Supplementary Materials

Hydrogeochemical Modeling to Identify Potential Risks of Underground Hydrogen Storage in Depleted Gas Fields

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Input file S1 for the transport model to calculate the reference scenario (for PHREEQC Version 3.1.4-8929; ready to copy, paste, and run.)

```
DATABASE phreeqc.dat
TITLE reference_scenario_UHS


SOLUTION_MASTER_SPECIES
Tracer          Tracer          0.0     1.0     1.0
Hydrogengas     Hydrogengas     0.0     1.0     1.0

SOLUTION_SPECIES
Tracer = Tracer
        -log_k          0.0
        #-delta_h -4.184 kJ
        #-analytic      -9.3114         4.6473e-3       -49.335         1.4341          1.2815e5
        #-T_c 33.2
        #-P_c 12.80
        #-Omega -0.225
        -dw     1.0e-9

Hydrogengas = Hydrogengas
        -log_k  0.0
        -gamma  5.0   0.1650
        -dw     0.793e-9
        -millero -19.69 0.1058 -0.001256 1.617 -0.075 0.0008262

PHASES
Dawsonite                                                       # from llnl.dat
    NaAlCO3(OH)2 +3.0000 H+ = + 1.0000 Al+++ + 1.0000 HCO3- + 1.0000 Na+ + 2.0000 H2O
    log_k               4.3464
    -delta_H            -76.3549        kJ/mol
# Enthalpy of formation: -1963.96 kJ/mol
    -analytic -1.1393e+002 -2.3487e-002 7.1758e+003 4.0900e+001 1.2189e+002
#-Range: 0-200

Hydrogengas(g)                                                  # = H2(g) from phreeqc.dat
Hydrogengas = Hydrogengas
    -log_k          -3.1050
    -delta_h -4.184 kJ
    -analytic       -9.3114         4.6473e-3       -49.335         1.4341          1.2815e5
    -T_c 33.2
    -P_c 12.80
    -Omega 0.225



Selected_Output
-file reference_scenario_UHS.xls
-temperature true
-totals C(4) C(-4) Tracer H(0) S(6) S(-2) Hydrogengas Na Cl N N(-3)
-equilibrium_phases K-feldspar Albite Kaolinite Quartz Calcite Pyrite Illite Barite Goethite Dawsonite Mackinawite Dolomite Anhydrite Gypsum Halite Sulfur
```

```
-kinetics H2
-gases CO2(g) CH4(g) H2S(g) H2(g) Hydrogengas(g) N2(g)
-water
-charge_balance true
-ionic_strength true

Rates

            H2
            -start
10 if (m < 0) then goto 70
20 rate = 2.3e-09*(TOT("C(4)")/1e-3 + TOT("C(4)")) + 9.26e-8*(TOT("S(6)")/(1.e-4 + TOT("S(6)")))
30 moles = rate * TIME
40 if (moles > m) then moles = m
70 SAVE moles
          -end

SOLUTION    1                                                    # cap rock
-temperature  33.994
-pH 6.377
-pe -3.391
units mol/kgw
Al    1.31E-007
Ba    5.85E-007
C     3.11E-002
Ca    3.63E-002
Cl    1.27E+000
Fe    5.69E-002
K     5.28E-001
Mg    8.73E-004
N     5.61E-002
Na    1.27E+000
S     1.01E+000
Si    8.73E-005
REACTION_TEMPERATURE     1
33.994
REACTION_PRESSURE      1
21.8
GAS_PHASE 1
-fixed_pressure
-pressure21.8
-temperature  33.994
-volume  3
Hydrogengas(g)    21.7
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    2
-temperature  34.027
-pH 6.377
-pe -3.391
```

```
units mol/kgw
Al   1.31E-007
Ba   5.85E-007
C    3.11E-002
Ca   3.63E-002
Cl   1.27E+000
Fe   5.69E-002
K    5.28E-001
Mg   8.73E-004
N    5.61E-002
Na   1.27E+000
S    1.01E+000
Si   8.73E-005
REACTION_TEMPERATURE    2
34.027
REACTION_PRESSURE     2
21.9
GAS_PHASE 2
-fixed_pressure
-pressure21.9
-temperature  34.027
-volume  3
Hydrogengas(g)    21.8
CO2(g)   0.0
CH4(g)   0.0
H2S(g)   0.0
#
SOLUTION   3
-temperature  34.06
-pH 6.377
-pe -3.391
units mol/kgw
Al   1.31E-007
Ba   5.85E-007
C    3.11E-002
Ca   3.63E-002
Cl   1.27E+000
Fe   5.69E-002
K    5.28E-001
Mg   8.73E-004
N    5.61E-002
Na   1.27E+000
S    1.01E+000
Si   8.73E-005
REACTION_TEMPERATURE    3
34.06
REACTION_PRESSURE     3
22
GAS_PHASE 3
-fixed_pressure
-pressure22
-temperature  34.06
```

```
-volume 3
Hydrogengas(g)  21.8
CO2(g)  0.0
CH4(g)  0.0
H2S(g)  0.0
#
SOLUTION  4
-temperature 34.093
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE  4
34.093
REACTION_PRESSURE  4
22.1
GAS_PHASE 4
-fixed_pressure
-pressure22.1
-temperature 34.093
-volume 3
Hydrogengas(g)  21.8
CO2(g)  0.0
CH4(g)  0.0
H2S(g)  0.0
#
SOLUTION  5
-temperature 34.126
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
```

```
S     1.01E+000
Si    8.73E-005
REACTION_TEMPERATURE     5
34.126
REACTION_PRESSURE      5
22.2
GAS_PHASE 5
-fixed_pressure
-pressure22.2
-temperature  34.126
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    6
-temperature  34.159
-pH 6.377
-pe -3.391
units mol/kgw
Al    1.31E-007
Ba    5.85E-007
C     3.11E-002
Ca    3.63E-002
Cl    1.27E+000
Fe    5.69E-002
K     5.28E-001
Mg  8.73E-004
N     5.61E-002
Na    1.27E+000
S     1.01E+000
Si    8.73E-005
REACTION_TEMPERATURE     6
34.159
REACTION_PRESSURE      6
22.3
GAS_PHASE 6
-fixed_pressure
-pressure22.3
-temperature  34.159
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    7
-temperature  34.192
-pH 6.377
-pe -3.391
units mol/kgw
```

```
Al   1.31E-007
Ba   5.85E-007
C    3.11E-002
Ca   3.63E-002
Cl   1.27E+000
Fe   5.69E-002
K    5.28E-001
Mg   8.73E-004
N    5.61E-002
Na   1.27E+000
S    1.01E+000
Si   8.73E-005
REACTION_TEMPERATURE    7
34.192
REACTION_PRESSURE     7
22.4
GAS_PHASE 7
-fixed_pressure
-pressure22.4
-temperature  34.192
-volume  3
Hydrogengas(g)    21.8
CO2(g)   0.0
CH4(g)   0.0
H2S(g)   0.0
#
SOLUTION   8
-temperature  34.225
-pH 6.377
-pe -3.391
units mol/kgw
Al   1.31E-007
Ba   5.85E-007
C    3.11E-002
Ca   3.63E-002
Cl   1.27E+000
Fe   5.69E-002
K    5.28E-001
Mg   8.73E-004
N    5.61E-002
Na   1.27E+000
S    1.01E+000
Si   8.73E-005
REACTION_TEMPERATURE    8
34.225
REACTION_PRESSURE     8
22.5
GAS_PHASE 8
-fixed_pressure
-pressure22.5
-temperature  34.225
-volume  3
```

```
Hydrogengas(g)  21.8
CO2(g)  0.0
CH4(g)  0.0
H2S(g)  0.0
#
SOLUTION  9
-temperature  34.258
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE  9
34.258
REACTION_PRESSURE  9
22.6
GAS_PHASE 9
-fixed_pressure
-pressure22.6
-temperature  34.258
-volume  3
Hydrogengas(g)  21.8
CO2(g)  0.0
CH4(g)  0.0
H2S(g)  0.0
#
SOLUTION  10
-temperature  34.291
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
```

```
Si    8.73E-005
REACTION_TEMPERATURE    10
34.291
REACTION_PRESSURE    10
22.7
GAS_PHASE 10
-fixed_pressure
-pressure22.7
-temperature  34.291
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    11
-temperature  34.324
-pH 6.377
-pe -3.391
units mol/kgw
Al    1.31E-007
Ba    5.85E-007
C    3.11E-002
Ca    3.63E-002
Cl    1.27E+000
Fe    5.69E-002
K    5.28E-001
Mg    8.73E-004
N    5.61E-002
Na    1.27E+000
S    1.01E+000
Si    8.73E-005
REACTION_TEMPERATURE    11
34.324
REACTION_PRESSURE    11
22.8
GAS_PHASE 11
-fixed_pressure
-pressure22.8
-temperature  34.324
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    12
-temperature  34.357
-pH 6.377
-pe -3.391
units mol/kgw
Al    1.31E-007
```

Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 12
34.357
REACTION_PRESSURE 12
22.9
GAS_PHASE 12
-fixed_pressure
-pressure22.9
-temperature 34.357
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 13
-temperature 34.39
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 13
34.39
REACTION_PRESSURE 13
23
GAS_PHASE 13
-fixed_pressure
-pressure23
-temperature 34.39
-volume 3
Hydrogengas(g) 21.8

```
CO2(g)  0.0
CH4(g)  0.0
H2S(g)  0.0
#
SOLUTION  14
-temperature  34.423
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE  14
34.423
REACTION_PRESSURE  14
23.1
GAS_PHASE 14
-fixed_pressure
-pressure23.1
-temperature  34.423
-volume  3
Hydrogengas(g)  21.8
CO2(g)  0.0
CH4(g)  0.0
H2S(g)  0.0
#
SOLUTION  15
-temperature  34.456
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
```

```
REACTION_TEMPERATURE    15
34.456
REACTION_PRESSURE    15
23.2
GAS_PHASE 15
-fixed_pressure
-pressure23.2
-temperature  34.456
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    16
-temperature  34.489
-pH 6.377
-pe -3.391
units mol/kgw
Al    1.31E-007
Ba    5.85E-007
C    3.11E-002
Ca    3.63E-002
Cl    1.27E+000
Fe    5.69E-002
K    5.28E-001
Mg    8.73E-004
N    5.61E-002
Na    1.27E+000
S    1.01E+000
Si    8.73E-005
REACTION_TEMPERATURE    16
34.489
REACTION_PRESSURE    16
23.3
GAS_PHASE 16
-fixed_pressure
-pressure23.3
-temperature  34.489
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    17
-temperature  34.522
-pH 6.377
-pe -3.391
units mol/kgw
Al    1.31E-007
Ba    5.85E-007
```

C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 17
34.522
REACTION_PRESSURE 17
23.4
GAS_PHASE 17
-fixed_pressure
-pressure23.4
-temperature 34.522
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 18
-temperature 34.555
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 18
34.555
REACTION_PRESSURE 18
23.5
GAS_PHASE 18
-fixed_pressure
-pressure23.5
-temperature 34.555
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0

```
CH4(g)  0.0
H2S(g)  0.0
#
SOLUTION  19
-temperature  34.588
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE  19
34.588
REACTION_PRESSURE  19
23.6
GAS_PHASE 19
-fixed_pressure
-pressure23.6
-temperature  34.588
-volume  3
Hydrogengas(g)  21.8
CO2(g)  0.0
CH4(g)  0.0
H2S(g)  0.0
#
SOLUTION  20
-temperature  34.621
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE  20
```

```
34.621
REACTION_PRESSURE      20
23.7
GAS_PHASE 20
-fixed_pressure
-pressure23.7
-temperature  34.621
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    21
-temperature  34.654
-pH 6.377
-pe -3.391
units mol/kgw
Al    1.31E-007
Ba    5.85E-007
C     3.11E-002
Ca    3.63E-002
Cl    1.27E+000
Fe    5.69E-002
K     5.28E-001
Mg    8.73E-004
N     5.61E-002
Na    1.27E+000
S     1.01E+000
Si    8.73E-005
REACTION_TEMPERATURE     21
34.654
REACTION_PRESSURE      21
23.8
GAS_PHASE 21
-fixed_pressure
-pressure23.8
-temperature  34.654
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    22
-temperature  34.687
-pH 6.377
-pe -3.391
units mol/kgw
Al    1.31E-007
Ba    5.85E-007
C     3.11E-002
```

```
Ca   3.63E-002
Cl   1.27E+000
Fe   5.69E-002
K    5.28E-001
Mg   8.73E-004
N    5.61E-002
Na   1.27E+000
S    1.01E+000
Si   8.73E-005
REACTION_TEMPERATURE    22
34.687
REACTION_PRESSURE    22
23.9
GAS_PHASE 22
-fixed_pressure
-pressure23.9
-temperature  34.687
-volume  3
Hydrogengas(g)    21.8
CO2(g)   0.0
CH4(g)   0.0
H2S(g)   0.0
#
SOLUTION    23
-temperature  34.72
-pH 6.377
-pe -3.391
units mol/kgw
Al   1.31E-007
Ba   5.85E-007
C    3.11E-002
Ca   3.63E-002
Cl   1.27E+000
Fe   5.69E-002
K    5.28E-001
Mg   8.73E-004
N    5.61E-002
Na   1.27E+000
S    1.01E+000
Si   8.73E-005
REACTION_TEMPERATURE    23
34.72
REACTION_PRESSURE    23
24
GAS_PHASE 23
-fixed_pressure
-pressure24
-temperature  34.72
-volume  3
Hydrogengas(g)    21.8
CO2(g)   0.0
CH4(g)   0.0
```

```
H2S(g)  0.0
#
SOLUTION  24
-temperature  34.753
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE  24
34.753
REACTION_PRESSURE  24
24.1
GAS_PHASE 24
-fixed_pressure
-pressure24.1
-temperature  34.753
-volume  3
Hydrogengas(g)  21.8
CO2(g)  0.0
CH4(g)  0.0
H2S(g)  0.0
#
SOLUTION  25
-temperature  34.786
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE  25
34.786
```

```
REACTION_PRESSURE      25
24.2
GAS_PHASE 25
-fixed_pressure
-pressure24.2
-temperature  34.786
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    26
-temperature  34.819
-pH 6.377
-pe -3.391
units mol/kgw
Al    1.31E-007
Ba    5.85E-007
C     3.11E-002
Ca    3.63E-002
Cl    1.27E+000
Fe    5.69E-002
K     5.28E-001
Mg    8.73E-004
N     5.61E-002
Na    1.27E+000
S     1.01E+000
Si    8.73E-005
REACTION_TEMPERATURE     26
34.819
REACTION_PRESSURE      26
24.3
GAS_PHASE 26
-fixed_pressure
-pressure24.3
-temperature  34.819
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    27
-temperature  34.852
-pH 6.377
-pe -3.391
units mol/kgw
Al    1.31E-007
Ba    5.85E-007
C     3.11E-002
Ca    3.63E-002
```

```
Cl   1.27E+000
Fe   5.69E-002
K    5.28E-001
Mg   8.73E-004
N    5.61E-002
Na   1.27E+000
S    1.01E+000
Si   8.73E-005
REACTION_TEMPERATURE    27
34.852
REACTION_PRESSURE    27
24.4
GAS_PHASE 27
-fixed_pressure
-pressure24.4
-temperature  34.852
-volume  3
Hydrogengas(g)    21.8
CO2(g)   0.0
CH4(g)   0.0
H2S(g)   0.0
#
SOLUTION   28
-temperature  34.885
-pH 6.377
-pe -3.391
units mol/kgw
Al   1.31E-007
Ba   5.85E-007
C    3.11E-002
Ca   3.63E-002
Cl   1.27E+000
Fe   5.69E-002
K    5.28E-001
Mg   8.73E-004
N    5.61E-002
Na   1.27E+000
S    1.01E+000
Si   8.73E-005
REACTION_TEMPERATURE    28
34.885
REACTION_PRESSURE    28
24.5
GAS_PHASE 28
-fixed_pressure
-pressure24.5
-temperature  34.885
-volume  3
Hydrogengas(g)    21.8
CO2(g)   0.0
CH4(g)   0.0
H2S(g)   0.0
```

```
#
SOLUTION  29
-temperature  34.918
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE  29
34.918
REACTION_PRESSURE  29
24.6
GAS_PHASE 29
-fixed_pressure
-pressure24.6
-temperature  34.918
-volume  3
Hydrogengas(g)  21.8
CO2(g)  0.0
CH4(g)  0.0
H2S(g)  0.0
#
SOLUTION  30
-temperature  34.951
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE  30
34.951
REACTION_PRESSURE  30
```

```
24.7
GAS_PHASE 30
-fixed_pressure
-pressure24.7
-temperature  34.951
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    31
-temperature  34.984
-pH 6.377
-pe -3.391
units mol/kgw
Al    1.31E-007
Ba    5.85E-007
C     3.11E-002
Ca    3.63E-002
Cl    1.27E+000
Fe    5.69E-002
K     5.28E-001
Mg  8.73E-004
N     5.61E-002
Na    1.27E+000
S     1.01E+000
Si    8.73E-005
REACTION_TEMPERATURE     31
34.984
REACTION_PRESSURE      31
24.8
GAS_PHASE 31
-fixed_pressure
-pressure24.8
-temperature  34.984
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    32
-temperature  35.017
-pH 6.377
-pe -3.391
units mol/kgw
Al    1.31E-007
Ba    5.85E-007
C     3.11E-002
Ca    3.63E-002
Cl    1.27E+000
```

```
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE  32
35.017
REACTION_PRESSURE  32
24.9
GAS_PHASE 32
-fixed_pressure
-pressure24.9
-temperature  35.017
-volume  3
Hydrogengas(g)  21.8
CO2(g)  0.0
CH4(g)  0.0
H2S(g)  0.0
#
SOLUTION  33
-temperature  35.05
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE  33
35.05
REACTION_PRESSURE  33
25
GAS_PHASE 33
-fixed_pressure
-pressure25
-temperature  35.05
-volume  3
Hydrogengas(g)  21.8
CO2(g)  0.0
CH4(g)  0.0
H2S(g)  0.0
#
```

```
SOLUTION  34
-temperature  35.083
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE  34
35.083
REACTION_PRESSURE  34
25.1
GAS_PHASE 34
-fixed_pressure
-pressure25.1
-temperature  35.083
-volume  3
Hydrogengas(g)  21.8
CO2(g)  0.0
CH4(g)  0.0
H2S(g)  0.0
#
SOLUTION  35
-temperature  35.116
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE  35
35.116
REACTION_PRESSURE  35
25.2
```

