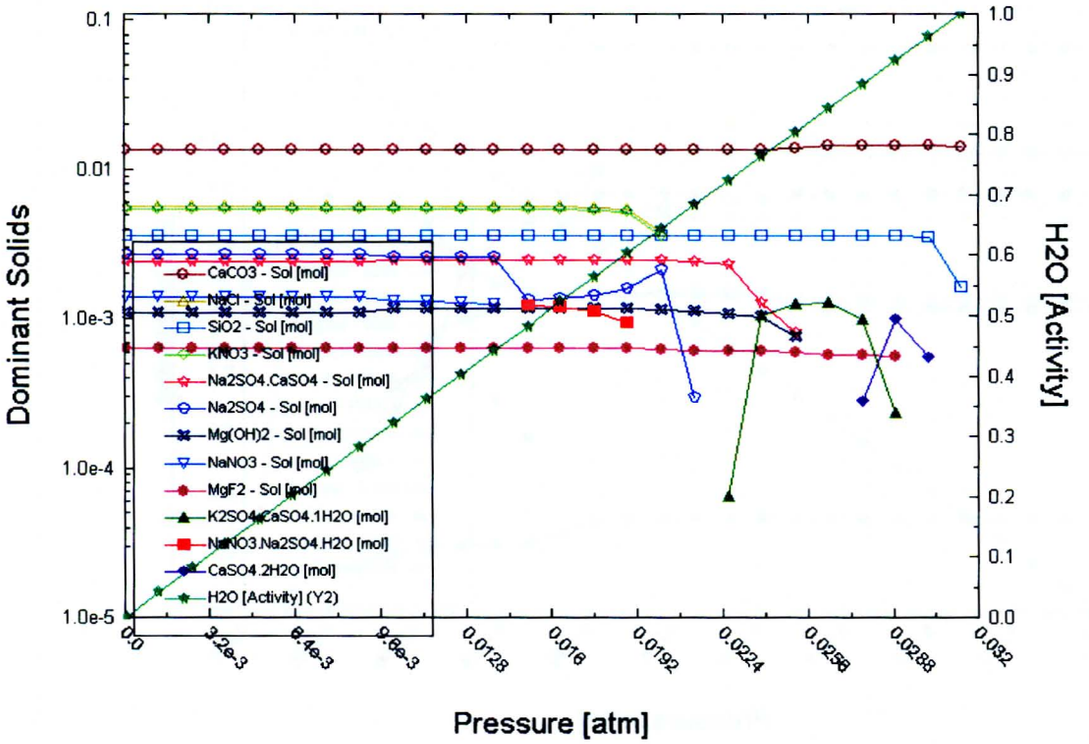
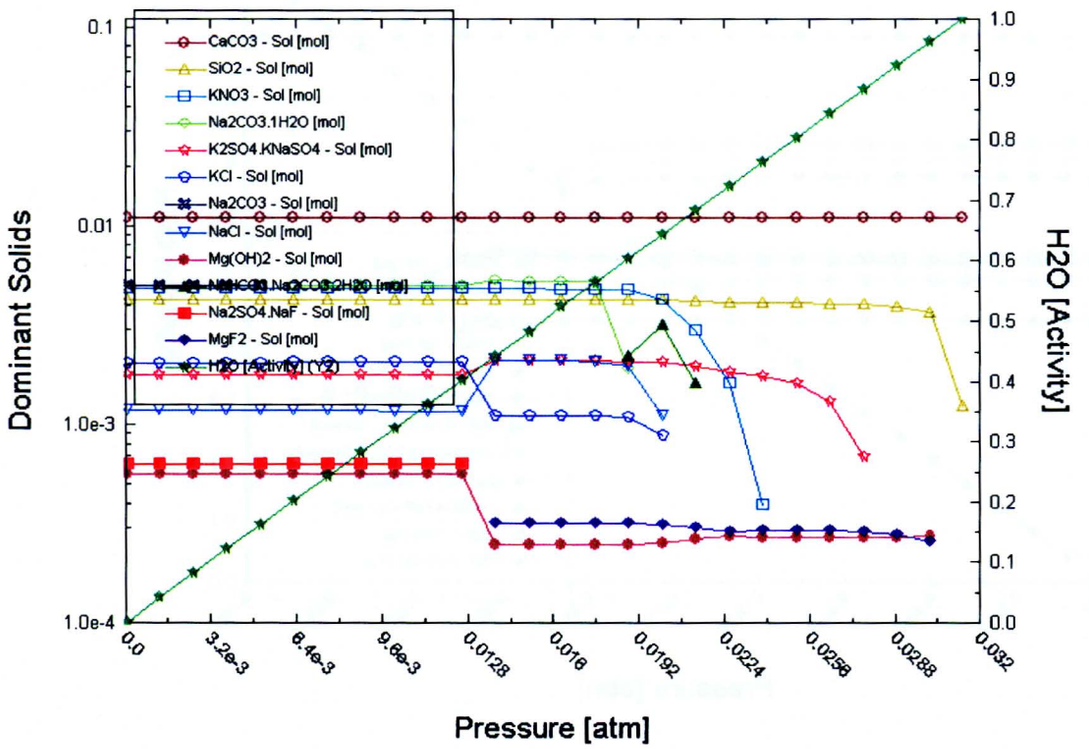
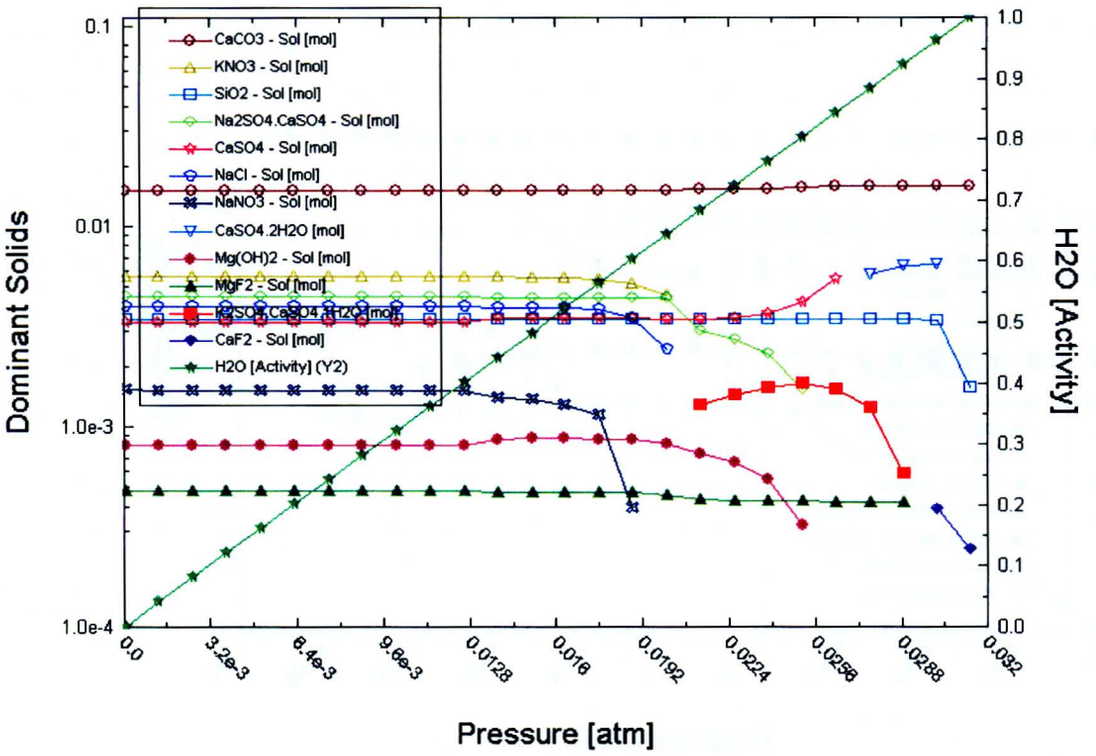
Lab sample C-186089



