3	4.25971E-13	3.49105E-18	-17.4570	3.48581E-19	-18.4577	9.98498E-02	0.000000
242	AS(OH)4-	-1	1.76905E-03	1.24659E-08	-7.9043	9.65028E-09	-8.0155	7.74134E-01	0.131220
243	AS(OH)3	0	1.10290E-01	8.82136E-07	-6.0545	9.00682E-07	-6.0454	1.02102E+00	9.285642
244	SB(OH)3	0	6.17269E-03	3.59898E-08	-7.4438	3.67465E-08	-7.4348	1.02102E+00	99.971777
245	SBOH+2	2	1.99312E-08	1.28898E-13	-12.8898	4.62928E-14	-13.3345	3.59141E-01	0.000358
246	SB(OH)4-	-1	1.88986E-06	1.00313E-11	-10.9986	7.76555E-12	-11.1098	7.74134E-01	0.027865
247	SB(OH)5	0	1.73814E-18	8.46707E-24	-23.0723	8.64508E-24	-23.0632	1.02102E+00	0.000000
248	SB(OH)6-	-1	4.02378E-14	1.81114E-19	-18.7420	1.40207E-19	-18.8532	7.74134E-01	0.000000
249	GE(OH)4	0	3.05436E-02	2.18797E-07	-6.6600	2.23397E-07	-6.6509	1.02102E+00	99.453187
250	GEO(OH)3	-1	1.66729E-04	1.20299E-09	-8.9197	9.31274E-10	-9.0309	7.74134E-01	0.546813

RAPPORTS MOLAIRES POUR LA MOLALITE ANALYTIQUE

CL/CA = 7.8862E+00
CL/MG = 2.3659E+01
CL/NA = 1.1200E-01
CL/K = 4.0182E+00
CL/AL = 3.7308E+03
CL/FE = 2.1556E+03
CL/SO4 = 4.8020E+00
CL/HCO3 = 1.2916E-01
CA/MG = 3.0000E+00
NA/K = 3.5878E+01

RAPPORTS MOLAIRES POUR LA MOLALITE CALCULEE

CL/CA = 1.5315E+01
CL/MG = 3.6236E+01
CL/NA = 1.1533E-01
CL/K = 4.0420E+00
CL/AL = 5.2356E+11
CL/FE = 1.2329E+04
CL/SO4 = 5.9345E+00
CL/HCO3 = 1.3522E-01
CA/MG = 2.3661E+00
NA/K = 3.5048E+01

RAPPORTS DES LOG D'ACTIVITE

LOG CA/H2 = 10.2399
LOG MG/H2 = 9.8831
LOG NA/H1 = 5.7442
LOG K/H1 = 4.1898
LOG AL/H3 = 6.0566
LOG FE/H2 = 7.3106
LOG CA/MG = 0.3567
LOG NA/K = 1.5544

NA/LI= 1.1704E+02 NA/LI= 1.1381E+02

ESPECE	CITOT/FETOT	CITOT/TDS
CD	0.6444E-03	0.3981E-12
ZN	0.1089E-01	0.6727E-11
PB	0.4000E-02	0.2471E-11
CO	0.5111E-02	0.3158E-11
NI	0.1333E-01	0.8237E-11
CR	0.1044E-02	0.6452E-12
CU	0.5556E-02	0.3432E-11
AS	0.2111E+01	0.1304E-08
SB	0.8000E-02	0.4942E-11
GE	0.4889E-01	0.3020E-10
MN	0.2333E+00	0.1441E-09

