ANEXO III

ESTUDIO DE MODELIZACIÓN GEOQUÍMICA MEDIANTE PHREEQC

-Cálculos de la modelización geoquímica mediante PHREEQC.
-Difractograma de un precipitado muestreado en la corta de Aznalcóllar.

		epilimnion		hipolimnion	
Elemento	**Especie**	**moles**	**%**	**moles**	**%**
Fe(III)	total	0,00005069	100	0,000007238	100
	$FeSO_4^+$	0,0000216	43	2,356E-07	3
	$FeOH^{2+}$	0,00001108	22	6,595E-07	9
	$Fe(SO4)_2^-$	0,000008397	17	8,925E-08	1
	$Fe(OH)_2^+$	0,000007409	15	0,000006224	86
	Fe^{+3}	0,000002138	4	2,722E-08	0,4
Al	total	0,003448	100	0,003184	100
	$AlSO_4^+$	0,002333	68	0,002132	67
	$Al(SO_4)_2^-$	0,0007769	23	0,0006962	22
	Al^{+3}	0,0003325	10	0,00033	10
Cd	total	0,00001799	100	0,00001798	100
	$CdSO_4$	0,00000759	42	0,000007451	41
	Cd^{+2}	0,00000695	39	0,000006986	39
	$Cd(SO_4)_2^{-2}$	0,00000345	19	0,000003544	20
Cu(II)	total	0,0005569	100	0,0006361	100
	Cu^{+2}	0,0003581	64	0,0004119	65
	$CuSO_4$	0,0001988	36	0,0002241	35
Ni	total	0,00004306	100	0,00004303	100
	Ni^{2+}	0,00002482	58	0,0000253	59
	$NiSO_4$	0,00001819	42	0,00001769	41
	$Ni(SO_4)_2^{-2}$	4,081E-08	0,1	4,25E-08	0,1
Pb	total	0,000003904	100	0,000003658	100
	$PbSO_4$	0,000002331	60	0,000002208	60
	Pb^{+2}	1,075E-07	3	9,838E-07	27
	$Pb(SO4)_2^{-2}$	4,979E-07	13	4,657E-07	13
Zn	total	0,01237	100	0,01159	100
	Zn^{+2}	0,005488	44	0,005212	45
	$ZnSO_4$	0,005144	42	0,004694	41
	$Zn(SO4)_2^{-2}$	0,001742	14	0,001688	15

Tabla; Especies químicas disueltas de algunos metales (epilimnion e hipolimnion), datos en moles y en porcentaje. Datos obtenidos por PHREEQC (junio de 2005).

		0m de profundidad		30m de profundidad	
Elemento	**Especie**	**moles**	**%**	**moles**	**%**
Fe(II)	total	0,0001989	100	0,01753	100
	Fe^{+2}	0,0001023	51	0,009474	54
	$FeSO_4$	0,00009663	49	0,00806	46
Fe(III)	total	0,001881	100	0,002541	100
	$FeSO_4^+$	0,001139	61	0,001448	57
	$Fe(SO4)_2^-$	0,0005769	31	0,0007776	31
	Fe^{+3}	0,00007975	4	0,0001183	5
	$FeOH^{2+}$	0,00007245	4	0,0001364	5
	$Fe(OH)_2^+$	0,000009293	0,5	0,00004428	2
Al	total	0,00539	100	0,007401	100
	$AlSO_4^+$	0,003519	65	0,004693	63
	$Al(SO_4)_2^-$	0,001511	28	0,002184	30
	Al^{+3}	0,0003595	7	0,0005225	7
Cd	total	0,00001186	100	0,00001218	100
	$CdSO_4$	0,000005333	45	0,000005159	42
	Cd^{+2}	0,000003545	30	0,000003503	29
	$Cd(SO_4)_2^{-2}$	0,000002982	25	0,000003513	29
Cu(II)	total	0,0004926	100	0,001021	100
	Cu^{+2}	0,0002721	55	0,0005916	58
	$CuSO_4$	0,0002206	45	0,0004293	0,42
Pb	total	0,000005152	100	0,000006473	100
	$PbSO_4$	0,000003233	62,7523292	0,000003957	61
	Pb^{+2}	0,000001075	20,8656832	0,000001299	20
	$Pb(SO4)_2^{-2}$	0,000000844	16,3819876	0,000001216	19
Zn	total	0,01149	100	0,01453	100
	$ZnSO_4$	0,005257	46	0,006268	43
	Zn^{+2}	0,004044	35	0,005049	35
	$Zn(SO4)_2$-^{2}	0,002193	19	0,003213	22

Tabla; Especies químicas disueltas de algunos metales (en superficie y profundidad), datos en moles y en porcentaje. Datos obtenidos por PHREEQC (mayo de 2006).

CÁLCULOS DE ESPECIACIÓN QUÍMICA DE METALES E ÍNDICES DE SATURACIÓN

AZNALCÓLLAR, EPILIMNION. JUNIO 2005

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Input file: C:\AMD-ODIEL\Calculo termodinámico\Aznalcóllar speciation.pqi
Output file: C:\AMD-ODIEL\Calculo termodinámico\Aznalcóllar speciation.pqo
Database file: C:\Archivos de programa\USGS\Phreeqc Interactive 2.7.1\minteq.dat

------------------
Reading data base.
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       SOLUTION_MASTER_SPECIES
       SOLUTION_SPECIES
       SOLUTION_SPECIES
       PHASES
       SURFACE_MASTER_SPECIES
       SURFACE_SPECIES
       END
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Reading input data for simulation 1.
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       DATABASE C:\Archivos de programa\USGS\Phreeqc Interactive 2.7.1\minteq.dat
       SOLUTION 1 T-1
           temp      22
           pH        3.6
           pe        8.5
           redox     pe
           units     mg/l
           density   1
           Ca        500
           Fe(3)     2.8
           K         12
           Mg        1100
           Mn        180
           Al        92
           S(6)      8200
           Cu        35
           Cd        2
           Zn        800
           Pb        0.8
           As        0.1
           V         6 ug/l
           Cr        18 ug/l
           Na        55
           Ni        2.5
           Fe(2)     0.7
           O(0)      7
           water    1 # kg
       SOLUTION_MASTER_SPECIES
           Fe(2)         Fe+2            0     Fe
           Fe(3)         Fe+3           -2     Fe
           Mg            Mg+2            0     Mg             24.312
           Na            Na+             0     Na             22.9898
           Ca            Ca+2            0     Ca             40.08
           S             SO4-2           0     SO4            32.064
           S(6)          SO4-2           0     SO4
           K             K+              0     K              39.102
           Al            Al+3            0     Al             26.9815
       SOLUTION_SPECIES
       H2O = OH- + H+
           log_k     -14
           delta_h   13.362 kcal
       Fe+2 = Fe+3 + e-
           log_k     -13.02
           delta_h   9.68 kcal
       Fe+3 + H2O = FeOH+2 + H+
           log_k     -2.19
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```
            delta_h   10.4 kcal
        H+ + SO4-2 = HSO4-
            log_k     1.988
            delta_h   3.85 kcal
        Al+3 + H2O = AlOH+2 + H+
            log_k     -5
            delta_h   11.49 kcal
        Al+3 + 3H2O = Al(OH)3 + 3H+
            log_k     -16.9
            delta_h   39.89 kcal
        Al+3 + SO4-2 = AlSO4+
            log_k     3.5
            delta_h   2.29 kcal
        PHASES
        Jarosite-K
            KFe3(SO4)2(OH)6 + 6H+ = 3Fe+3 + 6H2O + K+ + 2SO4-2
            log_k     -14.8
            delta_h   -31.28 kcal
        Jarosite-Na
            NaFe3(SO4)2(OH)6 + 6H+ = 3Fe+3 + 6H2O + Na+ + 2SO4-2
            log_k     -11.2
            delta_h   -36.18 kcal
        Schwertmannite
            Fe8O8(OH)6(SO4) + 22H+ = 8Fe+3 + 14H2O + SO4-2
            log_k     7
        Ferrihydrite
            Fe(OH)3 + 3H+ = Fe+3 + 3H2O
            log_k     5
        Goethite
            FeOOH + 3H+ = Fe+3 + 2H2O
            log_k     0.5
            delta_h   -14.48 kcal
        Jurbanite
            AlOHSO4 + H+ = Al+3 + H2O + SO4-2
            log_k     -3.23
        Basaluminite
            Al4(OH)10SO4 + 10H+ = 4Al+3 + 10H2O + SO4-2
            log_k     22.7
        Alunite
            KAl3(SO4)2(OH)6 + 6H+ = 3Al+3 + 6H2O + K+ + 2SO4-2
            log_k     -1.3
            delta_h   3.918 kcal
        END
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Beginning of initial solution calculations.
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Initial solution 1.   T-1

-----------------------------Solution composition------------------------------

        Elements           Molality       Moles

        Al               3.448e-003  3.448e-003
        As               1.350e-006  1.350e-006
        Ca               1.261e-002  1.261e-002
        Cd               1.799e-005  1.799e-005
        Cr               3.500e-007  3.500e-007
        Cu               5.569e-004  5.569e-004
        Fe(2)            1.267e-005  1.267e-005
        Fe(3)            5.069e-005  5.069e-005
        K                3.103e-004  3.103e-004
        Mg               4.575e-002  4.575e-002
        Mn               3.313e-003  3.313e-003
        Na               2.419e-003  2.419e-003
        Ni               4.306e-005  4.306e-005
        O(0)             4.424e-004  4.424e-004
        Pb               3.904e-006  3.904e-006
        S(6)             8.631e-002  8.631e-002
        V                1.191e-007  1.191e-007
        Zn               1.237e-002  1.237e-002

----------------------------Description of solution----------------------------
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```
                                    pH  =   3.600
                                    pe  =   8.500
                          Activity of water  =   0.998
                             Ionic strength  =  1.789e-001
                          Mass of water (kg)  =  1.000e+000
                 Total alkalinity (eq/kg)  = -7.645e-004
                    Total carbon (mol/kg)  =  0.000e+000
                       Total CO2 (mol/kg)  =  0.000e+000
                     Temperature (deg C)  =  22.000
                  Electrical balance (eq)  = -9.364e-003
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -5.15
                                Iterations  =  10
                                   Total H  = 1.110132e+002
                                   Total O  = 5.585193e+001

--------------------------------Redox couples--------------------------------

       Redox couple             pe  Eh (volts)

       Fe(2)/Fe(3)         11.9182      0.6979
       O(-2)/O(0)          17.2622      1.0109

--------------------------Distribution of species---------------------------

                                                 Log       Log         Log
       Species            Molality    Activity  Molality  Activity     Gamma

       H+               3.129e-004  2.512e-004    -3.505    -3.600    -0.095
       OH-              4.197e-011  3.159e-011   -10.377   -10.500    -0.123
       H2O              5.551e+001  9.978e-001     1.744    -0.001     0.000
Al              3.448e-003
       AlSO4+           2.333e-003  1.756e-003    -2.632    -2.755    -0.123
       Al(SO4)2-        7.769e-004  5.733e-004    -3.110    -3.242    -0.132
       Al+3             3.325e-004  4.610e-005    -3.478    -4.336    -0.858
       AlOH+2           4.687e-006  1.504e-006    -5.329    -5.823    -0.494
       Al(OH)2+         7.662e-008  5.778e-008    -7.116    -7.238    -0.123
       Al(OH)3          1.761e-011  1.835e-011   -10.754   -10.736     0.018
       Al(OH)4-         7.305e-014  5.391e-014   -13.136   -13.268    -0.132
As(3)           1.186e-012
       H3AsO3           1.186e-012  1.236e-012   -11.926   -11.908     0.018
       H4AsO3+          2.043e-016  1.538e-016   -15.690   -15.813    -0.123
       H2AsO3-          3.455e-018  2.600e-018   -17.462   -17.585    -0.123
       HAsO3-2          2.238e-026  7.179e-027   -25.650   -26.144    -0.494
       AsO3-3           1.282e-035  9.931e-037   -34.892   -36.003    -1.111
As(5)           1.350e-006
       H2AsO4-          1.307e-006  9.838e-007    -5.884    -6.007    -0.123
       H3AsO4           4.031e-008  4.201e-008    -7.395    -7.377     0.018
       HAsO4-2          2.103e-009  6.748e-010    -8.677    -9.171    -0.494
       AsO4-3           8.159e-017  6.320e-018   -16.088   -17.199    -1.111
Ca              1.261e-002
       Ca+2             6.744e-003  2.457e-003    -2.171    -2.610    -0.438
       CaSO4            5.869e-003  6.116e-003    -2.231    -2.214     0.018
       CaOH+            2.513e-012  1.920e-012   -11.600   -11.717    -0.117
Cd              1.799e-005
       CdSO4            7.591e-006  7.910e-006    -5.120    -5.102     0.018
       Cd+2             6.950e-006  2.230e-006    -5.158    -5.652    -0.494
       Cd(SO4)2-2       3.451e-006  1.107e-006    -5.462    -5.956    -0.494
       CdOH+            7.819e-013  5.885e-013   -12.107   -12.230    -0.123
       Cd2OH+3          8.615e-017  6.674e-018   -16.065   -17.176    -1.111
       Cd(OH)2          1.508e-019  1.572e-019   -18.821   -18.804     0.018
       Cd(OH)3-         9.309e-029  7.006e-029   -28.031   -28.155    -0.123
       Cd(OH)4-2        7.731e-039  2.480e-039   -38.112   -38.605    -0.494
Cr(2)           2.972e-023
       Cr+2             2.972e-023  9.537e-024   -22.527   -23.021    -0.494
Cr(3)           3.500e-007
       Cr+3             2.889e-007  2.238e-008    -6.539    -7.650    -1.111
       CrOHSO4          3.422e-008  3.566e-008    -7.466    -7.448     0.018
       Cr(OH)+2         1.961e-008  6.293e-009    -7.707    -8.201    -0.494
       CrSO4+           7.254e-009  5.459e-009    -8.139    -8.263    -0.123
       Cr(OH)2+         7.968e-011  5.996e-011   -10.099   -10.222    -0.123
       Cr2(OH)2SO4+2    1.272e-013  4.080e-014   -12.896   -13.389    -0.494
       Cr(OH)3          1.695e-014  1.766e-014   -13.771   -13.753     0.018
       Cr2(OH)2(SO4)2   1.157e-017  1.206e-017   -16.937   -16.919     0.018
       CrO2-            2.268e-021  1.707e-021   -20.644   -20.768    -0.123
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	Cr(OH)4-	8.901e-022	6.699e-022	-21.051	-21.174	-0.123
Cr(6)	5.764e-029					
	HCrO4-	5.731e-029	4.313e-029	-28.242	-28.365	-0.123
	CrO4-2	1.924e-031	5.403e-032	-30.716	-31.267	-0.551
	CrO3SO4-2	1.315e-031	4.219e-032	-30.881	-31.375	-0.494
	H2CrO4	1.466e-033	1.527e-033	-32.834	-32.816	0.018
	NaCrO4-	6.105e-034	4.595e-034	-33.214	-33.338	-0.123
	KCrO4-	9.232e-035	6.948e-035	-34.035	-34.158	-0.123
	Cr2O7-2	0.000e+000	0.000e+000	-54.661	-55.154	-0.494
Cu(1)	1.924e-010					
	Cu+	1.924e-010	1.334e-010	-9.716	-9.875	-0.159
Cu(2)	5.569e-004					
	Cu+2	3.581e-004	8.268e-005	-3.446	-4.083	-0.637
	CuSO4	1.988e-004	2.071e-004	-3.702	-3.684	0.018
	CuOH+	4.511e-009	3.284e-009	-8.346	-8.484	-0.138
	Cu(OH)2	2.616e-011	2.726e-011	-10.582	-10.564	0.018
	Cu2(OH)2+2	1.089e-011	3.494e-012	-10.963	-11.457	-0.494
	Cu(OH)3-	8.690e-021	6.540e-021	-20.061	-20.184	-0.123
	Cu(OH)4-2	1.612e-029	5.172e-030	-28.793	-29.286	-0.494
Fe(2)	1.267e-005					
	Fe+2	7.505e-006	2.555e-006	-5.125	-5.593	-0.468
	FeSO4	5.168e-006	5.386e-006	-5.287	-5.269	0.018
	FeOH+	3.425e-012	2.559e-012	-11.465	-11.592	-0.127
	Fe(OH)2	6.379e-020	6.648e-020	-19.195	-19.177	0.018
	Fe(OH)3-	1.275e-026	9.524e-027	-25.895	-26.021	-0.127
Fe(3)	5.069e-005					
	FeSO4+	2.160e-005	1.614e-005	-4.666	-4.792	-0.127
	FeOH+2	1.108e-005	3.553e-006	-4.956	-5.449	-0.494
	Fe(SO4)2-	8.397e-006	6.320e-006	-5.076	-5.199	-0.123
	Fe(OH)2+	7.409e-006	5.587e-006	-5.130	-5.253	-0.123
	Fe+3	2.138e-006	1.656e-007	-5.670	-6.781	-1.111
	Fe2(OH)2+4	3.635e-008	3.852e-010	-7.439	-9.414	-1.975
	Fe3(OH)4+5	5.403e-010	4.435e-013	-9.267	-12.353	-3.086
	Fe(OH)3	2.502e-010	2.608e-010	-9.602	-9.584	0.018
	Fe(OH)4-	1.374e-014	1.036e-014	-13.862	-13.985	-0.123
H(0)	8.836e-028					
	H2	4.418e-028	4.604e-028	-27.355	-27.337	0.018
K	3.103e-004					
	K+	2.877e-004	2.043e-004	-3.541	-3.690	-0.149
	KSO4-	2.262e-005	1.706e-005	-4.645	-4.768	-0.123
	KCrO4-	9.232e-035	6.948e-035	-34.035	-34.158	-0.123
Mg	4.575e-002					
	Mg+2	2.538e-002	9.757e-003	-1.596	-2.011	-0.415
	MgSO4	2.037e-002	2.123e-002	-1.691	-1.673	0.018
	MgOH+	6.336e-011	4.887e-011	-10.198	-10.311	-0.113
Mn(2)	3.313e-003					
	Mn+2	1.929e-003	6.566e-004	-2.715	-3.183	-0.468
	MnSO4	1.384e-003	1.442e-003	-2.859	-2.841	0.018
	MnOH+	7.009e-011	5.237e-011	-10.154	-10.281	-0.127
	Mn(OH)3-	8.731e-028	6.523e-028	-27.059	-27.186	-0.127
Mn(3)	7.250e-020					
	Mn+3	7.250e-020	1.005e-020	-19.140	-19.998	-0.858
Mn(6)	0.000e+000					
	MnO4-2	0.000e+000	0.000e+000	-59.438	-59.944	-0.506
Mn(7)	0.000e+000					
	MnO4-	0.000e+000	0.000e+000	-60.875	-61.026	-0.151
Na	2.419e-003					
	Na+	2.279e-003	1.711e-003	-2.642	-2.767	-0.124
	NaSO4-	1.398e-004	1.054e-004	-3.855	-3.977	-0.123
	NaCrO4-	6.105e-034	4.595e-034	-33.214	-33.338	-0.123
Ni	4.306e-005					
	Ni+2	2.482e-005	7.964e-006	-4.605	-5.099	-0.494
	NiSO4	1.819e-005	1.896e-005	-4.740	-4.722	0.018
	Ni(SO4)2-2	4.081e-008	1.309e-008	-7.389	-7.883	-0.494
	NiOH+	4.689e-012	3.529e-012	-11.329	-11.452	-0.123
	Ni(OH)2	1.206e-017	1.257e-017	-16.919	-16.901	0.018
	Ni(OH)3-	6.634e-025	4.992e-025	-24.178	-24.302	-0.123
O(0)	4.424e-004					
	O2	2.212e-004	2.305e-004	-3.655	-3.637	0.018
Pb	3.904e-006					
	PbSO4	2.331e-006	2.429e-006	-5.632	-5.614	0.018
	Pb+2	1.075e-006	3.448e-007	-5.969	-6.462	-0.494
	Pb(SO4)2-2	4.979e-007	1.598e-007	-6.303	-6.797	-0.494
	PbOH+	3.549e-011	2.671e-011	-10.450	-10.573	-0.123