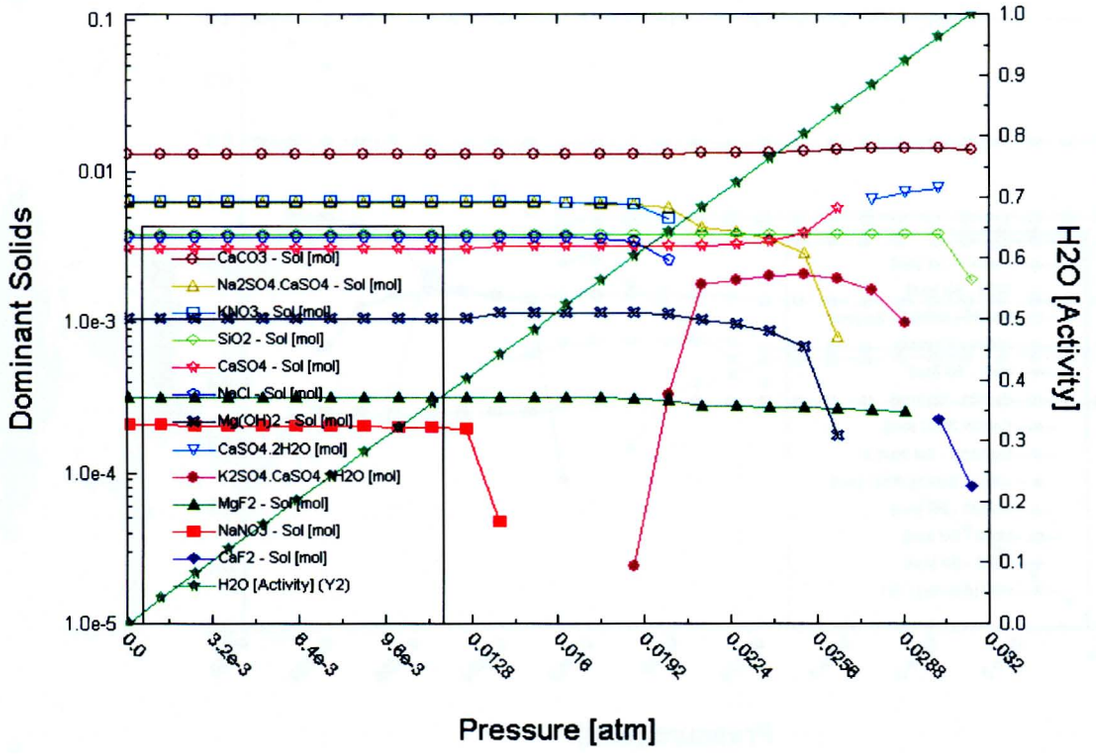
Lab sample C-186088



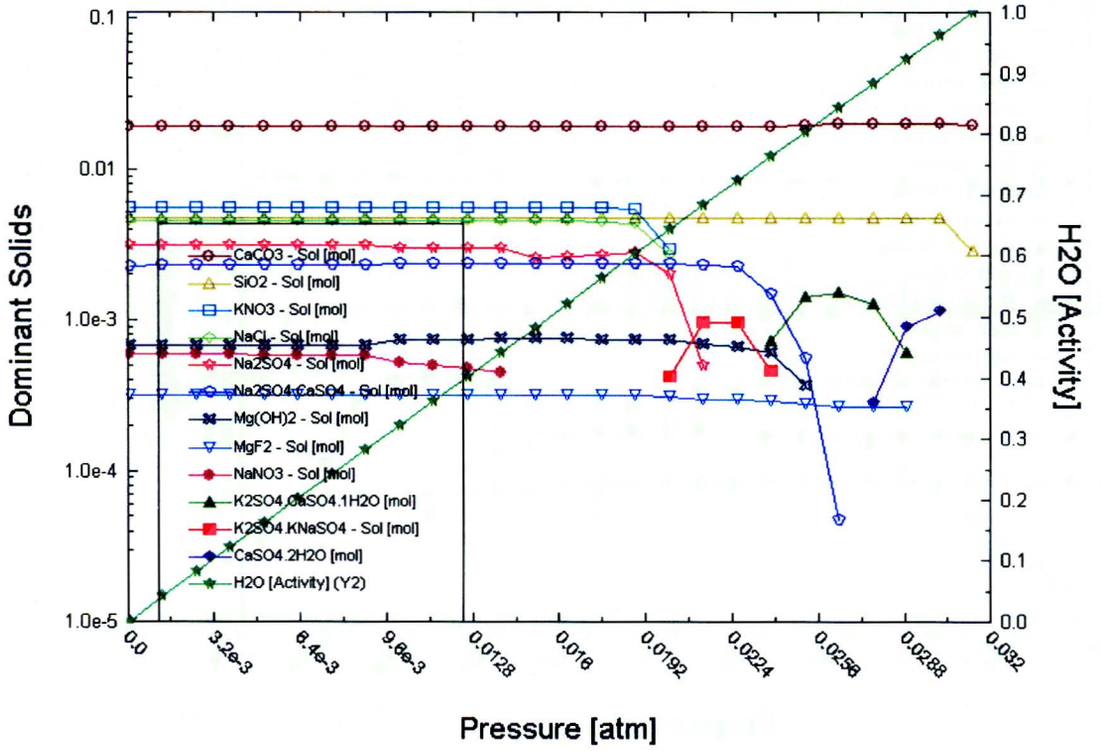
Lab sample C-186087



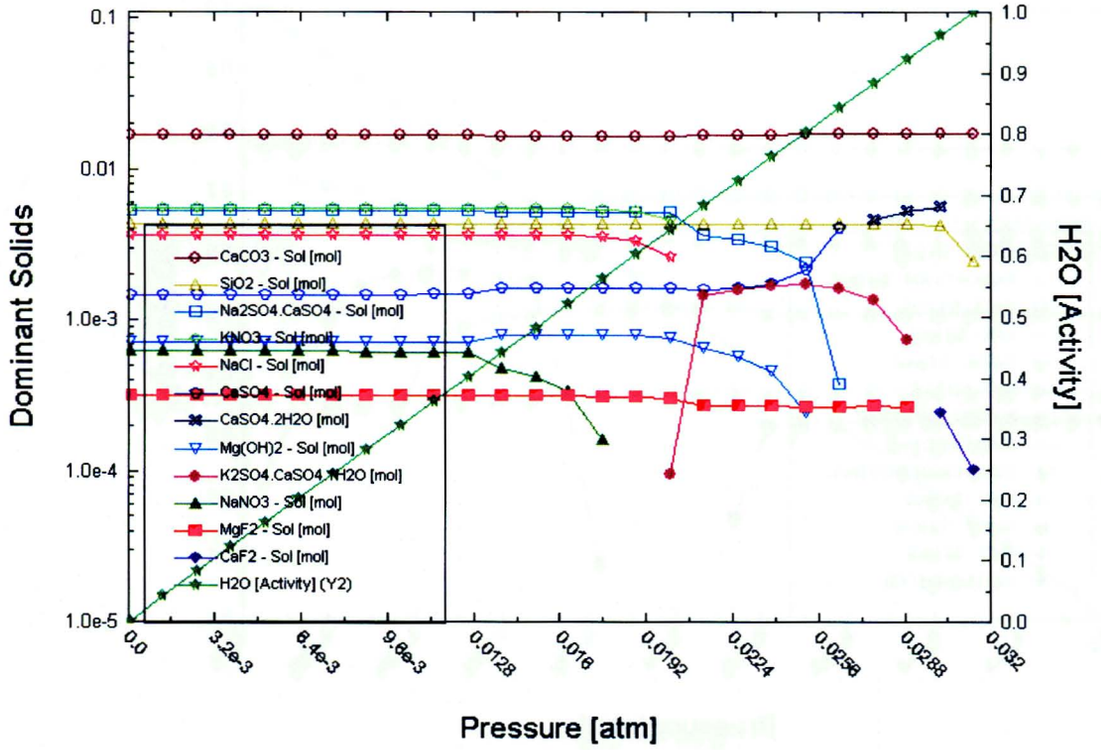
Lab sample C-186086



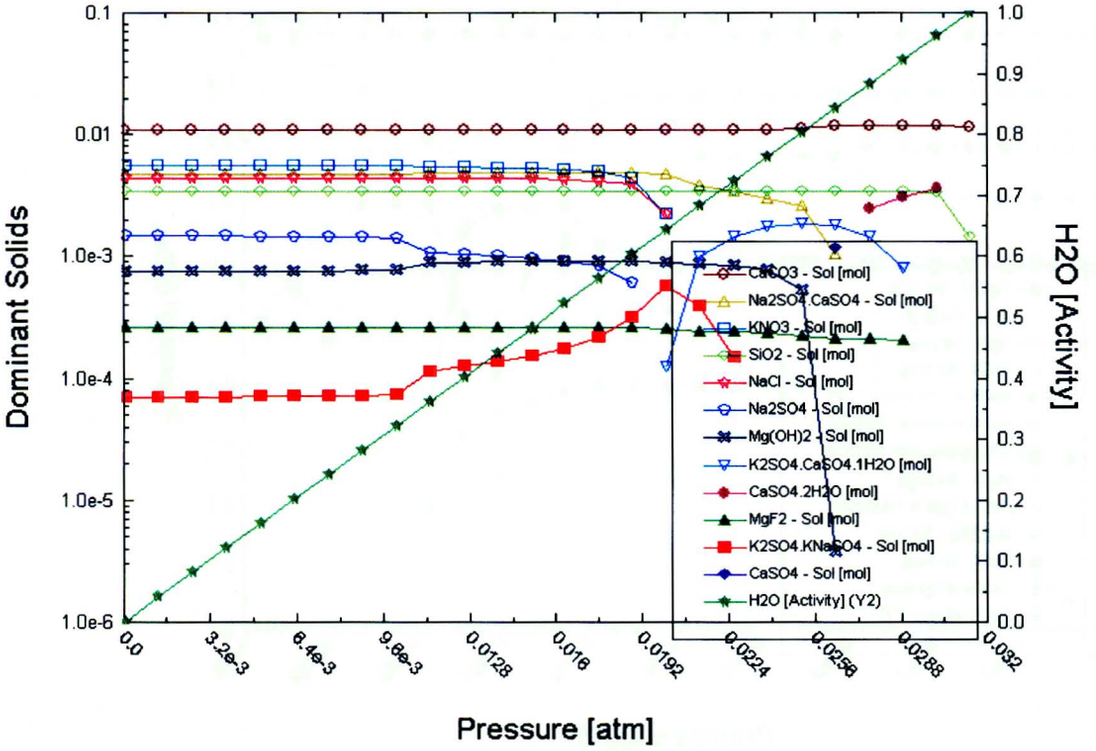
Lab sample C-186085



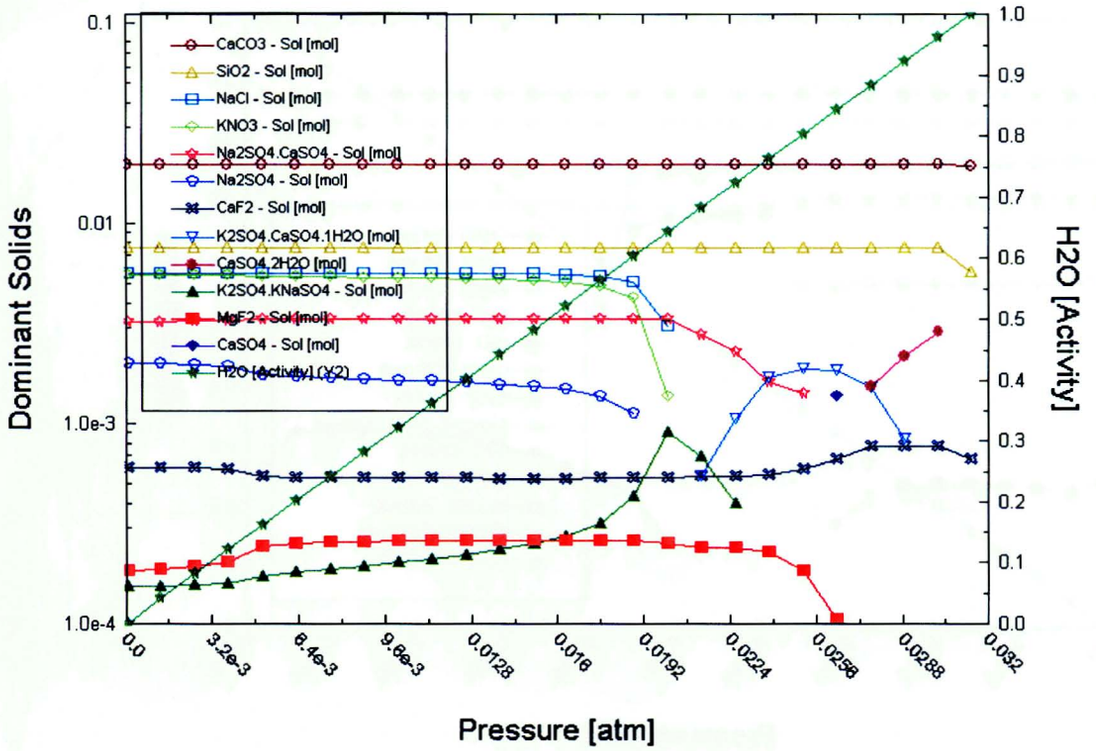
Lab sample C-186084



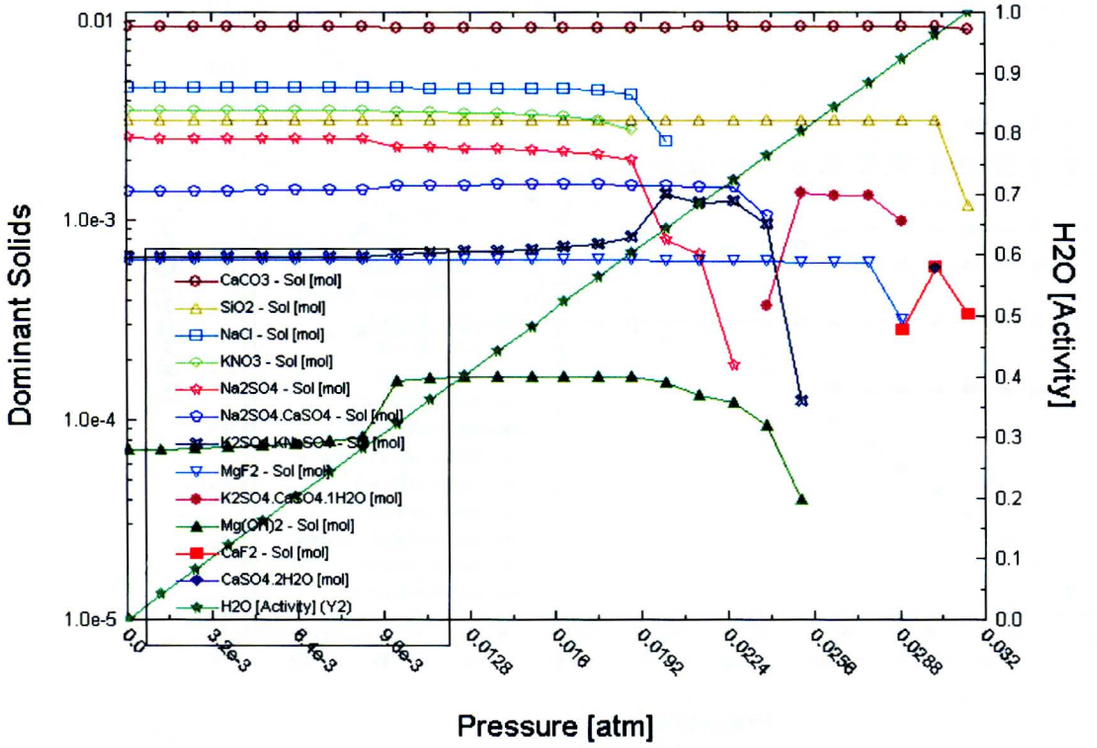
Lab sample C-186082



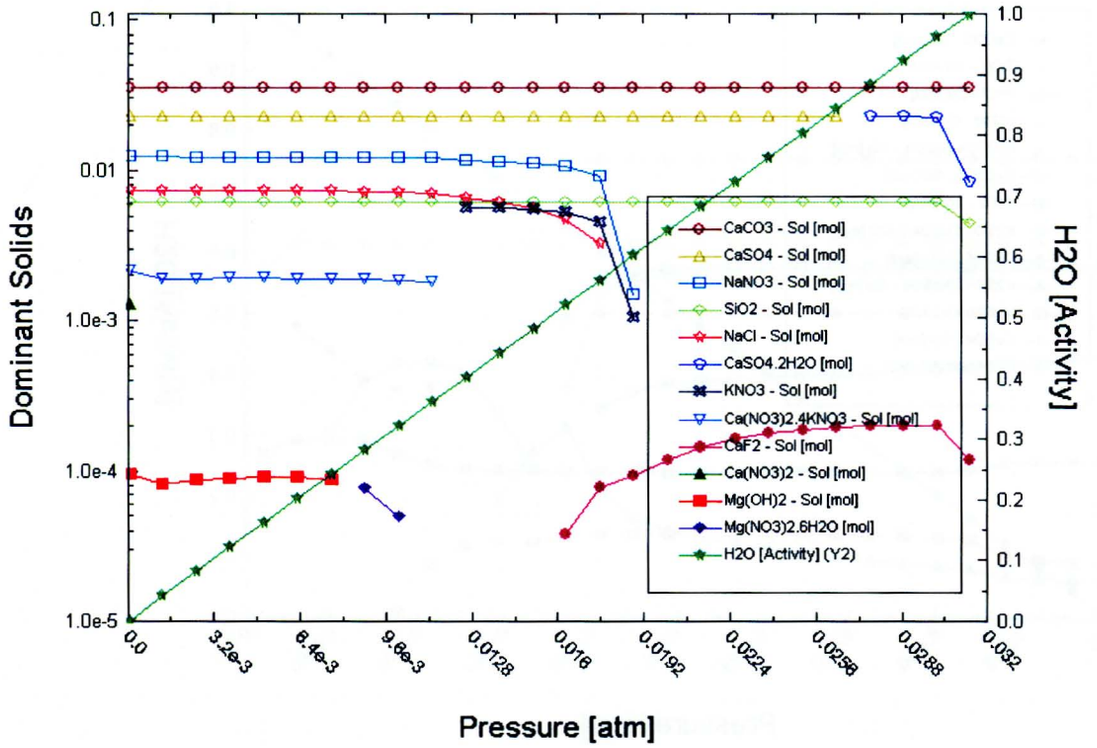
Lab sample C-186081



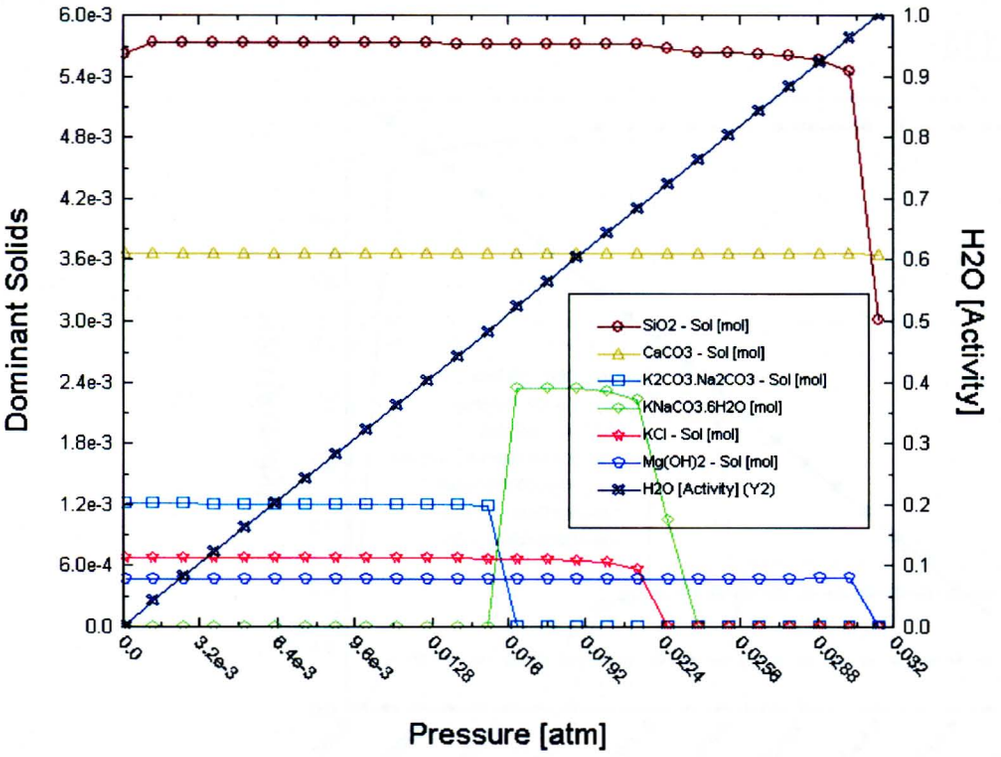
Lab sample C-186080



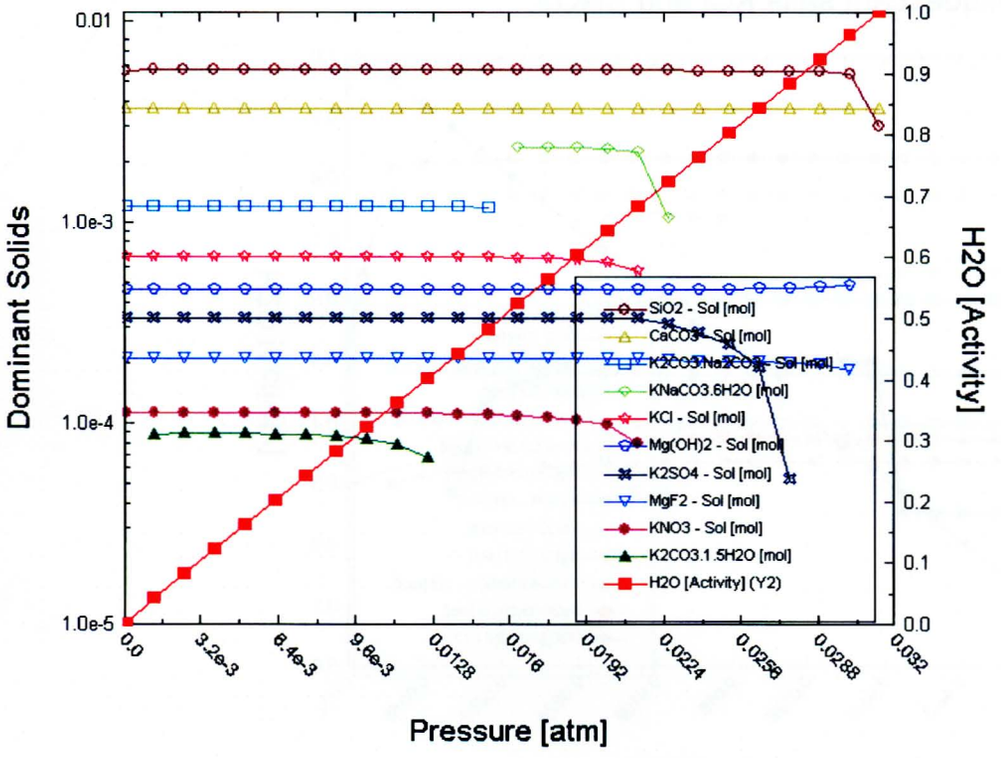
Lab sample C-186077



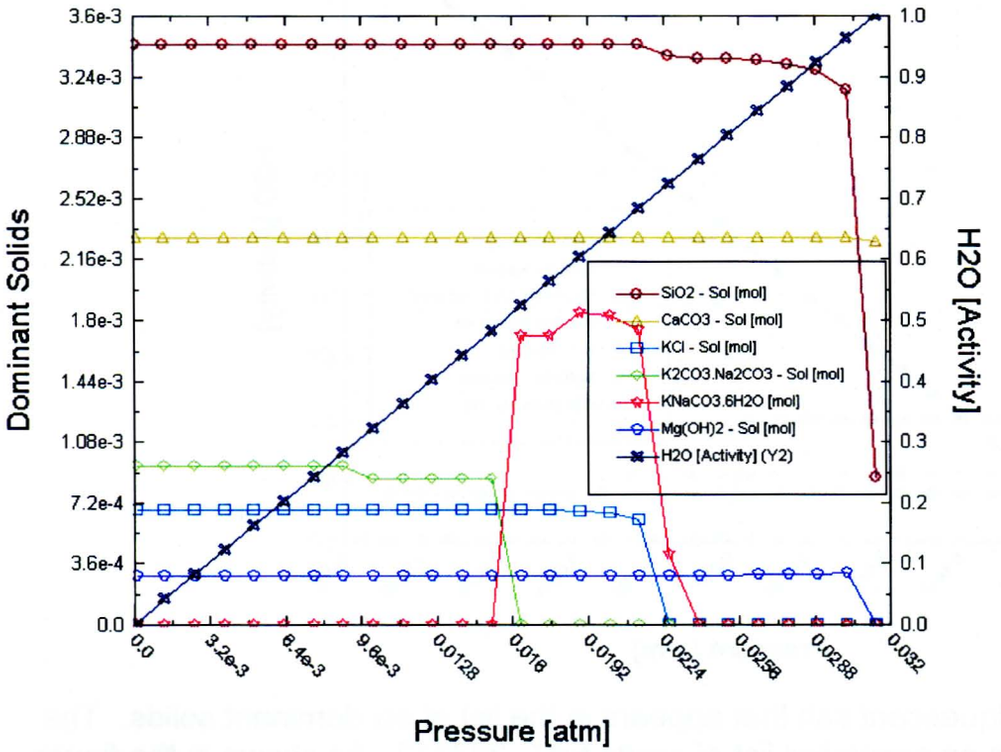
Lab sample C-203112



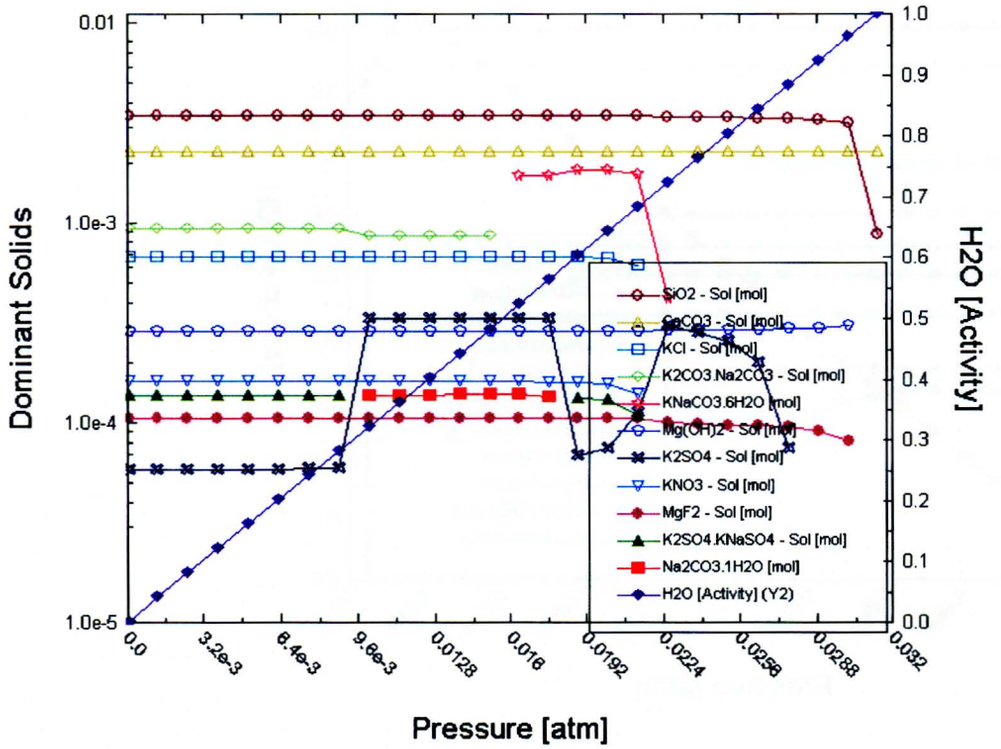
KCl is the only deliquescent salt that appears in the list of six dominant solids. The figure below shows an expanded list of solids for C-203112. As shown in the figure, KNO3 also is present, although in small amount only.



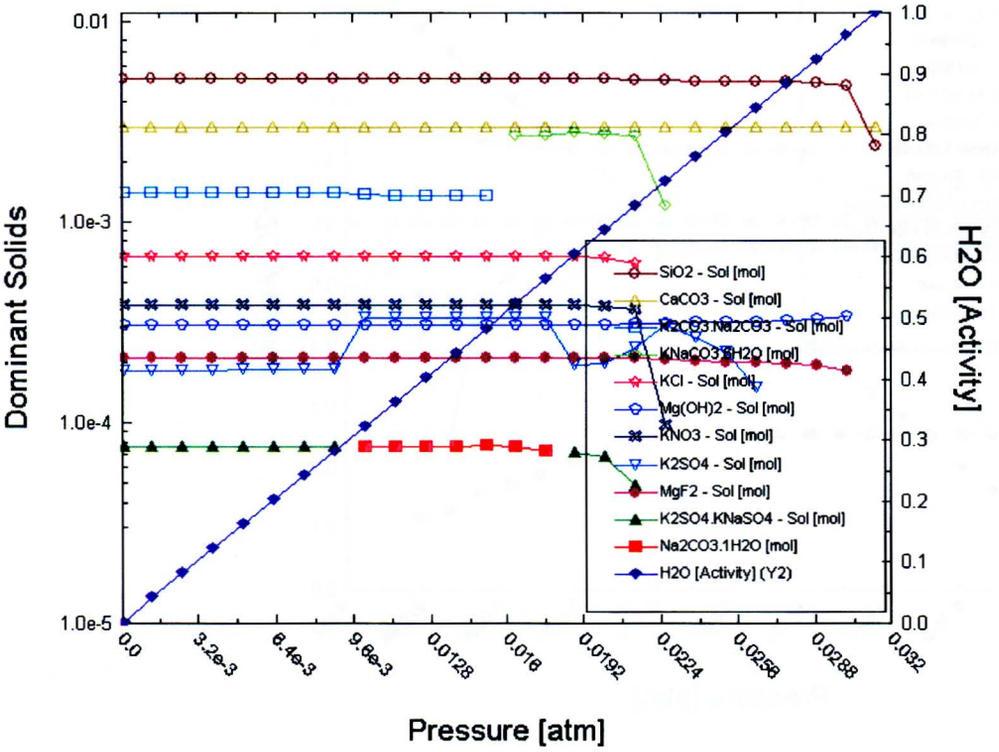
Lab sample C-203113



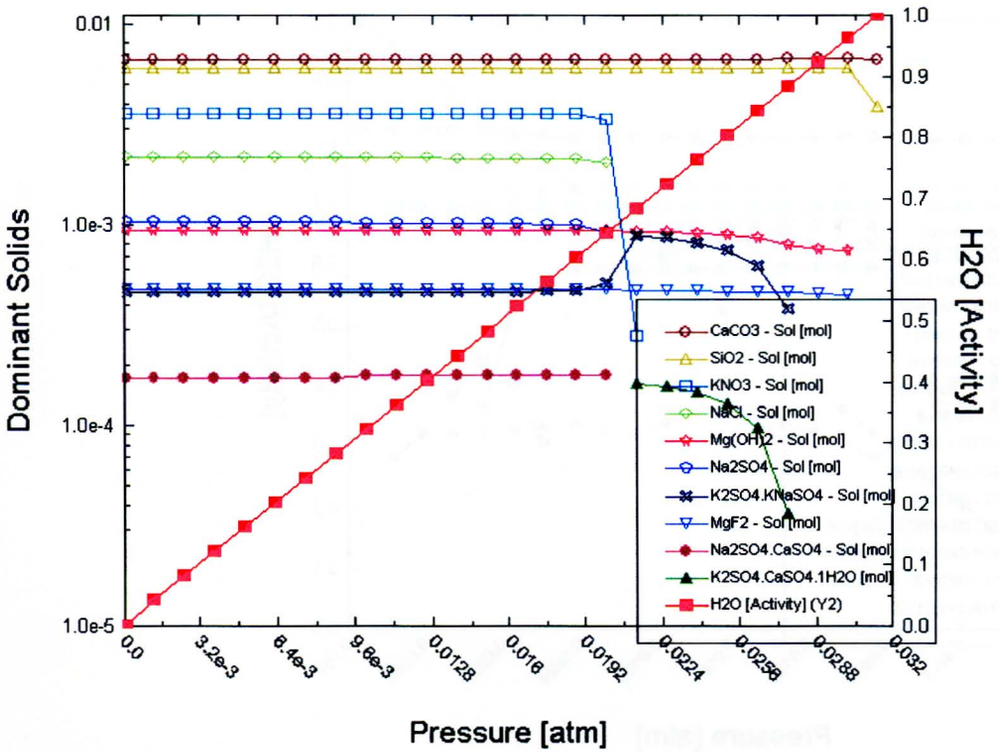
An expanded list of solids for C-203113 is shown in the next figure indicating the presence of the deliquescent salts KCl and KNO3:



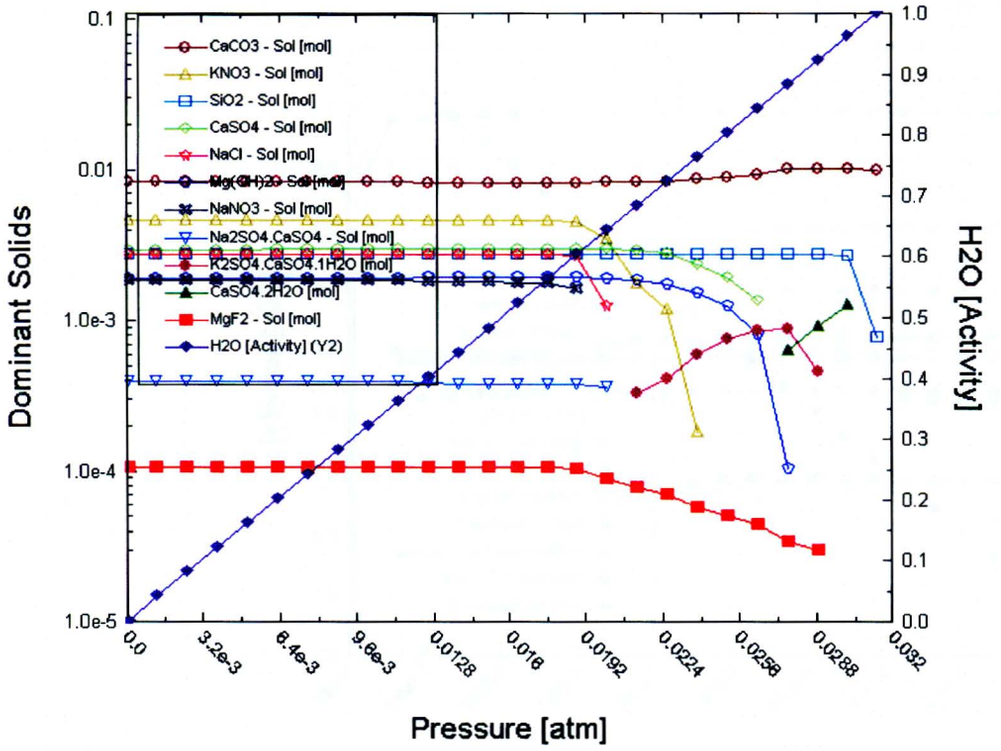
Lab sample C-203114



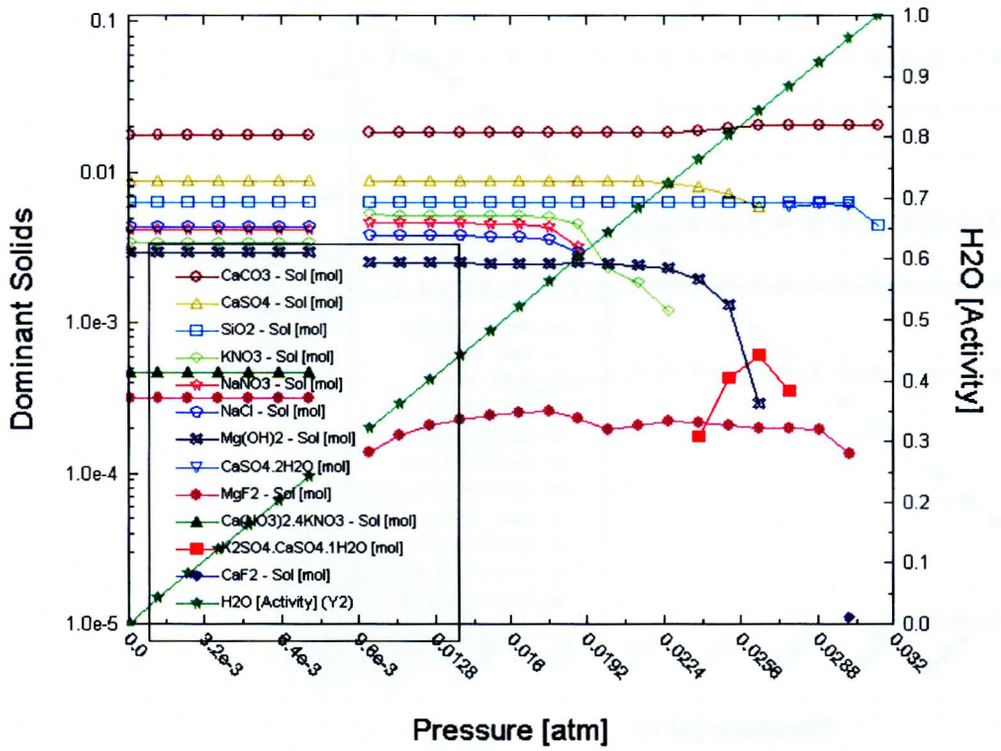
Lab sample C-203115



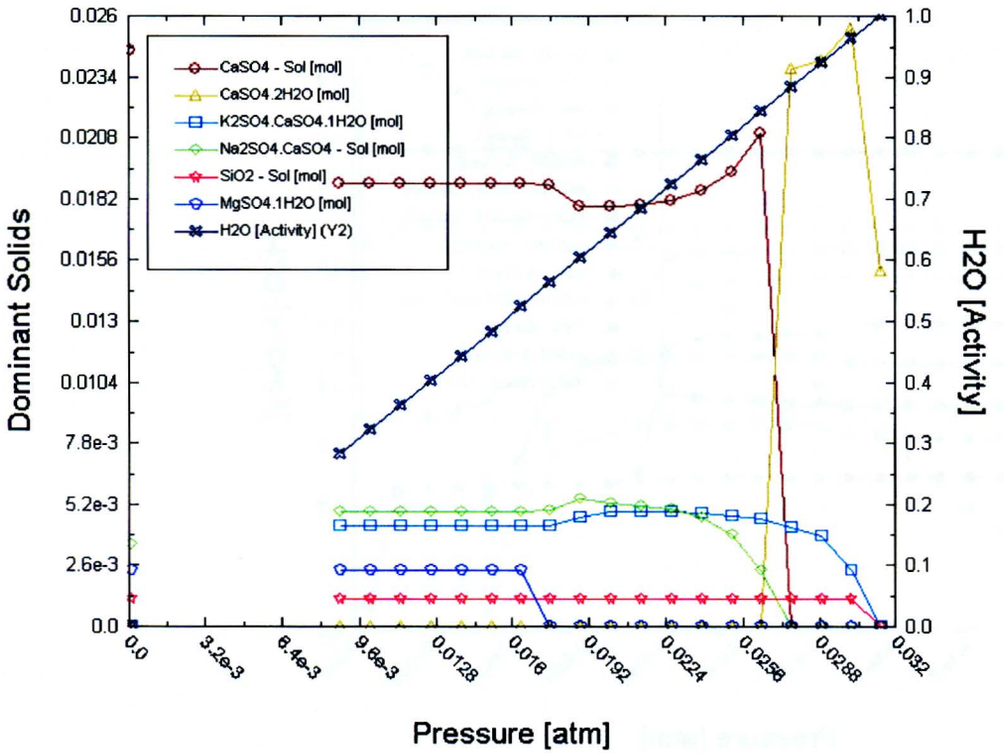
Lab sample C-203116



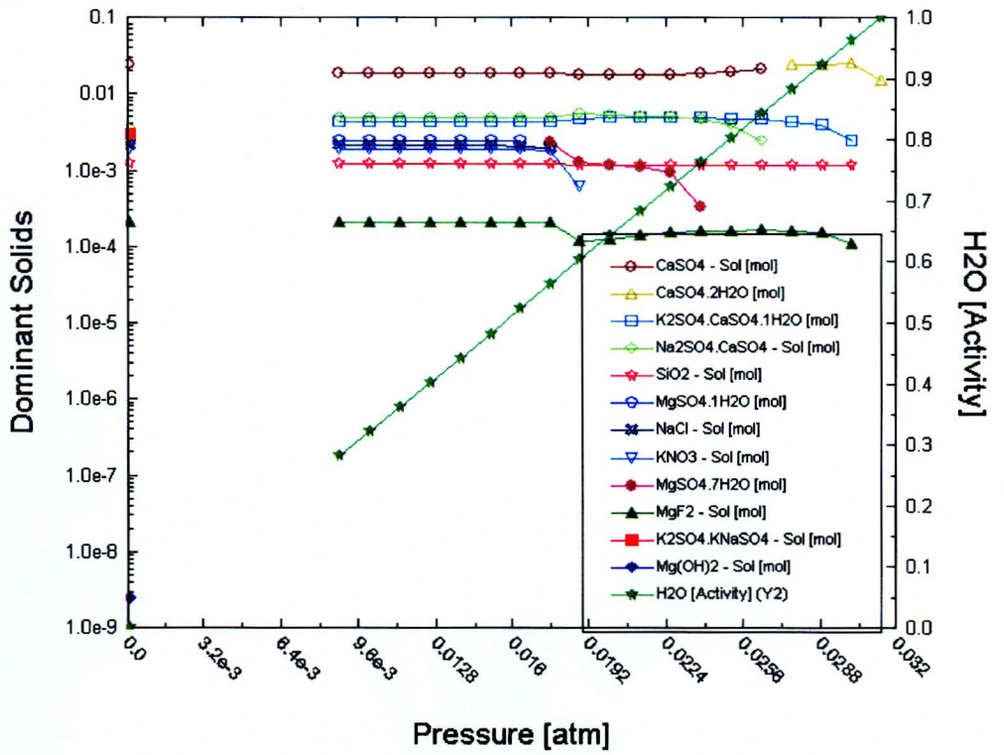
Lab sample C-203117



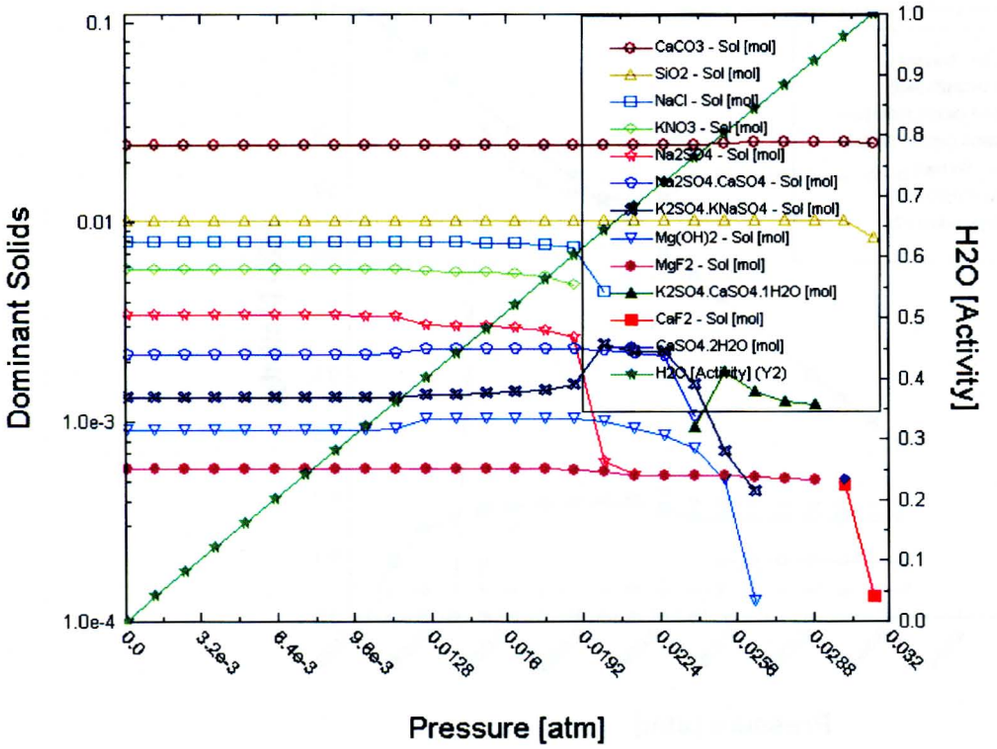
Lab sample C-203118



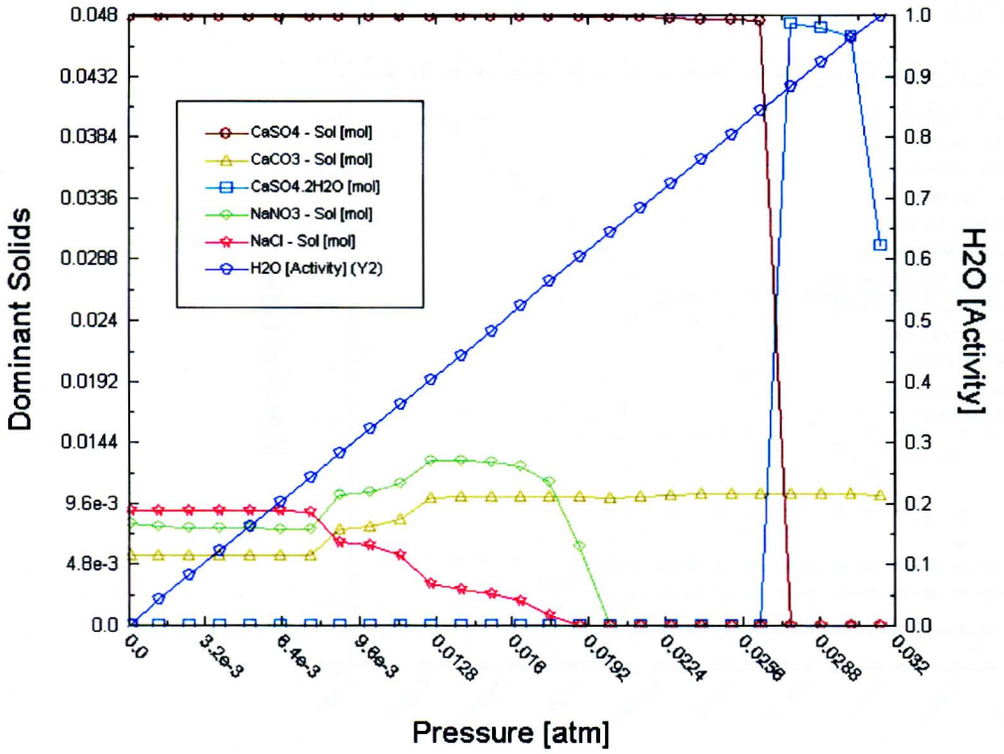
For the above system, the calculations did not converge at several points. It did converge at the last point. Below shows an expanded list of solids. NaCl and KNO3 are present.



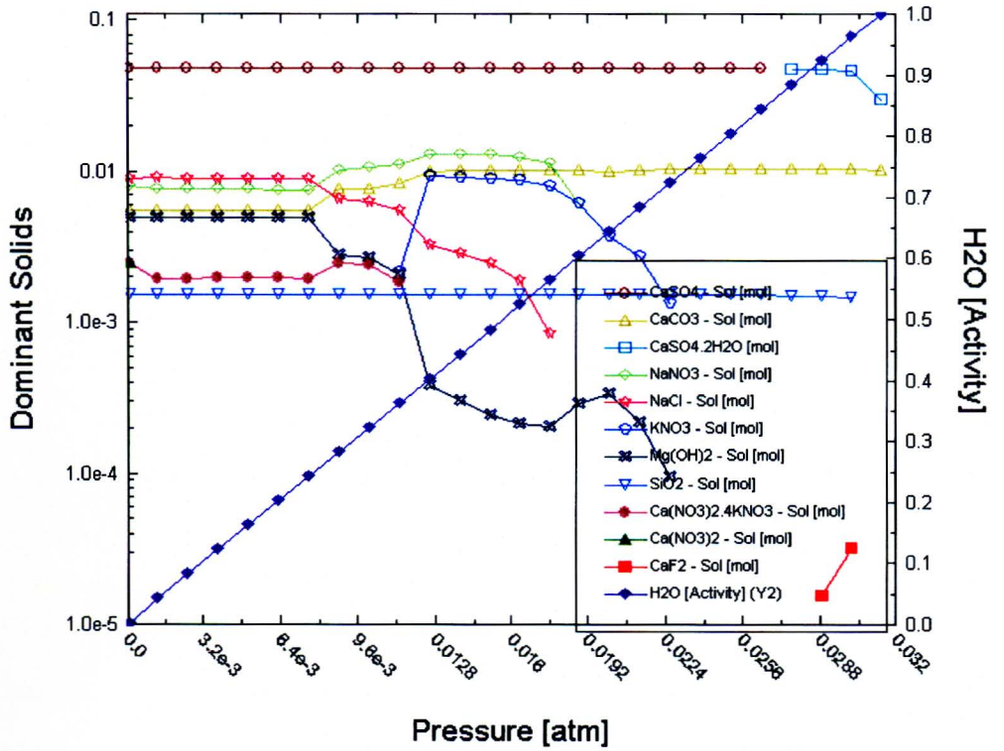
Lab sample C-203119



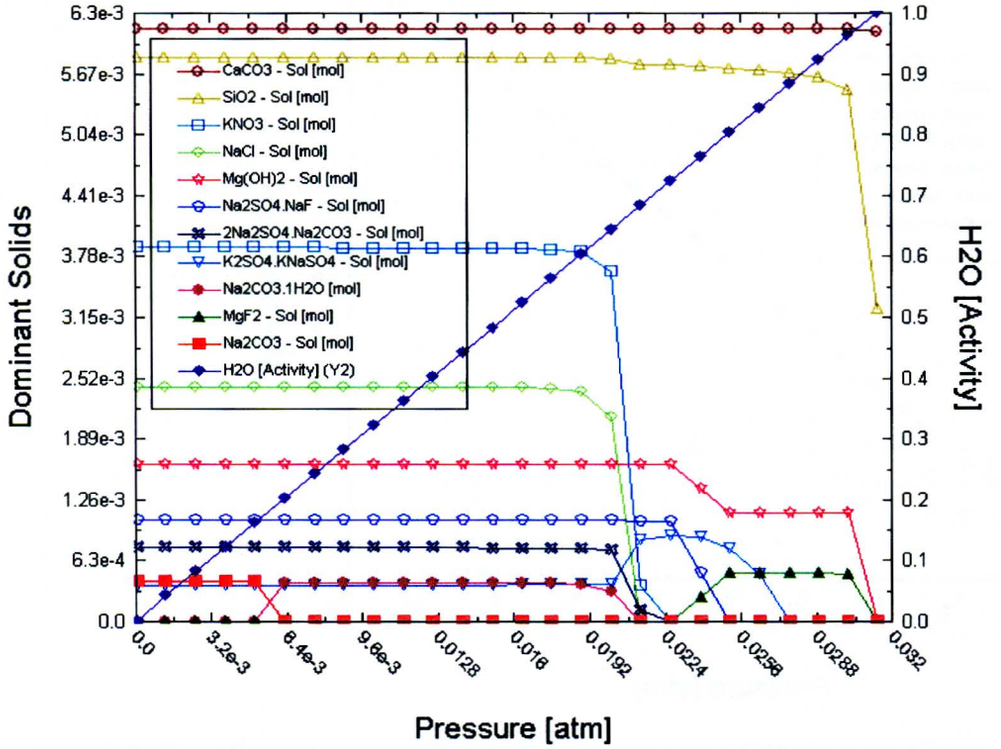
Lab sample C-203120



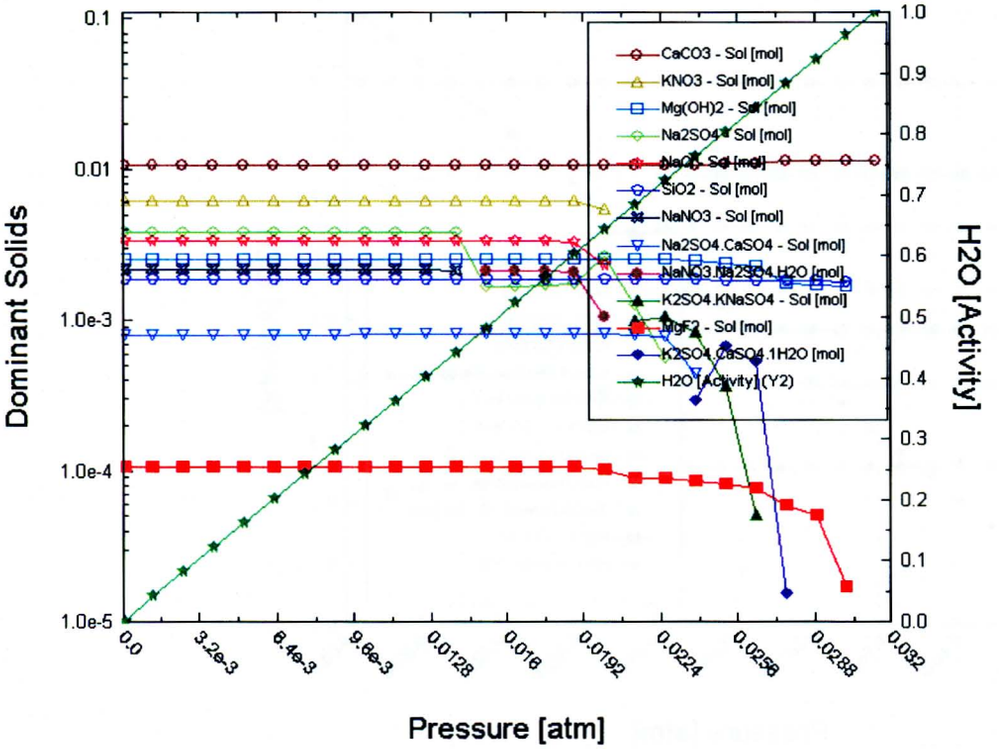
At first glance, only NaCl and NaNO3 appears as the deliquescent salts. The figure below with an expanded list of solids shows KNO3, Ca(NO3)2, and Ca(NO3)2·4KNO3 salts also are present.