GAS_PHASE 35
-fixed_pressure
-pressure25.2
-temperature 35.116
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 36
-temperature 35.149
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 36
35.149
REACTION_PRESSURE 36
25.3
GAS_PHASE 36
-fixed_pressure
-pressure25.3
-temperature 35.149
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 37
-temperature 35.182
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002

```
K    5.28E-001
Mg   8.73E-004
N    5.61E-002
Na   1.27E+000
S    1.01E+000
Si   8.73E-005
REACTION_TEMPERATURE    37
35.182
REACTION_PRESSURE    37
25.4
GAS_PHASE 37
-fixed_pressure
-pressure25.4
-temperature  35.182
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    38
-temperature  35.215
-pH 6.377
-pe -3.391
units mol/kgw
Al    1.31E-007
Ba    5.85E-007
C    3.11E-002
Ca    3.63E-002
Cl    1.27E+000
Fe    5.69E-002
K    5.28E-001
Mg   8.73E-004
N    5.61E-002
Na   1.27E+000
S    1.01E+000
Si   8.73E-005
REACTION_TEMPERATURE    38
35.215
REACTION_PRESSURE    38
25.5
GAS_PHASE 38
-fixed_pressure
-pressure25.5
-temperature  35.215
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    39
```

```
-temperature  35.248
-pH 6.377
-pe -3.391
units mol/kgw
Al   1.31E-007
Ba   5.85E-007
C    3.11E-002
Ca   3.63E-002
Cl   1.27E+000
Fe   5.69E-002
K    5.28E-001
Mg   8.73E-004
N    5.61E-002
Na   1.27E+000
S    1.01E+000
Si   8.73E-005
REACTION_TEMPERATURE    39
35.248
REACTION_PRESSURE     39
25.6
GAS_PHASE 39
-fixed_pressure
-pressure25.6
-temperature  35.248
-volume  3
Hydrogengas(g)   21.8
CO2(g)   0.0
CH4(g)   0.0
H2S(g)   0.0
#
SOLUTION   40
-temperature  35.281
-pH 6.377
-pe -3.391
units mol/kgw
Al   1.31E-007
Ba   5.85E-007
C    3.11E-002
Ca   3.63E-002
Cl   1.27E+000
Fe   5.69E-002
K    5.28E-001
Mg   8.73E-004
N    5.61E-002
Na   1.27E+000
S    1.01E+000
Si   8.73E-005
REACTION_TEMPERATURE    40
35.281
REACTION_PRESSURE     40
25.7
GAS_PHASE 40
```

-fixed_pressure
-pressure25.7
-temperature 35.281
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 41
-temperature 35.314
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 41
35.314
REACTION_PRESSURE 41
25.8
GAS_PHASE 41
-fixed_pressure
-pressure25.8
-temperature 35.314
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 42
-temperature 35.347
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001

```
Mg  8.73E-004
N   5.61E-002
Na  1.27E+000
S   1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE    42
35.347
REACTION_PRESSURE   42
25.9
GAS_PHASE 42
-fixed_pressure
-pressure25.9
-temperature  35.347
-volume  3
Hydrogengas(g)   21.8
CO2(g)   0.0
CH4(g)   0.0
H2S(g)   0.0
#
SOLUTION   43
-temperature  35.38
-pH 6.377
-pe -3.391
units mol/kgw
Al   1.31E-007
Ba   5.85E-007
C    3.11E-002
Ca   3.63E-002
Cl   1.27E+000
Fe   5.69E-002
K    5.28E-001
Mg  8.73E-004
N   5.61E-002
Na  1.27E+000
S   1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE    43
35.38
REACTION_PRESSURE   43
26
GAS_PHASE 43
-fixed_pressure
-pressure26
-temperature  35.38
-volume  3
Hydrogengas(g)   21.8
CO2(g)   0.0
CH4(g)   0.0
H2S(g)   0.0
#
SOLUTION   44
-temperature  35.413
```

-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 44
35.413
REACTION_PRESSURE 44
26.1
GAS_PHASE 44
-fixed_pressure
-pressure26.1
-temperature 35.413
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 45
-temperature 35.446
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 45
35.446
REACTION_PRESSURE 45
26.2
GAS_PHASE 45
-fixed_pressure

-pressure26.2
-temperature 35.446
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 46
-temperature 35.479
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 46
35.479
REACTION_PRESSURE 46
26.3
GAS_PHASE 46
-fixed_pressure
-pressure26.3
-temperature 35.479
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 47
-temperature 35.512
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004

N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 47
35.512
REACTION_PRESSURE 47
26.4
GAS_PHASE 47
-fixed_pressure
-pressure26.4
-temperature 35.512
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 48
-temperature 35.545
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 48
35.545
REACTION_PRESSURE 48
26.5
GAS_PHASE 48
-fixed_pressure
-pressure26.5
-temperature 35.545
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 49
-temperature 35.578
-pH 6.377

```
-pe -3.391
units mol/kgw
Al   1.31E-007
Ba   5.85E-007
C    3.11E-002
Ca   3.63E-002
Cl   1.27E+000
Fe   5.69E-002
K    5.28E-001
Mg   8.73E-004
N    5.61E-002
Na   1.27E+000
S    1.01E+000
Si   8.73E-005
REACTION_TEMPERATURE    49
35.578
REACTION_PRESSURE    49
26.6
GAS_PHASE 49
-fixed_pressure
-pressure26.6
-temperature  35.578
-volume  3
Hydrogengas(g)   21.8
CO2(g)   0.0
CH4(g)   0.0
H2S(g)   0.0
#
SOLUTION   50
-temperature  35.611
-pH 6.377
-pe -3.391
units mol/kgw
Al   1.31E-007
Ba   5.85E-007
C    3.11E-002
Ca   3.63E-002
Cl   1.27E+000
Fe   5.69E-002
K    5.28E-001
Mg   8.73E-004
N    5.61E-002
Na   1.27E+000
S    1.01E+000
Si   8.73E-005
REACTION_TEMPERATURE    50
35.611
REACTION_PRESSURE    50
26.7
GAS_PHASE 50
-fixed_pressure
-pressure26.7
```

-temperature 35.611
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 51
-temperature 35.644
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 51
35.644
REACTION_PRESSURE 51
26.8
GAS_PHASE 51
-fixed_pressure
-pressure26.8
-temperature 35.644
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 52
-temperature 35.677
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002

```
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE  52
35.677
REACTION_PRESSURE  52
26.9
GAS_PHASE 52
-fixed_pressure
-pressure26.9
-temperature  35.677
-volume  3
Hydrogengas(g)  21.8
CO2(g)  0.0
CH4(g)  0.0
H2S(g)  0.0
#
SOLUTION  53
-temperature  35.71
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE  53
35.71
REACTION_PRESSURE  53
27
GAS_PHASE 53
-fixed_pressure
-pressure27
-temperature  35.71
-volume  3
Hydrogengas(g)  21.8
CO2(g)  0.0
CH4(g)  0.0
H2S(g)  0.0
#
SOLUTION  54
-temperature  35.743
-pH 6.377
-pe -3.391
```

```
units mol/kgw
Al   1.31E-007
Ba   5.85E-007
C    3.11E-002
Ca   3.63E-002
Cl   1.27E+000
Fe   5.69E-002
K    5.28E-001
Mg   8.73E-004
N    5.61E-002
Na   1.27E+000
S    1.01E+000
Si   8.73E-005
REACTION_TEMPERATURE    54
35.743
REACTION_PRESSURE    54
27.1
GAS_PHASE 54
-fixed_pressure
-pressure27.1
-temperature  35.743
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    55
-temperature  35.776
-pH 6.377
-pe -3.391
units mol/kgw
Al   1.31E-007
Ba   5.85E-007
C    3.11E-002
Ca   3.63E-002
Cl   1.27E+000
Fe   5.69E-002
K    5.28E-001
Mg   8.73E-004
N    5.61E-002
Na   1.27E+000
S    1.01E+000
Si   8.73E-005
REACTION_TEMPERATURE    55
35.776
REACTION_PRESSURE    55
27.2
GAS_PHASE 55
-fixed_pressure
-pressure27.2
-temperature  35.776
```

-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 56
-temperature 35.809
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 56
35.809
REACTION_PRESSURE 56
27.3
GAS_PHASE 56
-fixed_pressure
-pressure27.3
-temperature 35.809
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 57
-temperature 35.842
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000

S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 57
35.842
REACTION_PRESSURE 57
27.4
GAS_PHASE 57
-fixed_pressure
-pressure27.4
-temperature 35.842
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 58
-temperature 35.875
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 58
35.875
REACTION_PRESSURE 58
27.5
GAS_PHASE 58
-fixed_pressure
-pressure27.5
-temperature 35.875
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 59
-temperature 35.908
-pH 6.377
-pe -3.391
units mol/kgw

Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 59
35.908
REACTION_PRESSURE 59
27.6
GAS_PHASE 59
-fixed_pressure
-pressure27.6
-temperature 35.908
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 60
-temperature 35.941
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 60
35.941
REACTION_PRESSURE 60
27.7
GAS_PHASE 60
-fixed_pressure
-pressure27.7
-temperature 35.941
-volume 3

Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 61
-temperature 35.974
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 61
35.974
REACTION_PRESSURE 61
27.8
GAS_PHASE 61
-fixed_pressure
-pressure27.8
-temperature 35.974
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 62
-temperature 36.007
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000

```
Si    8.73E-005
REACTION_TEMPERATURE    62
36.007
REACTION_PRESSURE    62
27.9
GAS_PHASE 62
-fixed_pressure
-pressure27.9
-temperature  36.007
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    63
-temperature  36.04
-pH 6.377
-pe -3.391
units mol/kgw
Al    1.31E-007
Ba    5.85E-007
C    3.11E-002
Ca    3.63E-002
Cl    1.27E+000
Fe    5.69E-002
K    5.28E-001
Mg    8.73E-004
N    5.61E-002
Na    1.27E+000
S    1.01E+000
Si    8.73E-005
REACTION_TEMPERATURE    63
36.04
REACTION_PRESSURE    63
28
GAS_PHASE 63
-fixed_pressure
-pressure28
-temperature  36.04
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    64
-temperature  36.073
-pH 6.377
-pe -3.391
units mol/kgw
Al    1.31E-007
```

Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 64
36.073
REACTION_PRESSURE 64
28.1
GAS_PHASE 64
-fixed_pressure
-pressure28.1
-temperature 36.073
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 65
-temperature 36.106
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 65
36.106
REACTION_PRESSURE 65
28.2
GAS_PHASE 65
-fixed_pressure
-pressure28.2
-temperature 36.106
-volume 3
Hydrogengas(g) 21.8

```
CO2(g)  0.0
CH4(g)  0.0
H2S(g)  0.0
#
SOLUTION  66
-temperature  36.139
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE  66
36.139
REACTION_PRESSURE  66
28.3
GAS_PHASE 66
-fixed_pressure
-pressure28.3
-temperature  36.139
-volume  3
Hydrogengas(g)  21.8
CO2(g)  0.0
CH4(g)  0.0
H2S(g)  0.0
#
SOLUTION  67
-temperature  36.172
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
```

```
REACTION_TEMPERATURE    67
36.172
REACTION_PRESSURE    67
28.4
GAS_PHASE 67
-fixed_pressure
-pressure28.4
-temperature  36.172
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    68
-temperature  36.205
-pH 6.377
-pe -3.391
units mol/kgw
Al    1.31E-007
Ba    5.85E-007
C    3.11E-002
Ca    3.63E-002
Cl    1.27E+000
Fe    5.69E-002
K    5.28E-001
Mg    8.73E-004
N    5.61E-002
Na    1.27E+000
S    1.01E+000
Si    8.73E-005
REACTION_TEMPERATURE    68
36.205
REACTION_PRESSURE    68
28.5
GAS_PHASE 68
-fixed_pressure
-pressure28.5
-temperature  36.205
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    69
-temperature  36.238
-pH 6.377
-pe -3.391
units mol/kgw
Al    1.31E-007
Ba    5.85E-007
```

C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 69
36.238
REACTION_PRESSURE 69
28.6
GAS_PHASE 69
-fixed_pressure
-pressure28.6
-temperature 36.238
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 70
-temperature 36.271
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 70
36.271
REACTION_PRESSURE 70
28.7
GAS_PHASE 70
-fixed_pressure
-pressure28.7
-temperature 36.271
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0

```
CH4(g)  0.0
H2S(g)  0.0
#
SOLUTION  71
-temperature  36.304
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE  71
36.304
REACTION_PRESSURE  71
28.8
GAS_PHASE 71
-fixed_pressure
-pressure28.8
-temperature  36.304
-volume  3
Hydrogengas(g)  21.8
CO2(g)  0.0
CH4(g)  0.0
H2S(g)  0.0
#
SOLUTION  72
-temperature  36.337
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE  72
```

```
36.337
REACTION_PRESSURE	72
28.9
GAS_PHASE 72
-fixed_pressure
-pressure28.9
-temperature  36.337
-volume  3
Hydrogengas(g)	21.8
CO2(g)	0.0
CH4(g)	0.0
H2S(g)	0.0
#
SOLUTION	73
-temperature  36.37
-pH 6.377
-pe -3.391
units mol/kgw
Al	1.31E-007
Ba	5.85E-007
C	3.11E-002
Ca	3.63E-002
Cl	1.27E+000
Fe	5.69E-002
K	5.28E-001
Mg	8.73E-004
N	5.61E-002
Na	1.27E+000
S	1.01E+000
Si	8.73E-005
REACTION_TEMPERATURE	73
36.37
REACTION_PRESSURE	73
29
GAS_PHASE 73
-fixed_pressure
-pressure29
-temperature  36.37
-volume  3
Hydrogengas(g)	21.8
CO2(g)	0.0
CH4(g)	0.0
H2S(g)	0.0
#
SOLUTION	74
-temperature  36.403
-pH 6.377
-pe -3.391
units mol/kgw
Al	1.31E-007
Ba	5.85E-007
C	3.11E-002
```

```
Ca   3.63E-002
Cl   1.27E+000
Fe   5.69E-002
K    5.28E-001
Mg   8.73E-004
N    5.61E-002
Na   1.27E+000
S    1.01E+000
Si   8.73E-005
REACTION_TEMPERATURE    74
36.403
REACTION_PRESSURE     74
29.1
GAS_PHASE 74
-fixed_pressure
-pressure29.1
-temperature  36.403
-volume  3
Hydrogengas(g)   21.8
CO2(g)   0.0
CH4(g)   0.0
H2S(g)   0.0
#
SOLUTION   75
-temperature  36.436
-pH 6.377
-pe -3.391
units mol/kgw
Al   1.31E-007
Ba   5.85E-007
C    3.11E-002
Ca   3.63E-002
Cl   1.27E+000
Fe   5.69E-002
K    5.28E-001
Mg   8.73E-004
N    5.61E-002
Na   1.27E+000
S    1.01E+000
Si   8.73E-005
REACTION_TEMPERATURE    75
36.436
REACTION_PRESSURE     75
29.2
GAS_PHASE 75
-fixed_pressure
-pressure29.2
-temperature  36.436
-volume  3
Hydrogengas(g)   21.8
CO2(g)   0.0
CH4(g)   0.0
```

```
H2S(g)  0.0
#
SOLUTION  76
-temperature  36.469
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE  76
36.469
REACTION_PRESSURE  76
29.3
GAS_PHASE 76
-fixed_pressure
-pressure29.3
-temperature  36.469
-volume  3
Hydrogengas(g)  21.8
CO2(g)  0.0
CH4(g)  0.0
H2S(g)  0.0
#
SOLUTION  77
-temperature  36.502
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE  77
36.502
```

```
REACTION_PRESSURE      77
29.4
GAS_PHASE 77
-fixed_pressure
-pressure29.4
-temperature  36.502
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    78
-temperature  36.535
-pH 6.377
-pe -3.391
units mol/kgw
Al    1.31E-007
Ba    5.85E-007
C     3.11E-002
Ca    3.63E-002
Cl    1.27E+000
Fe    5.69E-002
K     5.28E-001
Mg    8.73E-004
N     5.61E-002
Na    1.27E+000
S     1.01E+000
Si    8.73E-005
REACTION_TEMPERATURE     78
36.535
REACTION_PRESSURE      78
29.5
GAS_PHASE 78
-fixed_pressure
-pressure29.5
-temperature  36.535
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    79
-temperature  36.568
-pH 6.377
-pe -3.391
units mol/kgw
Al    1.31E-007
Ba    5.85E-007
C     3.11E-002
Ca    3.63E-002
```

```
Cl   1.27E+000
Fe   5.69E-002
K    5.28E-001
Mg   8.73E-004
N    5.61E-002
Na   1.27E+000
S    1.01E+000
Si   8.73E-005
REACTION_TEMPERATURE    79
36.568
REACTION_PRESSURE    79
29.6
GAS_PHASE 79
-fixed_pressure
-pressure29.6
-temperature  36.568
-volume  3
Hydrogengas(g)    21.8
CO2(g)   0.0
CH4(g)   0.0
H2S(g)   0.0
#
SOLUTION   80
-temperature  36.601
-pH 6.377
-pe -3.391
units mol/kgw
Al   1.31E-007
Ba   5.85E-007
C    3.11E-002
Ca   3.63E-002
Cl   1.27E+000
Fe   5.69E-002
K    5.28E-001
Mg   8.73E-004
N    5.61E-002
Na   1.27E+000
S    1.01E+000
Si   8.73E-005
REACTION_TEMPERATURE    80
36.601
REACTION_PRESSURE    80
29.7
GAS_PHASE 80
-fixed_pressure
-pressure29.7
-temperature  36.601
-volume  3
Hydrogengas(g)    21.8
CO2(g)   0.0
CH4(g)   0.0
H2S(g)   0.0
```

```
#
SOLUTION  81
-temperature  36.634
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE  81
36.634
REACTION_PRESSURE  81
29.8
GAS_PHASE 81
-fixed_pressure
-pressure29.8
-temperature  36.634
-volume  3
Hydrogengas(g)  21.8
CO2(g)  0.0
CH4(g)  0.0
H2S(g)  0.0
#
SOLUTION  82
-temperature  36.667
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE  82
36.667
REACTION_PRESSURE  82
```

```
29.9
GAS_PHASE 82
-fixed_pressure
-pressure29.9
-temperature  36.667
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    83
-temperature  36.7
-pH 6.377
-pe -3.391
units mol/kgw
Al    1.31E-007
Ba    5.85E-007
C     3.11E-002
Ca    3.63E-002
Cl    1.27E+000
Fe    5.69E-002
K     5.28E-001
Mg    8.73E-004
N     5.61E-002
Na    1.27E+000
S     1.01E+000
Si    8.73E-005
REACTION_TEMPERATURE     83
36.7
REACTION_PRESSURE      83
30
GAS_PHASE 83
-fixed_pressure
-pressure30
-temperature  36.7
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    84
-temperature  36.733
-pH 6.377
-pe -3.391
units mol/kgw
Al    1.31E-007
Ba    5.85E-007
C     3.11E-002
Ca    3.63E-002
Cl    1.27E+000
```

Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 84
36.733
REACTION_PRESSURE 84
30.1
GAS_PHASE 84
-fixed_pressure
-pressure30.1
-temperature 36.733
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 85
-temperature 36.766
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 85
36.766
REACTION_PRESSURE 85
30.2
GAS_PHASE 85
-fixed_pressure
-pressure30.2
-temperature 36.766
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#

```
SOLUTION  86
-temperature  36.799
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE  86
36.799
REACTION_PRESSURE  86
30.3
GAS_PHASE 86
-fixed_pressure
-pressure30.3
-temperature  36.799
-volume  3
Hydrogengas(g)  21.8
CO2(g)  0.0
CH4(g)  0.0
H2S(g)  0.0
#
SOLUTION  87
-temperature  36.832
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE  87
36.832
REACTION_PRESSURE  87
30.4
```

GAS_PHASE 87
-fixed_pressure
-pressure30.4
-temperature 36.832
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 88
-temperature 36.865
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 88
36.865
REACTION_PRESSURE 88
30.5
GAS_PHASE 88
-fixed_pressure
-pressure30.5
-temperature 36.865
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 89
-temperature 36.898
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002

K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 89
36.898
REACTION_PRESSURE 89
30.6
GAS_PHASE 89
-fixed_pressure
-pressure30.6
-temperature 36.898
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 90
-temperature 36.931
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 90
36.931
REACTION_PRESSURE 90
30.7
GAS_PHASE 90
-fixed_pressure
-pressure30.7
-temperature 36.931
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 91

```
-temperature  36.964
-pH 6.377
-pe -3.391
units mol/kgw
Al   1.31E-007
Ba   5.85E-007
C    3.11E-002
Ca   3.63E-002
Cl   1.27E+000
Fe   5.69E-002
K    5.28E-001
Mg   8.73E-004
N    5.61E-002
Na   1.27E+000
S    1.01E+000
Si   8.73E-005
REACTION_TEMPERATURE    91
36.964
REACTION_PRESSURE     91
30.8
GAS_PHASE 91
-fixed_pressure
-pressure30.8
-temperature  36.964
-volume  3
Hydrogengas(g)   21.8
CO2(g)   0.0
CH4(g)   0.0
H2S(g)   0.0
#
SOLUTION   92
-temperature  36.997
-pH 6.377
-pe -3.391
units mol/kgw
Al   1.31E-007
Ba   5.85E-007
C    3.11E-002
Ca   3.63E-002
Cl   1.27E+000
Fe   5.69E-002
K    5.28E-001
Mg   8.73E-004
N    5.61E-002
Na   1.27E+000
S    1.01E+000
Si   8.73E-005
REACTION_TEMPERATURE    92
36.997
REACTION_PRESSURE     92
30.9
GAS_PHASE 92
```

-fixed_pressure
-pressure30.9
-temperature 36.997
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 93
-temperature 37.03
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 93
37.03
REACTION_PRESSURE 93
31
GAS_PHASE 93
-fixed_pressure
-pressure31
-temperature 37.03
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 94
-temperature 37.063
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001

Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 94
37.063
REACTION_PRESSURE 94
31.1
GAS_PHASE 94
-fixed_pressure
-pressure31.1
-temperature 37.063
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 95
-temperature 37.096
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 95
37.096
REACTION_PRESSURE 95
31.2
GAS_PHASE 95
-fixed_pressure
-pressure31.2
-temperature 37.096
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 96
-temperature 37.129

-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 96
37.129
REACTION_PRESSURE 96
31.3
GAS_PHASE 96
-fixed_pressure
-pressure31.3
-temperature 37.129
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 97
-temperature 37.162
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 97
37.162
REACTION_PRESSURE 97
31.4
GAS_PHASE 97
-fixed_pressure

-pressure31.4
-temperature 37.162
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 98
-temperature 37.195
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 98
37.195
REACTION_PRESSURE 98
31.5
GAS_PHASE 98
-fixed_pressure
-pressure31.5
-temperature 37.195
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 99
-temperature 37.228
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004

```
N    5.61E-002
Na   1.27E+000
S    1.01E+000
Si   8.73E-005
REACTION_TEMPERATURE    99
37.228
REACTION_PRESSURE    99
31.6
GAS_PHASE 99
-fixed_pressure
-pressure31.6
-temperature  37.228
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    100
-temperature  37.261
-pH 6.377
-pe -3.391
units mol/kgw
Al    1.31E-007
Ba    5.85E-007
C    3.11E-002
Ca    3.63E-002
Cl    1.27E+000
Fe    5.69E-002
K    5.28E-001
Mg    8.73E-004
N    5.61E-002
Na    1.27E+000
S    1.01E+000
Si    8.73E-005
REACTION_TEMPERATURE    100
37.261
REACTION_PRESSURE    100
31.7
GAS_PHASE 100
-fixed_pressure
-pressure31.7
-temperature  37.261
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    101
-temperature  37.294
-pH 6.377
```

```
-pe -3.391
units mol/kgw
Al   1.31E-007
Ba   5.85E-007
C    3.11E-002
Ca   3.63E-002
Cl   1.27E+000
Fe   5.69E-002
K    5.28E-001
Mg   8.73E-004
N    5.61E-002
Na   1.27E+000
S    1.01E+000
Si   8.73E-005
REACTION_TEMPERATURE    101
37.294
REACTION_PRESSURE     101
31.8
GAS_PHASE 101
-fixed_pressure
-pressure31.8
-temperature  37.294
-volume  3
Hydrogengas(g)   21.8
CO2(g)   0.0
CH4(g)   0.0
H2S(g)   0.0
#
SOLUTION   102
-temperature  37.327
-pH 6.377
-pe -3.391
units mol/kgw
Al   1.31E-007
Ba   5.85E-007
C    3.11E-002
Ca   3.63E-002
Cl   1.27E+000
Fe   5.69E-002
K    5.28E-001
Mg   8.73E-004
N    5.61E-002
Na   1.27E+000
S    1.01E+000
Si   8.73E-005
REACTION_TEMPERATURE    102
37.327
REACTION_PRESSURE     102
31.9
GAS_PHASE 102
-fixed_pressure
-pressure31.9
```

-temperature 37.327
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 103
-temperature 37.36
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 103
37.36
REACTION_PRESSURE 103
32
GAS_PHASE 103
-fixed_pressure
-pressure32
-temperature 37.36
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 104
-temperature 37.393
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002

```
Na   1.27E+000
S    1.01E+000
Si   8.73E-005
REACTION_TEMPERATURE    104
37.393
REACTION_PRESSURE    104
32.1
GAS_PHASE 104
-fixed_pressure
-pressure32.1
-temperature  37.393
-volume  3
Hydrogengas(g)   21.8
CO2(g)   0.0
CH4(g)   0.0
H2S(g)   0.0
#
SOLUTION   105
-temperature  37.426
-pH 6.377
-pe -3.391
units mol/kgw
Al   1.31E-007
Ba   5.85E-007
C    3.11E-002
Ca   3.63E-002
Cl   1.27E+000
Fe   5.69E-002
K    5.28E-001
Mg   8.73E-004
N    5.61E-002
Na   1.27E+000
S    1.01E+000
Si   8.73E-005
REACTION_TEMPERATURE    105
37.426
REACTION_PRESSURE    105
32.2
GAS_PHASE 105
-fixed_pressure
-pressure32.2
-temperature  37.426
-volume  3
Hydrogengas(g)   21.8
CO2(g)   0.0
CH4(g)   0.0
H2S(g)   0.0
#
SOLUTION   106
-temperature  37.459
-pH 6.377
-pe -3.391
```

```
units mol/kgw
Al   1.31E-007
Ba   5.85E-007
C    3.11E-002
Ca   3.63E-002
Cl   1.27E+000
Fe   5.69E-002
K    5.28E-001
Mg   8.73E-004
N    5.61E-002
Na   1.27E+000
S    1.01E+000
Si   8.73E-005
REACTION_TEMPERATURE    106
37.459
REACTION_PRESSURE    106
32.3
GAS_PHASE 106
-fixed_pressure
-pressure32.3
-temperature  37.459
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    107
-temperature  37.492
-pH 6.377
-pe -3.391
units mol/kgw
Al   1.31E-007
Ba   5.85E-007
C    3.11E-002
Ca   3.63E-002
Cl   1.27E+000
Fe   5.69E-002
K    5.28E-001
Mg   8.73E-004
N    5.61E-002
Na   1.27E+000
S    1.01E+000
Si   8.73E-005
REACTION_TEMPERATURE    107
37.492
REACTION_PRESSURE    107
32.4
GAS_PHASE 107
-fixed_pressure
-pressure32.4
-temperature  37.492
```

```
-volume 3
Hydrogengas(g)  21.8
CO2(g)  0.0
CH4(g)  0.0
H2S(g)  0.0
#
SOLUTION  108
-temperature 37.525
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE  108
37.525
REACTION_PRESSURE  108
32.5
GAS_PHASE 108
-fixed_pressure
-pressure32.5
-temperature 37.525
-volume 3
Hydrogengas(g)  21.8
CO2(g)  0.0
CH4(g)  0.0
H2S(g)  0.0
#
SOLUTION  109
-temperature 37.558
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
```

```
S     1.01E+000
Si    8.73E-005
REACTION_TEMPERATURE     109
37.558
REACTION_PRESSURE      109
32.6
GAS_PHASE 109
-fixed_pressure
-pressure32.6
-temperature  37.558
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    110
-temperature  37.591
-pH 6.377
-pe -3.391
units mol/kgw
Al    1.31E-007
Ba    5.85E-007
C     3.11E-002
Ca    3.63E-002
Cl    1.27E+000
Fe    5.69E-002
K     5.28E-001
Mg    8.73E-004
N     5.61E-002
Na    1.27E+000
S     1.01E+000
Si    8.73E-005
REACTION_TEMPERATURE     110
37.591
REACTION_PRESSURE      110
32.7
GAS_PHASE 110
-fixed_pressure
-pressure32.7
-temperature  37.591
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    111
-temperature  37.624
-pH 6.377
-pe -3.391
units mol/kgw
```

```
Al   1.31E-007
Ba   5.85E-007
C    3.11E-002
Ca   3.63E-002
Cl   1.27E+000
Fe   5.69E-002
K    5.28E-001
Mg   8.73E-004
N    5.61E-002
Na   1.27E+000
S    1.01E+000
Si   8.73E-005
REACTION_TEMPERATURE    111
37.624
REACTION_PRESSURE     111
32.8
GAS_PHASE 111
-fixed_pressure
-pressure32.8
-temperature  37.624
-volume  3
Hydrogengas(g)    21.8
CO2(g)   0.0
CH4(g)   0.0
H2S(g)   0.0
#
SOLUTION   112
-temperature  37.657
-pH 6.377
-pe -3.391
units mol/kgw
Al   1.31E-007
Ba   5.85E-007
C    3.11E-002
Ca   3.63E-002
Cl   1.27E+000
Fe   5.69E-002
K    5.28E-001
Mg   8.73E-004
N    5.61E-002
Na   1.27E+000
S    1.01E+000
Si   8.73E-005
REACTION_TEMPERATURE    112
37.657
REACTION_PRESSURE     112
32.9
GAS_PHASE 112
-fixed_pressure
-pressure32.9
-temperature  37.657
-volume  3
```

Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 113
-temperature 37.69
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 113
37.69
REACTION_PRESSURE 113
33
GAS_PHASE 113
-fixed_pressure
-pressure33
-temperature 37.69
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 114
-temperature 37.723
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000

Si 8.73E-005
REACTION_TEMPERATURE 114
37.723
REACTION_PRESSURE 114
33.1
GAS_PHASE 114
-fixed_pressure
-pressure33.1
-temperature 37.723
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 115
-temperature 37.756
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 115
37.756
REACTION_PRESSURE 115
33.2
GAS_PHASE 115
-fixed_pressure
-pressure33.2
-temperature 37.756
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 116
-temperature 37.789
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007

Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 116
37.789
REACTION_PRESSURE 116
33.3
GAS_PHASE 116
-fixed_pressure
-pressure33.3
-temperature 37.789
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 117
-temperature 37.822
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 117
37.822
REACTION_PRESSURE 117
33.4
GAS_PHASE 117
-fixed_pressure
-pressure33.4
-temperature 37.822
-volume 3
Hydrogengas(g) 21.8

```
CO2(g)  0.0
CH4(g)  0.0
H2S(g)  0.0
#
SOLUTION  118
-temperature  37.855
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE  118
37.855
REACTION_PRESSURE  118
33.5
GAS_PHASE 118
-fixed_pressure
-pressure33.5
-temperature  37.855
-volume  3
Hydrogengas(g)  21.8
CO2(g)  0.0
CH4(g)  0.0
H2S(g)  0.0
#
SOLUTION  119
-temperature  37.888
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
```

```
REACTION_TEMPERATURE    119
37.888
REACTION_PRESSURE    119
33.6
GAS_PHASE 119
-fixed_pressure
-pressure33.6
-temperature  37.888
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    120
-temperature  37.921
-pH 6.377
-pe -3.391
units mol/kgw
Al    1.31E-007
Ba    5.85E-007
C    3.11E-002
Ca    3.63E-002
Cl    1.27E+000
Fe    5.69E-002
K    5.28E-001
Mg    8.73E-004
N    5.61E-002
Na    1.27E+000
S    1.01E+000
Si    8.73E-005
REACTION_TEMPERATURE    120
37.921
REACTION_PRESSURE    120
33.7
GAS_PHASE 120
-fixed_pressure
-pressure33.7
-temperature  37.921
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    121
-temperature  37.954
-pH 6.377
-pe -3.391
units mol/kgw
Al    1.31E-007
Ba    5.85E-007
```

C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 121
37.954
REACTION_PRESSURE 121
33.8
GAS_PHASE 121
-fixed_pressure
-pressure33.8
-temperature 37.954
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 122
-temperature 37.987
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 122
37.987
REACTION_PRESSURE 122
33.9
GAS_PHASE 122
-fixed_pressure
-pressure33.9
-temperature 37.987
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0

```
CH4(g)  0.0
H2S(g)  0.0
#
SOLUTION  123
-temperature  38.02
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE  123
38.02
REACTION_PRESSURE  123
34
GAS_PHASE 123
-fixed_pressure
-pressure34
-temperature  38.02
-volume  3
Hydrogengas(g)  21.8
CO2(g)  0.0
CH4(g)  0.0
H2S(g)  0.0
#
SOLUTION  124
-temperature  38.053
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE  124
```

```
38.053
REACTION_PRESSURE      124
34.1
GAS_PHASE 124
-fixed_pressure
-pressure34.1
-temperature  38.053
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    125
-temperature  38.086
-pH 6.377
-pe -3.391
units mol/kgw
Al    1.31E-007
Ba    5.85E-007
C     3.11E-002
Ca    3.63E-002
Cl    1.27E+000
Fe    5.69E-002
K     5.28E-001
Mg    8.73E-004
N     5.61E-002
Na    1.27E+000
S     1.01E+000
Si    8.73E-005
REACTION_TEMPERATURE     125
38.086
REACTION_PRESSURE      125
34.2
GAS_PHASE 125
-fixed_pressure
-pressure34.2
-temperature  38.086
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    126
-temperature  38.119
-pH 6.377
-pe -3.391
units mol/kgw
Al    1.31E-007
Ba    5.85E-007
C     3.11E-002
```

```
Ca   3.63E-002
Cl   1.27E+000
Fe   5.69E-002
K    5.28E-001
Mg   8.73E-004
N    5.61E-002
Na   1.27E+000
S    1.01E+000
Si   8.73E-005
REACTION_TEMPERATURE    126
38.119
REACTION_PRESSURE    126
34.3
GAS_PHASE 126
-fixed_pressure
-pressure34.3
-temperature  38.119
-volume  3
Hydrogengas(g)    21.8
CO2(g)   0.0
CH4(g)   0.0
H2S(g)   0.0
#
SOLUTION    127
-temperature  38.152
-pH 6.377
-pe -3.391
units mol/kgw
Al   1.31E-007
Ba   5.85E-007
C    3.11E-002
Ca   3.63E-002
Cl   1.27E+000
Fe   5.69E-002
K    5.28E-001
Mg   8.73E-004
N    5.61E-002
Na   1.27E+000
S    1.01E+000
Si   8.73E-005
REACTION_TEMPERATURE    127
38.152
REACTION_PRESSURE    127
34.4
GAS_PHASE 127
-fixed_pressure
-pressure34.4
-temperature  38.152
-volume  3
Hydrogengas(g)    21.8
CO2(g)   0.0
CH4(g)   0.0
```

```
H2S(g)  0.0
#
SOLUTION  128
-temperature  38.185
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE  128
38.185
REACTION_PRESSURE  128
34.5
GAS_PHASE 128
-fixed_pressure
-pressure34.5
-temperature  38.185
-volume  3
Hydrogengas(g)  21.8
CO2(g)  0.0
CH4(g)  0.0
H2S(g)  0.0
#
SOLUTION  129
-temperature  38.218
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE  129
38.218
```

```
REACTION_PRESSURE      129
34.6
GAS_PHASE 129
-fixed_pressure
-pressure34.6
-temperature  38.218
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    130
-temperature  38.251
-pH 6.377
-pe -3.391
units mol/kgw
Al    1.31E-007
Ba    5.85E-007
C     3.11E-002
Ca    3.63E-002
Cl    1.27E+000
Fe    5.69E-002
K     5.28E-001
Mg    8.73E-004
N     5.61E-002
Na    1.27E+000
S     1.01E+000
Si    8.73E-005
REACTION_TEMPERATURE     130
38.251
REACTION_PRESSURE      130
34.7
GAS_PHASE 130
-fixed_pressure
-pressure34.7
-temperature  38.251
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    131
-temperature  38.284
-pH 6.377
-pe -3.391
units mol/kgw
Al    1.31E-007
Ba    5.85E-007
C     3.11E-002
Ca    3.63E-002
```

Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 131
38.284
REACTION_PRESSURE 131
34.8
GAS_PHASE 131
-fixed_pressure
-pressure34.8
-temperature 38.284
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 132
-temperature 38.317
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 132
38.317
REACTION_PRESSURE 132
34.9
GAS_PHASE 132
-fixed_pressure
-pressure34.9
-temperature 38.317
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0

```
#
SOLUTION  133
-temperature  38.35
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE  133
38.35
REACTION_PRESSURE  133
35
GAS_PHASE 133
-fixed_pressure
-pressure35
-temperature  38.35
-volume  3
Hydrogengas(g)  21.8
CO2(g)  0.0
CH4(g)  0.0
H2S(g)  0.0
#
SOLUTION  134
-temperature  38.383
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE  134
38.383
REACTION_PRESSURE  134
```

```
35.1
GAS_PHASE 134
-fixed_pressure
-pressure35.1
-temperature  38.383
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    135
-temperature  38.416
-pH 6.377
-pe -3.391
units mol/kgw
Al    1.31E-007
Ba    5.85E-007
C     3.11E-002
Ca    3.63E-002
Cl    1.27E+000
Fe    5.69E-002
K     5.28E-001
Mg    8.73E-004
N     5.61E-002
Na    1.27E+000
S     1.01E+000
Si    8.73E-005
REACTION_TEMPERATURE     135
38.416
REACTION_PRESSURE      135
35.2
GAS_PHASE 135
-fixed_pressure
-pressure35.2
-temperature  38.416
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    136
-temperature  38.449
-pH 6.377
-pe -3.391
units mol/kgw
Al    1.31E-007
Ba    5.85E-007
C     3.11E-002
Ca    3.63E-002
Cl    1.27E+000
```

Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 136
38.449
REACTION_PRESSURE 136
35.3
GAS_PHASE 136
-fixed_pressure
-pressure35.3
-temperature 38.449
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 137
-temperature 38.482
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 137
38.482
REACTION_PRESSURE 137
35.4
GAS_PHASE 137
-fixed_pressure
-pressure35.4
-temperature 38.482
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#

```
SOLUTION  138
-temperature  38.515
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE  138
38.515
REACTION_PRESSURE  138
35.5
GAS_PHASE 138
-fixed_pressure
-pressure35.5
-temperature  38.515
-volume  3
Hydrogengas(g)  21.8
CO2(g)  0.0
CH4(g)  0.0
H2S(g)  0.0
#
SOLUTION  139
-temperature  38.548
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE  139
38.548
REACTION_PRESSURE  139
35.6
```

GAS_PHASE 139
-fixed_pressure
-pressure35.6
-temperature 38.548
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 140
-temperature 38.581
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 140
38.581
REACTION_PRESSURE 140
35.7
GAS_PHASE 140
-fixed_pressure
-pressure35.7
-temperature 38.581
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 141
-temperature 38.614
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002

K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 141
38.614
REACTION_PRESSURE 141
35.8
GAS_PHASE 141
-fixed_pressure
-pressure35.8
-temperature 38.614
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 142
-temperature 38.647
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 142
38.647
REACTION_PRESSURE 142
35.9
GAS_PHASE 142
-fixed_pressure
-pressure35.9
-temperature 38.647
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 143

-temperature 38.68
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 143
38.68
REACTION_PRESSURE 143
36
GAS_PHASE 143
-fixed_pressure
-pressure36
-temperature 38.68
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 144
-temperature 38.713
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 144
38.713
REACTION_PRESSURE 144
36.1
GAS_PHASE 144

-fixed_pressure
-pressure36.1
-temperature 38.713
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 145
-temperature 38.746
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 145
38.746
REACTION_PRESSURE 145
36.2
GAS_PHASE 145
-fixed_pressure
-pressure36.2
-temperature 38.746
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 146
-temperature 38.779
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001

Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 146
38.779
REACTION_PRESSURE 146
36.3
GAS_PHASE 146
-fixed_pressure
-pressure36.3
-temperature 38.779
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 147
-temperature 38.812
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 147
38.812
REACTION_PRESSURE 147
36.4
GAS_PHASE 147
-fixed_pressure
-pressure36.4
-temperature 38.812
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 148
-temperature 38.845

-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 148
38.845
REACTION_PRESSURE 148
36.5
GAS_PHASE 148
-fixed_pressure
-pressure36.5
-temperature 38.845
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 149
-temperature 38.878
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 149
38.878
REACTION_PRESSURE 149
36.6
GAS_PHASE 149
-fixed_pressure

-pressure36.6
-temperature 38.878
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 150
-temperature 38.911
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 150
38.911
REACTION_PRESSURE 150
36.7
GAS_PHASE 150
-fixed_pressure
-pressure36.7
-temperature 38.911
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 151
-temperature 38.944
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004

N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 151
38.944
REACTION_PRESSURE 151
36.8
GAS_PHASE 151
-fixed_pressure
-pressure36.8
-temperature 38.944
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 152
-temperature 38.977
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 152
38.977
REACTION_PRESSURE 152
36.9
GAS_PHASE 152
-fixed_pressure
-pressure36.9
-temperature 38.977
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 153
-temperature 39.01
-pH 6.377

-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 153
39.01
REACTION_PRESSURE 153
37
GAS_PHASE 153
-fixed_pressure
-pressure37
-temperature 39.01
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 154
-temperature 39.043
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 154
39.043
REACTION_PRESSURE 154
37.1
GAS_PHASE 154
-fixed_pressure
-pressure37.1

-temperature 39.043
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 155
-temperature 39.076
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 155
39.076
REACTION_PRESSURE 155
37.2
GAS_PHASE 155
-fixed_pressure
-pressure37.2
-temperature 39.076
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 156
-temperature 39.109
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002

```
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE  156
39.109
REACTION_PRESSURE  156
37.3
GAS_PHASE 156
-fixed_pressure
-pressure37.3
-temperature  39.109
-volume  3
Hydrogengas(g)  21.8
CO2(g)  0.0
CH4(g)  0.0
H2S(g)  0.0
#
SOLUTION  157
-temperature  39.142
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE  157
39.142
REACTION_PRESSURE  157
37.4
GAS_PHASE 157
-fixed_pressure
-pressure37.4
-temperature  39.142
-volume  3
Hydrogengas(g)  21.8
CO2(g)  0.0
CH4(g)  0.0
H2S(g)  0.0
#
SOLUTION  158
-temperature  39.175
-pH 6.377
-pe -3.391
```

```
units mol/kgw
Al   1.31E-007
Ba   5.85E-007
C    3.11E-002
Ca   3.63E-002
Cl   1.27E+000
Fe   5.69E-002
K    5.28E-001
Mg   8.73E-004
N    5.61E-002
Na   1.27E+000
S    1.01E+000
Si   8.73E-005
REACTION_TEMPERATURE    158
39.175
REACTION_PRESSURE    158
37.5
GAS_PHASE 158
-fixed_pressure
-pressure37.5
-temperature  39.175
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    159
-temperature  39.208
-pH 6.377
-pe -3.391
units mol/kgw
Al   1.31E-007
Ba   5.85E-007
C    3.11E-002
Ca   3.63E-002
Cl   1.27E+000
Fe   5.69E-002
K    5.28E-001
Mg   8.73E-004
N    5.61E-002
Na   1.27E+000
S    1.01E+000
Si   8.73E-005
REACTION_TEMPERATURE    159
39.208
REACTION_PRESSURE    159
37.6
GAS_PHASE 159
-fixed_pressure
-pressure37.6
-temperature  39.208
```

-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 160
-temperature 39.241
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 160
39.241
REACTION_PRESSURE 160
37.7
GAS_PHASE 160
-fixed_pressure
-pressure37.7
-temperature 39.241
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 161
-temperature 39.274
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000

S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 161
39.274
REACTION_PRESSURE 161
37.8
GAS_PHASE 161
-fixed_pressure
-pressure37.8
-temperature 39.274
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 162
-temperature 39.307
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 162
39.307
REACTION_PRESSURE 162
37.9
GAS_PHASE 162
-fixed_pressure
-pressure37.9
-temperature 39.307
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 163
-temperature 39.34
-pH 6.377
-pe -3.391
units mol/kgw

Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 163
39.34
REACTION_PRESSURE 163
38
GAS_PHASE 163
-fixed_pressure
-pressure38
-temperature 39.34
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 164
-temperature 39.373
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 164
39.373
REACTION_PRESSURE 164
38.1
GAS_PHASE 164
-fixed_pressure
-pressure38.1
-temperature 39.373
-volume 3

Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 165
-temperature 39.406
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 165
39.406
REACTION_PRESSURE 165
38.2
GAS_PHASE 165
-fixed_pressure
-pressure38.2
-temperature 39.406
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 166
-temperature 39.439
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000

```
Si    8.73E-005
REACTION_TEMPERATURE    166
39.439
REACTION_PRESSURE    166
38.3
GAS_PHASE 166
-fixed_pressure
-pressure38.3
-temperature  39.439
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    167
-temperature  39.472
-pH 6.377
-pe -3.391
units mol/kgw
Al    1.31E-007
Ba    5.85E-007
C    3.11E-002
Ca    3.63E-002
Cl    1.27E+000
Fe    5.69E-002
K    5.28E-001
Mg    8.73E-004
N    5.61E-002
Na    1.27E+000
S    1.01E+000
Si    8.73E-005
REACTION_TEMPERATURE    167
39.472
REACTION_PRESSURE    167
38.4
GAS_PHASE 167
-fixed_pressure
-pressure38.4
-temperature  39.472
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    168
-temperature  39.505
-pH 6.377
-pe -3.391
units mol/kgw
Al    1.31E-007
```

Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 168
39.505
REACTION_PRESSURE 168
38.5
GAS_PHASE 168
-fixed_pressure
-pressure38.5
-temperature 39.505
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 169
-temperature 39.538
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 169
39.538
REACTION_PRESSURE 169
38.6
GAS_PHASE 169
-fixed_pressure
-pressure38.6
-temperature 39.538
-volume 3
Hydrogengas(g) 21.8

```
CO2(g)  0.0
CH4(g)  0.0
H2S(g)  0.0
#
SOLUTION  170
-temperature  39.571
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE  170
39.571
REACTION_PRESSURE  170
38.7
GAS_PHASE 170
-fixed_pressure
-pressure38.7
-temperature  39.571
-volume  3
Hydrogengas(g)  21.8
CO2(g)  0.0
CH4(g)  0.0
H2S(g)  0.0
#
SOLUTION  171
-temperature  39.604
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
```

```
REACTION_TEMPERATURE    171
39.604
REACTION_PRESSURE    171
38.8
GAS_PHASE 171
-fixed_pressure
-pressure38.8
-temperature  39.604
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    172
-temperature  39.637
-pH 6.377
-pe -3.391
units mol/kgw
Al    1.31E-007
Ba    5.85E-007
C    3.11E-002
Ca    3.63E-002
Cl    1.27E+000
Fe    5.69E-002
K    5.28E-001
Mg    8.73E-004
N    5.61E-002
Na    1.27E+000
S    1.01E+000
Si    8.73E-005
REACTION_TEMPERATURE    172
39.637
REACTION_PRESSURE    172
38.9
GAS_PHASE 172
-fixed_pressure
-pressure38.9
-temperature  39.637
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    173
-temperature  39.67
-pH 6.377
-pe -3.391
units mol/kgw
Al    1.31E-007
Ba    5.85E-007
```