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* SATURATION MINERALE *
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	PHASE	IAP	KT	LOG IAP	LOG KT	IAP/KT	LOG IAP/KT	DEG DE SATURATION
40	ADULAIRE	2.9435E-18	6.0958E-19	-17.5311	-18.2150	4.8288E+00	0.68384	1.04153
41	ALBITE	1.0551E-16	9.5230E-17	-15.9767	-16.0212	1.1080E+00	0.04453	0.06781
141	ALOH3A	1.3110E-33	2.4132E-31	-32.8824	-30.6174	5.4324E-03	-2.26501	-3.44974
51	ALUNITE	2.0313E-90	9.0911E-84	-89.6922	-83.0414	2.2344E-07	-6.65084	-10.12963
43	ANALCIME	1.1248E-13	4.9109E-12	-12.9489	-11.3088	2.2903E-02	-1.64010	-2.49797
18	ANHYDRIT	1.4222E-07	1.4588E-05	-6.8470	-4.8360	9.7493E-03	-2.01103	-3.06291
114	ANNITE	3.3520E-74	3.4217E-80	-73.4747	-79.4658	9.7964E+05	5.99106	9.12474
42	ANORTHIT	8.2160E-22	1.0221E-18	-21.0853	-17.9905	8.0381E-04	-3.09485	-4.71363
22	ARAGONIT	8.2904E-09	3.6216E-09	-8.0814	-8.4411	2.2892E+00	0.35968	0.54782
151	ARTINITE	1.5665E-24	4.3456E-19	-23.8051	-18.3619	3.6047E-06	-5.44313	-8.29021
145	BARITE							
49	BEIDEL							
53	BOEHMITE	1.3152E-33	3.1600E-33	-32.8810	-32.5003	4.1620E-01	-0.38070	-0.57983
20	BRUCITE	8.3905E-17	4.5180E-12	-16.0762	-11.3450	1.8571E-05	-4.73116	-7.20584
13	CALCITE	8.2904E-09	1.5224E-09	-8.0814	-8.8175	5.4458E+00	0.73606	1.12107
144	CELESTIT							
98	CALCEDON	9.3506E-04	6.7553E-04	-3.0292	-3.1704	1.3842E+00	0.14120	0.21505
50	CHLORITE	1.6745E-89	3.7527E-87	-88.7761	-86.4257	4.4623E-03	-2.35044	-3.57986
21	CHRYSOTL	5.1813E-55	2.0316E-50	-54.2856	-49.6922	2.5504E-05	-4.59340	-6.99602
30	CLENSTIT	7.8709E-20	4.3657E-17	-19.1040	-16.3599	1.8029E-03	-2.74403	-4.17932
57	CLINOP	3.6220E-22	1.0000E+00	-21.4410	0.0000	3.6220E-22	-21.44105	-32.65598
100	CRISTOBA	9.3506E-04	6.8276E-04	-3.0292	-3.1657	1.3695E+00	0.13657	0.20801
29	DIOPSIDE	1.4086E-38	2.4677E-35	-37.8512	-34.6077	5.7082E-04	-3.24350	-4.94005
12	DOLOMITE	3.0228E-17	2.2210E-18	-16.5196	-17.6535	1.3610E+01	1.13386	1.72694
56	ERIONITE	3.1954E-18	1.0000E+00	-17.4955	0.0000	3.1954E-18	-17.49547	-26.64663
113	FEOH3A	3.2385E+01	7.6736E+04	1.5104	4.8850	4.2204E-04	-3.37465	-5.13979
120	FESPPT							
97	FLUAPT							
63	FLUORITE	2.4083E-11	4.1391E-11	-10.6183	-10.3831	5.8182E-01	-0.23521	-0.35824
28	FORSTRIT	6.6253E-36	1.8286E-28	-35.1788	-27.7379	3.6231E-08	-7.44092	-11.33296
52	GIBCRS	1.3110E-33	2.1661E-32	-32.8824	-31.6643	6.0521E-02	-1.21810	-1.85523
111	GOETHITE	3.7750E-38	5.6587E-40	-37.4231	-39.2473	6.6711E+01	1.82420	2.77836
112	GREENALI	9.9249E-63	6.4565E-64	-62.0033	-63.1900	1.5372E+01	1.18673	1.80745
119	GREGITE							
19	GYPSE	1.4131E-07	1.8237E-05	-6.8498	-4.7391	7.7488E-03	-2.11076	-3.21482
65	HALITE	4.7931E-04	4.4890E+01	-3.3194	1.6521	1.0678E-05	-4.97153	-7.57193
48	HALLOYSI	4.7139E-32	3.9274E-30	-31.3266	-29.4059	1.2003E-02	-1.92072	-2.92537
109	HEMATITE	1.0590E+03	4.3258E-07	3.0249	-6.3639	2.4481E+09	9.38883	14.29974
118	HUNTITE	4.0185E-34	3.3237E-33	-33.3959	-32.4784	1.2090E-01	-0.91756	-1.39749
39	HYDMAG	4.0279E-42	1.6981E-40	-41.3949	-39.7700	2.3720E-02	-1.62488	-2.47478
96	HYXAPT							
46	ILLITE	2.1140E-35	7.3881E-37	-34.6749	-36.1315	2.8614E+01	1.45657	2.21845
47	KAOLINIT	4.7139E-32	7.0092E-34	-31.3266	-33.1543	6.7253E+01	1.82771	2.78372
44	KMICA	1.5921E-43	1.2455E-44	-42.7980	-43.9047	1.2783E+01	1.10662	1.68545
129	LAUMONTI	7.0918E-28	1.1660E-29	-27.1492	-28.9333	6.0822E+01	1.78406	2.71723