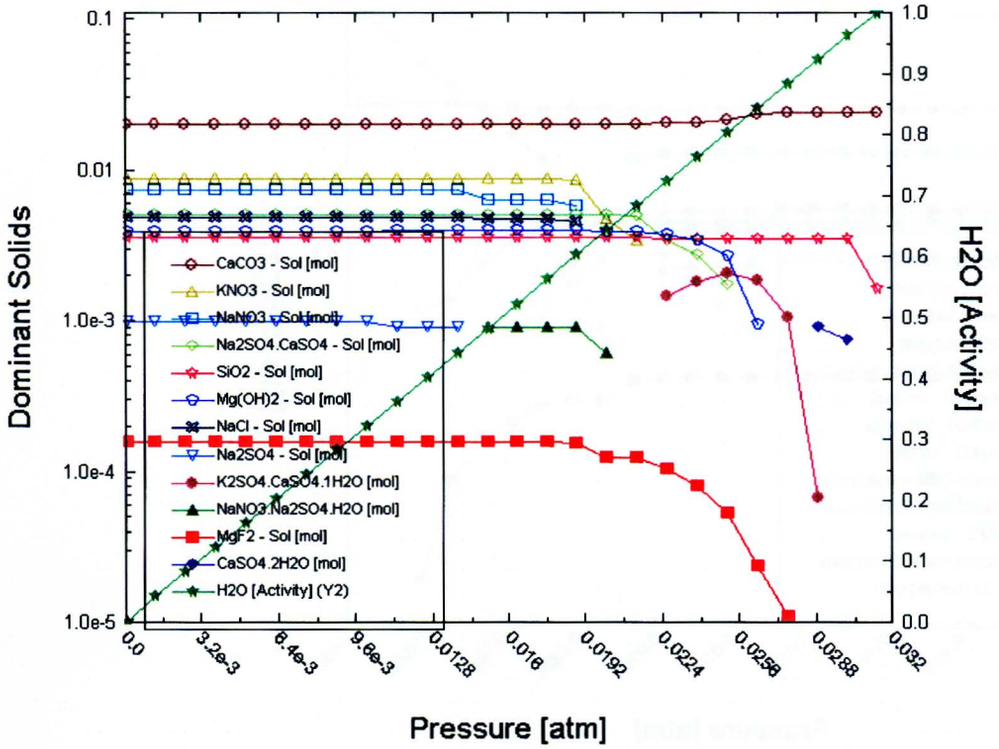
Lab sample C-203121



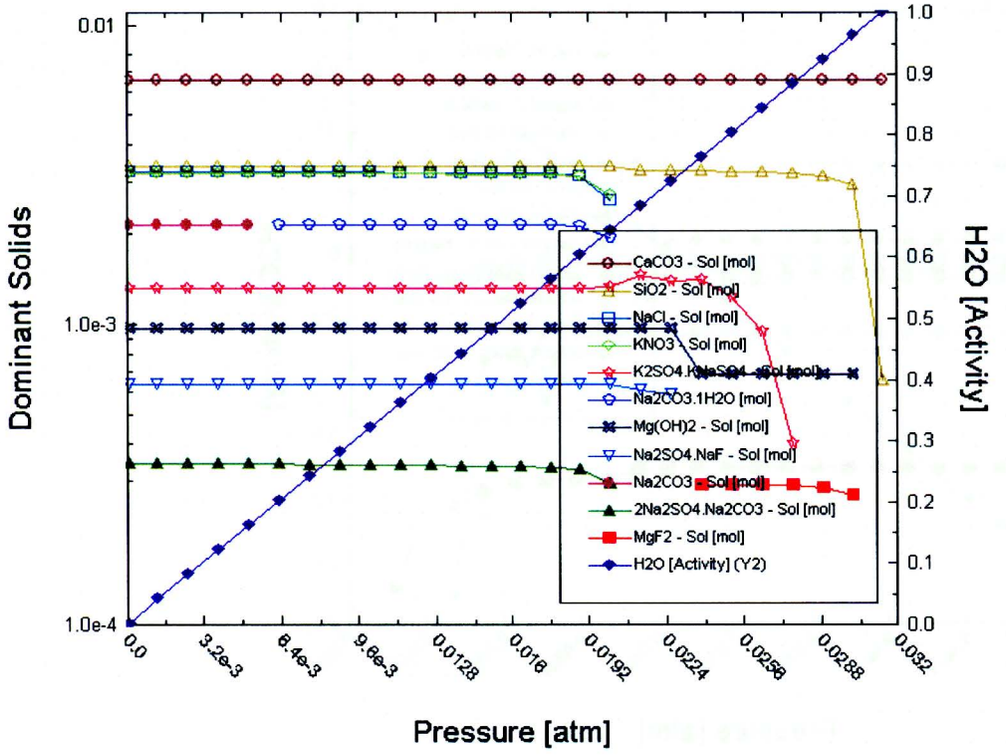
Lab sample C-203122



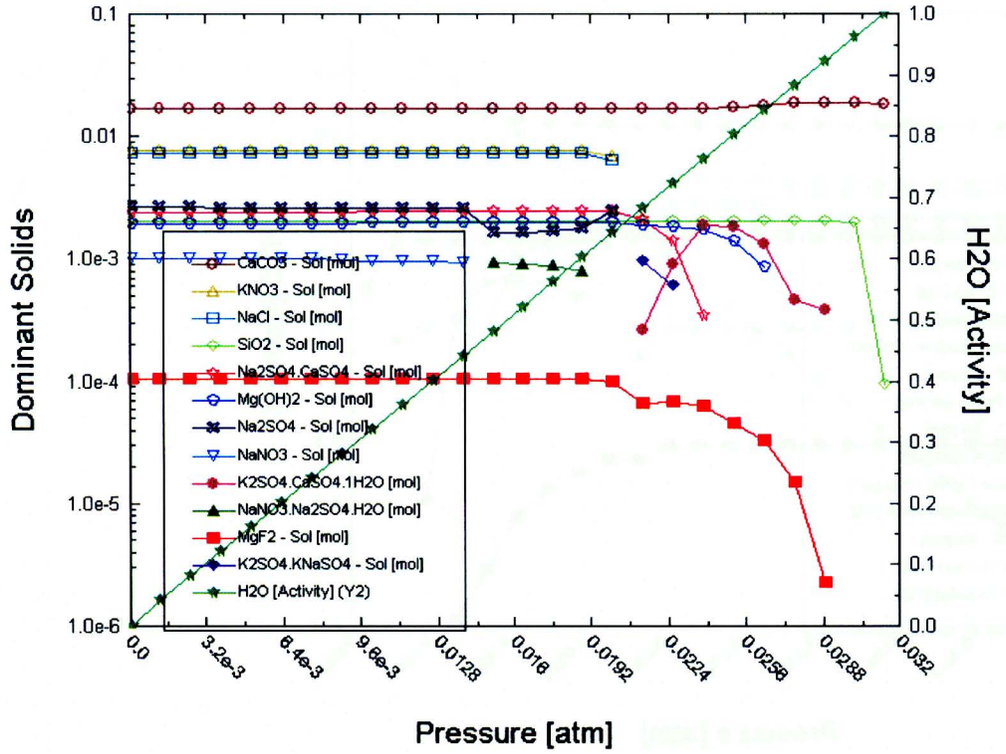
Lab sample C-203123



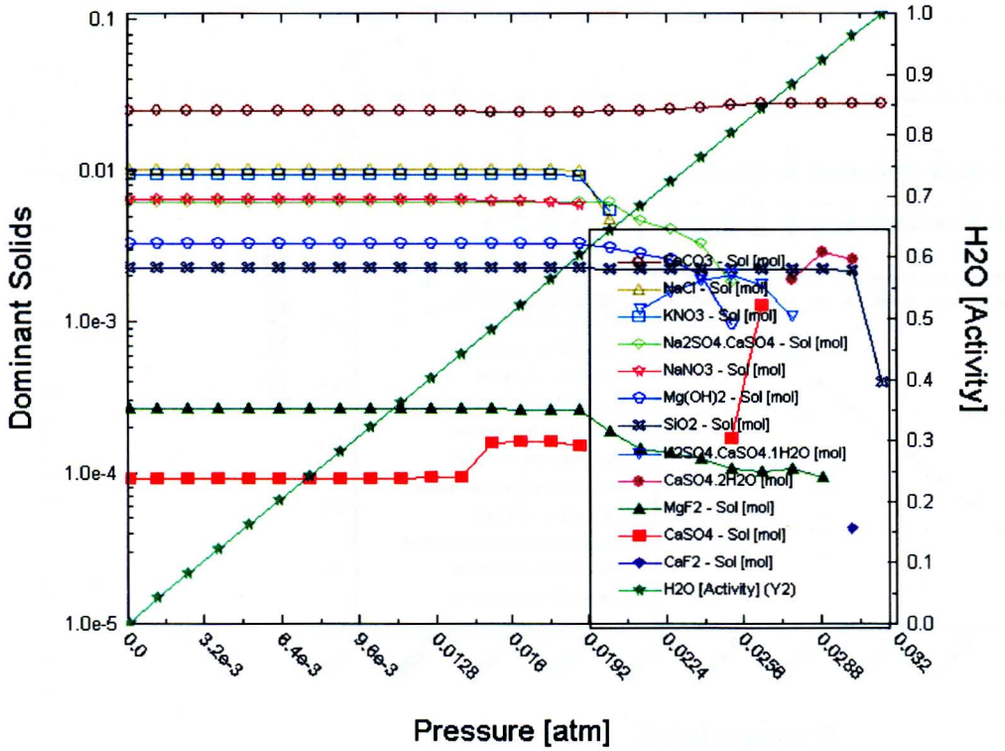
Lab sample C-203124



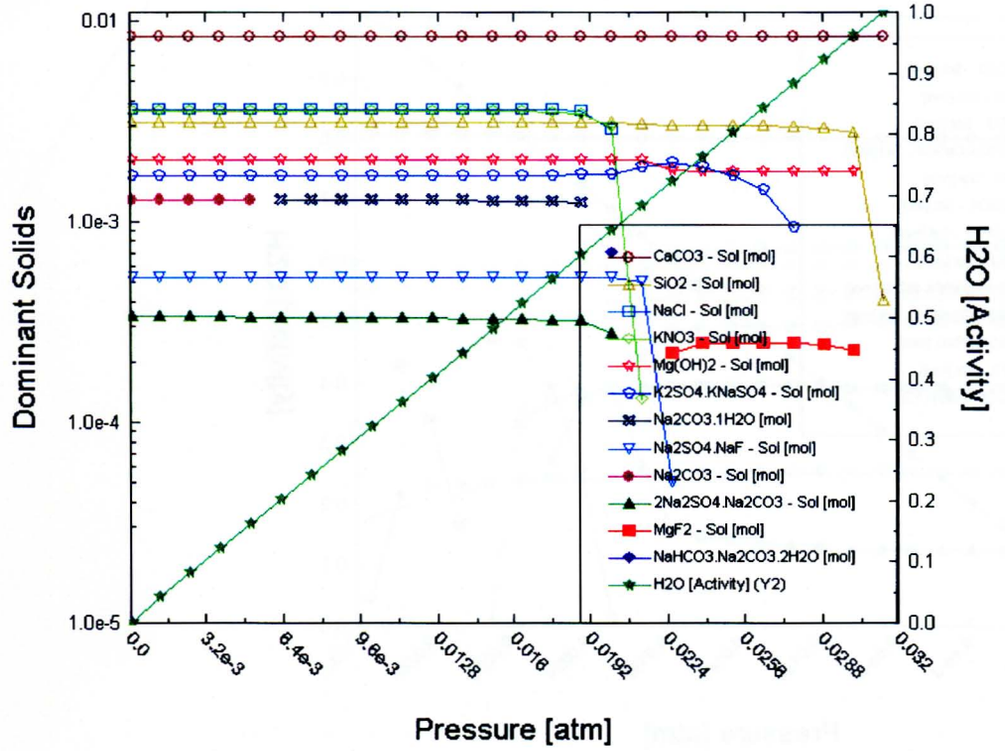
Lab sample C-203125



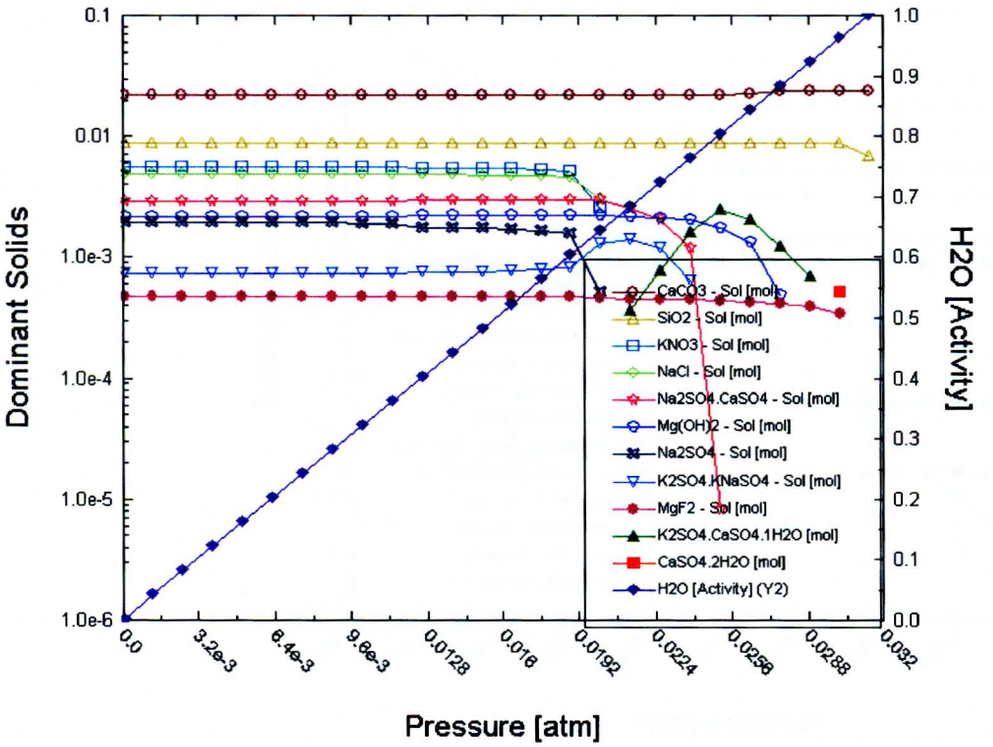
Lab sample C-203126



Lab sample C-203127



Lab sample C-203130



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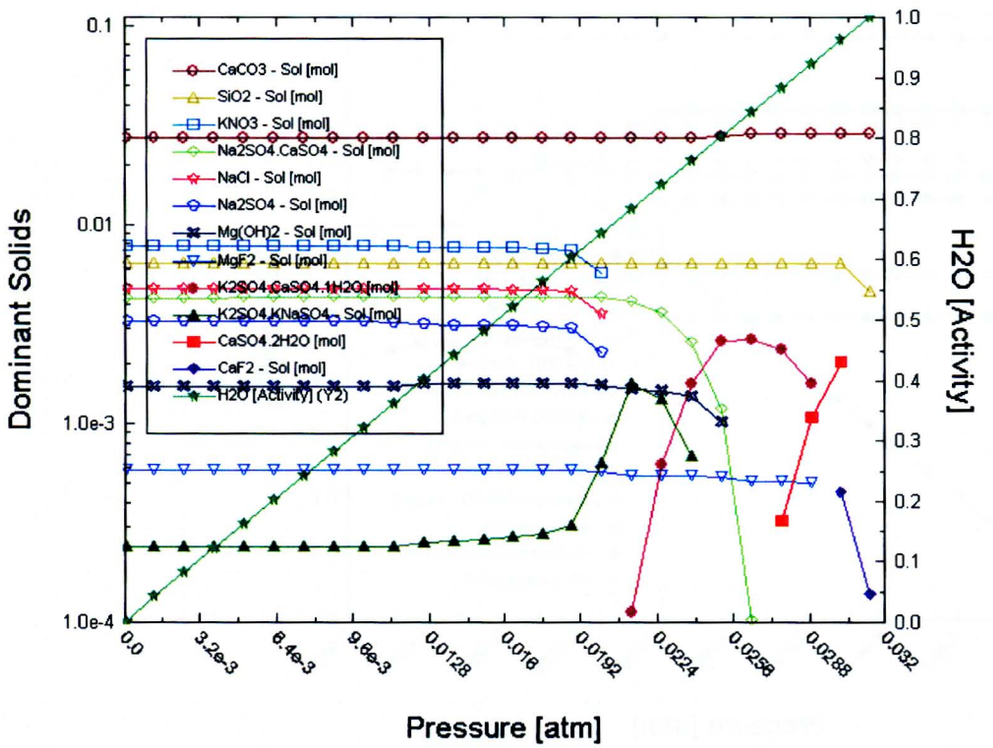

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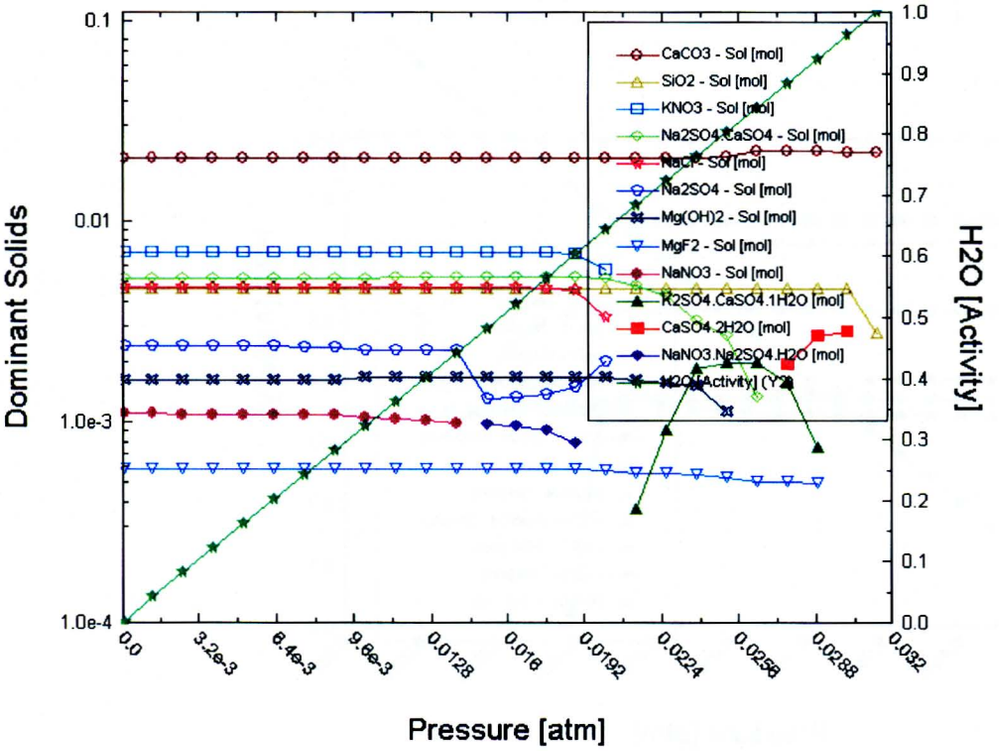