	Pb2OH+3	2.661e-015	2.062e-016	-14.575	-15.686	-1.111
	Pb(OH)2	3.961e-017	4.128e-017	-16.402	-16.384	0.018
	Pb(OH)3-	2.501e-024	1.883e-024	-23.602	-23.725	-0.123
	Pb3(OH)4+2	2.662e-029	8.541e-030	-28.575	-29.068	-0.494
	Pb(OH)4-2	5.352e-032	1.717e-032	-31.271	-31.765	-0.494
S(6)	8.631e-002					
	SO4-2	4.535e-002	1.253e-002	-1.343	-1.902	-0.559
	MgSO4	2.037e-002	2.123e-002	-1.691	-1.673	0.018
	CaSO4	5.869e-003	6.116e-003	-2.231	-2.214	0.018
	ZnSO4	5.144e-003	5.361e-003	-2.289	-2.271	0.018
	AlSO4+	2.333e-003	1.756e-003	-2.632	-2.755	-0.123
	Zn(SO4)2-2	1.742e-003	5.589e-004	-2.759	-3.253	-0.494
	MnSO4	1.384e-003	1.442e-003	-2.859	-2.841	0.018
	Al(SO4)2-	7.769e-004	5.733e-004	-3.110	-3.242	-0.132
	HSO4-	3.808e-004	2.866e-004	-3.419	-3.543	-0.123
	CuSO4	1.988e-004	2.071e-004	-3.702	-3.684	0.018
	NaSO4-	1.398e-004	1.054e-004	-3.855	-3.977	-0.123
	KSO4-	2.262e-005	1.706e-005	-4.645	-4.768	-0.123
	FeSO4+	2.160e-005	1.614e-005	-4.666	-4.792	-0.127
	NiSO4	1.819e-005	1.896e-005	-4.740	-4.722	0.018
	Fe(SO4)2-	8.397e-006	6.320e-006	-5.076	-5.199	-0.123
	CdSO4	7.591e-006	7.910e-006	-5.120	-5.102	0.018
	FeSO4	5.168e-006	5.386e-006	-5.287	-5.269	0.018
	Cd(SO4)2-2	3.451e-006	1.107e-006	-5.462	-5.956	-0.494
	PbSO4	2.331e-006	2.429e-006	-5.632	-5.614	0.018
	Pb(SO4)2-2	4.979e-007	1.598e-007	-6.303	-6.797	-0.494
	VOSO4	5.833e-008	6.078e-008	-7.234	-7.216	0.018
	Ni(SO4)2-2	4.081e-008	1.309e-008	-7.389	-7.883	-0.494
	CrOHSO4	3.422e-008	3.566e-008	-7.466	-7.448	0.018
	CrSO4+	7.254e-009	5.459e-009	-8.139	-8.263	-0.123
	VO2SO4-	5.566e-010	4.189e-010	-9.254	-9.378	-0.123
	Cr2(OH)2SO4+2	1.272e-013	4.080e-014	-12.896	-13.389	-0.494
	Cr2(OH)2(SO4)2	1.157e-017	1.206e-017	-16.937	-16.919	0.018
	VSO4+	1.040e-018	7.825e-019	-17.983	-18.107	-0.123
	CrO3SO4-2	1.315e-031	4.219e-032	-30.881	-31.375	-0.494
V(2)	1.134e-030					
	V+2	1.130e-030	3.624e-031	-29.947	-30.441	-0.494
	VOH+	4.382e-033	3.298e-033	-32.358	-32.482	-0.123
V(3)	2.218e-016					
	VOH+2	1.199e-016	3.845e-017	-15.921	-16.415	-0.494
	V(OH)2+	7.032e-017	5.292e-017	-16.153	-16.276	-0.123
	V+3	2.927e-017	2.267e-018	-16.534	-17.644	-1.111
	V(OH)3	1.303e-018	1.357e-018	-17.885	-17.867	0.018
	VSO4+	1.040e-018	7.825e-019	-17.983	-18.107	-0.123
	V2(OH)2+4	1.362e-030	1.443e-032	-29.866	-31.841	-1.975
	V2(OH)3+3	1.316e-031	1.019e-032	-30.881	-31.992	-1.111
V(4)	1.157e-007					
	VOSO4	5.833e-008	6.078e-008	-7.234	-7.216	0.018
	VO+2	5.718e-008	1.834e-008	-7.243	-7.736	-0.494
	V(OH)3+	2.066e-010	1.555e-010	-9.685	-9.808	-0.123
	H2V2O4+2	6.010e-015	1.928e-015	-14.221	-14.715	-0.494
V(5)	3.384e-009					
	H3VO4	1.036e-009	1.079e-009	-8.985	-8.967	0.018
	H2VO4-	9.147e-010	6.884e-010	-9.039	-9.162	-0.123
	VO2+	8.661e-010	6.518e-010	-9.062	-9.186	-0.123
	VO2SO4-	5.566e-010	4.189e-010	-9.254	-9.378	-0.123
	H3V2O7-	5.740e-012	4.320e-012	-11.241	-11.365	-0.123
	HVO4-2	6.994e-014	2.244e-014	-13.155	-13.649	-0.494
	HV2O7-3	2.608e-016	2.020e-017	-15.584	-16.695	-1.111
	V3O9-3	1.864e-021	1.444e-022	-20.730	-21.840	-1.111
	VO4-3	5.993e-023	4.642e-024	-22.222	-23.333	-1.111
	V2O7-4	1.319e-024	1.398e-026	-23.880	-25.855	-1.975
	V4O12-4	1.728e-027	1.831e-029	-26.762	-28.737	-1.975
	HV10O28-5	0.000e+000	0.000e+000	-46.291	-49.377	-3.086
	H2V10O28-4	0.000e+000	0.000e+000	-47.201	-49.176	-1.975
	V10O28-6	0.000e+000	0.000e+000	-47.353	-51.796	-4.443
Zn	1.237e-002					
	Zn+2	5.488e-003	1.868e-003	-2.261	-2.729	-0.468
	ZnSO4	5.144e-003	5.361e-003	-2.289	-2.271	0.018
	Zn(SO4)2-2	1.742e-003	5.589e-004	-2.759	-3.253	-0.494
	ZnOH+	8.592e-009	6.466e-009	-8.066	-8.189	-0.123
	Zn(OH)2	3.570e-013	3.720e-013	-12.447	-12.429	0.018
	Zn(OH)3-	6.209e-021	4.673e-021	-20.207	-20.330	-0.123
	Zn(OH)4-2	9.170e-030	2.942e-030	-29.038	-29.531	-0.494

----------Saturation indices----------

Phase	SI	log IAP	log KT	
Al(OH)3(a)	-4.12	6.46	10.58	Al(OH)3
Al2O3	-10.06	12.92	22.98	Al2O3
Al4(OH)10SO4	-5.96	16.74	22.70	Al4(OH)10SO4
AlAsO4:2H2O	-5.71	-0.91	4.80	AlAsO4:2H2O
AlOHSO4	0.59	-2.64	-3.23	AlOHSO4
AlumK	-6.62	-11.84	-5.22	KAl(SO4)2:12H2O
Alunite	2.42	1.09	-1.33	KAl3(SO4)2(OH)6
Anglesite	-0.56	-8.36	-7.81	PbSO4
Anhydrite	0.10	-4.51	-4.61	CaSO4
Antlerite	-8.04	0.25	8.29	Cu3(OH)4SO4
Arsenolite	-44.72	-126.30	-81.58	As4O6
As2O5	-21.49	-14.75	6.74	As2O5
Basaluminite	-5.96	16.74	22.70	Al4(OH)10SO4
Bianchite	-2.87	-4.64	-1.76	ZnSO4:6H2O
Birnessite	-15.19	28.22	43.41	MnO2
Bixbyite	-17.90	32.23	50.13	Mn2O3
Boehmite	-2.33	6.46	8.79	AlOOH
Brochantite	-11.98	3.36	15.34	Cu4(OH)6SO4
Brucite	-11.80	5.19	16.98	Mg(OH)2
Bunsenite	-10.53	2.10	12.63	NiO
Ca2V2O7	-9.89	-1.00	8.89	CaVO3.5
Ca3(AsO4)2:6H2O	-23.29	-0.99	22.30	Ca3(AsO4)2:6H2O
Ca3(VO4)2	-18.44	1.30	19.74	Ca1.5VO4
Ca_Vanadate	-6.20	-3.29	2.91	Ca0.5VO3
CaCrO4	-31.66	34.27	65.93	CaCrO4
Cd(Gamma)	-36.38	-22.65	13.73	Cd
Cd(OH)2(A)	-12.34	1.55	13.88	Cd(OH)2
Cd(OH)2(C)	-12.10	1.55	13.65	Cd(OH)2
Cd3(OH)2(SO4)2	-20.27	-13.56	6.71	Cd3(OH)2(SO4)2
Cd3(OH)4SO4	-27.02	-4.46	22.56	Cd3(OH)4SO4
Cd4(OH)6SO4	-31.31	-2.91	28.40	Cd4(OH)6SO4
CdMetal	-36.28	-22.65	13.62	Cd
CdSO4	-7.56	-7.55	0.01	CdSO4
CdSO4:2.67H2O	-5.72	-7.56	-1.84	CdSO4:2.67H2O
CdSO4:H2O	-5.95	-7.55	-1.60	CdSO4:H2O
Chalcanthite	-3.34	-5.99	-2.65	CuSO4:5H2O
Claudetite	-44.46	-126.30	-81.83	As4O6
Cr(OH)2	-26.70	-18.72	7.98	Cr(OH)2
Cr(OH)3(A)	-5.87	-6.62	-0.75	Cr(OH)3
Cr(OH)3(C)	-8.38	-6.62	1.75	Cr(OH)3
Cr2O3	-9.94	-13.24	-3.30	Cr2O3
CrMetal	-72.52	-42.92	29.60	Cr
CrO3	-35.27	29.68	64.94	CrO3
Cu(OH)2	-5.64	3.12	8.75	Cu(OH)2
Cu2SO4	-19.74	-27.07	-7.33	Cu2SO4
Cu3(AsO4)2:6H2O	-11.51	-5.41	6.10	Cu3(AsO4)2:6H2O
CuCrO4	-29.87	32.79	62.67	CuCrO4
CuMetal	-9.49	-21.08	-11.60	Cu
CuOCuSO4	-14.66	-2.87	11.80	CuO:CuSO4
CupricFerrite	4.98	11.15	6.17	CuFe2O4
Cuprite	-10.95	-17.97	-7.01	Cu2O
CuprousFerrite	6.63	-4.97	-11.60	CuFeO2
CuSO4	-9.13	-5.98	3.15	CuSO4
Diaspore	-0.59	6.46	7.06	AlOOH
Epsomite	-1.76	-3.92	-2.16	MgSO4:7H2O
Fe2(SO4)3	-23.29	-19.27	4.02	Fe2(SO4)3
Fe3(OH)8	-10.58	9.64	20.22	Fe3(OH)8
Fe_Vanadate	-2.98	-4.78	-1.81	Fe0.5VO3
FeAsO4:2H2O	-3.76	-3.36	0.40	FeAsO4:2H2O
FeCr2O4	-10.92	-11.64	-0.72	FeCr2O4
Ferrihydrite	-0.98	4.02	5.00	Fe(OH)3
Gibbsite(C)	-2.48	6.46	8.94	Al(OH)3
Goethite	3.41	4.02	0.61	FeOOH
Goslarite	-2.65	-4.64	-1.98	ZnSO4:7H2O
Gypsum	0.34	-4.51	-4.85	CaSO4:2H2O
Hausmannite	-25.89	36.25	62.14	Mn3O4
Hematite	11.81	8.04	-3.78	Fe2O3
Hercynite	-13.21	14.53	27.75	FeAl2O4
Jarosite-H	5.54	-6.15	-11.69	(H3O)Fe3(SO4)2(OH)6

Jarosite-K	8.32	-6.24	-14.57	KFe3(SO4)2(OH)6
Jarosite-Na	5.61	-5.32	-10.93	NaFe3(SO4)2(OH)6
Jurbanite	0.59	-2.64	-3.23	AlOHSO4
K2Cr2O7	-61.31	59.17	120.48	K2Cr2O7
K2CrO4	-38.62	29.50	68.12	K2CrO4
Langite	-13.72	3.36	17.09	Cu4(OH)6SO4:H2O
Larnakite	-7.40	-7.63	-0.23	PbO:PbSO4
Lepidocrocite	2.65	4.02	1.37	FeOOH
Lime	-28.55	4.59	33.14	CaO
Litharge	-12.11	0.74	12.84	PbO
Maghemite	1.65	8.04	6.39	Fe2O3
Magnetite	5.53	9.64	4.11	Fe3O4
Manganite	-8.96	16.12	25.08	MnOOH
Massicot	-12.30	0.74	13.04	PbO
Melanterite	-5.01	-7.50	-2.49	FeSO4:7H2O
Mg-Ferrite	-4.04	13.22	17.26	MgFe2O4
Mg2V2O7	-13.81	-0.40	13.41	MgVO3.5
Mg_Vanadate	-8.75	-2.99	5.76	Mg0.5VO3
MgCr2O4	-20.43	-8.05	12.38	MgCr2O4
MgCrO4	-38.82	34.87	73.68	MgCrO4
Minium	-48.05	26.41	74.46	Pb3O4
Mirabilite	-6.19	-7.44	-1.26	Na2SO4:10H2O
Mn2(SO4)3	-40.28	4.93	45.21	Mn2(SO4)3
Mn3(AsO4)2:8H2O	-15.21	-2.71	12.50	Mn3(AsO4)2:8H2O
Mn_Vanadate	-6.11	-3.58	2.53	Mn0.5VO3
MnSO4	-7.87	-5.08	2.78	MnSO4
Monteponite	-13.76	1.55	15.30	CdO
Morenosite	-4.63	-7.01	-2.38	NiSO4:7H2O
Na2Cr2O7	-65.33	61.02	126.35	Na2Cr2O7
Na2CrO4	-40.10	31.34	71.44	Na2CrO4
Na3VO4	-40.36	-3.09	37.27	Na3VO4
Na4V2O7	-22.80	-3.92	18.88	Na2VO3.5
Na_Vanadate	-8.52	-4.75	3.76	NaVO3
Ni(OH)2	-8.47	2.10	10.57	Ni(OH)2
Ni3(AsO4)2:8H2O	-24.16	-8.46	15.70	Ni3(AsO4)2:8H2O
Ni4(OH)6SO4	-32.70	-0.70	32.00	Ni4(OH)6SO4
Nsutite	-14.60	28.22	42.82	MnO2
O2(g)	-35.72	48.40	84.12	O2
Pb(OH)2(C)	-7.52	0.74	8.25	Pb(OH)2
Pb2O(OH)2	-24.73	1.47	26.20	Pb2O(OH)2
Pb2O3	-35.37	25.67	61.04	Pb2O3
Pb2V2O7	-3.92	-4.85	-0.93	PbVO3.5
Pb3(AsO4)2	-18.34	-12.54	5.80	Pb3(AsO4)2
Pb3(VO4)2	-7.62	-4.48	3.13	Pb1.5VO4
Pb3O2SO4	-17.45	-6.89	10.55	Pb3O2SO4
Pb4(OH)6SO4	-27.26	-6.16	21.10	Pb4(OH)6SO4
Pb4O3SO4	-28.52	-6.15	22.36	Pb4O3SO4
PbCrO4	-23.97	30.41	54.38	PbCrO4
PbMetal	-27.73	-23.46	4.27	Pb
PbO:0.3H2O	-12.24	0.74	12.98	PbO:0.33H2O
Periclase	-16.59	5.19	21.78	MgO
Plattnerite	-24.89	24.94	49.83	PbO2
Portlandite	-18.32	4.59	22.90	Ca(OH)2
Pyrocroite	-11.24	4.02	15.26	Mn(OH)2
Pyrolusite	-13.18	28.22	41.39	MnO2
Retgersite	-4.96	-7.01	-2.05	NiSO4:6H2O
Schwertmannite	16.04	23.04	7.00	Fe8O8(OH)6(SO4)
Spinel	-18.88	18.11	37.00	MgAl2O4
Tenorite	-4.62	3.12	7.73	CuO
Thenardite	-7.26	-7.44	-0.17	Na2SO4
V(OH)3	-14.50	-29.79	-15.29	V(OH)3
V2O3	-11.89	-29.79	-17.89	VO1.5
V2O4	-4.91	-17.69	-12.77	VO2
V2O5	-4.90	-5.59	-0.69	VO2.5
V3O5	-27.86	-77.26	-49.40	V3O5
V4O7	-33.78	-94.94	-61.16	V4O7
V6O13	-20.57	-81.92	-61.34	V6O13
VMetal	-85.96	-66.08	19.88	V
VO	-32.23	-41.88	-9.65	VO
VO(OH)2	-6.39	-17.69	-11.30	VO(OH)2
VOSO4(C)	-13.36	-26.79	-13.42	VOSO4
Zincite	-6.83	4.47	11.30	ZnO
Zincosite	-7.78	-4.63	3.15	ZnSO4
Zn(OH)2(A)	-7.98	4.47	12.45	Zn(OH)2

Zn(OH)2(B)	-7.28	4.47	11.75	Zn(OH)2
Zn(OH)2(C)	-7.73	4.47	12.20	Zn(OH)2
Zn(OH)2(E)	-7.03	4.47	11.50	Zn(OH)2
Zn(OH)2(G)	-7.24	4.47	11.71	Zn(OH)2
Zn2(OH)2SO4	-7.66	-0.16	7.50	Zn2(OH)2SO4
Zn3(AsO4)2:2.5H2O	-14.99	-1.34	13.65	Zn3(AsO4)2:2.5H2O
Zn3O(SO4)2	-24.27	-4.79	19.48	Zn3O(SO4)2
Zn4(OH)6SO4	-19.62	8.78	28.40	Zn4(OH)6SO4
ZnMetal	-45.76	-19.73	26.03	Zn
ZnO(Active)	-6.84	4.47	11.31	ZnO
ZnSO4:H2O	-4.14	-4.63	-0.49	ZnSO4:H2O

End of simulation.

Reading input data for simulation 2.

End of run.

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```
Input file: C:\AMD-ODIEL\Calculo termodinámico\Aznalcóllar speciation.pqi
  Output file: C:\AMD-ODIEL\Calculo termodinámico\Aznalcóllar speciation.pqo
Database file: C:\Archivos de programa\USGS\Phreeqc Interactive 2.7.1\minteq.dat

------------------
Reading data base.
------------------

       SOLUTION_MASTER_SPECIES
       SOLUTION_SPECIES
       SOLUTION_SPECIES
       PHASES
       SURFACE_MASTER_SPECIES
       SURFACE_SPECIES
       END
-----------------------------------
Reading input data for simulation 1.
-----------------------------------

       DATABASE C:\Archivos de programa\USGS\Phreeqc Interactive 2.7.1\minteq.dat
       SOLUTION 1 T-1
           temp      13
           pH        4.5
           pe        8.5
           redox     pe
           units     mg/l
           density   1
           Ca        450
           Fe(3)     0.4
           K         12
           Mg        1050
           Mn        180
           Al        85
           S(6)      7800
           Cu        40
           Cd        2
           Zn        750
           Pb        0.75
           As        0.1
           V         6 ug/l
           Cr        18 ug/l
           Na        55
           Ni        2.5
           O(0)      7
           water    1 # kg
       SOLUTION_MASTER_SPECIES
           Fe(2)         Fe+2            0     Fe
           Fe(3)         Fe+3           -2     Fe
           Mg            Mg+2            0     Mg              24.312
           Na            Na+             0     Na              22.9898
           Ca            Ca+2            0     Ca              40.08
           S             SO4-2           0     SO4             32.064
           S(6)          SO4-2           0     SO4
           K             K+              0     K               39.102
           Al            Al+3            0     Al              26.9815
       SOLUTION_SPECIES
       H2O = OH- + H+
           log_k     -14
           delta_h   13.362 kcal
       Fe+2 = Fe+3 + e-
           log_k     -13.02
           delta_h   9.68 kcal
       Fe+3 + H2O = FeOH+2 + H+
           log_k     -2.19
           delta_h   10.4 kcal
       H+ + SO4-2 = HSO4-
           log_k     1.988
           delta_h   3.85 kcal
       Al+3 + H2O = AlOH+2 + H+
```

```
            log_k     -5
            delta_h   11.49 kcal
        Al+3 + 3H2O = Al(OH)3 + 3H+
            log_k     -16.9
            delta_h   39.89 kcal
        Al+3 + SO4-2 = AlSO4+
            log_k     3.5
            delta_h   2.29 kcal
        PHASES
        Jarosite-K
            KFe3(SO4)2(OH)6 + 6H+ = 3Fe+3 + 6H2O + K+ + 2SO4-2
            log_k     -14.8
            delta_h   -31.28 kcal
        Jarosite-Na
            NaFe3(SO4)2(OH)6 + 6H+ = 3Fe+3 + 6H2O + Na+ + 2SO4-2
            log_k     -11.2
            delta_h   -36.18 kcal
        Schwertmannite
            Fe8O8(OH)6(SO4) + 22H+ = 8Fe+3 + 14H2O + SO4-2
            log_k     7
        Ferrihydrite
            Fe(OH)3 + 3H+ = Fe+3 + 3H2O
            log_k     5
        Goethite
            FeOOH + 3H+ = Fe+3 + 2H2O
            log_k     0.5
            delta_h   -14.48 kcal
        Jurbanite
            AlOHSO4 + H+ = Al+3 + H2O + SO4-2
            log_k     -3.23
        Basaluminite
            Al4(OH)10SO4 + 10H+ = 4Al+3 + 10H2O + SO4-2
            log_k     22.7
        Alunite
            KAl3(SO4)2(OH)6 + 6H+ = 3Al+3 + 6H2O + K+ + 2SO4-2
            log_k     -1.3
            delta_h   3.918 kcal
        END
-------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 1.   T-1

-----------------------------Solution composition------------------------------

        Elements           Molality       Moles

        Al               3.184e-003  3.184e-003
        As               1.349e-006  1.349e-006
        Ca               1.135e-002  1.135e-002
        Cd               1.798e-005  1.798e-005
        Cr               3.498e-007  3.498e-007
        Cu               6.361e-004  6.361e-004
        Fe(3)            7.238e-006  7.238e-006
        K                3.101e-004  3.101e-004
        Mg               4.364e-002  4.364e-002
        Mn               3.311e-003  3.311e-003
        Na               2.418e-003  2.418e-003
        Ni               4.303e-005  4.303e-005
        O(0)             4.421e-004  4.421e-004
        Pb               3.658e-006  3.658e-006
        S(6)             8.205e-002  8.205e-002
        V                1.190e-007  1.190e-007
        Zn               1.159e-002  1.159e-002