148	LEONHARD	5.0455E-55	2.0533E-63	-54.2971	-62.6875	2.4572E+08	8.39045	12.77915
68	MACKIT							
99	MAGARITE	9.5213E-18	5.0119E-15	-17.0213	-14.3000	1.8998E-03	-2.72130	-4.14470
110	MAGHEMIT	1.0590E+03	2.3442E+06	3.0249	6.3700	4.5174E-04	-3.34511	-5.09480
11	MAGNESIT	3.6461E-09	1.3141E-09	-8.4382	-8.8814	2.7747E+00	0.44322	0.67504
108	MAGNETIT	3.2846E-02	2.1285E-13	-1.4835	-12.6719	1.5431E+11	11.18841	17.04060
64	MONTCA	1.3470E-39	2.8868E-41	-38.8706	-40.5396	4.6662E+01	1.66897	2.54193
116	MONTBF	3.1324E-27	1.0715E-35	-26.5041	-34.9700	2.9233E+08	8.46588	12.89403
117	MONTAB	9.2505E-24	1.6596E-30	-23.0338	-29.7800	5.5740E+06	6.74616	10.27480
58	MORDENIT	1.1864E-20	1.0000E+00	-19.9258	0.0000	1.1864E-20	-19.92577	-30.34812
67	MIRABILI	2.4411E-06	2.1769E+00	-5.6124	0.3378	1.1213E-06	-5.95026	-9.06260
59	NAHCOLIT	3.6577E-03	5.8379E-01	-2.4368	-0.2337	6.2656E-03	-2.20304	-3.35536
61	NATRON	1.4229E-07	7.8003E-01	-6.8468	-0.1079	1.8242E-07	-6.73893	-10.26379
150	NESQUHO	3.6111E-09	2.7622E-06	-8.4424	-5.5588	1.3073E-03	-2.88361	-4.39191
55	PHILIST	1.7567E-17	1.3804E-20	-16.7553	-19.8600	1.2726E+03	3.10469	4.72862
45	PHLOGOPI	1.7499E-66	2.9512E-64	-65.7570	-63.5300	5.9295E-03	-2.22698	-3.39183
142	PREHNITE	1.3261E-14	1.8790E-11	-13.8774	-10.7261	7.0578E-04	-3.15133	-4.79966
115	PYRITE							
54	PYROPHYL	4.1348E-38	3.7154E-43	-37.3835	-42.4300	1.1129E+05	5.04646	7.68605
102	QUARTZ	9.3506E-04	2.9531E-04	-3.0292	-3.5297	3.1663E+00	0.50056	0.76238
37	SEPIOLIT	5.7279E-42	8.4600E-39	-41.2420	-38.0726	6.7706E-04	-3.16937	-4.82714
10	SIDERITE	9.7557E-12	1.1038E-11	-11.0107	-10.9571	8.8386E-01	-0.05362	-0.08166
101	SILGEL	9.3506E-04	2.1002E-03	-3.0292	-2.6777	4.4522E-01	-0.35143	-0.53525
147	STRENGIT							
143	STRONTIA							
38	TALC	4.5448E-61	1.4240E-59	-60.3425	-58.8465	3.1915E-02	-1.49601	-2.27851
66	THENARDI	2.5209E-06	5.9881E-01	-5.5985	-0.2227	4.2097E-06	-5.37574	-8.18758
62	THRNAT	1.4647E-07	8.1450E-01	-6.8342	-0.0891	1.7983E-07	-6.74514	-10.27324
32	TREMOLIT	9.0179-137	3.9223-134	-136.0449	-133.4065	2.2992E-03	-2.63843	-4.01848
60	TRONA	5.3404E-10	6.7543E-03	-9.2724	-2.1704	7.9067E-08	-7.10201	-10.81678
107	VIVIANIT							
146	WITHERIT							
154	SEP PT	5.7279E-42	6.1376E-38	-41.2420	-37.2120	9.3325E-05	-4.03000	-6.13793