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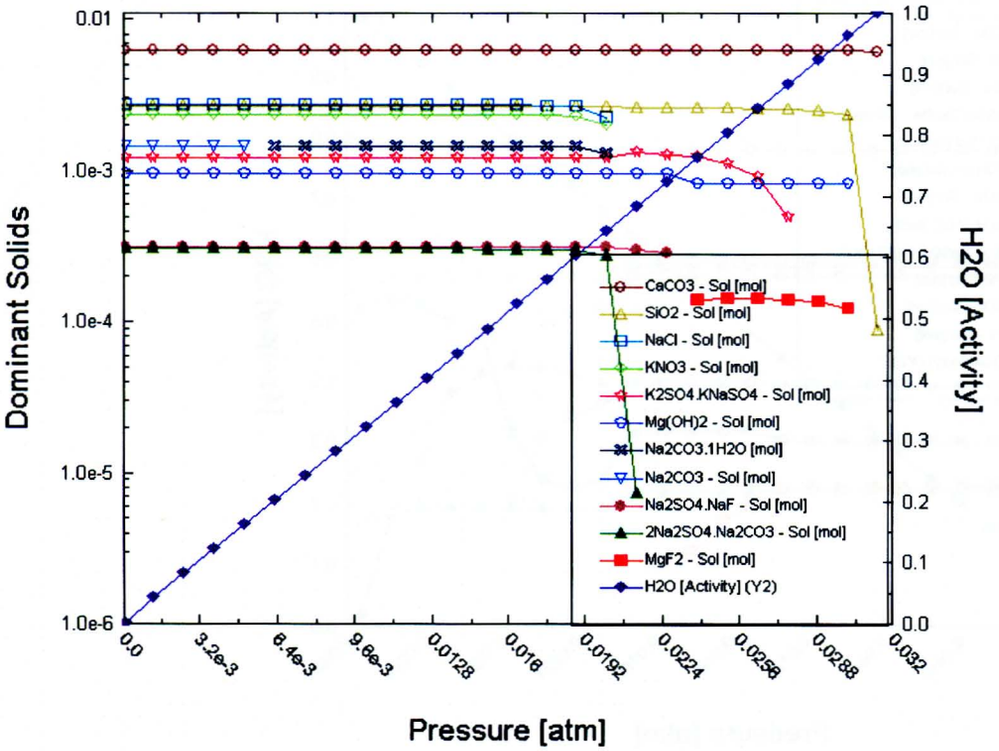

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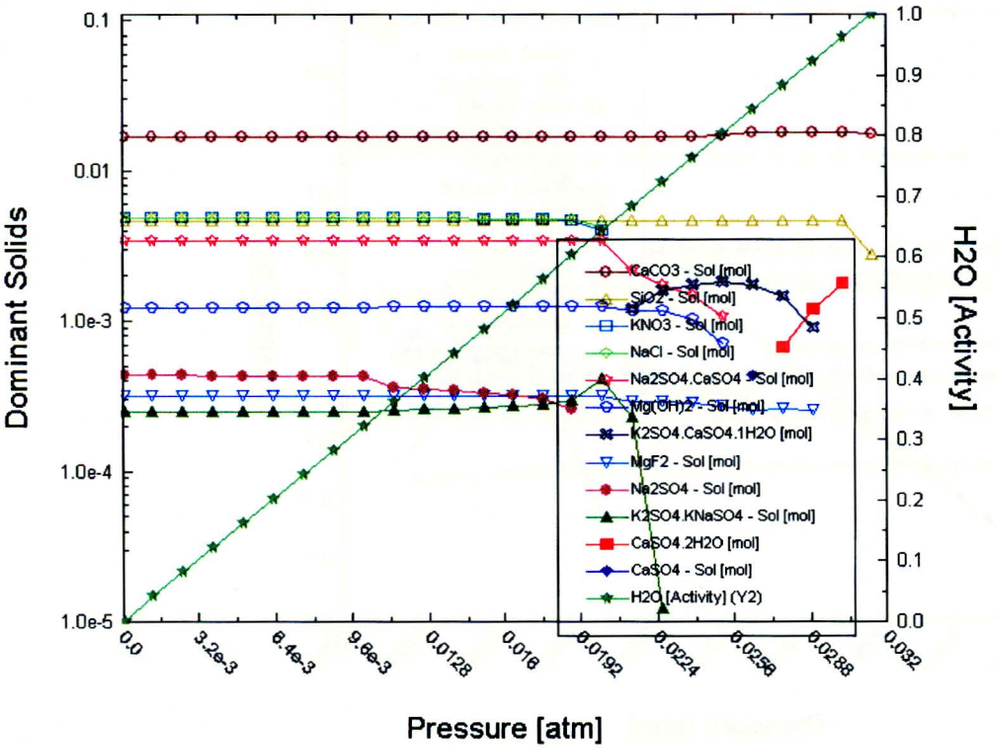
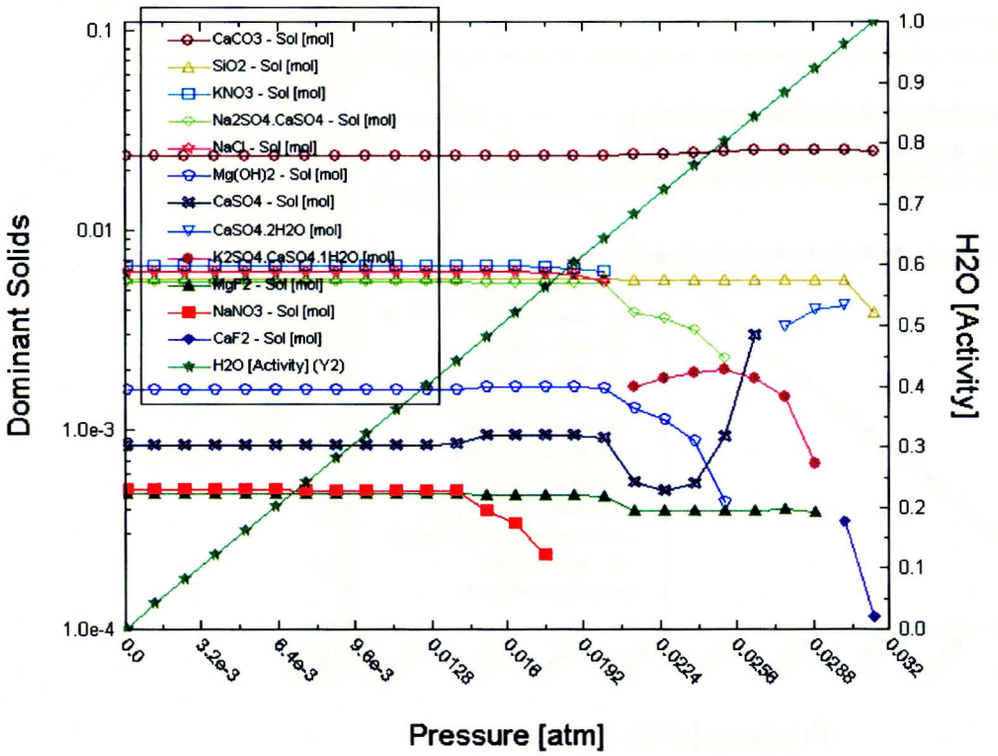
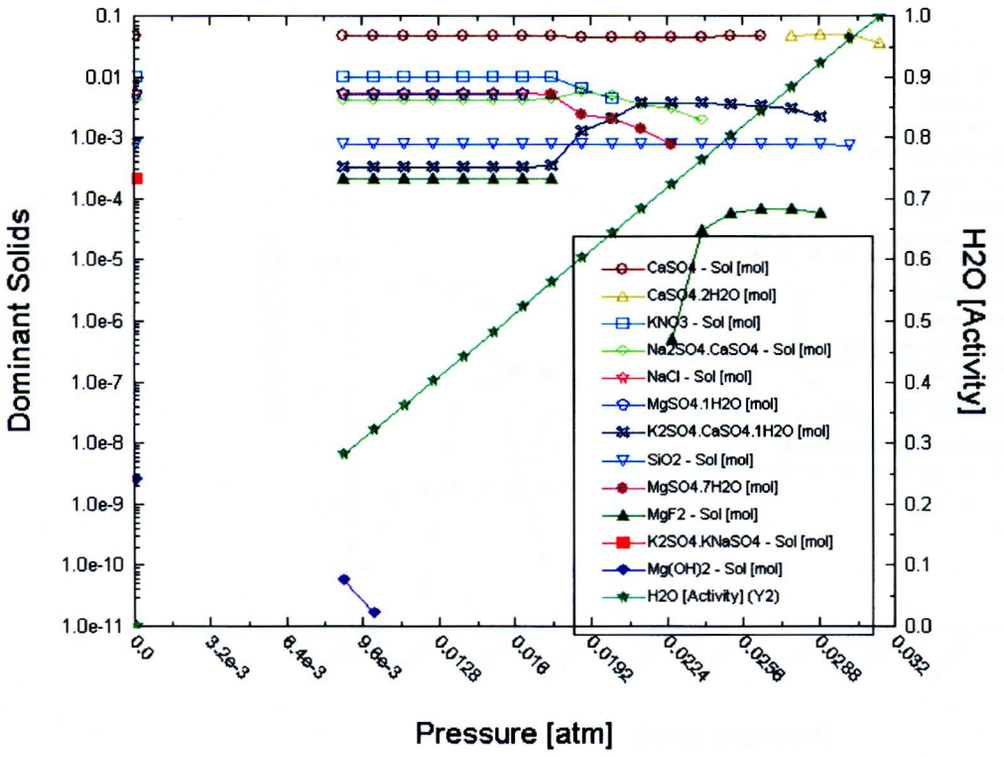