----------------------------Description of solution----------------------------

                                    pH  =   4.500
                                    pe  =   8.500
                       Activity of water  =   0.998
                          Ionic strength  =  1.740e-001
                       Mass of water (kg)  =  1.000e+000
                Total alkalinity (eq/kg)  = -4.966e-005
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                    Total carbon (mol/kg)  =  0.000e+000
                       Total CO2 (mol/kg)  =  0.000e+000
                      Temperature (deg C)  =  13.000
                  Electrical balance (eq)  = -1.058e-002
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -6.00
                                Iterations  =  10
                                   Total H  = 1.110126e+002
                                   Total O  = 5.583492e+001

---------------------------------Redox couples---------------------------------

       Redox couple             pe  Eh (volts)

       O(-2)/O(0)          17.1467      0.9735

---------------------------Distribution of species---------------------------

                                                    Log       Log         Log
       Species            Molality    Activity  Molality  Activity     Gamma

       H+               3.923e-005  3.162e-005    -4.406    -4.500    -0.094
       OH-              1.620e-010  1.226e-010    -9.791    -9.912    -0.121
       H2O              5.551e+001  9.979e-001     1.744    -0.001     0.000
Al              3.184e-003
       AlSO4+           2.132e-003  1.614e-003    -2.671    -2.792    -0.121
       Al(SO4)2-        6.962e-004  5.170e-004    -3.157    -3.286    -0.129
       Al+3             3.300e-004  4.738e-005    -3.481    -4.324    -0.843
       AlOH+2           2.021e-005  6.630e-006    -4.694    -5.178    -0.484
       Al(OH)2+         4.942e-006  3.748e-006    -5.306    -5.426    -0.120
       Al(OH)3          1.070e-009  1.114e-009    -8.971    -8.953     0.017
       Al(OH)4-         2.798e-011  2.078e-011   -10.553   -10.682    -0.129
As(3)           1.105e-014
       H3AsO3           1.105e-014  1.150e-014   -13.957   -13.939     0.017
       H4AsO3+          2.381e-019  1.802e-019   -18.623   -18.744    -0.121
       H2AsO3-          1.787e-019  1.352e-019   -18.748   -18.869    -0.121
       HAsO3-2          6.003e-027  1.969e-027   -26.222   -26.706    -0.484
       AsO3-3           1.920e-035  1.564e-036   -34.717   -35.806    -1.089
As(5)           1.349e-006
       H2AsO4-          1.328e-006  1.005e-006    -5.877    -5.998    -0.121
       HAsO4-2          1.602e-008  5.255e-009    -7.795    -8.279    -0.484
       H3AsO4           4.741e-009  4.935e-009    -8.324    -8.307     0.017
       AsO4-3           3.801e-015  3.096e-016   -14.420   -15.509    -1.089
Ca              1.135e-002
       Ca+2             6.201e-003  2.303e-003    -2.208    -2.638    -0.430
       CaSO4            5.145e-003  5.355e-003    -2.289    -2.271     0.017
       CaOH+            8.538e-012  6.556e-012   -11.069   -11.183    -0.115
Cd              1.798e-005
       CdSO4            7.451e-006  7.756e-006    -5.128    -5.110     0.017
       Cd+2             6.986e-006  2.292e-006    -5.156    -5.640    -0.484
       Cd(SO4)2-2       3.544e-006  1.163e-006    -5.451    -5.935    -0.484
       CdOH+            3.145e-012  2.380e-012   -11.502   -11.623    -0.121
       Cd2OH+3          3.833e-016  3.123e-017   -15.416   -16.505    -1.089
       Cd(OH)2          9.796e-018  1.020e-017   -17.009   -16.992     0.017
       Cd(OH)3-         4.770e-026  3.610e-026   -25.321   -25.442    -0.121
       Cd(OH)4-2        3.095e-035  1.015e-035   -34.509   -34.993    -0.484
Cr(2)           5.758e-024
       Cr+2             5.758e-024  1.889e-024   -23.240   -23.724    -0.484
Cr(3)           3.498e-007
       Cr+3             2.254e-007  1.836e-008    -6.647    -7.736    -1.089
       CrOHSO4          7.664e-008  7.977e-008    -7.116    -7.098     0.017
       Cr(OH)+2         4.245e-008  1.393e-008    -7.372    -7.856    -0.484
       CrSO4+           3.996e-009  3.025e-009    -8.398    -8.519    -0.121
       Cr(OH)2+         1.393e-009  1.054e-009    -8.856    -8.977    -0.121
       Cr(OH)3          2.369e-012  2.466e-012   -11.625   -11.608     0.017
       Cr2(OH)2SO4+2    6.156e-013  2.020e-013   -12.211   -12.695    -0.484
       Cr2(OH)2(SO4)2   5.798e-017  6.035e-017   -16.237   -16.219     0.017
       CrO2-            2.502e-018  1.894e-018   -17.602   -17.723    -0.121
       Cr(OH)4-         9.821e-019  7.433e-019   -18.008   -18.129    -0.121
Cr(6)           1.239e-025
       HCrO4-           1.206e-025  9.127e-026   -24.919   -25.040    -0.121
       CrO4-2           3.303e-027  9.530e-028   -26.481   -27.021    -0.540
       CrO3SO4-2        3.633e-029  1.192e-029   -28.440   -28.924    -0.484
       NaCrO4-          1.080e-029  8.170e-030   -28.967   -29.088    -0.121
       KCrO4-           1.648e-030  1.247e-030   -29.783   -29.904    -0.121
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	H2CrO4	4.102e-031	4.270e-031	-30.387	-30.370	0.017
	Cr2O7-2	0.000e+000	0.000e+000	-47.908	-48.392	-0.484
Cu(1)	2.078e-010					
	Cu+	2.078e-010	1.452e-010	-9.682	-9.838	-0.156
Cu(2)	6.361e-004					
	Cu+2	4.119e-004	9.835e-005	-3.385	-4.007	-0.622
	CuSO4	2.241e-004	2.333e-004	-3.650	-3.632	0.017
	CuOH+	4.235e-008	3.104e-008	-7.373	-7.508	-0.135
	Cu(OH)2	1.966e-009	2.046e-009	-8.706	-8.689	0.017
	Cu2(OH)2+2	3.713e-010	1.218e-010	-9.430	-9.914	-0.484
	Cu(OH)3-	5.153e-018	3.900e-018	-17.288	-17.409	-0.121
	Cu(OH)4-2	7.468e-026	2.450e-026	-25.127	-25.611	-0.484
Fe(3)	7.238e-006					
	Fe(OH)2+	6.224e-006	4.720e-006	-5.206	-5.326	-0.120
	FeOH+2	6.595e-007	2.164e-007	-6.181	-6.665	-0.484
	FeSO4+	2.356e-007	1.771e-007	-6.628	-6.752	-0.124
	Fe(SO4)2-	8.925e-008	6.754e-008	-7.049	-7.170	-0.121
	Fe+3	2.722e-008	2.217e-009	-7.565	-8.654	-1.089
	Fe(OH)3	1.681e-009	1.750e-009	-8.774	-8.757	0.017
	Fe2(OH)2+4	1.823e-010	2.112e-012	-9.739	-11.675	-1.936
	Fe3(OH)4+5	2.086e-012	1.969e-015	-11.681	-14.706	-3.025
	Fe(OH)4-	7.283e-013	5.523e-013	-12.138	-12.258	-0.120
H(0)	1.541e-029					
	H2	7.703e-030	8.018e-030	-29.113	-29.096	0.017
K	3.101e-004					
	K+	2.905e-004	2.079e-004	-3.537	-3.682	-0.145
	KSO4-	1.961e-005	1.487e-005	-4.708	-4.828	-0.120
	KCrO4-	1.648e-030	1.247e-030	-29.783	-29.904	-0.121
Mg	4.364e-002					
	Mg+2	2.470e-002	9.666e-003	-1.607	-2.015	-0.407
	MgSO4	1.894e-002	1.972e-002	-1.723	-1.705	0.017
	MgOH+	2.181e-010	1.690e-010	-9.661	-9.772	-0.111
Mn(2)	3.311e-003					
	Mn+2	1.994e-003	6.933e-004	-2.700	-3.159	-0.459
	MnSO4	1.317e-003	1.370e-003	-2.881	-2.863	0.017
	MnOH+	2.701e-010	2.030e-010	-9.569	-9.693	-0.124
	Mn(OH)3-	4.595e-025	3.453e-025	-24.338	-24.462	-0.124
Mn(3)	2.942e-019					
	Mn+3	2.942e-019	4.224e-020	-18.531	-19.374	-0.843
Mn(6)	0.000e+000					
	MnO4-2	0.000e+000	0.000e+000	-55.718	-56.214	-0.496
Mn(7)	0.000e+000					
	MnO4-	0.000e+000	0.000e+000	-57.768	-57.916	-0.148
Na	2.418e-003					
	Na+	2.284e-003	1.725e-003	-2.641	-2.763	-0.122
	NaSO4-	1.334e-004	1.012e-004	-3.875	-3.995	-0.120
	NaCrO4-	1.080e-029	8.170e-030	-28.967	-29.088	-0.121
Ni	4.303e-005					
	Ni+2	2.530e-005	8.301e-006	-4.597	-5.081	-0.484
	NiSO4	1.769e-005	1.841e-005	-4.752	-4.735	0.017
	Ni(SO4)2-2	4.250e-008	1.394e-008	-7.372	-7.856	-0.484
	NiOH+	1.984e-011	1.501e-011	-10.703	-10.824	-0.121
	Ni(OH)2	7.942e-016	8.267e-016	-15.100	-15.083	0.017
	Ni(OH)3-	3.447e-022	2.609e-022	-21.463	-21.584	-0.121
O(0)	4.421e-004					
	O2	2.211e-004	2.301e-004	-3.655	-3.638	0.017
Pb	3.658e-006					
	PbSO4	2.208e-006	2.299e-006	-5.656	-5.639	0.017
	Pb+2	9.838e-007	3.227e-007	-6.007	-6.491	-0.484
	Pb(SO4)2-2	4.657e-007	1.528e-007	-6.332	-6.816	-0.484
	PbOH+	2.624e-010	1.986e-010	-9.581	-9.702	-0.121
	Pb2OH+3	1.761e-014	1.435e-015	-13.754	-14.843	-1.089
	Pb(OH)2	2.342e-015	2.438e-015	-14.630	-14.613	0.017
	Pb(OH)3-	1.167e-021	8.834e-022	-20.933	-21.054	-0.121
	Pb3(OH)4+2	2.053e-026	6.736e-027	-25.688	-26.172	-0.484
	Pb(OH)4-2	1.951e-028	6.401e-029	-27.710	-28.194	-0.484
S(6)	8.205e-002					
	SO4-2	4.460e-002	1.267e-002	-1.351	-1.897	-0.547
	MgSO4	1.894e-002	1.972e-002	-1.723	-1.705	0.017
	CaSO4	5.145e-003	5.355e-003	-2.289	-2.271	0.017
	ZnSO4	4.694e-003	4.886e-003	-2.328	-2.311	0.017
	AlSO4+	2.132e-003	1.614e-003	-2.671	-2.792	-0.121
	Zn(SO4)2-2	1.688e-003	5.538e-004	-2.773	-3.257	-0.484
	MnSO4	1.317e-003	1.370e-003	-2.881	-2.863	0.017

Al(SO4)2-	6.962e-004	5.170e-004	-3.157	-3.286	-0.129
CuSO4	2.241e-004	2.333e-004	-3.650	-3.632	0.017
NaSO4-	1.334e-004	1.012e-004	-3.875	-3.995	-0.120
HSO4-	3.920e-005	2.967e-005	-4.407	-4.528	-0.121
KSO4-	1.961e-005	1.487e-005	-4.708	-4.828	-0.120
NiSO4	1.769e-005	1.841e-005	-4.752	-4.735	0.017
CdSO4	7.451e-006	7.756e-006	-5.128	-5.110	0.017
Cd(SO4)2-2	3.544e-006	1.163e-006	-5.451	-5.935	-0.484
PbSO4	2.208e-006	2.299e-006	-5.656	-5.639	0.017
Pb(SO4)2-2	4.657e-007	1.528e-007	-6.332	-6.816	-0.484
FeSO4+	2.356e-007	1.771e-007	-6.628	-6.752	-0.124
Fe(SO4)2-	8.925e-008	6.754e-008	-7.049	-7.170	-0.121
CrOHSO4	7.664e-008	7.977e-008	-7.116	-7.098	0.017
Ni(SO4)2-2	4.250e-008	1.394e-008	-7.372	-7.856	-0.484
VOSO4	7.660e-009	7.973e-009	-8.116	-8.098	0.017
CrSO4+	3.996e-009	3.025e-009	-8.398	-8.519	-0.121
VO2SO4-	1.161e-009	8.787e-010	-8.935	-9.056	-0.121
Cr2(OH)2SO4+2	6.156e-013	2.020e-013	-12.211	-12.695	-0.484
Cr2(OH)2(SO4)2	5.798e-017	6.035e-017	-16.237	-16.219	0.017
VSO4+	5.837e-021	4.418e-021	-20.234	-20.355	-0.121
CrO3SO4-2	3.633e-029	1.192e-029	-28.440	-28.924	-0.484
V(2)	3.948e-033				
V+2	3.828e-033	1.256e-033	-32.417	-32.901	-0.484
VOH+	1.200e-034	9.080e-035	-33.921	-34.042	-0.121
V(3)	3.161e-017				
V(OH)2+	2.465e-017	1.865e-017	-16.608	-16.729	-0.121
V(OH)3	3.652e-018	3.801e-018	-17.438	-17.420	0.017
VOH+2	3.150e-018	1.033e-018	-17.502	-17.986	-0.484
V+3	1.555e-019	1.266e-020	-18.808	-19.897	-1.089
VSO4+	5.837e-021	4.418e-021	-20.234	-20.355	-0.121
V2(OH)2+4	2.452e-033	2.840e-035	-32.611	-34.547	-1.936
V2(OH)3+3	1.957e-033	1.594e-034	-32.708	-33.798	-1.089
V(4)	1.678e-008				
VO+2	8.859e-009	2.906e-009	-8.053	-8.537	-0.484
VOSO4	7.660e-009	7.973e-009	-8.116	-8.098	0.017
V(OH)3+	2.586e-010	1.957e-010	-9.587	-9.708	-0.121
H2V2O4+2	9.310e-015	3.054e-015	-14.031	-14.515	-0.484
V(5)	1.023e-007				
H2VO4-	6.489e-008	4.911e-008	-7.188	-7.309	-0.121
H3V2O7-	1.232e-008	9.327e-009	-7.909	-8.030	-0.121
H3VO4	9.666e-009	1.006e-008	-8.015	-7.997	0.017
VO2+	1.787e-009	1.353e-009	-8.748	-8.869	-0.121
VO2SO4-	1.161e-009	8.787e-010	-8.935	-9.056	-0.121
HV2O7-3	3.379e-011	2.753e-012	-10.471	-11.560	-1.089
HVO4-2	3.195e-011	1.048e-011	-10.495	-10.980	-0.484
V3O9-3	3.981e-015	3.243e-016	-14.400	-15.489	-1.089
V2O7-4	1.306e-018	1.513e-020	-17.884	-19.820	-1.936
V4O12-4	4.649e-019	5.386e-021	-18.333	-20.269	-1.936
VO4-3	1.653e-019	1.346e-020	-18.782	-19.871	-1.089
V10O28-6	1.353e-030	5.957e-035	-29.869	-34.225	-4.356
HV10O28-5	6.587e-031	6.216e-034	-30.181	-33.206	-3.025
H2V10O28-4	3.397e-032	3.936e-034	-31.469	-33.405	-1.936
Zn	1.159e-002				
Zn+2	5.212e-003	1.812e-003	-2.283	-2.742	-0.459
ZnSO4	4.694e-003	4.886e-003	-2.328	-2.311	0.017
Zn(SO4)2-2	1.688e-003	5.538e-004	-2.773	-3.257	-0.484
ZnOH+	3.209e-008	2.429e-008	-7.494	-7.615	-0.121
Zn(OH)2	2.187e-011	2.277e-011	-10.660	-10.643	0.017
Zn(OH)3-	3.002e-018	2.272e-018	-17.523	-17.644	-0.121
Zn(OH)4-2	3.464e-026	1.136e-026	-25.460	-25.944	-0.484

Saturation indices

Phase	SI	log IAP	log KT	
Al(OH)3(a)	-2.04	9.17	11.21	Al(OH)3
Al2O3	-4.63	18.35	22.98	Al2O3
Al4(OH)10SO4	3.10	25.80	22.70	Al4(OH)10SO4
AlAsO4:2H2O	-3.93	0.87	4.80	AlAsO4:2H2O
AlOHSO4	1.51	-1.72	-3.23	AlOHSO4
AlumK	-6.42	-11.81	-5.39	KAl(SO4)2:12H2O
Alunite	7.96	6.54	-1.42	KAl3(SO4)2(OH)6
Anglesite	-0.53	-8.39	-7.86	PbSO4
Anhydrite	-0.01	-4.54	-4.52	CaSO4