155	DIASPORE	1.3152E-33	5.7925E-37	-32.8810	-36.2371	2.2705E+03	3.35612	5.11157
156	WAIRAKIT	7.1375E-28	2.3846E-25	-27.1465	-24.6226	2.9932E-03	-2.52387	-3.84400
172	MANGANO	8.7246E+06	1.2653E+16	6.9407	16.1022	6.8952E-10	-9.16145	-13.95343
173	PYROLUST	2.2505E-04	4.2785E+13	-3.6477	13.6313	5.2601E-18	-17.27901	-26.31695
174	RIRNESIT	2.2505E-04	1.2331E+18	-3.6477	18.0910	1.8251E-22	-21.73872	-33.10935
175	NUSTITE	2.2505E-04	3.1915E+17	-3.6477	17.5040	7.0515E-22	-21.15172	-32.21531
176	BIXBYITE	5.6807E-21	1.6753E-02	-20.2456	-1.7759	3.3909E-19	-18.46969	-28.13042
177	HAUSMANI	5.9209E+33	2.6081E+55	33.7724	55.4163	2.2702E-22	-21.64393	-32.96498
178	MNOH2	9.6115E-20	2.5194E-13	-19.0172	-12.5987	3.8151E-07	-6.41850	-9.77575
179	MNOH3	8.7151E-50	7.7826E-35	-49.0597	-34.1089	1.1198E-15	-14.95085	-22.77102
180	MANGANIT	7.5250E-11	5.7810E-01	-10.1235	-0.2380	1.3017E-10	-9.88550	-15.05619
181	RHODOCHR	4.1767E-12	2.0051E-11	-11.3792	-10.6979	2.0830E-01	-0.68131	-1.03767
183	MNCL2	6.5301E-12	2.5910E+07	-11.1851	7.4135	2.5204E-19	-18.59854	-28.32667
184	MNCL2,1W	6.5092E-12	9.4133E+04	-11.1865	4.9737	6.9149E-17	-16.16022	-24.61296
185	MNCL2,2W	6.4883E-12	1.2725E+04	-11.1879	4.1047	5.0988E-16	-15.29254	-23.29143
186	MNCL2,4W	6.4467E-12	1.0916E+04	-11.1907	4.0380	5.9059E-16	-15.22871	-23.19422
187	TEPHRITE	7.1175E+10	1.1506E+20	10.8523	20.0609	6.1859E-10	-9.20860	-14.02523
188	RHODONIT	9.8565E-04	7.0748E+07	-3.0063	7.8497	1.3932E-11	-10.85599	-16.53432
189	MNS GRN							
190	MNSO4	7.1652E-11	3.0629E+01	-10.1448	1.4861	2.3393E-12	-11.63091	-17.71456
191	MN2SO4,3	3.1468E-72	2.0153E-09	-71.5021	-8.6957	1.5615E-63	-62.80647	-95.65795
192	MN3PO4,2							
193	MNHPO4							
319	OTAVITE	7.4151E-15	1.6432E-14	-14.1299	-13.7843	4.5127E-01	-0.34557	-0.52632
320	CDCL2	1.5769E-12	9.5156E-02	-11.8022	-1.0216	1.6572E-11	-10.78062	-16.41953
321	CDCL2,W	1.1593E-14	1.4156E-02	-13.9358	-1.8491	8.1898E-13	-12.08673	-18.40879
322	CDCL25/2	1.1593E-14	1.5512E-02	-13.9358	-1.8093	7.4738E-13	-12.12646	-18.46931
323	CDF2	2.1540E-17	1.8935E-04	-16.6668	-3.7227	1.1375E-13	-12.94403	-19.71452
324	CD(OH)2A	1.5539E+04	1.3897E+12	4.1914	12.1429	1.1182E-08	-7.95150	-12.11060
325	CD(OH)2C	1.5539E+04	4.4668E+13	4.1914	13.6500	3.4787E-10	-9.45858	-14.40597