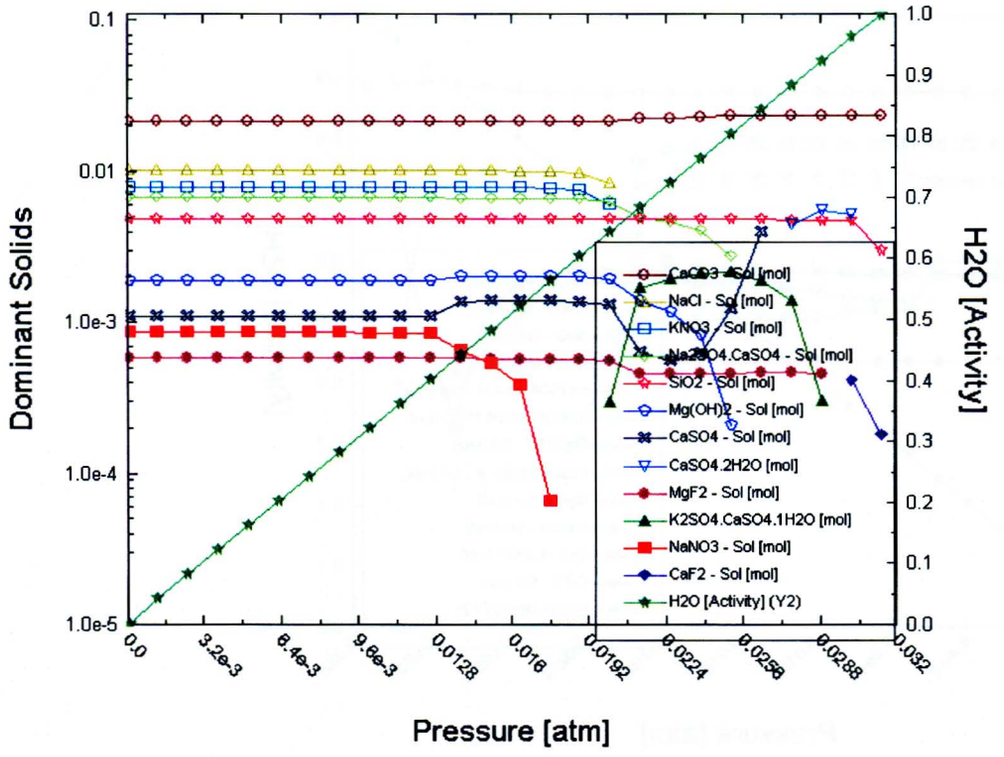
Lab sample C-203135



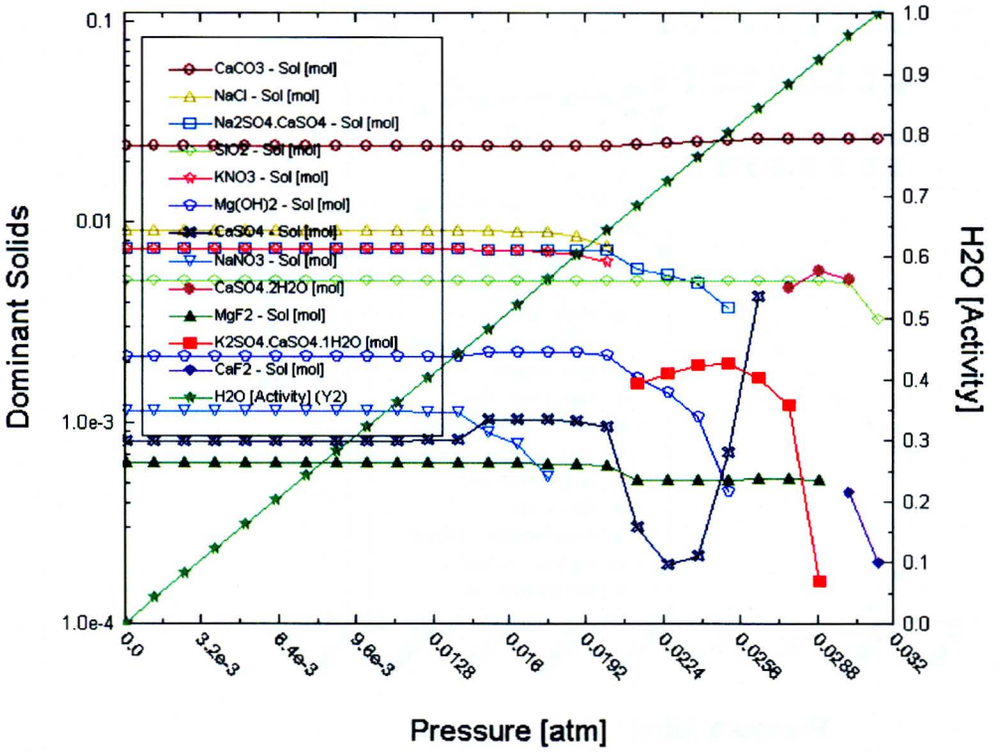
Lab sample C-203136



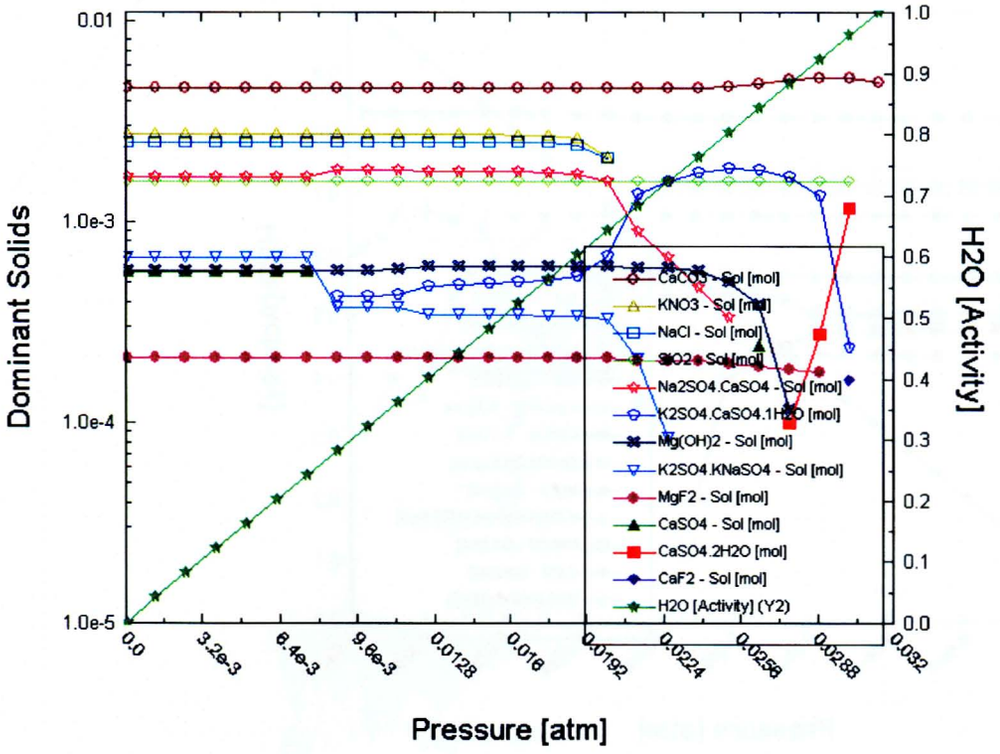
Lab sample C-203137



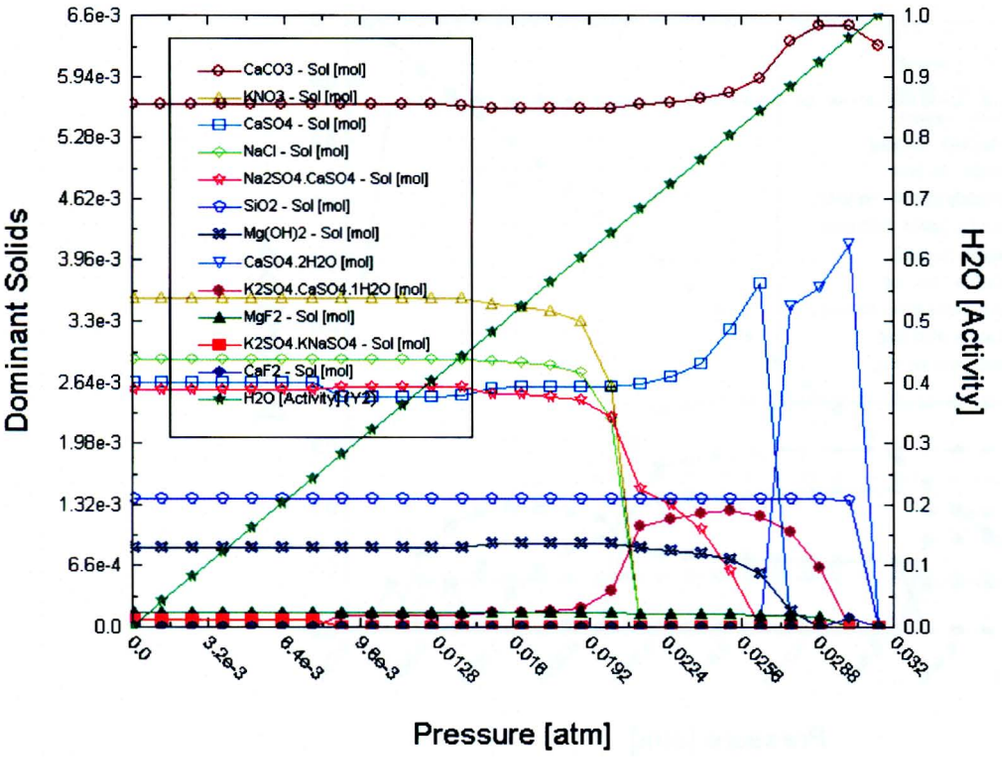
Lab sample C-203138



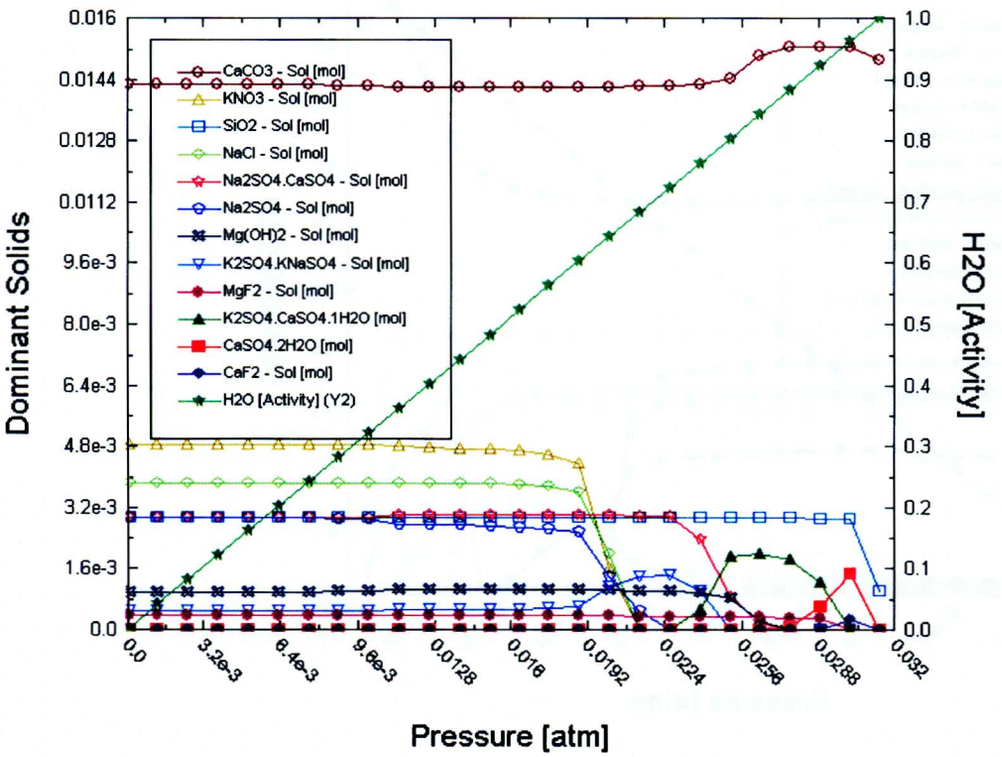
Lab sample C-203139



Lab sample C-203140



Lab sample C-203141



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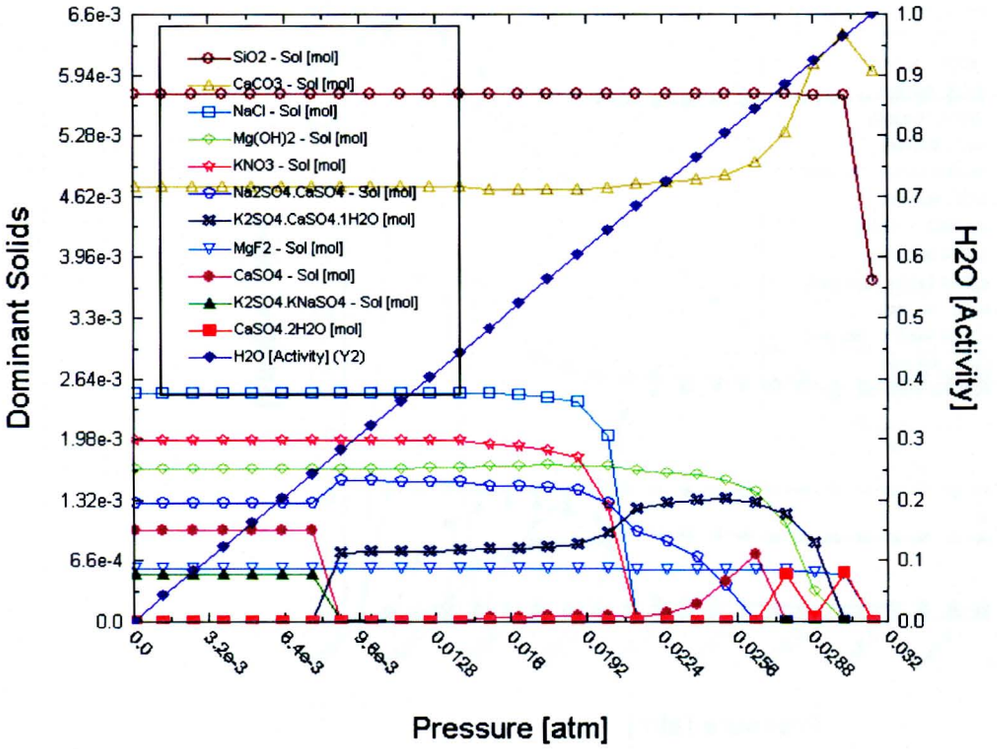
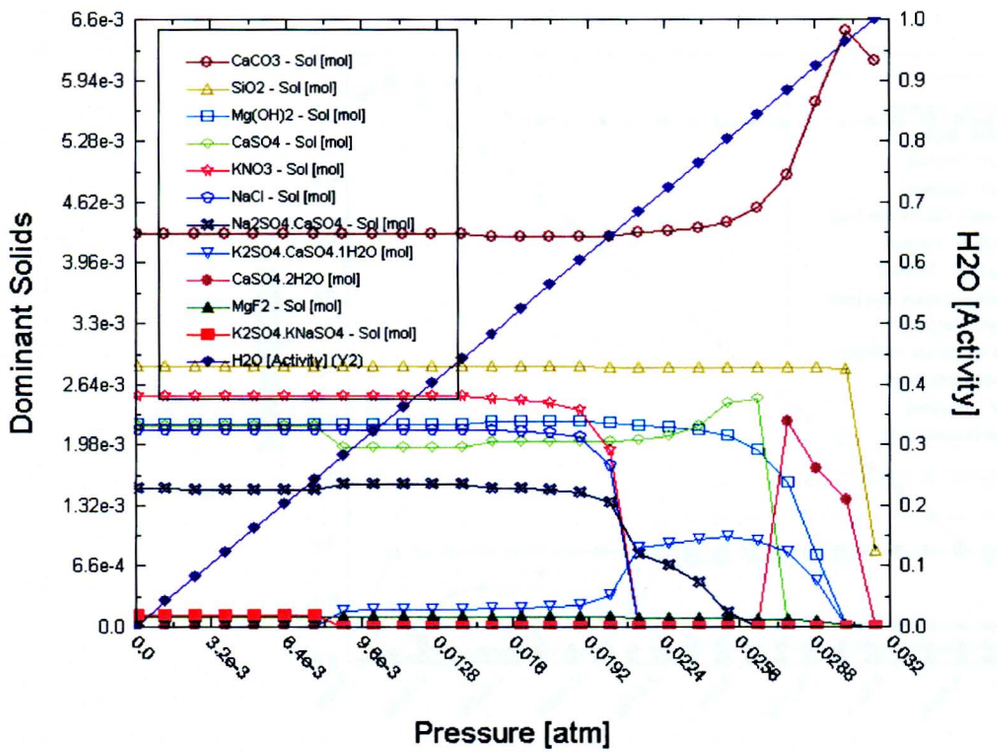


Lab sample C-203143



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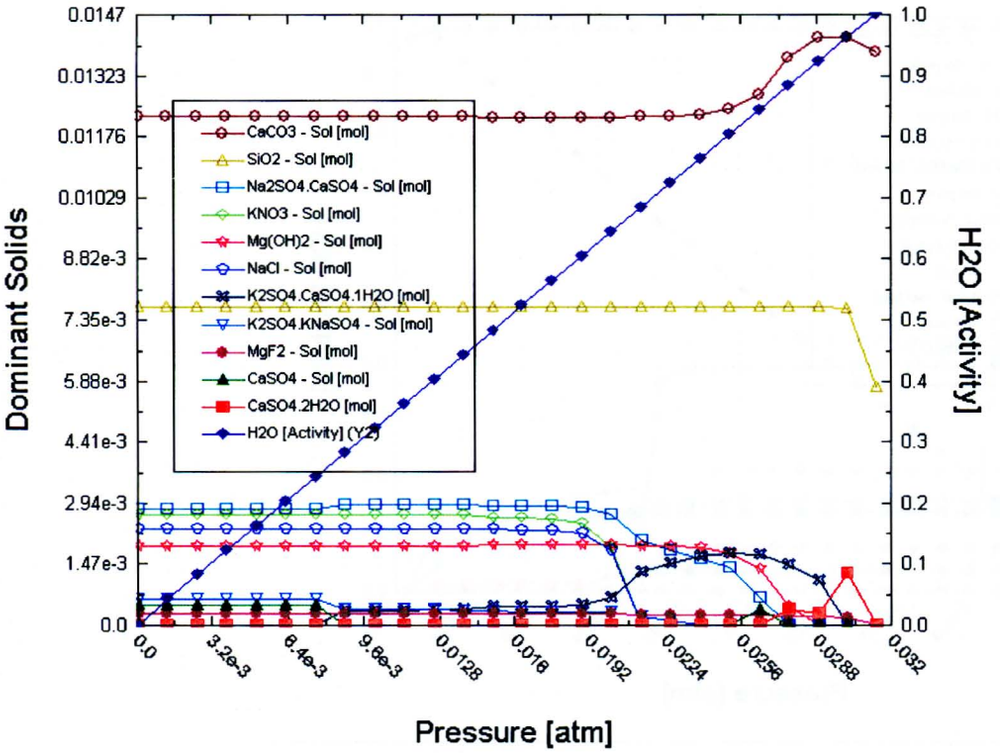

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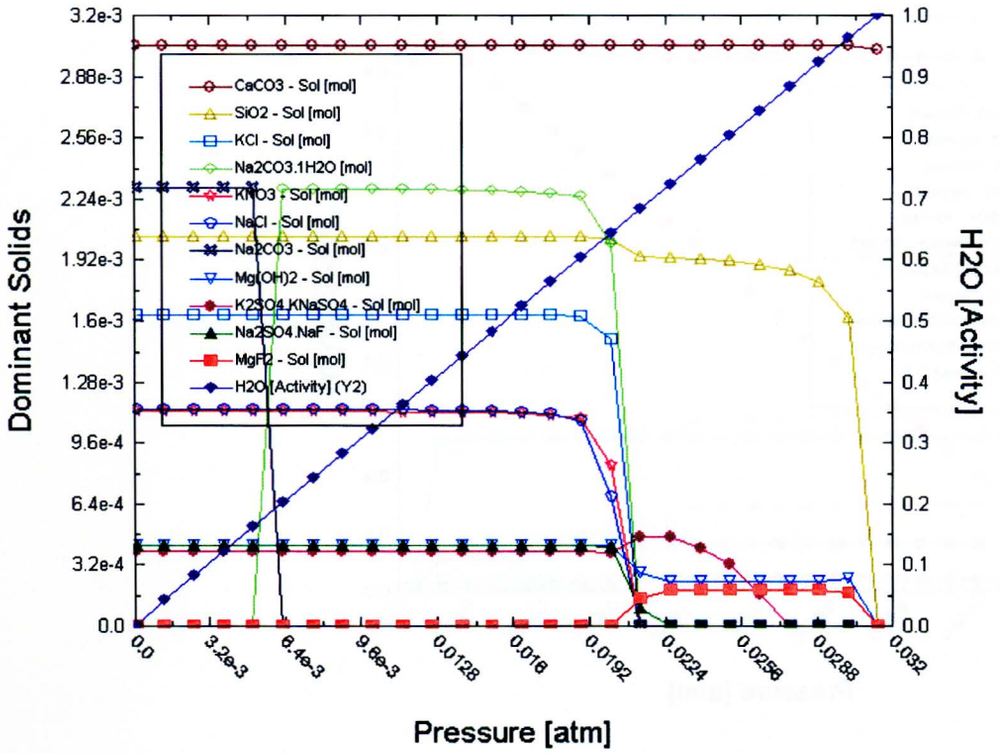

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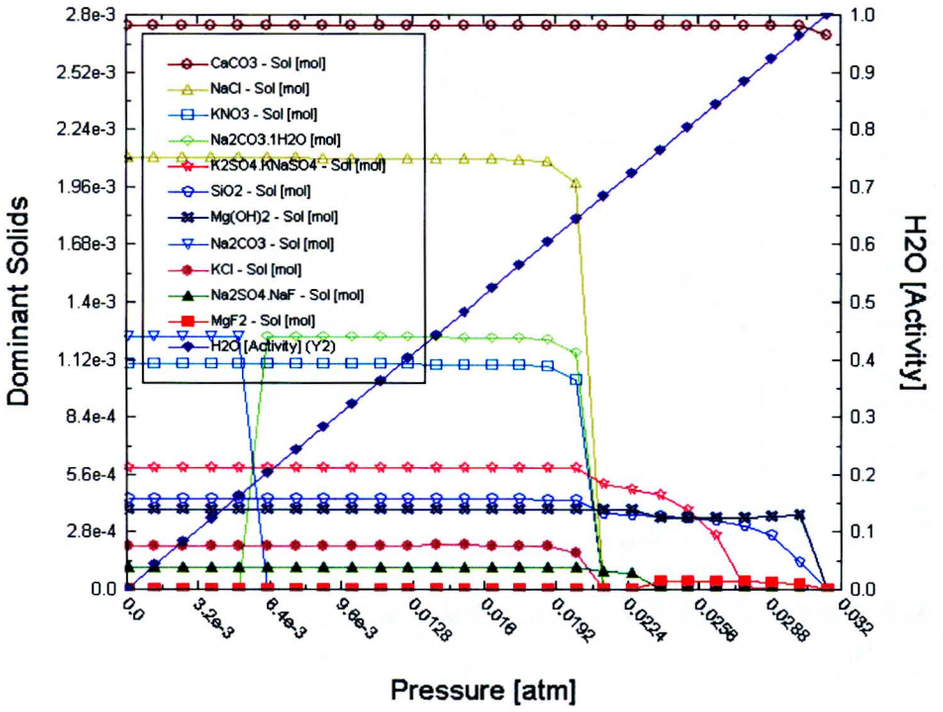

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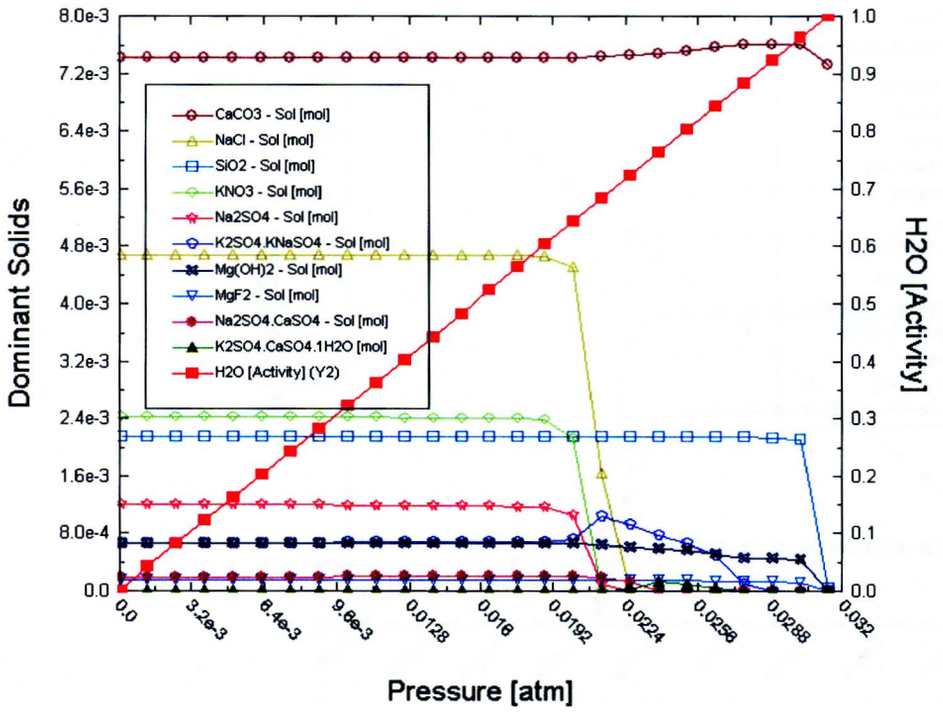
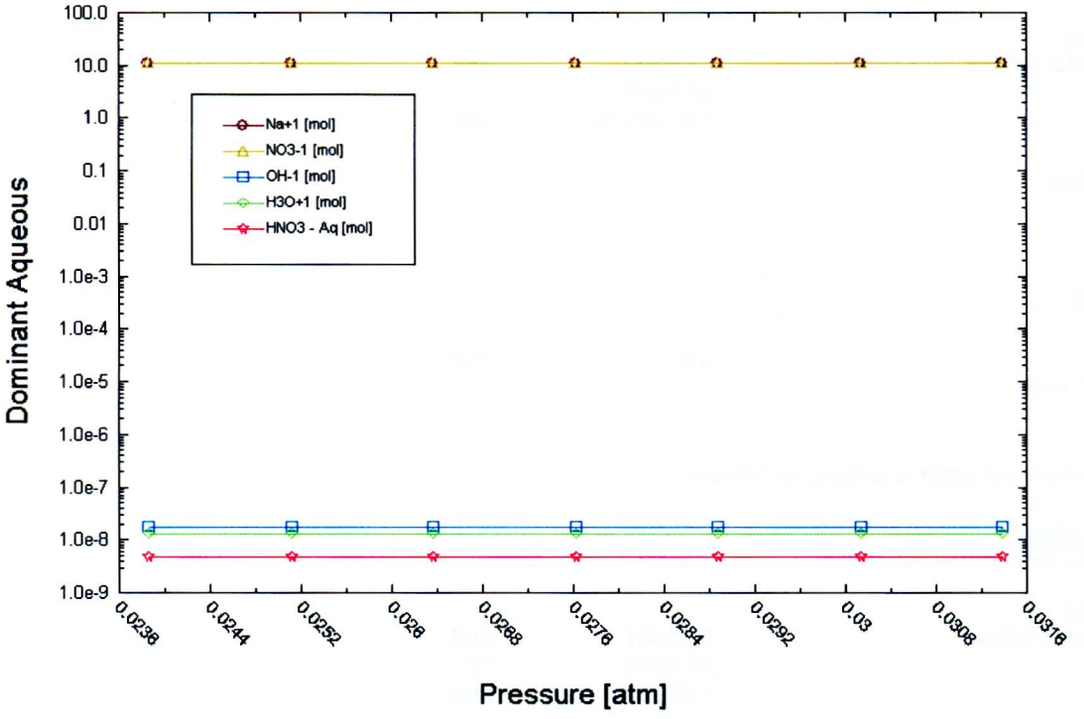
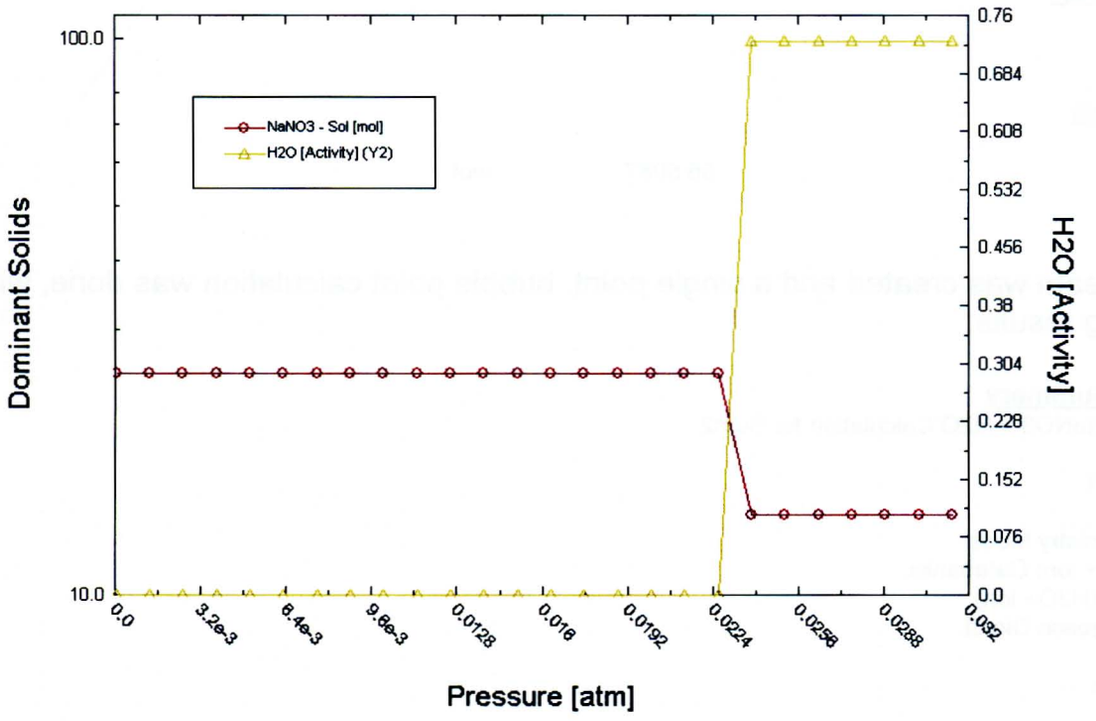


November 28, 2007

Evaporate at 25 C a NaNO3 solution:





The DRH of NaNO3 at 25 C is 72.57%. The drop off in water activity from 72.57 to 0 % indicates dryout.