Antlerite	-4.21	4.08	8.29	Cu3(OH)4SO4
Arsenolite	-52.51	-137.22	-84.71	As4O6
As2O5	-23.48	-16.61	6.87	As2O5
Basaluminite	3.10	25.80	22.70	Al4(OH)10SO4
Bianchite	-2.88	-4.64	-1.76	ZnSO4:6H2O
Birnessite	-10.97	31.84	42.81	MnO2
Bixbyite	-11.61	37.68	49.29	Mn2O3
Boehmite	-0.27	9.17	9.44	AlOOH
Brochantite	-6.27	9.07	15.34	Cu4(OH)6SO4
Brucite	-10.60	6.98	17.59	Mg(OH)2
Bunsenite	-9.27	3.92	13.19	NiO
Ca2V2O7	-7.34	1.99	9.34	CaVO3.5
Ca3(AsO4)2:6H2O	-19.83	2.47	22.30	Ca3(AsO4)2:6H2O
Ca3(VO4)2	-15.39	5.17	20.56	Ca1.5VO4
Ca_Vanadate	-4.33	-1.19	3.14	Ca0.5VO3
CaCrO4	-27.59	40.88	68.47	CaCrO4
Cd(Gamma)	-36.79	-22.64	14.15	Cd
Cd(OH)2(A)	-11.01	3.36	14.37	Cd(OH)2
Cd(OH)2(C)	-10.29	3.36	13.65	Cd(OH)2
Cd3(OH)2(SO4)2	-18.43	-11.72	6.71	Cd3(OH)2(SO4)2
Cd3(OH)4SO4	-23.38	-0.82	22.56	Cd3(OH)4SO4
Cd4(OH)6SO4	-25.86	2.54	28.40	Cd4(OH)6SO4
CdMetal	-36.68	-22.64	14.04	Cd
CdSO4	-7.89	-7.54	0.35	CdSO4
CdSO4:2.67H2O	-5.80	-7.54	-1.74	CdSO4:2.67H2O
CdSO4:H2O	-6.11	-7.54	-1.43	CdSO4:H2O
Chalcanthite	-3.22	-5.91	-2.68	CuSO4:5H2O
Claudetite	-52.28	-137.22	-84.94	As4O6
Cr(OH)2	-25.81	-17.48	8.33	Cr(OH)2
Cr(OH)3(A)	-3.73	-4.48	-0.75	Cr(OH)3
Cr(OH)3(C)	-6.40	-4.48	1.92	Cr(OH)3
Cr2O3	-5.93	-8.95	-3.02	Cr2O3
CrMetal	-74.02	-43.48	30.55	Cr
CrO3	-32.85	34.52	67.37	CrO3
Cu(OH)2	-4.12	4.99	9.11	Cu(OH)2
Cu2SO4	-19.76	-26.91	-7.15	Cu2SO4
Cu3(AsO4)2:6H2O	-7.74	-1.64	6.10	Cu3(AsO4)2:6H2O
CuCrO4	-25.55	39.51	65.07	CuCrO4
CuMetal	-9.05	-21.01	-11.96	Cu
CuOCuSO4	-13.54	-0.91	12.62	CuO:CuSO4
CupricFerrite	7.61	14.68	7.07	CuFe2O4
Cuprite	-8.93	-16.02	-7.08	Cu2O
CuprousFerrite	8.31	-3.16	-11.47	CuFeO2
CuSO4	-9.47	-5.90	3.57	CuSO4
Diaspore	1.54	9.17	7.63	AlOOH
Epsomite	-1.69	-3.92	-2.23	MgSO4:7H2O
Fe2(SO4)3	-28.40	-23.00	5.40	Fe2(SO4)3
FeAsO4:2H2O	-3.86	-3.46	0.40	FeAsO4:2H2O
Ferrihydrite	-0.16	4.84	5.00	Fe(OH)3
Gibbsite(C)	-0.30	9.17	9.47	Al(OH)3
Goethite	3.90	4.84	0.95	FeOOH
Goslarite	-2.58	-4.65	-2.06	ZnSO4:7H2O
Gypsum	0.32	-4.54	-4.86	CaSO4:2H2O
Hausmannite	-20.48	43.52	64.00	Mn3O4
Hematite	12.75	9.69	-3.06	Fe2O3
Jarosite-H	3.14	-7.26	-10.40	(H3O)Fe3(SO4)2(OH)6
Jarosite-K	7.39	-6.45	-13.84	KFe3(SO4)2(OH)6
Jarosite-Na	4.56	-5.53	-10.09	NaFe3(SO4)2(OH)6
Jurbanite	1.51	-1.72	-3.23	AlOHSO4
K2Cr2O7	-54.18	70.68	124.86	K2Cr2O7
K2CrO4	-34.26	36.16	70.42	K2CrO4
Langite	-8.94	9.07	18.01	Cu4(OH)6SO4:H2O
Larnakite	-5.80	-5.88	-0.08	PbO:PbSO4
Lepidocrocite	3.47	4.84	1.37	FeOOH
Lime	-27.86	6.36	34.22	CaO
Litharge	-10.72	2.51	13.22	PbO
Maghemite	3.30	9.69	6.39	Fe2O3
Manganite	-5.64	18.84	24.48	MnOOH
Massicot	-10.92	2.51	13.43	PbO
Mg-Ferrite	-2.14	16.67	18.81	MgFe2O4
Mg2V2O7	-11.50	2.62	14.12	MgVO3.5
Mg_Vanadate	-7.02	-0.88	6.14	Mg0.5VO3
MgCr2O4	-15.27	-1.97	13.30	MgCr2O4
MgCrO4	-35.07	41.51	76.58	MgCrO4

```
        Minium          -43.33   33.52   76.85  Pb3O4
        Mirabilite       -5.74   -7.43   -1.70  Na2SO4:10H2O
        Mn2(SO4)3       -39.93    4.99   44.92  Mn2(SO4)3
        Mn3(AsO4)2:8H2O -11.60    0.90   12.50  Mn3(AsO4)2:8H2O
        Mn_Vanadate      -4.24   -1.45    2.79  Mn0.5VO3
        MnSO4            -8.20   -5.06    3.14  MnSO4
        Monteponite     -12.52    3.36   15.88  CdO
        Morenosite       -4.53   -6.98   -2.45  NiSO4:7H2O
        Na2Cr2O7        -58.51   72.52  131.03  Na2Cr2O7
        Na2CrO4         -35.95   37.99   73.95  Na2CrO4
        Na3VO4          -37.47    0.84   38.31  Na3VO4
        Na4V2O7         -20.34   -0.90   19.44  Na2VO3.5
        Na_Vanadate      -6.56   -2.63    3.93  NaVO3
        Ni(OH)2          -5.95    3.92    9.86  Ni(OH)2
        Ni3(AsO4)2:8H2O -20.56   -4.86   15.70  Ni3(AsO4)2:8H2O
        Ni4(OH)6SO4     -27.23    4.77   32.00  Ni4(OH)6SO4
        Nsutite         -10.38   31.84   42.22  MnO2
        O2(g)           -35.24   52.00   87.23  O2
        Pb(OH)2(C)       -6.07    2.51    8.58  Pb(OH)2
        Pb2O(OH)2       -21.18    5.02   26.20  Pb2O(OH)2
        Pb2O3           -30.02   31.02   61.04  Pb2O3
        Pb2V2O7          -1.01   -1.86   -0.85  PbVO3.5
        Pb3(AsO4)2      -14.89   -9.09    5.80  Pb3(AsO4)2
        Pb3(VO4)2        -3.94   -0.61    3.34  Pb1.5VO4
        Pb3O2SO4        -14.41   -3.37   11.04  Pb3O2SO4
        Pb4(OH)6SO4     -21.97   -0.87   21.10  Pb4(OH)6SO4
        Pb4O3SO4        -24.04   -0.86   23.18  Pb4O3SO4
        PbCrO4          -19.51   37.03   56.54  PbCrO4
        PbMetal         -27.75  -23.49    4.26  Pb
        PbO:0.3H2O      -10.47    2.51   12.98  PbO:0.33H2O
        Periclase       -15.64    6.98   22.62  MgO
        Plattnerite     -22.97   28.51   51.47  PbO2
        Portlandite     -17.26    6.36   23.62  Ca(OH)2
        Pyrocroite       -9.94    5.84   15.78  Mn(OH)2
        Pyrolusite       -9.63   31.84   41.47  MnO2
        Retgersite       -4.91   -6.98   -2.07  NiSO4:6H2O
        Schwertmannite   20.86   27.86    7.00  Fe8O8(OH)6(SO4)
        Spinel          -13.74   25.33   39.07  MgAl2O4
        Tenorite         -3.10    4.99    8.09  CuO
        Thenardite       -7.26   -7.42   -0.16  Na2SO4
        V(OH)3          -14.05  -30.37  -16.32  V(OH)3
        V2O3            -11.90  -30.37  -18.46  VO1.5
        V2O4             -4.24  -17.37  -13.13  VO2
        V2O5             -3.78   -4.37   -0.59  VO2.5
        V3O5            -27.20  -78.11  -50.90  V3O5
        V4O7            -32.49  -95.47  -62.98  V4O7
        V6O13           -15.36  -78.21  -62.85  V6O13
        VMetal          -89.68  -69.37   20.31  V
        VO              -33.34  -43.37  -10.03  VO
        VO(OH)2          -5.39  -17.37  -11.98  VO(OH)2
        VOSO4(C)        -14.64  -28.27  -13.62  VOSO4
        Zincite          -5.55    6.26   11.81  ZnO
        Zincosite        -8.24   -4.64    3.60  ZnSO4
        Zn(OH)2(A)       -6.19    6.26   12.45  Zn(OH)2
        Zn(OH)2(B)       -5.49    6.26   11.75  Zn(OH)2
        Zn(OH)2(C)       -5.94    6.26   12.20  Zn(OH)2
        Zn(OH)2(E)       -5.24    6.26   11.50  Zn(OH)2
        Zn(OH)2(G)       -5.45    6.26   11.71  Zn(OH)2
        Zn2(OH)2SO4      -5.88    1.62    7.50  Zn2(OH)2SO4
        Zn3(AsO4)2:2.5H2O -11.49    2.16   13.65  Zn3(AsO4)2:2.5H2O
        Zn3O(SO4)2      -23.95   -3.02   20.93  Zn3O(SO4)2
        Zn4(OH)6SO4     -14.27   14.13   28.40  Zn4(OH)6SO4
        ZnMetal         -46.63  -19.74   26.89  Zn
        ZnO(Active)      -5.05    6.26   11.31  ZnO
        ZnSO4:H2O        -4.40   -4.64   -0.24  ZnSO4:H2O
------------------
End of simulation.
------------------
------------------------------------
Reading input data for simulation 2.
------------------------------------
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End of run.
-----------
```

CÁLCULOS DE ESPECIACIÓN QUÍMICA DE METALES E ÍNDICES DE SATURACIÓN

AZNALCÓLLAR, MUESTRA SUPERFICIAL (0M). MAYO 2006

```
Input file: C:\TRABAJO\Compartida\MODELIZACIÓN\Especiación Aznalcóllar Mayo 2006.pqi
  Output file: C:\TRABAJO\Compartida\MODELIZACIÓN\Especiación Aznalcóllar Mayo 2006.pqo
Database file: C:\Archivos de programa\USGS\Phreeqc Interactive 2.7.1\minteq.dat

------------------
Reading data base.
------------------

       SOLUTION_MASTER_SPECIES
       SOLUTION_SPECIES
       SOLUTION_SPECIES
       PHASES
       SURFACE_MASTER_SPECIES
       SURFACE_SPECIES
       END
-----------------------------------
Reading input data for simulation 1.
-----------------------------------

       DATABASE C:\Archivos de programa\USGS\Phreeqc Interactive 2.7.1\minteq.dat
       SOLUTION 2 Muestra superficial (m. 0)
           temp      21
           pH        2.84
           pe        4
           redox     Fe(2)/Fe(3)
           units     mg/l
           density   1
           S(6)      7.98 g/L
           Al        144
           Fe(2)     11
           Fe(3)     104
           Zn        744
           Cu        31
           Mn        170
           K         17
           Na        65.8
           Ca        478
           Cd        1.32
           Ni        2.4
           O(0)      5.17
           As        82 ug/L
           Pb        1057 ug/L
           water    1 # kg
       SOLUTION_MASTER_SPECIES
           Fe(2)         Fe+2            0     Fe
           Fe(3)         Fe+3           -2     Fe
           Mg            Mg+2            0     Mg              24.312
           Na            Na+             0     Na              22.9898
           Ca            Ca+2            0     Ca              40.08
           S             SO4-2           0     SO4             32.064
           S(6)          SO4-2           0     SO4
           K             K+              0     K               39.102
           Al            Al+3            0     Al              26.9815
       SOLUTION_SPECIES
       H2O = OH- + H+
           log_k     -14
           delta_h   13.362 kcal
       Fe+2 = Fe+3 + e-
           log_k     -13.02
           delta_h   9.68 kcal
       Fe+3 + H2O = FeOH+2 + H+
           log_k     -2.19
           delta_h   10.4 kcal
       H+ + SO4-2 = HSO4-
           log_k     1.988
```

```
            delta_h   3.85 kcal
        Al+3 + H2O = AlOH+2 + H+
            log_k     -5
            delta_h   11.49 kcal
        Al+3 + 3H2O = Al(OH)3 + 3H+
            log_k     -16.9
            delta_h   39.89 kcal
        Al+3 + SO4-2 = AlSO4+
            log_k     3.5
            delta_h   2.29 kcal
        PHASES
        Jarosite-K
            KFe3(SO4)2(OH)6 + 6H+ = 3Fe+3 + 6H2O + K+ + 2SO4-2
            log_k     -14.8
            delta_h   -31.28 kcal
        Jarosite-Na
            NaFe3(SO4)2(OH)6 + 6H+ = 3Fe+3 + 6H2O + Na+ + 2SO4-2
            log_k     -11.2
            delta_h   -36.18 kcal
        Schwertmannite
            Fe8O8(OH)6(SO4) + 22H+ = 8Fe+3 + 14H2O + SO4-2
            log_k     7
        Ferrihydrite
            Fe(OH)3 + 3H+ = Fe+3 + 3H2O
            log_k     5
        Goethite
            FeOOH + 3H+ = Fe+3 + 2H2O
            log_k     0.5
            delta_h   -14.48 kcal
        Jurbanite
            AlOHSO4 + H+ = Al+3 + H2O + SO4-2
            log_k     -3.23
        Basaluminite
            Al4(OH)10SO4 + 10H+ = 4Al+3 + 10H2O + SO4-2
            log_k     22.7
        Alunite
            KAl3(SO4)2(OH)6 + 6H+ = 3Al+3 + 6H2O + K+ + 2SO4-2
            log_k     -1.3
            delta_h   3.918 kcal
        END
------------------------------------------
Beginning of initial solution calculations.
------------------------------------------

Initial solution 2.   Muestra superficial (m. 0)

-----------------------------Solution composition----------------------

        Elements           Molality       Moles

        Al               5.390e-003  5.390e-003
        As               1.105e-006  1.105e-006
        Ca               1.204e-002  1.204e-002
        Cd               1.186e-005  1.186e-005
        Cu               4.926e-004  4.926e-004
        Fe(2)            1.989e-004  1.989e-004
        Fe(3)            1.881e-003  1.881e-003
        K                4.390e-004  4.390e-004
        Mn               3.125e-003  3.125e-003
        Na               2.890e-003  2.890e-003
        Ni               4.128e-005  4.128e-005
        O(0)             3.263e-004  3.263e-004
        Pb               5.152e-006  5.152e-006
        S(6)             8.389e-002  8.389e-002
        Zn               1.149e-002  1.149e-002

---------------------------Description of solution-------------------

                                    pH  =   2.840
                                    pe  =   4.000
                       Activity of water  =   0.998
                          Ionic strength  =  1.448e-001
                       Mass of water (kg)  =  1.000e+000
                Total alkalinity (eq/kg)  = -8.199e-003
```

```
                    Total carbon (mol/kg)  =  0.000e+000
                       Total CO2 (mol/kg)  =  0.000e+000
                      Temperature (deg C)  =  21.000
                  Electrical balance (eq)  = -8.338e-002
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  = -55.07
                                Iterations  =  14
                                   Total H  = 1.110171e+002
                                   Total O  = 5.584219e+001

---------------------------------Redox couples-------------------------

       Redox couple             pe  Eh (volts)

       Fe(2)/Fe(3)         12.4069      0.7241
       O(-2)/O(0)          18.0730      1.0548

----------------------------Distribution of species--------------------

                                                    Log       Log         Log
       Species             Molality    Activity  Molality  Activity     Gamma

       H+                1.781e-003  1.445e-003    -2.749    -2.840    -0.091
       OH-               6.661e-012  5.083e-012   -11.176   -11.294    -0.117
       H2O               5.551e+001  9.984e-001     1.744    -0.001     0.000
Al               5.390e-003
       AlSO4+            3.519e-003  2.685e-003    -2.454    -2.571    -0.117
       Al(SO4)2-         1.511e-003  1.137e-003    -2.821    -2.944    -0.123
       Al+3              3.595e-004  5.486e-005    -3.444    -4.261    -0.816
       AlOH+2            8.588e-007  2.911e-007    -6.066    -6.536    -0.470
       Al(OH)2+          2.709e-009  2.079e-009    -8.567    -8.682    -0.115
       Al(OH)3           8.811e-014  9.110e-014   -13.055   -13.040     0.014
       Al(OH)4-          6.033e-017  4.542e-017   -16.219   -16.343    -0.123
As(3)            2.995e-018
       H3AsO3            2.992e-018  3.093e-018   -17.524   -17.510     0.014
       H4AsO3+           2.903e-021  2.215e-021   -20.537   -20.655    -0.117
       H2AsO3-           1.427e-024  1.089e-024   -23.846   -23.963    -0.117
       HAsO3-2           1.475e-033  4.999e-034   -32.831   -33.301    -0.470
       AsO3-3            0.000e+000  0.000e+000   -42.878   -43.935    -1.057
As(5)            1.105e-006
       H2AsO4-           9.368e-007  7.148e-007    -6.028    -6.146    -0.117
       H3AsO4            1.682e-007  1.739e-007    -6.774    -6.760     0.014
       HAsO4-2           2.502e-010  8.482e-011    -9.602   -10.071    -0.470
       AsO4-3            1.536e-018  1.346e-019   -17.814   -18.871    -1.057
Ca               1.204e-002
       CaSO4             6.546e-003  6.768e-003    -2.184    -2.170     0.014
       Ca+2              5.498e-003  2.107e-003    -2.260    -2.676    -0.417
       CaOH+             3.390e-013  2.630e-013   -12.470   -12.580    -0.110
Cd               1.186e-005
       CdSO4             5.333e-006  5.513e-006    -5.273    -5.259     0.014
       Cd+2              3.545e-006  1.201e-006    -5.450    -5.920    -0.470
       Cd(SO4)2-2        2.982e-006  1.011e-006    -5.525    -5.995    -0.470
       CdOH+             6.697e-014  5.110e-014   -13.174   -13.292    -0.117
       Cd2OH+3           3.608e-018  3.163e-019   -17.443   -18.500    -1.057
       Cd(OH)2           2.476e-021  2.560e-021   -20.606   -20.592     0.014
       Cd(OH)3-          2.600e-031  1.984e-031   -30.585   -30.702    -0.117
       Cd(OH)4-2         0.000e+000  0.000e+000   -41.443   -41.913    -0.470
Cu(1)            1.955e-014
       Cu+               1.955e-014  1.394e-014   -13.709   -13.856    -0.147
Cu(2)            4.926e-004
       Cu+2              2.721e-004  7.042e-005    -3.565    -4.152    -0.587
       CuSO4             2.206e-004  2.280e-004    -3.656    -3.642     0.014
       CuOH+             6.538e-010  4.864e-010    -9.185    -9.313    -0.128
       Cu(OH)2           6.789e-013  7.019e-013   -12.168   -12.154     0.014
       Cu2(OH)2+2        2.042e-013  6.921e-014   -12.690   -13.160    -0.470
       Cu(OH)3-          3.837e-023  2.928e-023   -22.416   -22.533    -0.117
       Cu(OH)4-2         1.188e-032  4.026e-033   -31.925   -32.395    -0.470
Fe(2)            1.989e-004
       Fe+2              1.023e-004  3.709e-005    -3.990    -4.431    -0.440
       FeSO4             9.663e-005  9.990e-005    -4.015    -4.000     0.014
       FeOH+             7.863e-012  5.985e-012   -11.104   -11.223    -0.119
       Fe(OH)2           2.392e-020  2.473e-020   -19.621   -19.607     0.014
       Fe(OH)3-          8.012e-028  6.098e-028   -27.096   -27.215    -0.119
Fe(3)            1.881e-003
       FeSO4+            1.139e-003  8.670e-004    -2.943    -3.062    -0.119
```