326	CDOHCL	1.3422E-05	8.7953E+02	-4.8722	2.9540	1.4921E-08	-7.82620	-11.91977
327	CD3OH4SO	3.0715E-05	3.6308E+22	-4.5126	22.5600	8.4596E-28	-27.07265	-41.23324
328	CD3OH2SO	2.5144E-22	5.1286E+06	-21.5996	6.7100	4.9028E-29	-28.30956	-43.11712
329	CD3OH6SO	4.7728E-01	2.5119E+28	-0.3212	28.4000	1.9001E-29	-28.72123	-43.74412
330	MONTEPON	1.5539E+04	1.6906E+13	4.1914	13.2280	9.1916E-10	-9.03661	-13.76329
331	CDSIO3	1.4437E+01	6.1555E+07	1.1595	7.7893	2.3453E-07	-6.62980	-10.09757
332	CDSO4	1.2721E-13	5.9386E-02	-12.8955	-1.2263	2.1420E-12	-11.66917	-17.77284
333	CDSO4,W	2.7648E+06	5.8261E-03	6.4417	-2.2346	4.7456E+08	8.67629	13.21450
334	CDSO48/3	1.2721E-13	6.3303E-03	-12.8955	-2.1986	2.0095E-11	-10.69692	-16.29203
335	ZDCL2	1.3845E-13	4.9467E+05	-12.8587	5.6943	2.7989E-19	-18.55302	-28.25734
336	SMITHSON	8.8554E-14	4.6435E-11	-13.0528	-10.3332	1.9071E-03	-2.71964	-4.14216
337	ZNCO3,W	8.8554E-14	5.4954E-11	-13.0528	-10.2600	1.6114E-03	-2.79279	-4.25359
338	ZN(OH)2A	1.8557E+05	2.8184E+12	5.2685	12.4500	6.5844E-08	-7.18149	-10.93783
339	ZN(OH)2C	1.8557E+05	1.5849E+12	5.2685	12.2000	1.1709E-07	-6.93149	-10.55706
340	ZN(OH)2B	1.8557E+05	5.6234E+11	5.2685	11.7500	3.3900E-07	-6.48149	-9.87169
341	ZN(OH)2G	1.8557E+05	5.1286E+11	5.2685	11.7100	3.6184E-07	-6.44149	-9.81076
342	ZN(OH)2E	1.8557E+05	3.1623E+11	5.2685	11.5000	5.8683E-07	-6.23149	-9.49092
343	ZN2OH3CL	2.9745E+01	1.5849E+15	1.4734	15.2000	1.8768E-14	-13.72658	-20.90639
344	ZN5OH8CL	1.6419E+08	3.1623E+38	8.2154	38.5000	5.1922E-31	-30.28465	-46.12530
345	ZN2OH2SO	2.8191E-07	3.1623E+07	-6.5499	7.5000	8.9149E-15	-14.04988	-21.39880
346	ZN4OH6SO	9.7083E+03	2.5119E+28	3.9871	28.4000	3.8649E-25	-24.41286	-37.18222
347	ZNNO326W							
348	ZNO ACT	1.8557E+05	2.0417E+11	5.2685	11.3100	9.0889E-07	-6.04149	-9.20154
349	ZNO CRYS	1.8557E+05	2.9487E+09	5.2685	9.4696	6.2934E-05	-4.20111	-6.39854
350	ZN3OSO42	4.2827E-19	1.9162E+14	-18.3683	14.2824	2.2350E-33	-32.65072	-49.72896
351	ZNS AM							
352	SPHALERI							
353	WURTZITE							
354	ZNSIO3	1.7241E+02	3.4194E+01	2.2366	1.5339	5.0421E+00	0.70261	1.07012
355	WILLEMIT	3.1994E+07	6.0273E+12	7.5051	12.7801	5.3083E-06	-5.27505	-8.03421
356	ZINCOSIT	1.5192E-12	3.4905E+01	-11.8184	1.5429	4.3523E-14	-13.36128	-20.35002
357	ZNSO4,W	1.5192E-12	4.1397E-02	-11.8184	-1.3830	3.6697E-11	-10.43537	-15.89368