C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 173
39.67
REACTION_PRESSURE 173
39
GAS_PHASE 173
-fixed_pressure
-pressure39
-temperature 39.67
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 174
-temperature 39.703
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 174
39.703
REACTION_PRESSURE 174
39.1
GAS_PHASE 174
-fixed_pressure
-pressure39.1
-temperature 39.703
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0

```
CH4(g)  0.0
H2S(g)  0.0
#
SOLUTION  175
-temperature  39.736
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE  175
39.736
REACTION_PRESSURE  175
39.2
GAS_PHASE 175
-fixed_pressure
-pressure39.2
-temperature  39.736
-volume  3
Hydrogengas(g)  21.8
CO2(g)  0.0
CH4(g)  0.0
H2S(g)  0.0
#
SOLUTION  176
-temperature  39.769
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE  176
```

```
39.769
REACTION_PRESSURE	176
39.3
GAS_PHASE 176
-fixed_pressure
-pressure39.3
-temperature 39.769
-volume 3
Hydrogengas(g)	21.8
CO2(g)	0.0
CH4(g)	0.0
H2S(g)	0.0
#
SOLUTION	177
-temperature 39.802
-pH 6.377
-pe -3.391
units mol/kgw
Al	1.31E-007
Ba	5.85E-007
C	3.11E-002
Ca	3.63E-002
Cl	1.27E+000
Fe	5.69E-002
K	5.28E-001
Mg	8.73E-004
N	5.61E-002
Na	1.27E+000
S	1.01E+000
Si	8.73E-005
REACTION_TEMPERATURE	177
39.802
REACTION_PRESSURE	177
39.4
GAS_PHASE 177
-fixed_pressure
-pressure39.4
-temperature 39.802
-volume 3
Hydrogengas(g)	21.8
CO2(g)	0.0
CH4(g)	0.0
H2S(g)	0.0
#
SOLUTION	178
-temperature 39.835
-pH 6.377
-pe -3.391
units mol/kgw
Al	1.31E-007
Ba	5.85E-007
C	3.11E-002
```

Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 178
39.835
REACTION_PRESSURE 178
39.5
GAS_PHASE 178
-fixed_pressure
-pressure39.5
-temperature 39.835
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0
H2S(g) 0.0
#
SOLUTION 179
-temperature 39.868
-pH 6.377
-pe -3.391
units mol/kgw
Al 1.31E-007
Ba 5.85E-007
C 3.11E-002
Ca 3.63E-002
Cl 1.27E+000
Fe 5.69E-002
K 5.28E-001
Mg 8.73E-004
N 5.61E-002
Na 1.27E+000
S 1.01E+000
Si 8.73E-005
REACTION_TEMPERATURE 179
39.868
REACTION_PRESSURE 179
39.6
GAS_PHASE 179
-fixed_pressure
-pressure39.6
-temperature 39.868
-volume 3
Hydrogengas(g) 21.8
CO2(g) 0.0
CH4(g) 0.0

```
H2S(g)  0.0
#
SOLUTION  180
-temperature  39.901
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE  180
39.901
REACTION_PRESSURE  180
39.7
GAS_PHASE 180
-fixed_pressure
-pressure39.7
-temperature  39.901
-volume  3
Hydrogengas(g)  21.8
CO2(g)  0.0
CH4(g)  0.0
H2S(g)  0.0
#
SOLUTION  181
-temperature  39.934
-pH 6.377
-pe -3.391
units mol/kgw
Al  1.31E-007
Ba  5.85E-007
C  3.11E-002
Ca  3.63E-002
Cl  1.27E+000
Fe  5.69E-002
K  5.28E-001
Mg  8.73E-004
N  5.61E-002
Na  1.27E+000
S  1.01E+000
Si  8.73E-005
REACTION_TEMPERATURE  181
39.934
```

```
REACTION_PRESSURE      181
39.8
GAS_PHASE 181
-fixed_pressure
-pressure39.8
-temperature  39.934
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0
#
SOLUTION    182
-temperature  39.967
-pH 6.377
-pe -3.391
units mol/kgw
Al    1.31E-007
Ba    5.85E-007
C     3.11E-002
Ca    3.63E-002
Cl    1.27E+000
Fe    5.69E-002
K     5.28E-001
Mg    8.73E-004
N     5.61E-002
Na    1.27E+000
S     1.01E+000
Si    8.73E-005
REACTION_TEMPERATURE     182
39.967
REACTION_PRESSURE      182
39.9
GAS_PHASE 182
-fixed_pressure
-pressure39.9
-temperature  39.967
-volume  3
Hydrogengas(g)    21.8
CO2(g)    0.0
CH4(g)    0.0
H2S(g)    0.0

EQUILIBRIUM_PHASES 1-182
Halite              0.0             76.74
Quartz              0.0             746.42
Illite              0.0             46.73
Dolomite            0.0             24.32
Anhydrite           0.0             131.77

Dawsonite           0.0             0.00 # potential secondary phase
Mackinawite         0.0             0.00 # potential secondary phase
```

```
Sulfur          0.0         0.00 # potential secondary phase
Albite          0.0         0.00 # potential secondary phase
Pyrite          0.0         0.00 # potential secondary phase

KINETICS 1-182
H2
-tol  1e-8
-m0 0.0
-m   0.0

EXCHANGE 1-182
-equilibrate with solution 1-182
X 3.907

END

SOLUTION 183-850                # reservoir rock
-temperature 40.0
-pH 6.392
-pe -3.481
units mol/kgw
Al   2.209e-08
Ba   3.922e-07
C    1.762e-02
Ca   1.186e-02
Cl   1.123e+00
Fe   6.572e-02
K    6.151e-01
Mg   2.579e-03
N    6.485e-02
Na   1.123e+00
S    1.143e+00
Si   9.878e-05
Tracer    0.001

EQUILIBRIUM_PHASES 183-850
K-feldspar      0.0         103.90
Kaolinite       0.0         3.73
Quartz          0.0         882.43
Calcite         0.0         4.82
Dolomite        0.0         0.03
Illite          0.0         28.88
Barite          0.0         0.0009
Goethite        0.0         0.002
Anhydrite       0.0         0.132

Dawsonite       0.0         0.00 # potential secondary phase
Mackinawite     0.0         0.00 # potential secondary phase
Sulfur          0.0         0.00 # potential secondary phase
Albite          0.0         0.00 # potential secondary phase
Pyrite          0.0         0.00 # potential secondary phase
```

```
GAS_PHASE 183-850
-fixed_pressure
-pressure          40.0
-temperature       40.0
-volume            3.0
Hydrogengas(g)     34.56
CH4(g)             3.56
N2(g)              0.4
CO2(g)             1.48
H2S(g)             0.0

REACTION_PRESSURE 183-850
40.0
REACTION_TEMPERATURE 183-850
40.0

EXCHANGE 183-850
-equilibrate with solution 183-850
X 3.722

KINETICS 183-850
H2
-tol  1e-8
-m0 4.3
-m   4.3

SAVE SOLUTION    183-850

END

SOLUTION 851-1488                          # underlying rock
-temperature 60.0
-pH 5.995
-pe -4.233
units mol/kgw
Al    1.776e-08
Ba    2.206e-05
C     7.405e-03
Ca    1.562e-02
Cl    5.396e+00
Fe    4.263e-11
K     4.604e-01
Mg    1.142e-02
N     5.081e-02
Na    5.396e+00
S     7.540e-01
Si    1.509e-04

EQUILIBRIUM_PHASES 851-1488
Dolomite          0.0          0.03
Calcite           0.0          53.14
Anhydrite         0.0          66.11
```

```
Halite                  0.0         758.46
Quartz                  0.0         118.04
Pyrite                  0.0         7.39

Dawsonite               0.0         0.00 # potential secondary phase
Mackinawite             0.0         0.00 # potential secondary phase
Sulfur                  0.0         0.00 # potential secondary phase
Barite                  0.0         0.00 # potential secondary phase

GAS_PHASE 851-1488
-fixed_pressure
-pressure           106.7
-temperature        60.0
-volume         3.0
Hydrogengas(g)      0.0
CH4(g)              81.1
N2(g)               4.3
CO2(g)              10.7
H2S(g)              10.7

REACTION_PRESSURE 851-1488
106.7
REACTION_TEMPERATURE 851-1488
60.0

KINETICS 851-1488
H2
-tol  1e-8
-m0 0.0
-m   0.0

SAVE SOLUTION 851-1488
END

TRANSPORT
-cells                  1488
-shifts                 10
-flow_direction         diffusion_only
-time_step              94608000            # (10*3a =30 a)
-multi_d                true
-length                 1488*1.0
-dispersivity           1488*0.0
-boundary_conditions    flux flux

END
```