	Fe(SO4)2-	5.769e-004	4.402e-004	-3.239	-3.356	-0.117
	Fe+3	7.975e-005	6.991e-006	-4.098	-5.155	-1.057
	FeOH+2	7.245e-005	2.456e-005	-4.140	-4.610	-0.470
	Fe(OH)2+	9.293e-006	7.130e-006	-5.032	-5.147	-0.115
	Fe2(OH)2+4	1.454e-006	1.919e-008	-5.837	-7.717	-1.879
	Fe3(OH)4+5	2.426e-008	2.807e-011	-7.615	-10.552	-2.937
	Fe(OH)3	5.597e-011	5.786e-011	-10.252	-10.238	0.014
	Fe(OH)4-	5.209e-016	3.997e-016	-15.283	-15.398	-0.115
H(0)	4.574e-034					
	H2	2.287e-034	2.364e-034	-33.641	-33.626	0.014
K	4.390e-004					
	K+	3.987e-004	2.902e-004	-3.399	-3.537	-0.138
	KSO4-	4.038e-005	3.099e-005	-4.394	-4.509	-0.115
Mn(2)	3.125e-003					
	Mn+2	1.570e-003	5.694e-004	-2.804	-3.245	-0.440
	MnSO4	1.555e-003	1.608e-003	-2.808	-2.794	0.014
	MnOH+	9.544e-012	7.264e-012	-11.020	-11.139	-0.119
	Mn(OH)3-	3.907e-030	2.973e-030	-29.408	-29.527	-0.119
Mn(3)	5.351e-016					
	Mn+3	5.351e-016	8.167e-017	-15.272	-16.088	-0.816
Mn(6)	0.000e+000					
	MnO4-2	0.000e+000	0.000e+000	-50.361	-50.835	-0.474
Mn(7)	0.000e+000					
	MnO4-	0.000e+000	0.000e+000	-47.937	-48.077	-0.140
Na	2.890e-003					
	Na+	2.678e-003	2.043e-003	-2.572	-2.690	-0.118
	NaSO4-	2.121e-004	1.628e-004	-3.673	-3.788	-0.115
Ni	4.128e-005					
	NiSO4	2.068e-005	2.138e-005	-4.684	-4.670	0.014
	Ni+2	2.054e-005	6.963e-006	-4.687	-5.157	-0.470
	Ni(SO4)2-2	5.722e-008	1.940e-008	-7.242	-7.712	-0.470
	NiOH+	6.542e-013	4.992e-013	-12.184	-12.302	-0.117
	Ni(OH)2	3.213e-019	3.322e-019	-18.493	-18.479	0.014
	Ni(OH)3-	3.007e-027	2.294e-027	-26.522	-26.639	-0.117
O(0)	3.263e-004					
	O2	1.632e-004	1.687e-004	-3.787	-3.773	0.014
Pb	5.152e-006					
	PbSO4	3.233e-006	3.342e-006	-5.490	-5.476	0.014
	Pb+2	1.075e-006	3.644e-007	-5.969	-6.438	-0.470
	Pb(SO4)2-2	8.441e-007	2.861e-007	-6.074	-6.543	-0.470
	PbOH+	6.432e-012	4.908e-012	-11.192	-11.309	-0.117
	Pb2OH+3	4.567e-016	4.003e-017	-15.340	-16.398	-1.057
	Pb(OH)2	1.275e-018	1.319e-018	-17.894	-17.880	0.014
	Pb(OH)3-	1.371e-026	1.046e-026	-25.863	-25.981	-0.117
	Pb3(OH)4+2	2.331e-032	7.902e-033	-31.632	-32.102	-0.470
	Pb(OH)4-2	4.893e-035	1.659e-035	-34.310	-34.780	-0.470
S(6)	8.389e-002					
	SO4-2	5.395e-002	1.631e-002	-1.268	-1.788	-0.520
	CaSO4	6.546e-003	6.768e-003	-2.184	-2.170	0.014
	ZnSO4	5.257e-003	5.435e-003	-2.279	-2.265	0.014
	AlSO4+	3.519e-003	2.685e-003	-2.454	-2.571	-0.117
	HSO4-	2.751e-003	2.099e-003	-2.560	-2.678	-0.117
	Zn(SO4)2-2	2.193e-003	7.434e-004	-2.659	-3.129	-0.470
	MnSO4	1.555e-003	1.608e-003	-2.808	-2.794	0.014
	Al(SO4)2-	1.511e-003	1.137e-003	-2.821	-2.944	-0.123
	FeSO4+	1.139e-003	8.670e-004	-2.943	-3.062	-0.119
	Fe(SO4)2-	5.769e-004	4.402e-004	-3.239	-3.356	-0.117
	CuSO4	2.206e-004	2.280e-004	-3.656	-3.642	0.014
	NaSO4-	2.121e-004	1.628e-004	-3.673	-3.788	-0.115
	FeSO4	9.663e-005	9.990e-005	-4.015	-4.000	0.014
	KSO4-	4.038e-005	3.099e-005	-4.394	-4.509	-0.115
	NiSO4	2.068e-005	2.138e-005	-4.684	-4.670	0.014
	CdSO4	5.333e-006	5.513e-006	-5.273	-5.259	0.014
	PbSO4	3.233e-006	3.342e-006	-5.490	-5.476	0.014
	Cd(SO4)2-2	2.982e-006	1.011e-006	-5.525	-5.995	-0.470
	Pb(SO4)2-2	8.441e-007	2.861e-007	-6.074	-6.543	-0.470
	Ni(SO4)2-2	5.722e-008	1.940e-008	-7.242	-7.712	-0.470
Zn	1.149e-002					
	ZnSO4	5.257e-003	5.435e-003	-2.279	-2.265	0.014
	Zn+2	4.044e-003	1.467e-003	-2.393	-2.834	-0.440
	Zn(SO4)2-2	2.193e-003	7.434e-004	-2.659	-3.129	-0.470
	ZnOH+	1.070e-009	8.166e-010	-8.971	-9.088	-0.117
	Zn(OH)2	8.538e-015	8.828e-015	-14.069	-14.054	0.014
	Zn(OH)3-	2.527e-023	1.928e-023	-22.597	-22.715	-0.117

```
        Zn(OH)4-2        6.227e-033  2.111e-033   -32.206   -32.676    -0.470

------------------------------Saturation indices----------------------

        Phase               SI log IAP  log KT

        Al(OH)3(a)       -6.39    4.26   10.65  Al(OH)3
        Al2O3           -14.46    8.52   22.98  Al2O3
        Al4(OH)10SO4    -13.14    9.56   22.70  Al4(OH)10SO4
        AlAsO4:2H2O      -7.30   -2.50    4.80  AlAsO4:2H2O
        AlOHSO4           0.02   -3.21   -3.23  AlOHSO4
        AlumK            -6.14  -11.38   -5.24  KAl(SO4)2:12H2O
        Alunite          -1.52   -2.86   -1.34  KAl3(SO4)2(OH)6
        Anglesite        -0.41   -8.23   -7.81  PbSO4
        Anhydrite         0.14   -4.46   -4.60  CaSO4
        Antlerite       -11.18   -2.89    8.29  Cu3(OH)4SO4
        Arsenolite      -67.09  -43.95   23.14  As4O6
        As2O5           -20.27  -13.52    6.75  As2O5
        Basaluminite    -13.14    9.56   22.70  Al4(OH)10SO4
        Bianchite        -2.86   -4.63   -1.76  ZnSO4:6H2O
        Birnessite      -10.41    6.66   17.08  MnO2
        Bixbyite        -14.68    9.10   23.78  Mn2O3
        Boehmite         -4.60    4.26    8.86  AlOOH
        Brochantite     -16.70   -1.36   15.34  Cu4(OH)6SO4
        Bunsenite       -12.17    0.52   12.69  NiO
        Ca3(AsO4)2:6H2O -26.81   -4.51   22.30  Ca3(AsO4)2:6H2O
        Cd(Gamma)       -44.50   -4.47   40.03  Cd
        Cd(OH)2(A)      -14.18   -0.24   13.94  Cd(OH)2
        Cd(OH)2(C)      -13.89   -0.24   13.65  Cd(OH)2
        Cd3(OH)2(SO4)2  -22.37  -15.66    6.71  Cd3(OH)2(SO4)2
        Cd3(OH)4SO4     -30.75   -8.19   22.56  Cd3(OH)4SO4
        Cd4(OH)6SO4     -36.83   -8.43   28.40  Cd4(OH)6SO4
        CdMetal         -44.40   -4.47   39.93  Cd
        CdSO4            -7.75   -7.71    0.05  CdSO4
        CdSO4:2.67H2O    -5.88   -7.71   -1.83  CdSO4:2.67H2O
        CdSO4:H2O        -6.13   -7.71   -1.58  CdSO4:H2O
        Chalcanthite     -3.29   -5.94   -2.65  CuSO4:5H2O
        Claudetite      -66.84  -43.95   22.88  As4O6
        Cu(OH)2          -7.27    1.53    8.79  Cu(OH)2
        Cu2SO4          -27.59   -8.64   18.95  Cu2SO4
        Cu3(AsO4)2:6H2O -15.04   -8.94    6.10  Cu3(AsO4)2:6H2O
        CuMetal         -17.33   -2.70   14.63  Cu
        CuOCuSO4        -16.30   -4.41   11.88  CuO:CuSO4
        CupricFerrite     1.99    8.25    6.27  CuFe2O4
        Cuprite         -20.42   -1.18   19.24  Cu2O
        CuprousFerrite    1.23    2.78    1.55  CuFeO2
        CuSO4            -9.13   -5.94    3.19  CuSO4
        Diaspore         -2.86    4.26    7.12  AlOOH
        Fe2(SO4)3       -19.84  -15.67    4.17  Fe2(SO4)3
        Fe3(OH)8        -12.25    7.97   20.22  Fe3(OH)8
        FeAsO4:2H2O      -3.80   -3.40    0.40  FeAsO4:2H2O
        Ferrihydrite     -1.64    3.36    5.00  Fe(OH)3
        Gibbsite(C)      -4.74    4.26    9.00  Al(OH)3
        Goethite          2.72    3.36    0.64  FeOOH
        Goslarite        -2.63   -4.63   -1.99  ZnSO4:7H2O
        Gypsum            0.39   -4.47   -4.85  CaSO4:2H2O
        Hausmannite     -24.54   11.53   36.08  Mn3O4
        Hematite         10.43    6.73   -3.70  Fe2O3
        Hercynite       -18.18    9.76   27.94  FeAl2O4
        Jarosite-H        6.70   -4.85  -11.55  (H3O)Fe3(SO4)2(OH)6
        Jarosite-K        8.95   -5.54  -14.49  KFe3(SO4)2(OH)6
        Jarosite-Na       6.14   -4.70  -10.84  NaFe3(SO4)2(OH)6
        Jurbanite         0.02   -3.21   -3.23  AlOHSO4
        Langite         -18.55   -1.36   17.18  Cu4(OH)6SO4:H2O
        Larnakite        -8.77   -8.99   -0.22  PbO:PbSO4
        Lepidocrocite     1.99    3.36    1.37  FeOOH
        Lime            -30.26    3.00   33.26  CaO
        Litharge        -13.64   -0.76   12.88  PbO
        Maghemite         0.34    6.73    6.39  Fe2O3
        Magnetite         3.74    7.98    4.24  Fe3O4
        Manganite        -7.33    4.55   11.88  MnOOH
        Massicot        -13.84   -0.76   13.08  PbO
        Melanterite      -3.72   -6.22   -2.50  FeSO4:7H2O
        Minium          -46.50    1.95   48.45  Pb3O4
```

Mirabilite	-5.87	-7.17	-1.30	Na2SO4:10H2O
Mn2(SO4)3	-32.22	-13.30	18.92	Mn2(SO4)3
Mn3(AsO4)2:8H2O	-18.72	-6.22	12.50	Mn3(AsO4)2:8H2O
MnSO4	-7.86	-5.03	2.82	MnSO4
Monteponite	-15.61	-0.24	15.37	CdO
Morenosite	-4.56	-6.95	-2.39	NiSO4:7H2O
Ni(OH)2	-9.98	0.52	10.50	Ni(OH)2
Ni3(AsO4)2:8H2O	-27.66	-11.96	15.70	Ni3(AsO4)2:8H2O
Ni4(OH)6SO4	-37.38	-5.38	32.00	Ni4(OH)6SO4
Nsutite	-9.83	6.66	16.49	MnO2
O2(g)	-23.47	8.46	31.93	O2
Pb(OH)2(C)	-9.05	-0.76	8.29	Pb(OH)2
Pb2O(OH)2	-27.72	-1.52	26.20	Pb2O(OH)2
Pb2O3	-32.07	2.71	34.78	Pb2O3
Pb3(AsO4)2	-21.59	-15.79	5.80	Pb3(AsO4)2
Pb3O2SO4	-20.35	-9.74	10.61	Pb3O2SO4
Pb4(OH)6SO4	-31.61	-10.51	21.10	Pb4(OH)6SO4
Pb4O3SO4	-32.95	-10.50	22.45	Pb4O3SO4
PbMetal	-35.52	-4.99	30.53	Pb
PbO:0.3H2O	-13.74	-0.76	12.98	PbO:0.33H2O
Plattnerite	-20.27	3.47	23.74	PbO2
Portlandite	-19.98	3.00	22.98	Ca(OH)2
Pyrocroite	-12.88	2.43	15.31	Mn(OH)2
Pyrolusite	-8.47	6.66	15.14	MnO2
Retgersite	-4.90	-6.95	-2.05	NiSO4:6H2O
Schwertmannite	12.44	19.44	7.00	Fe8O8(OH)6(SO4)
Tenorite	-6.24	1.53	7.77	CuO
Thenardite	-6.99	-7.17	-0.17	Na2SO4
Zincite	-8.51	2.85	11.36	ZnO
Zincosite	-7.82	-4.62	3.20	ZnSO4
Zn(OH)2(A)	-9.61	2.84	12.45	Zn(OH)2
Zn(OH)2(B)	-8.91	2.84	11.75	Zn(OH)2
Zn(OH)2(C)	-9.36	2.84	12.20	Zn(OH)2
Zn(OH)2(E)	-8.66	2.84	11.50	Zn(OH)2
Zn(OH)2(G)	-8.87	2.84	11.71	Zn(OH)2
Zn2(OH)2SO4	-9.28	-1.78	7.50	Zn2(OH)2SO4
Zn3(AsO4)2:2.5H2O	-18.63	-4.98	13.65	Zn3(AsO4)2:2.5H2O
Zn3O(SO4)2	-26.03	-6.40	19.64	Zn3O(SO4)2
Zn4(OH)6SO4	-24.49	3.91	28.40	Zn4(OH)6SO4
ZnMetal	-53.77	-1.38	52.39	Zn
ZnO(Active)	-8.46	2.85	11.31	ZnO
ZnSO4:H2O	-4.16	-4.62	-0.46	ZnSO4:H2O

End of simulation.

AZNALCÓLLAR, MUESTRA EN PROFUNDIDAD (30M). MAYO 2006

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-----------------------------------
Reading input data for simulation 2.
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        SOLUTION 2 Muestra profundidad (m. 30)
            temp      15.7
            pH        3.12
            pe        4
            redox     Fe(2)/Fe(3)
            units     mg/l
            density   1
            S(6)      10.4 g/l
            Al        197
            Fe(2)     966
            Fe(3)     140
            Zn        937
            Cu        64
            Mn        170
            K         19.9
            Na        66.8
            Ca        524
            Cd        1.35
            Ni        2.22
            O(0)      0.3
            As        2286 ug/l
            Pb        1323 ug/l
            water    1 # kg
        SOLUTION_MASTER_SPECIES
            Fe(2)         Fe+2             0     Fe
            Fe(3)         Fe+3            -2     Fe
            Mg            Mg+2             0     Mg              24.312
            Na            Na+              0     Na              22.9898
            Ca            Ca+2             0     Ca              40.08
            S             SO4-2            0     SO4             32.064
            S(6)          SO4-2            0     SO4
            K             K+               0     K               39.102
            Al            Al+3             0     Al              26.9815
        SOLUTION_SPECIES
        H2O = OH- + H+
            log_k     -14
            delta_h   13.362 kcal
        Fe+2 = Fe+3 + e-
            log_k     -13.02
            delta_h   9.68 kcal
        Fe+3 + H2O = FeOH+2 + H+
            log_k     -2.19
            delta_h   10.4 kcal
        H+ + SO4-2 = HSO4-
            log_k     1.988
            delta_h   3.85 kcal
        Al+3 + H2O = AlOH+2 + H+
            log_k     -5
            delta_h   11.49 kcal
        Al+3 + 3H2O = Al(OH)3 + 3H+
            log_k     -16.9
            delta_h   39.89 kcal
        Al+3 + SO4-2 = AlSO4+
            log_k     3.5
            delta_h   2.29 kcal
        PHASES
        Jarosite-K
            KFe3(SO4)2(OH)6 + 6H+ = 3Fe+3 + 6H2O + K+ + 2SO4-2
            log_k     -14.8
            delta_h   -31.28 kcal
        Jarosite-Na
            NaFe3(SO4)2(OH)6 + 6H+ = 3Fe+3 + 6H2O + Na+ + 2SO4-2
            log_k     -11.2
            delta_h   -36.18 kcal
        Schwertmannite
            Fe8O8(OH)6(SO4) + 22H+ = 8Fe+3 + 14H2O + SO4-2
            log_k     7
```

```
        Ferrihydrite
            Fe(OH)3 + 3H+ = Fe+3 + 3H2O
            log_k     5
        Goethite
            FeOOH + 3H+ = Fe+3 + 2H2O
            log_k     0.5
            delta_h   -14.48 kcal
        Jurbanite
            AlOHSO4 + H+ = Al+3 + H2O + SO4-2
            log_k     -3.23
        Basaluminite
            Al4(OH)10SO4 + 10H+ = 4Al+3 + 10H2O + SO4-2
            log_k     22.7
        Alunite
            KAl3(SO4)2(OH)6 + 6H+ = 3Al+3 + 6H2O + K+ + 2SO4-2
            log_k     -1.3
            delta_h   3.918 kcal
        END
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------

Initial solution 2.   Muestra profundidad (m. 30)

-----------------------------Solution composition----------------------

        Elements           Molality       Moles

        Al                7.401e-003  7.401e-003
        As                3.093e-005  3.093e-005
        Ca                1.325e-002  1.325e-002
        Cd                1.218e-005  1.218e-005
        Cu                1.021e-003  1.021e-003
        Fe(2)             1.753e-002  1.753e-002
        Fe(3)             2.541e-003  2.541e-003
        K                 5.159e-004  5.159e-004
        Mn                3.137e-003  3.137e-003
        Na                2.945e-003  2.945e-003
        Ni                3.833e-005  3.833e-005
        O(0)              1.901e-005  1.901e-005
        Pb                6.473e-006  6.473e-006
        S(6)              1.097e-001  1.097e-001
        Zn                1.453e-002  1.453e-002

---------------------------Description of solution-------------------

                                     pH  =   3.120
                                     pe  =   4.000
                        Activity of water  =   0.998
                           Ionic strength  =  1.953e-001
                       Mass of water (kg)  =  1.000e+000
                Total alkalinity (eq/kg)  = -7.208e-003
                   Total carbon (mol/kg)  =  0.000e+000
                      Total CO2 (mol/kg)  =  0.000e+000
                     Temperature (deg C)  =  15.700
                  Electrical balance (eq)  = -8.504e-002
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  = -42.14
                                Iterations  =  13
                                   Total H  = 1.110151e+002
                                   Total O  = 5.594557e+001

---------------------------------Redox couples-----------------------

        Redox couple             pe  Eh (volts)

        Fe(2)/Fe(3)         10.7202      0.6144
        O(-2)/O(0)          17.9451      1.0284

---------------------------Distribution of species-------------------

                                                 Log       Log         Log
        Species            Molality    Activity  Molality  Activity     Gamma