The solid precipitate from StreamAnalyzer was separated into a different stream, as follows:

Stream Parameters
Row Filter Applied: Only Non Zero Values

Mixture Properties

Stream Amt - Total Inflow	13.9500	mol
Temperature	25.0000	°C
Pressure	0.0226933	atm

Aqueous Properties

Stream Inflows

H2O	0.0	mol
NaNO3 13.9500 mol		

A new stream comprising water is added, as follows:

Stream Parameters
Row Filter Applied: Only Non Zero Values

Mixture Properties

Stream Amt - Total Inflow	55.5087	mol
Temperature	25.0000	°C
Pressure	1.00000	atm

Aqueous Properties

Stream Inflows

H2O	55.5087	mol

A mixed stream was created and a single point, bubble point calculation was done, with the following results:

Calculation Summary
Mixed stream: NaNO3 + H2O Calculation for Sum2

Unit Set: Default

Automatic Chemistry Model
MSE (H30+ ion) Databanks:
MSE (H3O+ ion)
Using Helgeson Direct

Single Point Mix

Bubble Point Calculation

Stream Inflows

H2O	5.55087e-3	mol
NaNO3	13.9500	mol

Stream Parameters

Row Filter Applied: Only Non Zero Values

Mixture Properties

Stream Amt - Total Inflow	13.9556	mol
Temperature	25.0000	°C
Pressure	0.0226932	atm

Aqueous Properties

pH	7.04984	pH
Ionic Strength	0.142381	mol/mol
Osmotic Pressure	441.327	atm
Electrical Cond, specific	0.186010	1/(ohm-cm)
Viscosity, absolute	2.67102	cP

Vapor Properties

Viscosity, absolute	9.89124e-3	cP
Thermoconductivity	19.7246	cal/(hr-C-m)

	Total	Aqueous	Vapor	Solid	2nd Liquid	
		g/ml	g/ml	g/ml	g/ml	
Density		1.37347	1.67192e-5	2.25690	0.0	
	cal	cal	cal	cal	cal	
Enthalpy	-1.55388e6	-499.343	-8.06617e-5	-1.55338e6	0.0	
	cal/g K	cal/g K	cal/g K	cal/g K	cal/g K	
Heat Capacity	0.0	0.0	0.0	0.0	0.0	
		cal	cal	cal	cal	
Gibbs Free Energy			0.0	0.0	0.0	0.0
		cal	cal	cal	cal	
Gibbs Std State		0.0	0.0	0.0	0.0	
		cal/K	cal/K	cal/K	cal/K	
Entropy		0.0	0.0	0.0	0.0	
		cal/K	cal/K	cal/K	cal/K	
Entropy Std State		0.0	0.0	0.0	0.0	

Total and Phase Flows (Amounts)

	Total	Aqueous	Vapor	Solid	2nd Liquid
	mol	mol	mol	mol	mol
Mole (True)	13.9567	7.76086e-3	1.39556e-9	13.9489	0.0
Mole (App)	13.9556	6.65586e-3	1.39556e-9	13.9489	0.0

	Total	Aqueous	Vapor	Solid	2nd Liquid
	g	g	g	g	g
Mass	1185.78	0.193920	2.51415e-8	1185.59	0.0

	Total	Aqueous	Vapor	Solid	2nd Liquid
	L	L	L	L	L
Volume	0.525459	1.41190e-4	1.50375e-6	0.525317	0.0

Scaling Tendencies

Row Filter Applied: Only Non Zero Values

solids within temperature range	**Temperature Range**

NaNO3	1.00000	data valid through range	inside range
NaOH.4H2O	5.01383e-10	data valid through range	inside range
NaOH.3.5H2O	4.10958e-10	data valid through range	inside range
NaOH.5H2O	2.97507e-10	data valid through range	inside range
NaOH.7H2O	2.26262e-10	data valid through range	inside range
NaOH.2H2O	3.68610e-11	data valid through range	inside range
NaOH.1H2O	4.79273e-12	data valid through range	inside range
NaOH	1.28967e-14	data valid through range	inside range

Species Output (True Species)

Row Filter Applied: Only Non Zero Values

	Total	**Aqueous**	**Vapor**	**Solid**	**2nd**
	mol	mol	mol	mol	n/a
H2O	5.55087e-3	5.55087e-3	1.39556e-9	0.0	0.0
NaNO3	13.9489	0.0	0.0		
	13.9489	0.0			
HNO3	4.76481e-13	4.76481e-13	7.26864e-21	0.0	0.0
N2O5	1.49979e-32	1.49979e-32	1.03894e-38	0.0	0.0
H3O+1	1.29782e-12	1.29782e-12	0.0	0.0	0.0
Na+1	1.105e-3	1.105e-3	0.0	0.0	0.0
NO3-1	1.105e-3	1.105e-3	0.0	0.0	0.0
OH-1	1.7743e-12	1.7743e-12	0.0	0.0	0.0
Total (by phase)	13.9567	7.76086e-3	1.39556e-9		
	13.9489	0.0			

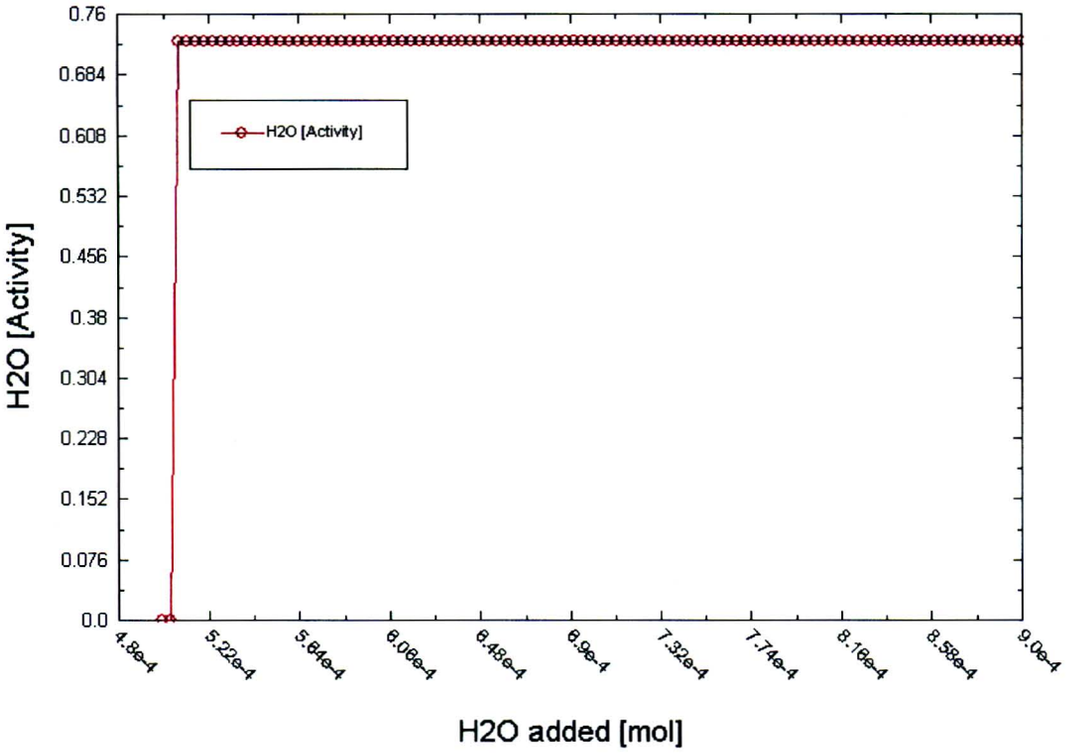
Species Activity/Fugacity Coefficients

Species	γ **x-based**	γ **m-based**
H2O	1.01464	0.725713*
HNO3 - Aq	5.88354	4.20814
N2O5 - Aq	8.38451	5.99693
Na+1	0.486683	0.348094
NO3-1	0.486683	0.348094
H3O+1	6.97046	4.98554
OH-1	6.48160	4.63589

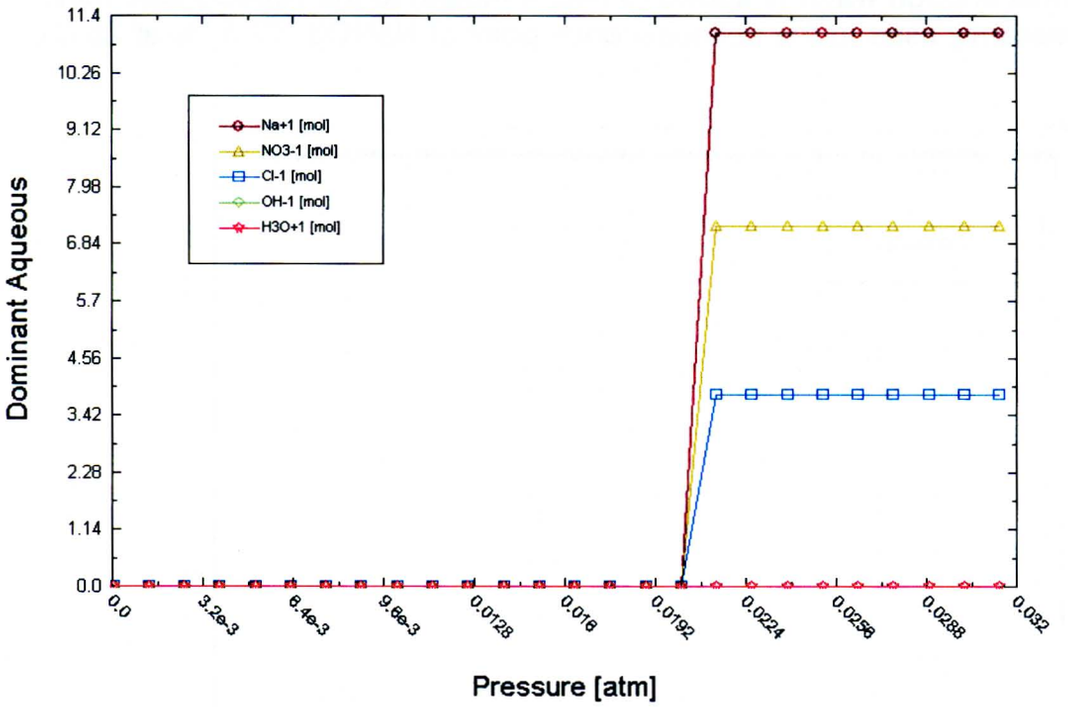
** - Value is an Activity not an Activity Coefficient.*

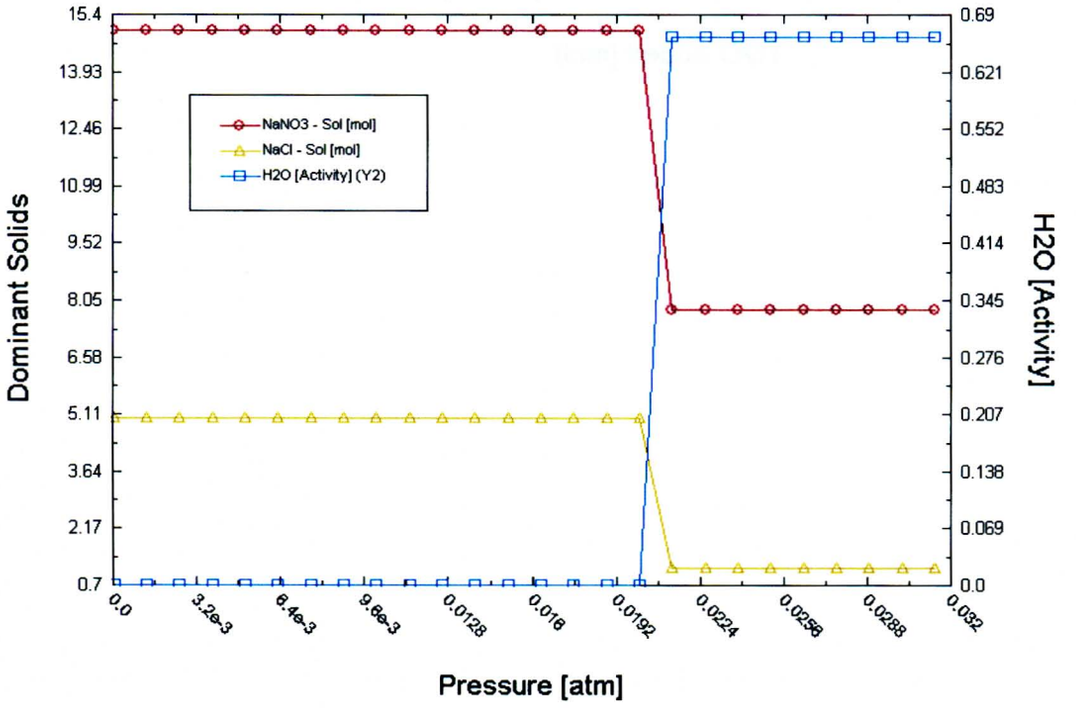
N2O5 - Vap Fug.Coef. 0.999653

The following is a plot of results of bubble point survey at 25 C for a NaNO3 solution as a function of water added (range from 0.0005 to 0.0009 moles H2O). The water activity remains zero until enough water is added (5.04E-4 moles) to the NaNO3 salt; then water activity instantly rises to the deliquescence point of NaNO3 (72.57% at 25 C).



NaCl-NaNO3 mixture (5 mol:15 mol)





The MDRH of NaCl+NaNO3 at 25 C is 66.19 %. The drop to zero at lower pressure indicates dryout.

Mixed streams:

NaCl+NaNO3 Stream Parameters
Row Filter Applied: Only Non Zero Values

Mixture Properties

Stream Amt - Total Inflow	8.96043	mol
Temperature	25.0000	°C
Pressure	0.0206981	atm

Aqueous Properties

Stream Inflows

H2O	0.0	mol
NaCl	1.16059	mol
NaNO3	7.79984	mol

H2O Stream Parameters
Row Filter Applied: Only Non Zero Values

Mixture Properties

Stream Amt - Total Inflow	55.5087	mol
Temperature	25.0000	°C
Pressure	1.00000	atm

Aqueous Properties

Stream Inflows

H2O	55.5087	mol

Results:

Calculation Summary
MixedStream H2O + NaCl/NaNO3 Calculation for Sum2

Unit Set: Default

Automatic Chemistry Model
MSE (H30+ ion) Databanks:
MSE (H3O+ ion)
Using Helgeson Direct

Single Point Mix

Isothermal Calculation

Stream Inflows

H2O	5.55087e-3	mol
NaCl	1.16059	mol
NaNO3	7.79984	mol

Stream Parameters

Row Filter Applied: Only Non Zero Values

Mixture Properties

Stream Amt - Total Inflow	8.96598	mol
Temperature	25.0000	°C
Pressure	1.00000	atm

Aqueous Properties

pH	6.87755	pH
Ionic Strength	0.142305	mol/mol
Osmotic Pressure	583.859	atm
Electrical Cond, specific	0.193746	1/(ohm-cm)
Viscosity, absolute	3.15614	cP

	Total	Aqueous	Vapor	Solid	2nd Liquid	
		g/ml	g/ml	g/ml	g/ml	
Density		1.35521	0.0	2.24792	0.0	
	cal	cal	cal	cal	cal	
Enthalpy	-9.83202e5	-495.105	0.0	-9.82707e5	0.0	
	cal/g K	cal/g K	cal/g K	cal/g K	cal/g K	
Heat Capacity	0.0	0.0	0.0	0.0	0.0	
		cal	cal	cal	cal	
Gibbs Free Energy			0.0	0.0	0.0	0.0
		cal	cal	cal	cal	
Gibbs Std State		0.0	0.0	0.0	0.0	
		cal/K	cal/K	cal/K	cal/K	
Entropy		0.0	0.0	0.0	0.0	
		cal/K	cal/K	cal/K	cal/K	
Entropy Std State		0.0	0.0	0.0	0.0	

Total and Phase Flows (Amounts)

	Total	Aqueous	Vapor	Solid	2nd Liquid
	mol	mol	mol	mol	mol
Mole (True)	8.96709	7.75922e-3	0.0	8.95933	0.0
Mole (App)	8.96598	6.65504e-3	0.0	8.95933	0.0

	Total	Aqueous	Vapor	Solid	2nd Liquid
	g	g	g	g	g
Mass	730.875	0.183655	0.0	730.691	0.0

	Total	Aqueous	Vapor	Solid	2nd Liquid
	L	L	L	L	L
Volume	0.325188	1.35518e-4	0.0	0.325052	0.0

Scaling Tendencies

Row Filter Applied: Only Non Zero Values

solids within temperature range		**Temperature Range**	
NaCl	1.00000	data valid through range	inside range
NaNO3	1.00000	data valid through range	inside range
NaCl.2H2O	0.468109	data valid through range	inside range
NaOH.4H2O	3.66024e-10	data valid through range	inside range

NaOH.3.5H2O	3.14094e-10	data valid through range	inside range
NaOH.5H2O	1.98149e-10	data valid through range	inside range
NaOH.7H2O	1.25460e-10	data valid through range	inside range
NaOH.2H2O	3.23228e-11	data valid through range	inside range
HCL.3H2O	1.62179e-11	data valid through range	inside range
NaOH.1H2O	4.60833e-12	data valid through range	inside range
HCL.2H2O	3.34622e-12	data valid through range	inside range
HCL.1H2O	7.03256e-14	data valid through range	inside range
NaOH	1.35873e-14	data valid through range	inside range

Species Output (True Species)

Row Filter Applied: Only Non Zero Values

	Total	**Aqueous**	**Vapor**	**Solid**	**2nd**
	mol	mol	mol	mol	n/a
H2O	5.55087e-3	5.55087e-3	0.0	0.0	0.0
NaCl	1.16021	0.0	0.0		
	1.16021	0.0			
NaNO3	7.79912	0.0	0.0		
	7.79912	0.0			
HCl	6.00652e-18	6.00652e-18	0.0	0.0	0.0
HNO3	3.30534e-13	3.30534e-13	0.0	0.0	0.0
N2O5	1.66531e-32	1.66531e-32	0.0	0.0	0.0
Cl-1	3.83961e-4	3.83961e-4	0.0	0.0	0.0
H3O+1	1.30354e-12	1.30354e-12	0.0	0.0	0.0
Na+1	1.10417e-3	1.10417e-3	0.0	0.0	0.0
NO3-1	7.20214e-4	7.20214e-4	0.0	0.0	0.0
OH-1	1.63408e-12	1.63408e-12	0.0	0.0	0.0
Total (by phase)	8.96709	7.75922e-3	0.0		
	8.95933	0.0			