358	BIANCHIT	1.5192E-12	1.6702E-02	-11.8184	-1.7772	9.0955E-11	-10.04117	-15.29329
359	GOSLARIT	1.5192E-12	1.9596E-02	-11.8184	-1.7078	7.7525E-11	-10.11056	-15.39897
360	COTUNNIT	2.0628E-15	4.5489E-05	-14.6855	-4.3421	4.5346E-11	-10.34346	-15.75369
361	MATLOCKI	8.8914E-17	1.5048E-09	-16.0510	-8.8225	5.9087E-08	-7.22851	-11.00944
362	PHOSGENI	2.7215E-30	1.5488E-20	-29.5652	-19.8100	1.7572E-10	-9.75518	-14.85772
363	CERRUSIT	1.3194E-15	1.7433E-13	-14.8796	-12.7586	7.5683E-03	-2.12100	-3.23041
364	PBF2	3.8325E-18	3.2100E-08	-17.4165	-7.4935	1.1939E-10	-9.92302	-15.11335
365	MASSICOT	2.7648E+03	4.2443E+11	3.4417	11.6278	6.5143E-09	-8.18613	-12.46796
366	LITHARGE	2.7648E+03	2.9401E+11	3.4417	11.4684	9.4038E-09	-8.02670	-12.22513
367	PBO,W/3	2.7648E+03	9.5499E+12	3.4417	12.9800	2.8951E-10	-9.53833	-14.52744
368	PB2OCO3	3.6478E-12	4.2103E-02	-11.4380	-1.3757	8.6640E-11	-10.06228	-15.32545
369	LARNAKIT	6.2579E-11	1.6901E-01	-10.2036	-0.7721	3.7027E-10	-9.43148	-14.36469
370	PB3O2SO4	1.7302E-07	6.5230E+08	-6.7619	8.8144	2.6525E-16	-15.57635	-23.72369
371	PB4O3SO4	4.7837E-04	2.6316E+19	-3.3202	19.4202	1.8178E-23	-22.74045	-34.63505
372	PBHPO4							
373	PB3O2CO3	1.0086E-08	1.0010E+09	-7.9963	9.0004	1.0076E-17	-16.99672	-25.88701
374	PBSIO3	2.5687E+00	4.0966E+06	0.4097	6.6124	6.2704E-07	-6.20271	-9.44709
375	PB2SIO4	7.1021E+03	5.9331E+17	3.8514	17.7733	1.1970E-14	-13.92189	-21.20386
376	ANGLESIT	2.2634E-14	2.3675E-08	-13.6452	-7.6257	9.5603E-07	-6.01953	-9.16809
377	GALENE							
378	PLATTNER	2.4730E+16	7.8588E+43	16.3932	43.8954	3.1468E-28	-27.50213	-41.88737
379	PB2O3	6.8374E+19	1.0965E+61	19.8349	61.0400	6.2358E-42	-41.20511	-62.75780
380	PB(OH)2	2.7648E+03	1.2050E+07	3.4417	7.0810	2.2944E-04	-3.63932	-5.54290
381	LAURIONI	2.3881E-06	4.1776E+00	-5.6219	0.6230	5.6893E-07	-6.24494	-9.51141
382	PB2OH3CL	6.6028E-03	6.1660E+08	-2.1803	8.7900	1.0709E-11	-10.97027	-16.70837
383	HYDCERRU	4.8128E-27	3.4674E-18	-26.3176	-17.4600	1.3880E-09	-8.85760	-13.49065
384	PB2OOH2	7.6443E+06	1.5849E+26	6.8833	26.2000	4.8232E-20	-19.31666	-29.42041
385	PB4OH4SO	4.7837E-04	1.2589E+21	-3.3202	21.1000	3.7999E-25	-24.42023	-37.19345
386	MELANOTH	3.0040E-17	6.1461E+02	-16.5223	2.7886	4.8877E-20	-19.31090	-29.41163
387	CUCO3	1.9214E-17	2.3442E-10	-16.7164	-9.6300	8.1962E-08	-7.08639	-10.79298
388	CUF2	5.5813E-20	4.2873E-01	-19.2533	-0.3678	1.3018E-19	-18.88545	-28.76365