        H+                9.471e-004  7.586e-004    -3.024    -3.120    -0.096
```

	OH-	8.474e-012	6.363e-012	-11.072	-11.196	-0.124
	H2O	5.551e+001	9.978e-001	1.744	-0.001	0.000
Al		7.401e-003				
	AlSO4+	4.693e-003	3.525e-003	-2.329	-2.453	-0.124
	Al(SO4)2-	2.184e-003	1.602e-003	-2.661	-2.795	-0.134
	Al+3	5.225e-004	7.088e-005	-3.282	-4.149	-0.868
	AlOH+2	1.570e-006	4.993e-007	-5.804	-6.302	-0.497
	Al(OH)2+	1.298e-008	9.740e-009	-7.887	-8.011	-0.125
	Al(OH)3	2.222e-013	2.324e-013	-12.653	-12.634	0.020
	Al(OH)4-	2.638e-016	1.936e-016	-15.579	-15.713	-0.134
As(3)		7.350e-014				
	H3AsO3	7.346e-014	7.684e-014	-13.134	-13.114	0.020
	H4AsO3+	3.846e-017	2.888e-017	-16.415	-16.539	-0.124
	H2AsO3-	5.587e-020	4.196e-020	-19.253	-19.377	-0.124
	HAsO3-2	9.078e-029	2.887e-029	-28.042	-28.539	-0.497
	AsO3-3	1.390e-038	1.056e-039	-37.857	-38.976	-1.119
As(5)		3.093e-005				
	H2AsO4-	2.844e-005	2.136e-005	-4.546	-4.670	-0.124
	H3AsO4	2.473e-006	2.586e-006	-5.607	-5.587	0.020
	HAsO4-2	1.482e-008	4.714e-009	-7.829	-8.327	-0.497
	AsO4-3	1.637e-016	1.244e-017	-15.786	-16.905	-1.119
Ca		1.325e-002				
	CaSO4	7.103e-003	7.429e-003	-2.149	-2.129	0.020
	Ca+2	6.150e-003	2.218e-003	-2.211	-2.654	-0.443
	CaOH+	4.393e-013	3.342e-013	-12.357	-12.476	-0.119
Cd		1.218e-005				
	CdSO4	5.159e-006	5.396e-006	-5.287	-5.268	0.020
	Cd(SO4)2-2	3.513e-006	1.117e-006	-5.454	-5.952	-0.497
	Cd+2	3.503e-006	1.114e-006	-5.456	-5.953	-0.497
	CdOH+	7.965e-014	5.981e-014	-13.099	-13.223	-0.124
	Cd2OH+3	4.842e-018	3.678e-019	-17.315	-18.434	-1.119
	Cd(OH)2	8.231e-021	8.610e-021	-20.085	-20.065	0.020
	Cd(OH)3-	1.692e-030	1.271e-030	-29.772	-29.896	-0.124
	Cd(OH)4-2	0.000e+000	0.000e+000	-40.329	-40.827	-0.497
Cu(1)		1.755e-012				
	Cu+	1.755e-012	1.206e-012	-11.756	-11.919	-0.163
Cu(2)		1.021e-003				
	Cu+2	5.916e-004	1.320e-004	-3.228	-3.880	-0.652
	CuSO4	4.293e-004	4.491e-004	-3.367	-3.348	0.020
	CuOH+	2.399e-009	1.736e-009	-8.620	-8.761	-0.141
	Cu(OH)2	4.560e-012	4.770e-012	-11.341	-11.322	0.020
	Cu2(OH)2+2	1.598e-012	5.082e-013	-11.796	-12.294	-0.497
	Cu(OH)3-	5.045e-022	3.789e-022	-21.297	-21.421	-0.124
	Cu(OH)4-2	3.119e-031	9.921e-032	-30.506	-31.003	-0.497
Fe(2)		1.753e-002				
	Fe+2	9.474e-003	3.173e-003	-2.023	-2.499	-0.475
	FeSO4	8.060e-003	8.430e-003	-2.094	-2.074	0.020
	FeOH+	8.664e-010	6.441e-010	-9.062	-9.191	-0.129
	Fe(OH)2	2.991e-018	3.129e-018	-17.524	-17.505	0.020
	Fe(OH)3-	1.871e-025	1.391e-025	-24.728	-24.857	-0.129
Fe(3)		2.541e-003				
	FeSO4+	1.448e-003	1.076e-003	-2.839	-2.968	-0.129
	Fe(SO4)2-	7.776e-004	5.840e-004	-3.109	-3.234	-0.124
	FeOH+2	1.364e-004	4.337e-005	-3.865	-4.363	-0.497
	Fe+3	1.183e-004	8.987e-006	-3.927	-5.046	-1.119
	Fe(OH)2+	4.428e-005	3.324e-005	-4.354	-4.478	-0.125
	Fe2(OH)2+4	7.357e-006	7.529e-008	-5.133	-7.123	-1.990
	Fe3(OH)4+5	6.440e-007	5.007e-010	-6.191	-9.300	-3.109
	Fe(OH)3	4.911e-010	5.137e-010	-9.309	-9.289	0.020
	Fe(OH)4-	9.001e-015	6.757e-015	-14.046	-14.170	-0.125
H(0)		3.109e-031				
	H2	1.554e-031	1.626e-031	-30.808	-30.789	0.020
K		5.159e-004				
	K+	4.692e-004	3.309e-004	-3.329	-3.480	-0.152
	KSO4-	4.665e-005	3.502e-005	-4.331	-4.456	-0.125
Mn(2)		3.137e-003				
	Mn+2	1.632e-003	5.465e-004	-2.787	-3.262	-0.475
	MnSO4	1.505e-003	1.574e-003	-2.823	-2.803	0.020
	MnOH+	1.136e-011	8.449e-012	-10.944	-11.073	-0.129
	Mn(OH)3-	2.651e-029	1.971e-029	-28.577	-28.705	-0.129
Mn(3)		2.669e-017				
	Mn+3	2.669e-017	3.620e-018	-16.574	-17.441	-0.868
Mn(6)		0.000e+000				
	MnO4-2	0.000e+000	0.000e+000	-56.891	-57.406	-0.515

Mn(7)	0.000e+000					
MnO4-	0.000e+000	0.000e+000	-56.543	-56.697	-0.155
Na	2.945e-003					
Na+	2.718e-003	2.034e-003	-2.566	-2.692	-0.126
NaSO4-	2.276e-004	1.708e-004	-3.643	-3.767	-0.125
Ni	3.833e-005					
Ni+2	1.940e-005	6.171e-006	-4.712	-5.210	-0.497
NiSO4	1.886e-005	1.973e-005	-4.724	-4.705	0.020
Ni(SO4)2-2	6.444e-008	2.050e-008	-7.191	-7.688	-0.497
NiOH+	7.597e-013	5.705e-013	-12.119	-12.244	-0.124
Ni(OH)2	1.021e-018	1.068e-018	-17.991	-17.972	0.020
Ni(OH)3-	1.870e-026	1.404e-026	-25.728	-25.853	-0.124
O(0)	1.901e-005					
O2	9.503e-006	9.940e-006	-5.022	-5.003	0.020
Pb	6.473e-006					
PbSO4	3.957e-006	4.139e-006	-5.403	-5.383	0.020
Pb+2	1.299e-006	4.133e-007	-5.886	-6.384	-0.497
Pb(SO4)2-2	1.216e-006	3.869e-007	-5.915	-6.412	-0.497
PbOH+	1.411e-011	1.060e-011	-10.850	-10.975	-0.124
Pb2OH+3	1.291e-015	9.807e-017	-14.889	-16.008	-1.119
Pb(OH)2	5.185e-018	5.424e-018	-17.285	-17.266	0.020
Pb(OH)3-	1.091e-025	8.191e-026	-24.962	-25.087	-0.124
Pb3(OH)4+2	2.075e-031	6.599e-032	-30.683	-31.181	-0.497
Pb(OH)4-2	7.778e-034	2.474e-034	-33.109	-33.607	-0.497
S(6)	1.097e-001					
SO4-2	6.616e-002	1.781e-002	-1.179	-1.749	-0.570
FeSO4	8.060e-003	8.430e-003	-2.094	-2.074	0.020
CaSO4	7.103e-003	7.429e-003	-2.149	-2.129	0.020
ZnSO4	6.268e-003	6.556e-003	-2.203	-2.183	0.020
AlSO4+	4.693e-003	3.525e-003	-2.329	-2.453	-0.124
Zn(SO4)2-2	3.213e-003	1.022e-003	-2.493	-2.991	-0.497
Al(SO4)2-	2.184e-003	1.602e-003	-2.661	-2.795	-0.134
MnSO4	1.505e-003	1.574e-003	-2.823	-2.803	0.020
FeSO4+	1.448e-003	1.076e-003	-2.839	-2.968	-0.129
HSO4-	1.420e-003	1.066e-003	-2.848	-2.972	-0.124
Fe(SO4)2-	7.776e-004	5.840e-004	-3.109	-3.234	-0.124
CuSO4	4.293e-004	4.491e-004	-3.367	-3.348	0.020
NaSO4-	2.276e-004	1.708e-004	-3.643	-3.767	-0.125
KSO4-	4.665e-005	3.502e-005	-4.331	-4.456	-0.125
NiSO4	1.886e-005	1.973e-005	-4.724	-4.705	0.020
CdSO4	5.159e-006	5.396e-006	-5.287	-5.268	0.020
PbSO4	3.957e-006	4.139e-006	-5.403	-5.383	0.020
Cd(SO4)2-2	3.513e-006	1.117e-006	-5.454	-5.952	-0.497
Pb(SO4)2-2	1.216e-006	3.869e-007	-5.915	-6.412	-0.497
Ni(SO4)2-2	6.444e-008	2.050e-008	-7.191	-7.688	-0.497
Zn	1.453e-002					
ZnSO4	6.268e-003	6.556e-003	-2.203	-2.183	0.020
Zn+2	5.049e-003	1.691e-003	-2.297	-2.772	-0.475
Zn(SO4)2-2	3.213e-003	1.022e-003	-2.493	-2.991	-0.497
ZnOH+	1.568e-009	1.177e-009	-8.805	-8.929	-0.124
Zn(OH)2	3.529e-014	3.691e-014	-13.452	-13.433	0.020
Zn(OH)3-	2.044e-022	1.535e-022	-21.689	-21.814	-0.124
Zn(OH)4-2	1.006e-031	3.200e-032	-30.997	-31.495	-0.497

----------Saturation indices----------

Phase	SI	log IAP	log KT	
Al(OH)3(a)	-5.81	5.21	11.02	Al(OH)3
Al2O3	-12.56	10.42	22.98	Al2O3
Al4(OH)10SO4	-9.86	12.84	22.70	Al4(OH)10SO4
AlAsO4:2H2O	-5.18	-0.38	4.80	AlAsO4:2H2O
AlOHSO4	0.45	-2.78	-3.23	AlOHSO4
AlumK	-5.80	-11.14	-5.34	KAl(SO4)2:12H2O
Alunite	0.68	-0.71	-1.39	KAl3(SO4)2(OH)6
Anglesite	-0.29	-8.13	-7.84	PbSO4
Anhydrite	0.14	-4.40	-4.55	CaSO4
Antlerite	-9.20	-0.91	8.29	Cu3(OH)4SO4
Arsenolite	-49.31	-26.92	22.40	As4O6
As2O5	-18.00	-11.17	6.83	As2O5
Basaluminite	-9.86	12.84	22.70	Al4(OH)10SO4
Bianchite	-2.77	-4.53	-1.76	ZnSO4:6H2O
Birnessite	-12.33	4.12	16.45	MnO2
Bixbyite	-15.91	7.10	23.01	Mn2O3

Boehmite	-4.03	5.21	9.24	AlOOH
Brochantite	-13.89	1.45	15.34	Cu4(OH)6SO4
Bunsenite	-11.99	1.03	13.01	NiO
Ca3(AsO4)2:6H2O	-22.72	-0.42	22.30	Ca3(AsO4)2:6H2O
Cd(Gamma)	-41.41	-0.86	40.55	Cd
Cd(OH)2(A)	-13.94	0.28	14.22	Cd(OH)2
Cd(OH)2(C)	-13.37	0.28	13.65	Cd(OH)2
Cd3(OH)2(SO4)2	-21.83	-15.12	6.71	Cd3(OH)2(SO4)2
Cd3(OH)4SO4	-29.69	-7.13	22.56	Cd3(OH)4SO4
Cd4(OH)6SO4	-35.25	-6.85	28.40	Cd4(OH)6SO4
CdMetal	-41.31	-0.86	40.45	Cd
CdSO4	-7.95	-7.70	0.25	CdSO4
CdSO4:2.67H2O	-5.93	-7.71	-1.77	CdSO4:2.67H2O
CdSO4:H2O	-6.22	-7.70	-1.48	CdSO4:H2O
Chalcanthite	-2.96	-5.63	-2.67	CuSO4:5H2O
Claudetite	-49.07	-26.92	22.16	As4O6
Cu(OH)2	-6.64	2.36	9.00	Cu(OH)2
Cu2SO4	-23.74	-4.41	19.33	Cu2SO4
Cu3(AsO4)2:6H2O	-10.20	-4.10	6.10	Cu3(AsO4)2:6H2O
CuMetal	-13.47	1.22	14.69	Cu
CuOCuSO4	-15.64	-3.27	12.37	CuO:CuSO4
CupricFerrite	4.19	10.98	6.79	CuFe2O4
Cuprite	-15.90	3.58	19.48	Cu2O
CuprousFerrite	4.34	6.10	1.76	CuFeO2
CuSO4	-9.07	-5.63	3.44	CuSO4
Diaspore	-2.25	5.21	7.45	AlOOH
Fe2(SO4)3	-20.32	-15.34	4.98	Fe2(SO4)3
Fe3(OH)8	-7.86	12.36	20.22	Fe3(OH)8
FeAsO4:2H2O	-1.68	-1.28	0.40	FeAsO4:2H2O
Ferrihydrite	-0.69	4.31	5.00	Fe(OH)3
Gibbsite(C)	-4.10	5.21	9.31	Al(OH)3
Goethite	3.47	4.31	0.84	FeOOH
Goslarite	-2.49	-4.53	-2.04	ZnSO4:7H2O
Gypsum	0.45	-4.41	-4.85	CaSO4:2H2O
Hausmannite	-26.82	10.07	36.90	Mn3O4
Hematite	11.90	8.62	-3.28	Fe2O3
Hercynite	-14.85	14.16	29.01	FeAl2O4
Jarosite-H	7.75	-3.04	-10.80	(H3O)Fe3(SO4)2(OH)6
Jarosite-K	10.66	-3.40	-14.06	KFe3(SO4)2(OH)6
Jarosite-Na	7.73	-2.62	-10.35	NaFe3(SO4)2(OH)6
Jurbanite	0.45	-2.78	-3.23	AlOHSO4
Langite	-16.28	1.45	17.72	Cu4(OH)6SO4:H2O
Larnakite	-8.15	-8.28	-0.13	PbO:PbSO4
Lepidocrocite	2.94	4.31	1.37	FeOOH
Lime	-30.30	3.59	33.89	CaO
Litharge	-13.25	-0.14	13.11	PbO
Maghemite	2.24	8.62	6.39	Fe2O3
Magnetite	7.44	12.36	4.93	Fe3O4
Manganite	-7.85	3.55	11.39	MnOOH
Massicot	-13.45	-0.14	13.31	PbO
Melanterite	-1.72	-4.25	-2.54	FeSO4:7H2O
Minium	-48.87	0.71	49.58	Pb3O4
Mirabilite	-5.58	-7.14	-1.56	Na2SO4:10H2O
Mn2(SO4)3	-35.34	-16.87	18.47	Mn2(SO4)3
Mn3(AsO4)2:8H2O	-14.75	-2.25	12.50	Mn3(AsO4)2:8H2O
MnSO4	-8.05	-5.01	3.03	MnSO4
Monteponite	-15.42	0.29	15.70	CdO
Morenosite	-4.54	-6.97	-2.43	NiSO4:7H2O
Ni(OH)2	-9.05	1.03	10.08	Ni(OH)2
Ni3(AsO4)2:8H2O	-23.79	-8.09	15.70	Ni3(AsO4)2:8H2O
Ni4(OH)6SO4	-35.87	-3.87	32.00	Ni4(OH)6SO4
Nsutite	-11.75	4.12	15.87	MnO2
O2(g)	-30.92	2.29	33.21	O2
Pb(OH)2(C)	-8.63	-0.15	8.48	Pb(OH)2
Pb2O(OH)2	-26.49	-0.29	26.20	Pb2O(OH)2
Pb2O3	-33.65	0.85	34.50	Pb2O3
Pb3(AsO4)2	-17.41	-11.61	5.80	Pb3(AsO4)2
Pb3O2SO4	-19.31	-8.42	10.89	Pb3O2SO4
Pb4(OH)6SO4	-29.67	-8.57	21.10	Pb4(OH)6SO4
Pb4O3SO4	-31.49	-8.57	22.93	Pb4O3SO4
PbMetal	-32.08	-1.29	30.80	Pb
PbO:0.3H2O	-13.13	-0.15	12.98	PbO:0.33H2O
Plattnerite	-23.43	1.00	24.43	PbO2
Portlandite	-19.82	3.58	23.40	Ca(OH)2

Pyrocroite	-12.65	2.98	15.62	Mn(OH)2
Pyrolusite	-10.79	4.12	14.91	MnO2
Retgersite	-4.90	-6.96	-2.07	NiSO4:6H2O
Schwertmannite	19.51	26.51	7.00	Fe8O8(OH)6(SO4)
Tenorite	-5.62	2.36	7.98	CuO
Thenardite	-6.97	-7.13	-0.17	Na2SO4
Zincite	-8.19	3.47	11.66	ZnO
Zincosite	-7.98	-4.52	3.46	ZnSO4
Zn(OH)2(A)	-8.98	3.47	12.45	Zn(OH)2
Zn(OH)2(B)	-8.28	3.47	11.75	Zn(OH)2
Zn(OH)2(C)	-8.73	3.47	12.20	Zn(OH)2
Zn(OH)2(E)	-8.03	3.47	11.50	Zn(OH)2
Zn(OH)2(G)	-8.24	3.47	11.71	Zn(OH)2
Zn2(OH)2SO4	-8.56	-1.06	7.50	Zn2(OH)2SO4
Zn3(AsO4)2:2.5H2O	-14.42	-0.77	13.65	Zn3(AsO4)2:2.5H2O
Zn3O(SO4)2	-26.06	-5.58	20.48	Zn3O(SO4)2
Zn4(OH)6SO4	-22.52	5.88	28.40	Zn4(OH)6SO4
ZnMetal	-50.84	2.32	53.16	Zn
ZnO(Active)	-7.84	3.47	11.31	ZnO
ZnSO4:H2O	-4.20	-4.52	-0.32	ZnSO4:H2O

End of simulation.

Reading input data for simulation 3.

End of run.

CÁLCULOS DE ESPECIACIÓN QUÍMICA DE METALES E ÍNDICES DE SATURACIÓN

AZNALCÓLLAR, EPILIMNION. MAYO 2007

```
  Input file: C:\PHEEQC\MODELIZACIÓN\Especiación Aznalcóllar Mayo 2007.pqi
  Output file: C:\PHEEQC\MODELIZACIÓN\Especiación Aznalcóllar Mayo 2007.pqo
Database file: C:\Archivos de programa\USGS\Phreeqc Interactive 2.7.1\minteq.dat

------------------
Reading data base.
------------------

       SOLUTION_MASTER_SPECIES
       SOLUTION_SPECIES
       SOLUTION_SPECIES
       PHASES
       SURFACE_MASTER_SPECIES
       SURFACE_SPECIES
       END
-----------------------------------
Reading input data for simulation 1.
-----------------------------------

       DATABASE C:\Archivos de programa\USGS\Phreeqc Interactive 2.7.1\minteq.dat
       SOLUTION 2 Muestra superficial (m. 0)
           temp      23
           pH        2.9
           pe        4
           redox     Fe(2)/Fe(3)
           units     mg/l
           density   1
           S(6)      12.3 g/l
           Al        251
           Fe(2)     820
           Fe(3)     120
           Zn        1173
           Cu        44.4
           Mn        201
           K         13.5
           Na        71.9
           Ca        519
           Cd        4.83
           Ni        2.96
           O(0)      0.25
           As        125 ug/l
           Pb        1331 ug/l
           water    1 # kg
       SOLUTION_MASTER_SPECIES
           Fe(2)         Fe+2            0     Fe
           Fe(3)         Fe+3           -2     Fe
           Mg            Mg+2            0     Mg              24.312
           Na            Na+             0     Na              22.9898
           Ca            Ca+2            0     Ca              40.08
           S             SO4-2           0     SO4             32.064
           S(6)          SO4-2           0     SO4
           K             K+              0     K               39.102
           Al            Al+3            0     Al              26.9815
       SOLUTION_SPECIES
       H2O = OH- + H+
           log_k     -14
           delta_h   13.362 kcal
       Fe+2 = Fe+3 + e-
           log_k     -13.02
           delta_h   9.68 kcal
       Fe+3 + H2O = FeOH+2 + H+
           log_k     -2.19
           delta_h   10.4 kcal
       H+ + SO4-2 = HSO4-
           log_k     1.988
           delta_h   3.85 kcal
```

```
        Al+3 + H2O = AlOH+2 + H+
            log_k     -5
            delta_h   11.49 kcal
        Al+3 + 3H2O = Al(OH)3 + 3H+
            log_k     -16.9
            delta_h   39.89 kcal
        Al+3 + SO4-2 = AlSO4+
            log_k     3.5
            delta_h   2.29 kcal
        PHASES
        Jarosite-K
            KFe3(SO4)2(OH)6 + 6H+ = 3Fe+3 + 6H2O + K+ + 2SO4-2
            log_k     -14.8
            delta_h   -31.28 kcal
        Jarosite-Na
            NaFe3(SO4)2(OH)6 + 6H+ = 3Fe+3 + 6H2O + Na+ + 2SO4-2
            log_k     -11.2
            delta_h   -36.18 kcal
        Schwertmannite
            Fe8O8(OH)6(SO4) + 22H+ = 8Fe+3 + 14H2O + SO4-2
            log_k     7
        Ferrihydrite
            Fe(OH)3 + 3H+ = Fe+3 + 3H2O
            log_k     5
        Goethite
            FeOOH + 3H+ = Fe+3 + 2H2O
            log_k     0.5
            delta_h   -14.48 kcal
        Jurbanite
            AlOHSO4 + H+ = Al+3 + H2O + SO4-2
            log_k     -3.23
        Basaluminite
            Al4(OH)10SO4 + 10H+ = 4Al+3 + 10H2O + SO4-2
            log_k     22.7
        Alunite
            KAl3(SO4)2(OH)6 + 6H+ = 3Al+3 + 6H2O + K+ + 2SO4-2
            log_k     -1.3
            delta_h   3.918 kcal
        END
-------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 2.   Muestra superficial (m. 0)

-----------------------------Solution composition------------------------------

        Elements           Molality       Moles

        Al               9.449e-003  9.449e-003
        As               1.695e-006  1.695e-006
        Ca               1.315e-002  1.315e-002
        Cd               4.365e-005  4.365e-005
        Cu               7.097e-004  7.097e-004
        Fe(2)            1.491e-002  1.491e-002
        Fe(3)            2.183e-003  2.183e-003
        K                3.507e-004  3.507e-004
        Mn               3.716e-003  3.716e-003
        Na               3.177e-003  3.177e-003
        Ni               5.121e-005  5.121e-005
        O(0)             1.587e-005  1.587e-005
        Pb               6.525e-006  6.525e-006
        S(6)             1.301e-001  1.301e-001
        Zn               1.823e-002  1.823e-002

----------------------------Description of solution----------------------------

                                    pH  =   2.900
                                    pe  =   4.000
                       Activity of water  =   0.997
                          Ionic strength  =  2.194e-001
                       Mass of water (kg)  =  1.000e+000
                 Total alkalinity (eq/kg)  = -8.929e-003
                    Total carbon (mol/kg)  =  0.000e+000
```

```
                      Total CO2 (mol/kg)  =  0.000e+000
                     Temperature (deg C)  =  23.000
                   Electrical balance (eq)  = -1.155e-001
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  = -50.66
                                Iterations  =  11
                                   Total H  = 1.110172e+002
                                   Total O  = 5.602659e+001

---------------------------------Redox couples---------------------------------

       Redox couple             pe  Eh (volts)

       Fe(2)/Fe(3)         10.4750      0.6155
       O(-2)/O(0)          17.5177      1.0293

--------------------------Distribution of species--------------------------

                                                  Log       Log         Log
       Species             Molality    Activity  Molality  Activity     Gamma

       H+                1.584e-003  1.259e-003    -2.800    -2.900    -0.100
       OH-               9.147e-012  6.804e-012   -11.039   -11.167    -0.129
       H2O               5.551e+001  9.975e-001     1.744    -0.001     0.000
Al               9.449e-003
       AlSO4+            5.814e-003  4.325e-003    -2.236    -2.364    -0.129
       Al(SO4)2-         3.068e-003  2.220e-003    -2.513    -2.654    -0.141
       Al+3              5.654e-004  7.149e-005    -3.248    -4.146    -0.898
       AlOH+2            1.623e-006  4.969e-007    -5.790    -6.304    -0.514
       Al(OH)2+          4.809e-009  3.565e-009    -8.318    -8.448    -0.130
       Al(OH)3           2.701e-013  2.841e-013   -12.568   -12.546     0.022
       Al(OH)4-          2.357e-016  1.705e-016   -15.628   -15.768    -0.141
As(3)            1.569e-014
       H3AsO3            1.567e-014  1.649e-014   -13.805   -13.783     0.022
       H4AsO3+           1.382e-017  1.028e-017   -16.859   -16.988    -0.129
       H2AsO3-           9.664e-021  7.188e-021   -20.015   -20.143    -0.129
       HAsO3-2           1.352e-029  4.138e-030   -28.869   -29.383    -0.514
       AsO3-3            1.696e-039  1.183e-040   -38.771   -39.927    -1.157
As(5)            1.695e-006
       H2AsO4-           1.470e-006  1.093e-006    -5.833    -5.961    -0.129
       H3AsO4            2.246e-007  2.362e-007    -6.649    -6.627     0.022
       HAsO4-2           4.908e-010  1.503e-010    -9.309    -9.823    -0.514
       AsO4-3            4.129e-018  2.880e-019   -17.384   -18.541    -1.157
Ca               1.315e-002
       CaSO4             7.436e-003  7.821e-003    -2.129    -2.107     0.022
       Ca+2              5.717e-003  1.988e-003    -2.243    -2.701    -0.459
       CaOH+             4.479e-013  3.369e-013   -12.349   -12.473    -0.124
Cd               4.365e-005
       CdSO4             1.847e-005  1.943e-005    -4.733    -4.712     0.022
       Cd(SO4)2-2        1.383e-005  4.235e-006    -4.859    -5.373    -0.514
       Cd+2              1.134e-005  3.474e-006    -4.945    -5.459    -0.514
       CdOH+             2.651e-013  1.972e-013   -12.577   -12.705    -0.129
       Cd2OH+3           4.932e-017  3.440e-018   -16.307   -17.464    -1.157
       Cd(OH)2           9.261e-021  9.740e-021   -20.033   -20.011     0.022
       Cd(OH)3-          1.164e-030  8.659e-031   -29.934   -30.063    -0.129
       Cd(OH)4-2         0.000e+000  0.000e+000   -40.700   -41.214    -0.514
Cu(1)            2.109e-012
       Cu+               2.109e-012  1.420e-012   -11.676   -11.848    -0.172
Cu(2)            7.097e-004
       Cu+2              4.004e-004  8.229e-005    -3.398    -4.085    -0.687
       CuSO4             3.093e-004  3.254e-004    -3.510    -3.488     0.022
       CuOH+             9.152e-010  6.520e-010    -9.038    -9.186    -0.147
       Cu(OH)2           1.026e-012  1.079e-012   -11.989   -11.967     0.022
       Cu2(OH)2+2        4.975e-013  1.523e-013   -12.303   -12.817    -0.514
       Cu(OH)3-          6.944e-023  5.165e-023   -22.158   -22.287    -0.129
       Cu(OH)4-2         2.661e-032  8.147e-033   -31.575   -32.089    -0.514
Fe(2)            1.491e-002
       FeSO4             7.545e-003  7.936e-003    -2.122    -2.100     0.022
       Fe+2              7.369e-003  2.358e-003    -2.133    -2.627    -0.495
       FeOH+             6.928e-010  5.083e-010    -9.159    -9.294    -0.134
       Fe(OH)2           2.735e-018  2.877e-018   -17.563   -17.541     0.022
       Fe(OH)3-          1.132e-025  8.304e-026   -24.946   -25.081    -0.134
Fe(3)            2.183e-003
       FeSO4+            1.242e-003  9.114e-004    -2.906    -3.040    -0.134
       Fe(SO4)2-         7.548e-004  5.615e-004    -3.122    -3.251    -0.129
```

	FeOH+2	8.659e-005	2.651e-005	-4.063	-4.577	-0.514
	Fe+3	8.367e-005	5.835e-006	-4.077	-5.234	-1.157
	Fe(OH)2+	1.056e-005	7.831e-006	-4.976	-5.106	-0.130
	Fe2(OH)2+4	2.339e-006	2.056e-008	-5.631	-7.687	-2.056
	Fe3(OH)4+5	5.438e-008	3.333e-011	-7.265	-10.477	-3.213
	Fe(OH)3	6.931e-011	7.290e-011	-10.159	-10.137	0.022
	Fe(OH)4-	7.791e-016	5.776e-016	-15.108	-15.238	-0.130
H(0)	2.443e-030					
	H2	1.221e-030	1.285e-030	-29.913	-29.891	0.022
K	3.507e-004					
	K+	3.119e-004	2.160e-004	-3.506	-3.665	-0.159
	KSO4-	3.882e-005	2.878e-005	-4.411	-4.541	-0.130
Mn(2)	3.716e-003					
	MnSO4	1.913e-003	2.012e-003	-2.718	-2.696	0.022
	Mn+2	1.804e-003	5.772e-004	-2.744	-3.239	-0.495
	MnOH+	1.359e-011	9.975e-012	-10.867	-11.001	-0.134
	Mn(OH)3-	6.201e-030	4.550e-030	-29.208	-29.342	-0.134
Mn(3)	5.686e-018					
	Mn+3	5.686e-018	7.190e-019	-17.245	-18.143	-0.898
Mn(6)	0.000e+000					
	MnO4-2	0.000e+000	0.000e+000	-56.788	-57.326	-0.538
Mn(7)	0.000e+000					
	MnO4-	0.000e+000	0.000e+000	-56.204	-56.367	-0.163
Na	3.177e-003					
	Na+	2.896e-003	2.143e-003	-2.538	-2.669	-0.131
	NaSO4-	2.808e-004	2.082e-004	-3.552	-3.682	-0.130
Ni	5.121e-005					
	NiSO4	2.672e-005	2.810e-005	-4.573	-4.551	0.022
	Ni+2	2.439e-005	7.469e-006	-4.613	-5.127	-0.514
	Ni(SO4)2-2	9.848e-008	3.015e-008	-7.007	-7.521	-0.514
	NiOH+	9.532e-013	7.091e-013	-12.021	-12.149	-0.129
	Ni(OH)2	4.458e-019	4.689e-019	-18.351	-18.329	0.022
	Ni(OH)3-	4.994e-027	3.715e-027	-26.302	-26.430	-0.129
O(0)	1.587e-005					
	O2	7.936e-006	8.347e-006	-5.100	-5.078	0.022
Pb	6.525e-006					
	PbSO4	3.919e-006	4.122e-006	-5.407	-5.385	0.022
	Pb(SO4)2-2	1.387e-006	4.248e-007	-5.858	-6.372	-0.514
	Pb+2	1.219e-006	3.733e-007	-5.914	-6.428	-0.514
	PbOH+	7.753e-012	5.767e-012	-11.111	-11.239	-0.129
	Pb2OH+3	6.911e-016	4.820e-017	-15.160	-16.317	-1.157
	Pb(OH)2	1.690e-018	1.778e-018	-17.772	-17.750	0.022
	Pb(OH)3-	2.174e-026	1.617e-026	-25.663	-25.791	-0.129
	Pb3(OH)4+2	6.525e-032	1.998e-032	-31.185	-31.699	-0.514
	Pb(OH)4-2	9.609e-035	2.942e-035	-34.017	-34.531	-0.514
S(6)	1.301e-001					
	SO4-2	7.778e-002	1.964e-002	-1.109	-1.707	-0.598
	ZnSO4	7.987e-003	8.401e-003	-2.098	-2.076	0.022
	FeSO4	7.545e-003	7.936e-003	-2.122	-2.100	0.022
	CaSO4	7.436e-003	7.821e-003	-2.129	-2.107	0.022
	AlSO4+	5.814e-003	4.325e-003	-2.236	-2.364	-0.129
	Zn(SO4)2-2	4.448e-003	1.362e-003	-2.352	-2.866	-0.514
	HSO4-	3.094e-003	2.301e-003	-2.510	-2.638	-0.129
	Al(SO4)2-	3.068e-003	2.220e-003	-2.513	-2.654	-0.141
	MnSO4	1.913e-003	2.012e-003	-2.718	-2.696	0.022
	FeSO4+	1.242e-003	9.114e-004	-2.906	-3.040	-0.134
	Fe(SO4)2-	7.548e-004	5.615e-004	-3.122	-3.251	-0.129
	CuSO4	3.093e-004	3.254e-004	-3.510	-3.488	0.022
	NaSO4-	2.808e-004	2.082e-004	-3.552	-3.682	-0.130
	KSO4-	3.882e-005	2.878e-005	-4.411	-4.541	-0.130
	NiSO4	2.672e-005	2.810e-005	-4.573	-4.551	0.022
	CdSO4	1.847e-005	1.943e-005	-4.733	-4.712	0.022
	Cd(SO4)2-2	1.383e-005	4.235e-006	-4.859	-5.373	-0.514
	PbSO4	3.919e-006	4.122e-006	-5.407	-5.385	0.022
	Pb(SO4)2-2	1.387e-006	4.248e-007	-5.858	-6.372	-0.514
	Ni(SO4)2-2	9.848e-008	3.015e-008	-7.007	-7.521	-0.514
Zn	1.823e-002					
	ZnSO4	7.987e-003	8.401e-003	-2.098	-2.076	0.022
	Zn+2	5.792e-003	1.854e-003	-2.237	-2.732	-0.495
	Zn(SO4)2-2	4.448e-003	1.362e-003	-2.352	-2.866	-0.514
	ZnOH+	1.858e-009	1.382e-009	-8.731	-8.859	-0.129
	Zn(OH)2	1.396e-014	1.468e-014	-13.855	-13.833	0.022
	Zn(OH)3-	4.946e-023	3.679e-023	-22.306	-22.434	-0.129
	Zn(OH)4-2	1.509e-032	4.620e-033	-31.821	-32.335	-0.514

----------Saturation indices----------

Phase	SI	log IAP	log KT	
Al(OH)3(a)	-5.96	4.55	10.51	Al(OH)3
Al2O3	-13.87	9.11	22.98	Al2O3
Al4(OH)10SO4	-12.00	10.70	22.70	Al4(OH)10SO4
AlAsO4:2H2O	-6.87	-2.07	4.80	AlAsO4:2H2O
AlOHSO4	0.28	-2.95	-3.23	AlOHSO4
AlumK	-6.03	-11.24	-5.21	KAl(SO4)2:12H2O
Alunite	-0.80	-2.12	-1.32	KAl3(SO4)2(OH)6
Anglesite	-0.33	-8.13	-7.80	PbSO4
Anhydrite	0.21	-4.41	-4.62	CaSO4
Antlerite	-10.66	-2.37	8.29	Cu3(OH)4SO4
Arsenolite	-52.25	-28.84	23.41	As4O6
As2O5	-19.98	-13.25	6.73	As2O5
Basaluminite	-12.00	10.70	22.70	Al4(OH)10SO4
Bianchite	-2.68	-4.45	-1.76	ZnSO4:6H2O
Birnessite	-14.16	3.15	17.31	MnO2
Bixbyite	-18.35	5.71	24.06	Mn2O3
Boehmite	-4.17	4.55	8.72	AlOOH
Brochantite	-15.99	-0.65	15.34	Cu4(OH)6SO4
Bunsenite	-11.90	0.67	12.57	NiO
Ca3(AsO4)2:6H2O	-26.26	-3.96	22.30	Ca3(AsO4)2:6H2O
Cd(Gamma)	-40.09	-0.25	39.84	Cd
Cd(OH)2(A)	-13.49	0.34	13.83	Cd(OH)2
Cd(OH)2(C)	-13.31	0.34	13.65	Cd(OH)2
Cd3(OH)2(SO4)2	-20.70	-13.99	6.71	Cd3(OH)2(SO4)2
Cd3(OH)4SO4	-29.05	-6.49	22.56	Cd3(OH)4SO4
Cd4(OH)6SO4	-34.55	-6.15	28.40	Cd4(OH)6SO4
CdMetal	-39.99	-0.25	39.74	Cd
CdSO4	-7.14	-7.17	-0.03	CdSO4
CdSO4:2.67H2O	-5.32	-7.17	-1.85	CdSO4:2.67H2O
CdSO4:H2O	-5.55	-7.17	-1.62	CdSO4:H2O
Chalcanthite	-3.15	-5.80	-2.65	CuSO4:5H2O
Claudetite	-51.99	-28.84	23.15	As4O6
Cu(OH)2	-7.00	1.71	8.72	Cu(OH)2
Cu2SO4	-23.48	-4.66	18.81	Cu2SO4
Cu3(AsO4)2:6H2O	-14.21	-8.11	6.10	Cu3(AsO4)2:6H2O
CuMetal	-13.48	1.13	14.61	Cu
CuOCuSO4	-15.78	-4.08	11.71	CuO:CuSO4
CupricFerrite	2.57	8.64	6.07	CuFe2O4
Cuprite	-16.32	2.84	19.16	Cu2O
CuprousFerrite	3.42	4.89	1.47	CuFeO2
CuSO4	-8.89	-5.79	3.10	CuSO4
Diaspore	-2.44	4.55	6.99	AlOOH
Fe2(SO4)3	-19.46	-15.59	3.87	Fe2(SO4)3
Fe3(OH)8	-10.13	10.10	20.22	Fe3(OH)8
FeAsO4:2H2O	-3.56	-3.16	0.40	FeAsO4:2H2O
Ferrihydrite	-1.54	3.46	5.00	Fe(OH)3
Gibbsite(C)	-4.33	4.55	8.88	Al(OH)3
Goethite	2.89	3.46	0.57	FeOOH
Goslarite	-2.47	-4.45	-1.98	ZnSO4:7H2O
Gypsum	0.44	-4.41	-4.85	CaSO4:2H2O
Hausmannite	-27.51	8.27	35.77	Mn3O4
Hematite	10.78	6.93	-3.86	Fe2O3
Hercynite	-15.27	12.28	27.55	FeAl2O4
Jarosite-H	7.20	-4.62	-11.83	(H3O)Fe3(SO4)2(OH)6
Jarosite-K	9.26	-5.39	-14.65	KFe3(SO4)2(OH)6
Jarosite-Na	6.63	-4.39	-11.02	NaFe3(SO4)2(OH)6
Jurbanite	0.28	-2.95	-3.23	AlOHSO4
Langite	-17.64	-0.65	16.99	Cu4(OH)6SO4:H2O
Larnakite	-8.52	-8.76	-0.25	PbO:PbSO4
Lepidocrocite	2.09	3.46	1.37	FeOOH
Lime	-29.93	3.10	33.03	CaO
Litharge	-13.43	-0.63	12.80	PbO
Maghemite	0.54	6.93	6.39	Fe2O3
Magnetite	6.11	10.10	3.99	Fe3O4
Manganite	-9.21	2.85	12.06	MnOOH
Massicot	-13.62	-0.63	12.99	PbO
Melanterite	-1.86	-4.34	-2.48	FeSO4:7H2O
Minium	-49.34	-1.30	48.04	Pb3O4
Mirabilite	-5.85	-7.06	-1.21	Na2SO4:10H2O

Mn2(SO4)3	-35.89	-16.81	19.08	Mn2(SO4)3
Mn3(AsO4)2:8H2O	-18.08	-5.58	12.50	Mn3(AsO4)2:8H2O
MnSO4	-7.69	-4.95	2.75	MnSO4
Monteponite	-14.90	0.34	15.24	CdO
Morenosite	-4.47	-6.84	-2.37	NiSO4:7H2O
Ni(OH)2	-9.98	0.67	10.65	Ni(OH)2
Ni3(AsO4)2:8H2O	-26.94	-11.24	15.70	Ni3(AsO4)2:8H2O
Ni4(OH)6SO4	-36.82	-4.82	32.00	Ni4(OH)6SO4
Nsutite	-13.57	3.15	16.72	MnO2
O2(g)	-30.28	1.17	31.46	O2
Pb(OH)2(C)	-8.85	-0.63	8.22	Pb(OH)2
Pb2O(OH)2	-27.46	-1.26	26.20	Pb2O(OH)2
Pb2O3	-35.55	-0.67	34.88	Pb2O3
Pb3(AsO4)2	-20.94	-15.14	5.80	Pb3(AsO4)2
Pb3O2SO4	-19.90	-9.39	10.50	Pb3O2SO4
Pb4(OH)6SO4	-31.13	-10.03	21.10	Pb4(OH)6SO4
Pb4O3SO4	-32.30	-10.02	22.27	Pb4O3SO4
PbMetal	-31.65	-1.21	30.43	Pb
PbO:0.3H2O	-13.61	-0.63	12.98	PbO:0.33H2O
Plattnerite	-23.53	-0.04	23.49	PbO2
Portlandite	-19.73	3.10	22.83	Ca(OH)2
Pyrocroite	-12.64	2.56	15.20	Mn(OH)2
Pyrolusite	-12.08	3.15	15.22	MnO2
Retgersite	-4.79	-6.84	-2.05	NiSO4:6H2O
Schwertmannite	13.21	20.21	7.00	Fe8O8(OH)6(SO4)
Tenorite	-5.98	1.71	7.70	CuO
Thenardite	-6.87	-7.04	-0.18	Na2SO4
Zincite	-8.18	3.07	11.25	ZnO
Zincosite	-7.54	-4.44	3.11	ZnSO4
Zn(OH)2(A)	-9.38	3.07	12.45	Zn(OH)2
Zn(OH)2(B)	-8.68	3.07	11.75	Zn(OH)2
Zn(OH)2(C)	-9.13	3.07	12.20	Zn(OH)2
Zn(OH)2(E)	-8.43	3.07	11.50	Zn(OH)2
Zn(OH)2(G)	-8.64	3.07	11.71	Zn(OH)2
Zn2(OH)2SO4	-8.87	-1.37	7.50	Zn2(OH)2SO4
Zn3(AsO4)2:2.5H2O	-17.70	-4.05	13.65	Zn3(AsO4)2:2.5H2O
Zn3O(SO4)2	-25.14	-5.81	19.33	Zn3O(SO4)2
Zn4(OH)6SO4	-23.64	4.76	28.40	Zn4(OH)6SO4
ZnMetal	-49.62	2.48	52.10	Zn
ZnO(Active)	-8.24	3.07	11.31	ZnO
ZnSO4:H2O	-3.92	-4.44	-0.52	ZnSO4:H2O

End of simulation.

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```
Reading input data for simulation 2.
-----------------------------------

        SOLUTION 2 Muestra profundidad (m. 30)
            temp      17
            pH        4.3
            pe        4
            redox     Fe(2)/Fe(3)
            units     mg/l
            density   1
            S(6)      12.3 g/l
            Al        203
            Fe(2)     1252
            Fe(3)     1
            Zn        1232
            Cu        47.3
            Mn        213
            K         14.2
            Na        72.4
            Ca        557
            Cd        4.75
            Ni        2.75
            O(0)      0.07
            As        123 ug/l
            Pb        1322 ug/l
            water    1 # kg
        SOLUTION_MASTER_SPECIES
            Fe(2)         Fe+2             0     Fe
            Fe(3)         Fe+3            -2     Fe
            Mg            Mg+2             0     Mg              24.312
            Na            Na+              0     Na              22.9898
            Ca            Ca+2             0     Ca              40.08
            S             SO4-2            0     SO4             32.064
            S(6)          SO4-2            0     SO4
            K             K+               0     K               39.102
            Al            Al+3             0     Al              26.9815
        SOLUTION_SPECIES
        H2O = OH- + H+
            log_k     -14
            delta_h   13.362 kcal
        Fe+2 = Fe+3 + e-
            log_k     -13.02
            delta_h   9.68 kcal
        Fe+3 + H2O = FeOH+2 + H+
            log_k     -2.19
            delta_h   10.4 kcal
        H+ + SO4-2 = HSO4-
            log_k     1.988
            delta_h   3.85 kcal
        Al+3 + H2O = AlOH+2 + H+
            log_k     -5
            delta_h   11.49 kcal
        Al+3 + 3H2O = Al(OH)3 + 3H+
            log_k     -16.9
            delta_h   39.89 kcal
        Al+3 + SO4-2 = AlSO4+
            log_k     3.5
            delta_h   2.29 kcal
        PHASES
        Jarosite-K
            KFe3(SO4)2(OH)6 + 6H+ = 3Fe+3 + 6H2O + K+ + 2SO4-2
            log_k     -14.8
            delta_h   -31.28 kcal
        Jarosite-Na
            NaFe3(SO4)2(OH)6 + 6H+ = 3Fe+3 + 6H2O + Na+ + 2SO4-2
            log_k     -11.2
            delta_h   -36.18 kcal
        Schwertmannite
            Fe8O8(OH)6(SO4) + 22H+ = 8Fe+3 + 14H2O + SO4-2
            log_k     7
        Ferrihydrite
```

```
            Fe(OH)3 + 3H+ = Fe+3 + 3H2O
            log_k     5
        Goethite
            FeOOH + 3H+ = Fe+3 + 2H2O
            log_k     0.5
            delta_h   -14.48 kcal
        Jurbanite
            AlOHSO4 + H+ = Al+3 + H2O + SO4-2
            log_k     -3.23
        Basaluminite
            Al4(OH)10SO4 + 10H+ = 4Al+3 + 10H2O + SO4-2
            log_k     22.7
        Alunite
            KAl3(SO4)2(OH)6 + 6H+ = 3Al+3 + 6H2O + K+ + 2SO4-2
            log_k     -1.3
            delta_h   3.918 kcal
        END
-------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 2.   Muestra profundidad (m. 30)

-----------------------------Solution composition------------------------------

        Elements           Molality       Moles

        Al                7.645e-003  7.645e-003
        As                1.668e-006  1.668e-006
        Ca                1.412e-002  1.412e-002
        Cd                4.294e-005  4.294e-005
        Cu                7.564e-004  7.564e-004
        Fe(2)             2.278e-002  2.278e-002
        Fe(3)             1.820e-005  1.820e-005
        K                 3.690e-004  3.690e-004
        Mn                3.940e-003  3.940e-003
        Na                3.200e-003  3.200e-003
        Ni                4.760e-005  4.760e-005
        O(0)              4.446e-006  4.446e-006
        Pb                6.484e-006  6.484e-006
        S(6)              1.301e-001  1.301e-001
        Zn                1.915e-002  1.915e-002

----------------------------Description of solution----------------------------

                                     pH  =   4.300
                                     pe  =   4.000
                        Activity of water  =   0.997
                           Ionic strength  =  2.326e-001
                        Mass of water (kg)  =  1.000e+000
                Total alkalinity (eq/kg)  = -1.547e-004
                   Total carbon (mol/kg)  =  0.000e+000
                      Total CO2 (mol/kg)  =  0.000e+000
                     Temperature (deg C)  =  17.000
                  Electrical balance (eq)  = -1.118e-001
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  = -47.14
                                Iterations  =  11
                                   Total H  = 1.110127e+002
                                   Total O  = 5.602672e+001

---------------------------------Redox couples---------------------------------

        Redox couple             pe  Eh (volts)

        Fe(2)/Fe(3)          7.6830      0.4423
        O(-2)/O(0)          16.4941      0.9495

----------------------------Distribution of species----------------------------

                                                 Log       Log         Log
        Species            Molality    Activity  Molality  Activity     Gamma

        H+                6.312e-005  5.012e-005    -4.200    -4.300    -0.100
        OH-               1.437e-010  1.069e-010    -9.843    -9.971    -0.128
```