389	CUF2,2W	5.5813E-20	1.4928E-05	-19.2533	-4.8289	3.7639E-15	-14.42436	-21.96915
390	CU(OH)2	4.0264E+01	2.9834E+07	1.6049	7.4747	1.3496E-06	-5.86979	-8.94004
391	MALACHIT	1.0686E-05	4.3661E+03	-4.9712	3.6401	2.4475E-09	-8.61127	-13.11547
392	AZURITE	2.8361E-12	2.4612E+01	-11.5473	1.3912	1.1523E-13	-12.93842	-19.70598
393	ATACAMIT	1.4003E-06	8.1631E+05	-5.8538	5.9119	1.7154E-12	-11.76562	-17.91974
394	ANTLERIT	5.3438E-13	1.9498E+08	-12.2722	8.2900	2.7406E-21	-20.56215	-31.31737
395	CU2OH3NO							
396	BROCHANT	2.1516E-11	2.1878E+15	-10.6672	15.3400	9.8348E-27	-26.00723	-39.61055
397	LANGITE	2.1516E-11	5.7984E+13	-10.6672	13.7633	3.7107E-25	-24.43054	-37.20915
398	TENORITE	4.0264E+01	2.8541E+06	1.6049	6.4555	1.4107E-05	-4.85056	-7.38768
399	CU2OSO4	2.3879E-02	6.7189E+08	-1.6220	8.8273	3.5540E-11	-10.44929	-15.91488
400	CUSO4	3.2962E-16	4.2061E+01	-15.4820	1.6239	7.8366E-18	-17.10587	-26.05325
401	CHALCAN	3.2962E-16	2.9514E-03	-15.4820	-2.5300	1.1168E-13	-12.95202	-19.72670
402	CUPRIFER	4.3053E+04	8.3870E+02	4.6340	2.9236	5.1333E+01	1.71039	2.60503
403	NICO3	8.6848E-14	2.5146E-08	-13.0612	-7.5995	3.4538E-06	-5.46170	-8.31849
404	NI(OH)2	1.8200E+05	1.8050E+09	5.2601	9.2565	1.0083E-04	-3.99641	-6.08676
405	NI4OH4SO	8.9816E+03	1.0000E+32	3.9534	32.0000	8.9816E-29	-28.04665	-42.71669
406	BUNSENIT	1.8200E+05	4.1900E+10	5.2601	10.6222	4.3436E-06	-5.36215	-8.16687
407	RETGERSI	1.4899E-12	1.1068E-02	-11.8268	-1.9559	1.3462E-10	-9.87090	-15.03396
408	MORENOSI	1.4899E-12	7.3224E-03	-11.8268	-2.1353	2.0347E-10	-9.69150	-14.76072
409	NI2SIO4	3.0774E+07	9.7923E+11	7.4882	11.9909	3.1426E-05	-4.50271	-6.85789
410	NISO4	1.4899E-12	6.8970E+02	-11.8268	2.8387	2.1602E-15	-14.66551	-22.33643
411	COO	8.6065E+04	5.1718E+11	4.9348	11.7136	1.6641E-07	-6.77882	-10.32454
412	COOH2PIN	8.6065E+04	3.1627E+11	4.9348	11.5001	2.7213E-07	-6.56523	-9.99923
413	COOH2TRA	8.6065E+04	2.2387E+12	4.9348	12.3500	3.8444E-08	-7.41517	-11.29374
414	JAIPURIT							
415	COSO4	7.0456E-13	2.4918E+01	-12.1521	1.3965	2.8276E-14	-13.54859	-20.63530
416	COSO4,W	7.0456E-13	1.0553E-02	-12.1521	-1.9766	6.6763E-11	-10.17547	-15.49783