	H2O	5.551e+001	9.974e-001	1.744	-0.001	0.000
Al		7.645e-003				
	AlSO4+	4.657e-003	3.464e-003	-2.332	-2.460	-0.128
	Al(SO4)2-	2.480e-003	1.789e-003	-2.606	-2.747	-0.142
	Al+3	4.826e-004	6.050e-005	-3.316	-4.218	-0.902
	AlOH+2	2.303e-005	7.054e-006	-4.638	-5.152	-0.514
	Al(OH)2+	2.573e-006	1.903e-006	-5.590	-5.720	-0.131
	Al(OH)3	8.891e-010	9.380e-010	-9.051	-9.028	0.023
	Al(OH)4-	1.693e-011	1.221e-011	-10.771	-10.913	-0.142
As(3)		1.146e-012				
	H3AsO3	1.146e-012	1.209e-012	-11.941	-11.918	0.023
	H4AsO3+	4.036e-017	3.002e-017	-16.394	-16.523	-0.128
	H2AsO3-	1.414e-017	1.052e-017	-16.850	-16.978	-0.128
	HAsO3-2	3.797e-025	1.163e-025	-24.421	-24.935	-0.514
	AsO3-3	9.673e-034	6.748e-035	-33.014	-34.171	-1.156
As(5)		1.668e-006				
	H2AsO4-	1.645e-006	1.224e-006	-5.784	-5.912	-0.128
	HAsO4-2	1.343e-008	4.114e-009	-7.872	-8.386	-0.514
	H3AsO4	9.405e-009	9.923e-009	-8.027	-8.003	0.023
	AsO4-3	2.436e-015	1.699e-016	-14.613	-15.770	-1.156
Ca		1.412e-002				
	CaSO4	7.873e-003	8.306e-003	-2.104	-2.081	0.023
	Ca+2	6.249e-003	2.167e-003	-2.204	-2.664	-0.460
	CaOH+	7.373e-012	5.534e-012	-11.132	-11.257	-0.125
Cd		4.294e-005				
	CdSO4	1.772e-005	1.869e-005	-4.752	-4.728	0.023
	Cd(SO4)2-2	1.418e-005	4.341e-006	-4.848	-5.362	-0.514
	Cd+2	1.105e-005	3.383e-006	-4.957	-5.471	-0.514
	CdOH+	4.092e-012	3.044e-012	-11.388	-11.517	-0.128
	Cd2OH+3	8.011e-016	5.589e-017	-15.096	-16.253	-1.156
	Cd(OH)2	5.673e-018	5.985e-018	-17.246	-17.223	0.023
	Cd(OH)3-	1.797e-026	1.336e-026	-25.746	-25.874	-0.128
	Cd(OH)4-2	7.740e-036	2.370e-036	-35.111	-35.625	-0.514
Cu(1)		1.317e-009				
	Cu+	1.317e-009	8.825e-010	-8.880	-9.054	-0.174
Cu(2)		7.564e-004				
	Cu+2	4.340e-004	8.751e-005	-3.362	-4.058	-0.695
	CuSO4	3.223e-004	3.400e-004	-3.492	-3.468	0.023
	CuOH+	2.452e-008	1.741e-008	-7.610	-7.759	-0.149
	Cu(OH)2	6.863e-010	7.241e-010	-9.163	-9.140	0.023
	Cu2(OH)2+2	1.916e-010	5.867e-011	-9.718	-10.232	-0.514
	Cu(OH)3-	1.170e-018	8.702e-019	-17.932	-18.060	-0.128
	Cu(OH)4-2	1.126e-026	3.448e-027	-25.949	-26.462	-0.514
Fe(2)		2.278e-002				
	Fe+2	1.182e-002	3.752e-003	-1.927	-2.426	-0.498
	FeSO4	1.096e-002	1.157e-002	-1.960	-1.937	0.023
	FeOH+	1.746e-008	1.278e-008	-7.758	-7.894	-0.136
	Fe(OH)2	1.003e-015	1.059e-015	-14.999	-14.975	0.023
	Fe(OH)3-	9.865e-022	7.220e-022	-21.006	-21.141	-0.136
Fe(3)		1.820e-005				
	Fe(OH)2+	1.207e-005	8.931e-006	-4.918	-5.049	-0.131
	FeOH+2	2.728e-006	8.353e-007	-5.564	-6.078	-0.514
	FeSO4+	2.013e-006	1.473e-006	-5.696	-5.832	-0.136
	Fe(SO4)2-	1.222e-006	9.089e-007	-5.913	-6.042	-0.128
	Fe+3	1.512e-007	1.055e-008	-6.820	-7.977	-1.156
	Fe2(OH)2+4	2.999e-009	2.638e-011	-8.523	-10.579	-2.056
	Fe(OH)3	1.979e-009	2.088e-009	-8.703	-8.680	0.023
	Fe3(OH)4+5	7.729e-011	4.742e-014	-10.112	-13.324	-3.212
	Fe(OH)4-	5.618e-013	4.156e-013	-12.250	-12.381	-0.131
H(0)		1.575e-027				
	H2	7.877e-028	8.310e-028	-27.104	-27.080	0.023
K		3.690e-004				
	K+	3.311e-004	2.285e-004	-3.480	-3.641	-0.161
	KSO4-	3.788e-005	2.802e-005	-4.422	-4.552	-0.131
Mn(2)		3.940e-003				
	Mn+2	1.973e-003	6.263e-004	-2.705	-3.203	-0.498
	MnSO4	1.967e-003	2.075e-003	-2.706	-2.683	0.023
	MnOH+	2.240e-010	1.639e-010	-9.650	-9.785	-0.136
	Mn(OH)3-	1.069e-025	7.824e-026	-24.971	-25.107	-0.136
Mn(3)		2.484e-020				
	Mn+3	2.484e-020	3.114e-021	-19.605	-20.507	-0.902
Mn(6)		0.000e+000				
	MnO4-2	0.000e+000	0.000e+000	-59.006	-59.548	-0.542
Mn(7)		0.000e+000				

	MnO4-	0.000e+000	0.000e+000	-61.622	-61.786	-0.165
Na	3.200e-003					
	Na+	2.920e-003	2.159e-003	-2.535	-2.666	-0.131
	NaSO4-	2.797e-004	2.069e-004	-3.553	-3.684	-0.131
Ni	4.760e-005					
	NiSO4	2.447e-005	2.581e-005	-4.611	-4.588	0.023
	Ni+2	2.303e-005	7.054e-006	-4.638	-5.152	-0.514
	Ni(SO4)2-2	9.786e-008	2.997e-008	-7.009	-7.523	-0.514
	NiOH+	1.461e-011	1.087e-011	-10.835	-10.964	-0.128
	Ni(OH)2	2.648e-016	2.793e-016	-15.577	-15.554	0.023
	Ni(OH)3-	7.473e-023	5.559e-023	-22.127	-22.255	-0.128
O(0)	4.446e-006					
	O2	2.223e-006	2.345e-006	-5.653	-5.630	0.023
Pb	6.484e-006					
	PbSO4	3.886e-006	4.100e-006	-5.410	-5.387	0.023
	Pb(SO4)2-2	1.415e-006	4.334e-007	-5.849	-6.363	-0.514
	Pb+2	1.182e-006	3.619e-007	-5.927	-6.441	-0.514
	PbOH+	1.888e-010	1.404e-010	-9.724	-9.852	-0.128
	Pb2OH+3	1.631e-014	1.138e-015	-13.787	-14.944	-1.156
	Pb(OH)2	1.031e-015	1.087e-015	-14.987	-14.964	0.023
	Pb(OH)3-	3.340e-022	2.485e-022	-21.476	-21.605	-0.128
	Pb3(OH)4+2	9.328e-027	2.857e-027	-26.030	-26.544	-0.514
	Pb(OH)4-2	3.707e-029	1.135e-029	-28.431	-28.945	-0.514
S(6)	1.301e-001					
	SO4-2	8.092e-002	2.014e-002	-1.092	-1.696	-0.604
	FeSO4	1.096e-002	1.157e-002	-1.960	-1.937	0.023
	ZnSO4	8.148e-003	8.596e-003	-2.089	-2.066	0.023
	CaSO4	7.873e-003	8.306e-003	-2.104	-2.081	0.023
	Zn(SO4)2-2	4.896e-003	1.499e-003	-2.310	-2.824	-0.514
	AlSO4+	4.657e-003	3.464e-003	-2.332	-2.460	-0.128
	Al(SO4)2-	2.480e-003	1.789e-003	-2.606	-2.747	-0.142
	MnSO4	1.967e-003	2.075e-003	-2.706	-2.683	0.023
	CuSO4	3.223e-004	3.400e-004	-3.492	-3.468	0.023
	NaSO4-	2.797e-004	2.069e-004	-3.553	-3.684	-0.131
	HSO4-	1.104e-004	8.210e-005	-3.957	-4.086	-0.128
	KSO4-	3.788e-005	2.802e-005	-4.422	-4.552	-0.131
	NiSO4	2.447e-005	2.581e-005	-4.611	-4.588	0.023
	CdSO4	1.772e-005	1.869e-005	-4.752	-4.728	0.023
	Cd(SO4)2-2	1.418e-005	4.341e-006	-4.848	-5.362	-0.514
	PbSO4	3.886e-006	4.100e-006	-5.410	-5.387	0.023
	FeSO4+	2.013e-006	1.473e-006	-5.696	-5.832	-0.136
	Pb(SO4)2-2	1.415e-006	4.334e-007	-5.849	-6.363	-0.514
	Fe(SO4)2-	1.222e-006	9.089e-007	-5.913	-6.042	-0.128
	Ni(SO4)2-2	9.786e-008	2.997e-008	-7.009	-7.523	-0.514
Zn	1.915e-002					
	ZnSO4	8.148e-003	8.596e-003	-2.089	-2.066	0.023
	Zn+2	6.107e-003	1.939e-003	-2.214	-2.712	-0.498
	Zn(SO4)2-2	4.896e-003	1.499e-003	-2.310	-2.824	-0.514
	ZnOH+	3.049e-008	2.268e-008	-7.516	-7.644	-0.128
	Zn(OH)2	9.186e-012	9.691e-012	-11.037	-11.014	0.023
	Zn(OH)3-	8.198e-019	6.099e-019	-18.086	-18.215	-0.128
	Zn(OH)4-2	6.281e-027	1.924e-027	-26.202	-26.716	-0.514

Saturation indices

Phase	SI	log IAP	log KT	
Al(OH)3(a)	-2.25	8.68	10.93	Al(OH)3
Al2O3	-5.62	17.36	22.98	Al2O3
Al4(OH)10SO4	1.72	24.42	22.70	Al4(OH)10SO4
AlAsO4:2H2O	-4.12	0.68	4.80	AlAsO4:2H2O
AlOHSO4	1.61	-1.62	-3.23	AlOHSO4
AlumK	-5.95	-11.26	-5.32	KAl(SO4)2:12H2O
Alunite	7.48	6.11	-1.38	KAl3(SO4)2(OH)6
Anglesite	-0.30	-8.14	-7.83	PbSO4
Anhydrite	0.20	-4.36	-4.56	CaSO4
Antlerite	-4.96	3.33	8.29	Cu3(OH)4SO4
Arsenolite	-44.57	-21.99	22.58	As4O6
As2O5	-22.81	-16.00	6.81	As2O5
Basaluminite	1.72	24.42	22.70	Al4(OH)10SO4
Bianchite	-2.65	-4.42	-1.76	ZnSO4:6H2O
Birnessite	-13.72	2.89	16.61	MnO2
Bixbyite	-14.91	8.29	23.20	Mn2O3
Boehmite	-0.47	8.68	9.15	AlOOH

Brochantite	-7.47	7.87	15.34	Cu4(OH)6SO4
Bunsenite	-9.49	3.45	12.93	NiO
Ca3(AsO4)2:6H2O	-20.51	1.79	22.30	Ca3(AsO4)2:6H2O
Cd(Gamma)	-34.79	5.63	40.42	Cd
Cd(OH)2(A)	-11.02	3.13	14.15	Cd(OH)2
Cd(OH)2(C)	-10.52	3.13	13.65	Cd(OH)2
Cd3(OH)2(SO4)2	-17.92	-11.21	6.71	Cd3(OH)2(SO4)2
Cd3(OH)4SO4	-23.47	-0.91	22.56	Cd3(OH)4SO4
Cd4(OH)6SO4	-26.19	2.21	28.40	Cd4(OH)6SO4
CdMetal	-34.69	5.63	40.32	Cd
CdSO4	-7.36	-7.17	0.20	CdSO4
CdSO4:2.67H2O	-5.38	-7.17	-1.79	CdSO4:2.67H2O
CdSO4:H2O	-5.66	-7.17	-1.51	CdSO4:H2O
Chalcanthite	-3.09	-5.76	-2.67	CuSO4:5H2O
Claudetite	-44.33	-21.99	22.34	As4O6
Cu(OH)2	-4.41	4.54	8.95	Cu(OH)2
Cu2SO4	-17.95	1.29	19.24	Cu2SO4
Cu3(AsO4)2:6H2O	-8.49	-2.39	6.10	Cu3(AsO4)2:6H2O
CuMetal	-7.63	7.04	14.68	Cu
CuOCuSO4	-13.46	-1.21	12.25	CuO:CuSO4
CupricFerrite	7.72	14.38	6.66	CuFe2O4
Cuprite	-7.83	11.59	19.42	Cu2O
CuprousFerrite	9.01	10.71	1.70	CuFeO2
CuSO4	-9.13	-5.75	3.38	CuSO4
Diaspore	1.31	8.68	7.37	AlOOH
Fe2(SO4)3	-25.82	-21.04	4.77	Fe2(SO4)3
Fe3(OH)8	-4.21	16.01	20.22	Fe3(OH)8
FeAsO4:2H2O	-3.48	-3.08	0.40	FeAsO4:2H2O
Ferrihydrite	-0.08	4.92	5.00	Fe(OH)3
Gibbsite(C)	-0.55	8.68	9.23	Al(OH)3
Goethite	4.13	4.92	0.79	FeOOH
Goslarite	-2.39	-4.42	-2.03	ZnSO4:7H2O
Gypsum	0.49	-4.36	-4.85	CaSO4:2H2O
Hausmannite	-23.01	13.68	36.69	Mn3O4
Hematite	13.23	9.84	-3.38	Fe2O3
Hercynite	-5.21	23.53	28.75	FeAl2O4
Jarosite-H	5.16	-5.83	-10.99	(H3O)Fe3(SO4)2(OH)6
Jarosite-K	9.00	-5.17	-14.17	KFe3(SO4)2(OH)6
Jarosite-Na	6.27	-4.19	-10.47	NaFe3(SO4)2(OH)6
Jurbanite	1.61	-1.62	-3.23	AlOHSO4
Langite	-9.73	7.86	17.59	Cu4(OH)6SO4:H2O
Larnakite	-5.83	-5.98	-0.15	PbO:PbSO4
Lepidocrocite	3.55	4.92	1.37	FeOOH
Lime	-27.80	5.93	33.73	CaO
Litharge	-10.89	2.16	13.05	PbO
Maghemite	3.46	9.84	6.39	Fe2O3
Magnetite	11.26	16.02	4.76	Fe3O4
Manganite	-7.37	4.14	11.51	MnOOH
Massicot	-11.09	2.16	13.25	PbO
Melanterite	-1.60	-4.13	-2.53	FeSO4:7H2O
Minium	-45.33	3.97	49.30	Pb3O4
Mirabilite	-5.54	-7.04	-1.50	Na2SO4:10H2O
Mn2(SO4)3	-41.18	-22.60	18.58	Mn2(SO4)3
Mn3(AsO4)2:8H2O	-12.33	0.17	12.50	Mn3(AsO4)2:8H2O
MnSO4	-7.88	-4.90	2.98	MnSO4
Monteponite	-12.49	3.13	15.62	CdO
Morenosite	-4.44	-6.86	-2.42	NiSO4:7H2O
Ni(OH)2	-6.74	3.45	10.18	Ni(OH)2
Ni3(AsO4)2:8H2O	-21.37	-5.67	15.70	Ni3(AsO4)2:8H2O
Ni4(OH)6SO4	-28.51	3.49	32.00	Ni4(OH)6SO4
Nsutite	-13.13	2.89	16.02	MnO2
O2(g)	-37.90	-5.01	32.89	O2
Pb(OH)2(C)	-6.28	2.16	8.43	Pb(OH)2
Pb2O(OH)2	-21.89	4.31	26.20	Pb2O(OH)2
Pb2O3	-32.76	1.81	34.57	Pb2O3
Pb3(AsO4)2	-15.33	-9.53	5.80	Pb3(AsO4)2
Pb3O2SO4	-14.64	-3.82	10.82	Pb3O2SO4
Pb4(OH)6SO4	-22.77	-1.67	21.10	Pb4(OH)6SO4
Pb4O3SO4	-24.47	-1.66	22.81	Pb4O3SO4
PbMetal	-26.07	4.66	30.73	Pb
PbO:0.3H2O	-10.82	2.16	12.98	PbO:0.33H2O
Plattnerite	-24.61	-0.35	24.26	PbO2
Portlandite	-17.36	5.93	23.30	Ca(OH)2
Pyrocroite	-10.15	5.39	15.54	Mn(OH)2

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        Pyrolusite      -12.08    2.89   14.97  MnO2
        Retgersite       -4.79   -6.85   -2.06  NiSO4:6H2O
        Schwertmannite   22.07   29.07    7.00  Fe8O8(OH)6(SO4)
        Tenorite         -3.39    4.54    7.93  CuO
        Thenardite       -6.86   -7.03   -0.17  Na2SO4
        Zincite          -5.70    5.89   11.58  ZnO
        Zincosite        -7.81   -4.41    3.40  ZnSO4
        Zn(OH)2(A)       -6.56    5.89   12.45  Zn(OH)2
        Zn(OH)2(B)       -5.86    5.89   11.75  Zn(OH)2
        Zn(OH)2(C)       -6.31    5.89   12.20  Zn(OH)2
        Zn(OH)2(E)       -5.61    5.89   11.50  Zn(OH)2
        Zn(OH)2(G)       -5.82    5.89   11.71  Zn(OH)2
        Zn2(OH)2SO4      -6.02    1.48    7.50  Zn2(OH)2SO4
        Zn3(AsO4)2:2.5H2O -12.00    1.65   13.65  Zn3(AsO4)2:2.5H2O
        Zn3O(SO4)2      -23.20   -2.93   20.27  Zn3O(SO4)2
        Zn4(OH)6SO4     -15.15   13.25   28.40  Zn4(OH)6SO4
        ZnMetal         -44.58    8.39   52.97  Zn
        ZnO(Active)      -5.42    5.89   11.31  ZnO
        ZnSO4:H2O        -4.05   -4.41   -0.35  ZnSO4:H2O

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End of simulation.
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Reading input data for simulation 3.
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        END
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End of simulation.
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Reading input data for simulation 4.
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End of run.
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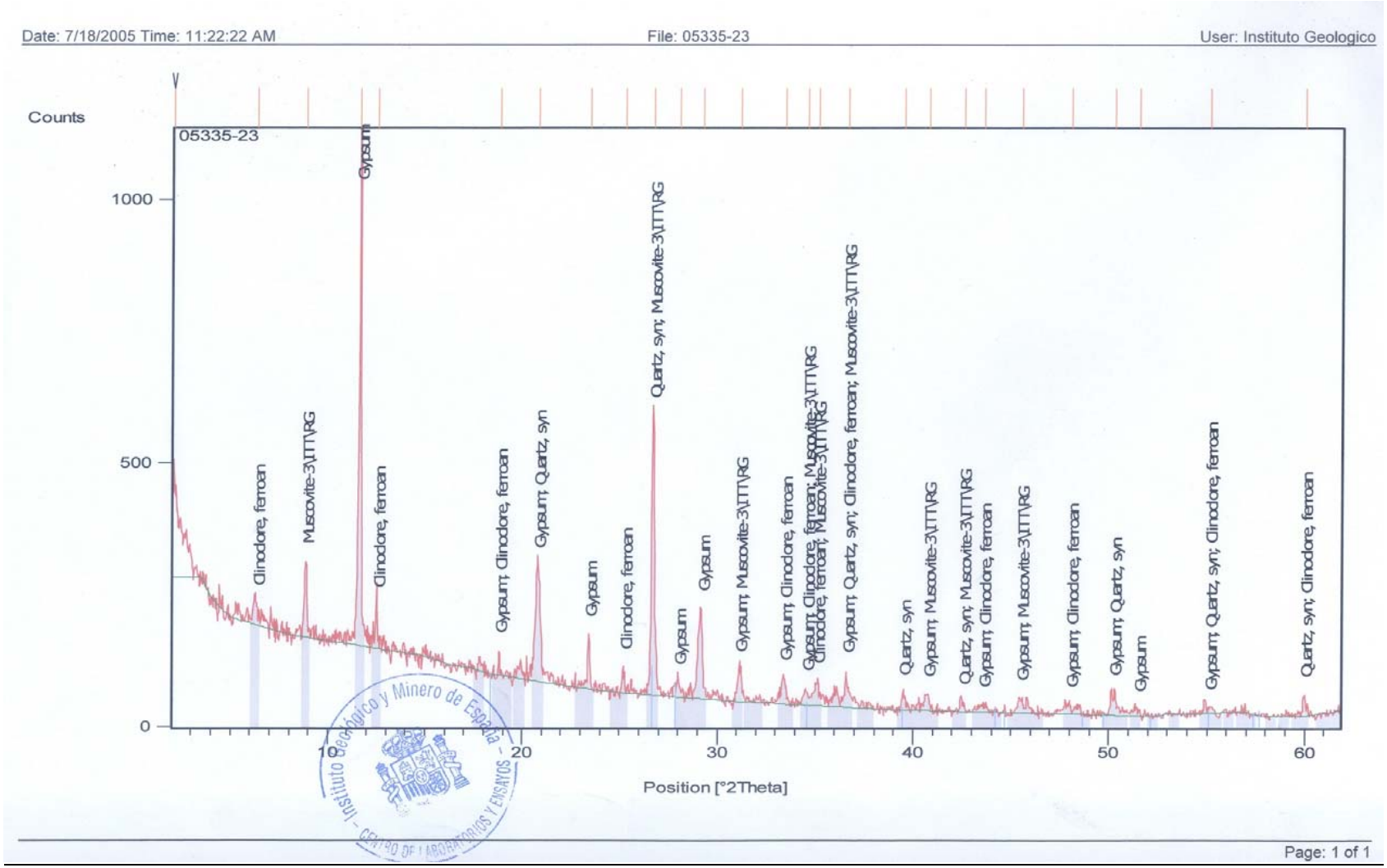

Difractograma; precipitado obtenido en la corta de Aznalcóllar.