417	COSO4,6W	7.0456E-13	7.1158E-03	-12.1521	-2.1478	9.9013E-11	-10.00431	-15.23715
418	BIEBERIT	7.0456E-13	5.6225E-39	-12.1521	-38.2501	1.2531E+26	26.09799	39.74878
419	COCO3	4.1070E-14	7.1060E-11	-13.3865	-10.1484	5.7796E-04	-3.23810	-4.93182
420	CO3ARS8W	2.6789E-47	9.5499E-29	-46.5720	-28.0200	2.8051E-19	-18.55205	-28.25586
421	AS2O5	2.8793E-21	1.9381E+06	-20.5407	6.2874	1.4856E-27	-26.82809	-40.86076
422	CU3ARS6W	2.7430E-57	7.5858E-36	-56.5618	-35.1200	3.6160E-22	-21.44177	-32.65708
423	NI3ARS8W	2.5332E-46	3.0903E-26	-45.5963	-25.5100	8.1972E-21	-20.08633	-30.59267
424	PB3ARS2	8.8813E-52	3.9811E-36	-51.0515	-35.4000	2.2309E-16	-15.65152	-23.83819
425	ZN3ARS2	2.6854E-46	2.8184E-28	-45.5710	-27.5500	9.5282E-19	-18.02099	-27.44703
426	ARSENOLI	6.5809E-25	1.9724E-02	-24.1817	-1.7050	3.3366E-23	-22.47670	-34.23334
427	CLAUDETI	6.5809E-25	9.0265E-03	-24.1817	-2.0445	7.2907E-23	-22.13723	-33.71631
428	ORPIMENT							
429	REALGAR							
430	SENARMON	1.3503E-15	2.8141E-10	-14.8696	-9.5507	4.7984E-06	-5.31891	-8.10101
431	VALENTIN	1.3503E-15	6.8693E-09	-14.8696	-8.1631	1.9657E-07	-6.70648	-10.21436
432	SB2O5	7.4737E-47	3.9811E-08	-46.1265	-7.4000	1.8773E-39	-38.72646	-58.98268
433	SB(OH)3	2.7213E+07	1.4797E-04	7.4348	-3.8298	1.8391E+11	11.26462	17.15667
434	STIBNITE							
435	CR(OH)3	4.1429E+06	1.7904E+10	6.6173	10.2529	2.3140E-04	-3.63564	-5.53729
436	ALASO4W2	2.3353E-25	1.4454E-16	-24.6317	-15.8400	1.6157E-09	-8.79165	-13.39020
437	CA3ASO42	2.2035E-31	1.2589E-19	-30.6569	-18.9000	1.7503E-12	-11.75688	-17.90642
438	FEASO4W2	6.7031E-30	5.6234E-21	-29.1737	-20.2500	1.1920E-09	-8.92372	-13.59136
439	MN3ASO42	2.8177E-41	1.9498E-29	-40.5501	-28.7100	1.4451E-12	-11.84011	-18.03318
440	HYDROZIN	6.6360E-89	6.3096E-74	-88.1781	-73.2000	1.0517E-15	-14.97809	-22.81252

*** CONVERGENCE DES ITERATIONS ***

	ITERATION	S1-CO2ATM	S2-SO4TOT	S3-PTOT	S4-PTOT	S5-CLTOT
ITER 2	ITMIN 1	XMAX 0.51700E-10	IMAX 1			
ITER 3	ITMIN 1	XMAX 0.42443E-12	IMAX 6			
ITER 4	ITMIN 1	XMAX 0.14806E-12	IMAX 1			
ITER 5	ITMIN 1	XMAX 0.52229E-15	IMAX 1			
ITER 6	ITMIN 1	XMAX 0.30415E-15	IMAX 1			

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