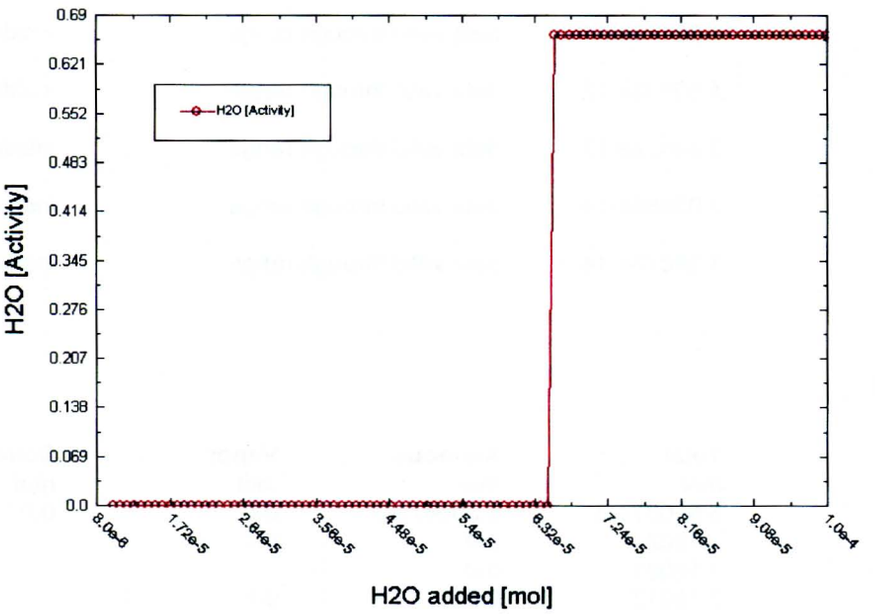
Species Activity/Fugacity Coefficients

Species	**x-based**	**m-based**
H2O	0.925210	0.661887*
HNO3 - Aq	7.35159	5.25925
HCl - Aq	0.341935	0.244617
N2O5 - Aq	6.21728	4.44778
Na+1	0.836457	0.598393
NO3-1	0.434773	0.311032
H3O+1	9.40956	6.73151
OH-1	4.31965	3.09024
Cl-1	1.95468	1.39836

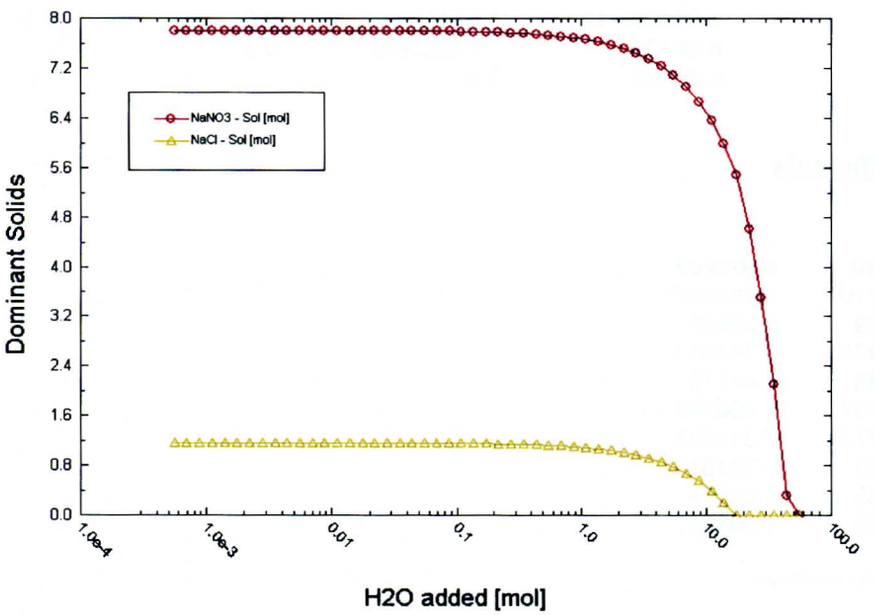
** - Value is an Activity not an Activity Coefficient.*

N2O5 - Vap Fug.Coef. 1.00000

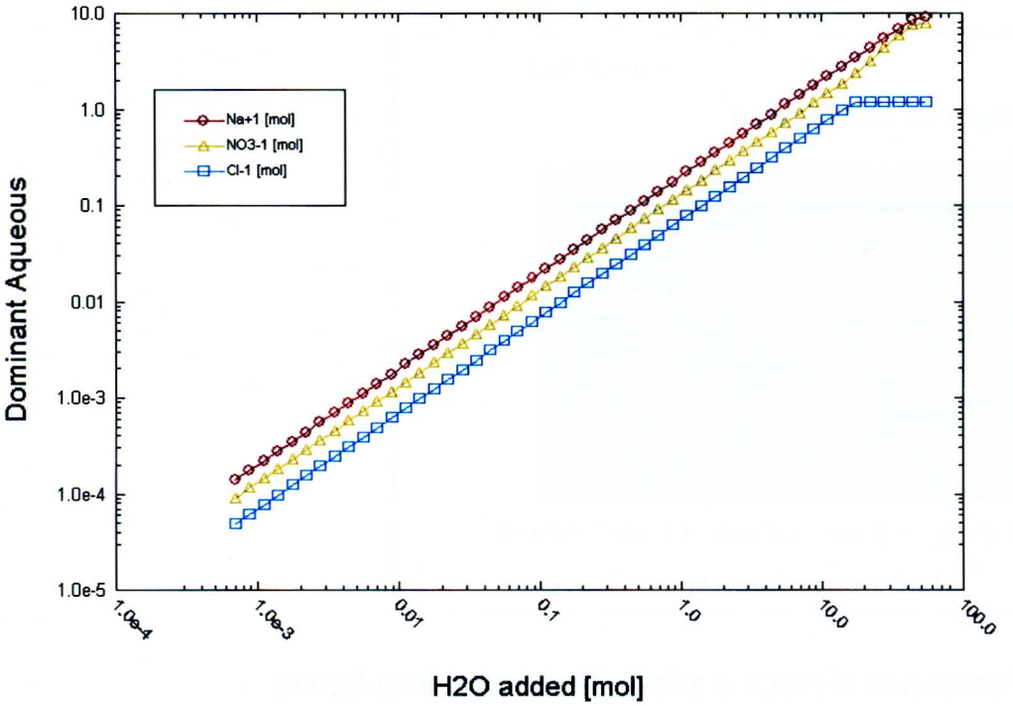
The following plots the results of bubble point survey at 25 C for a 5 mole NaCl + 15 mole NaNO3 mixture as a function of water added to the salt mixture. The water activity is zero until enough water has been added to form an aqueous phase (6.58E-5 moles H2O). Then water activity jumps to the deliquescence point value of 66.19 % RH.



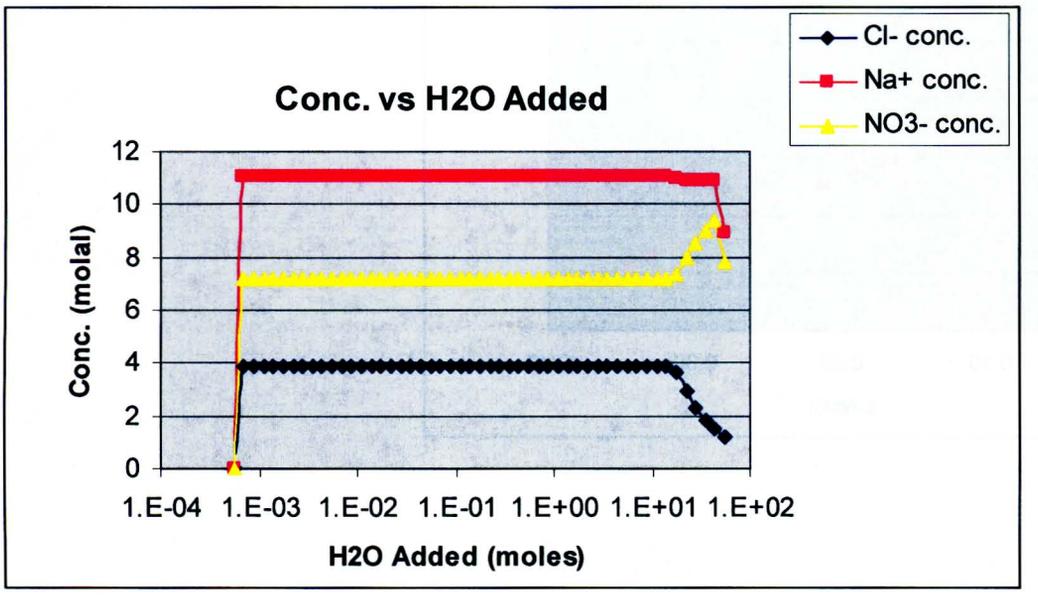
The following is a plot of dominant solids vs amount of H2O added to an NaCl/NaNO3 mixture (bubble point survey at 25 C):



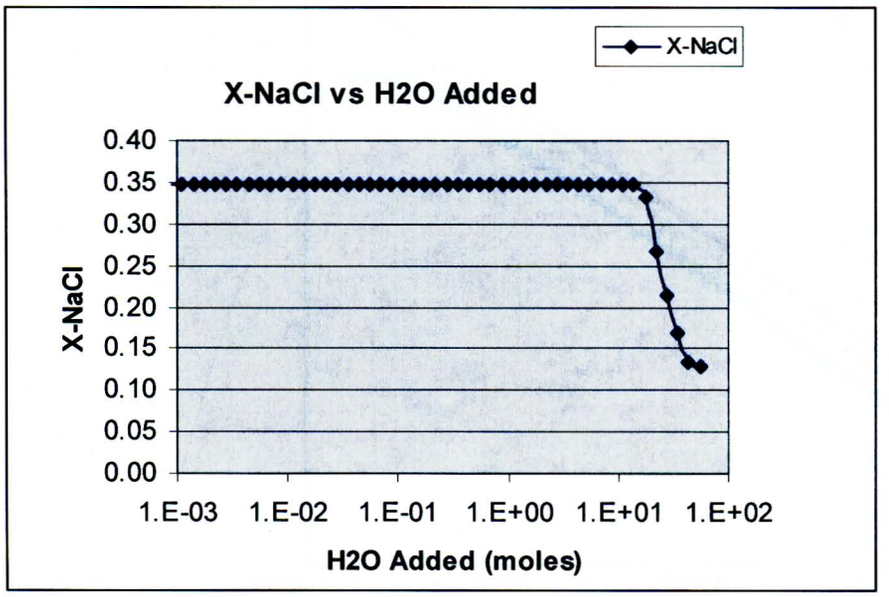
The aqueous composition (in moles) as a function of H2O added is shown below:



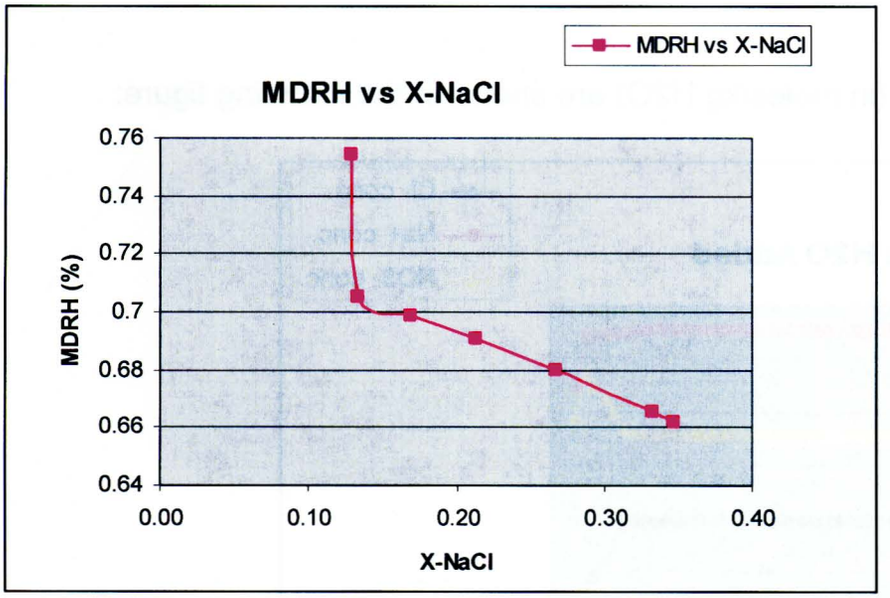
The aqueous concentration (in moles/kg H2O) are shown in the following figure:



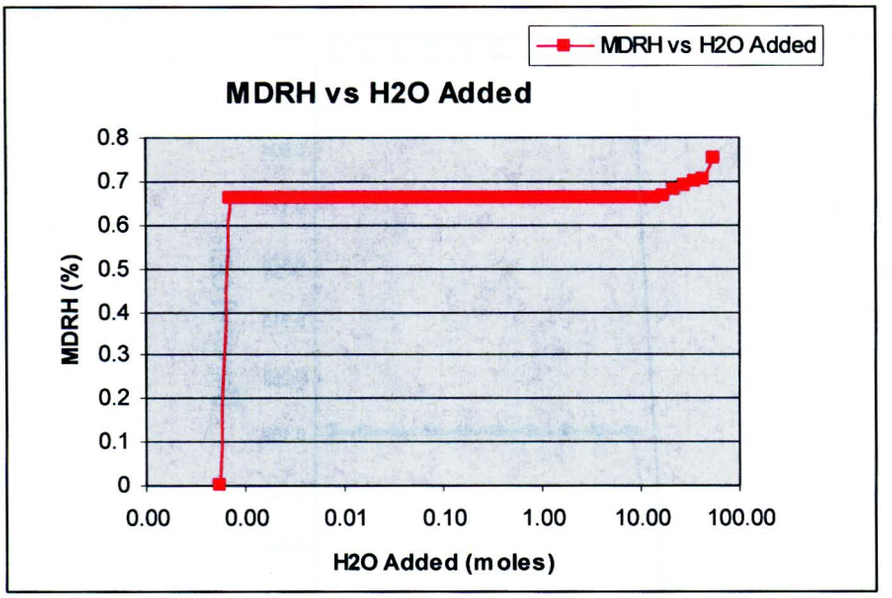
The mole fraction of NaCl (X-NaCl) as a function of H2O added is shown in the following figure;



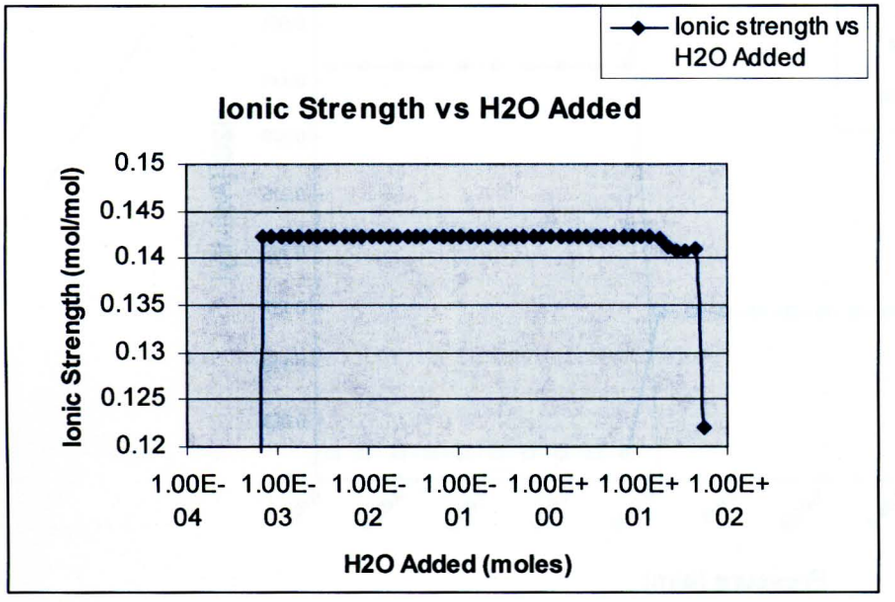
The MDRH as a function of X-NaCl is shown in the following figure:



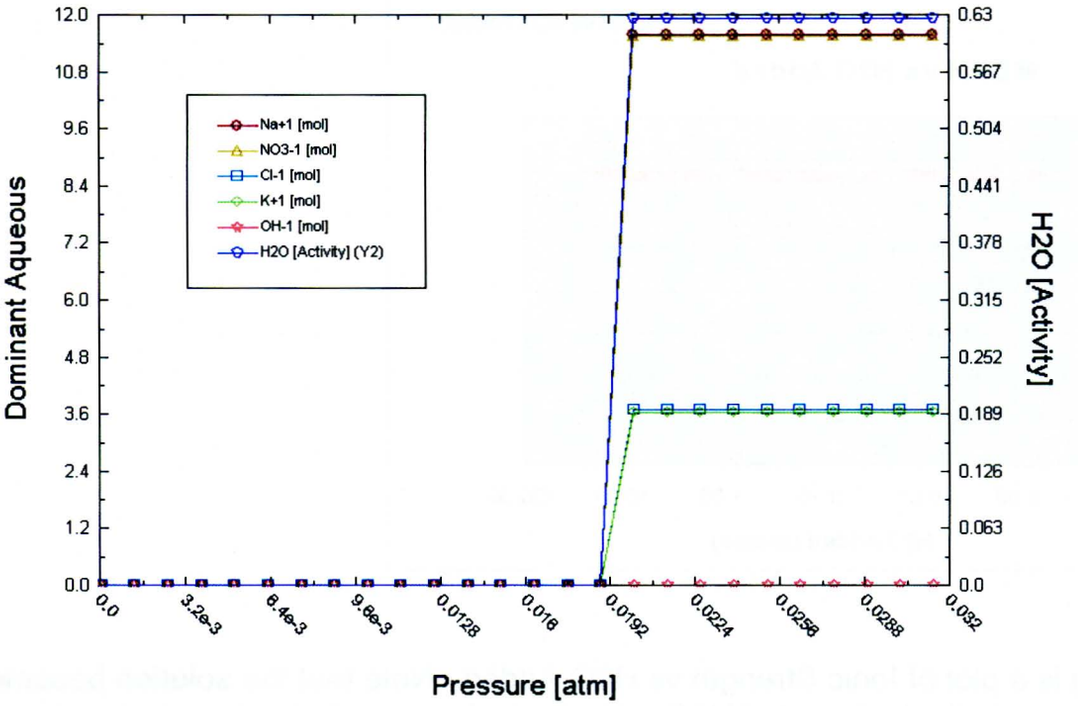
The following is a plot of MDRH vs H2O added:

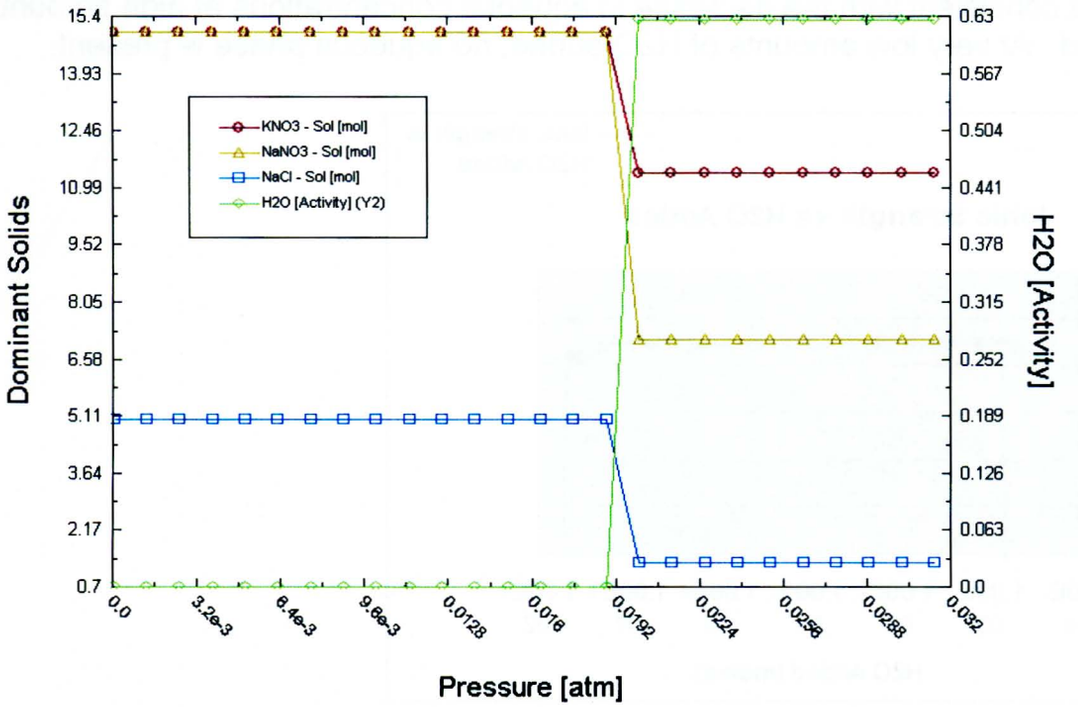


The following is a plot of Ionic Strength vs H2O Added. Note that the solution becomes more dilute towards the high end of H2O added, which accounts for the increase in MDRH and is consistent with the decrease in aqueous concentrations at high amounts of H2O added. At very low amounts of H2O added, no aqueous phase is present.



NaCl+NaNO3+KNO3 mixture





The MDRH of NaCl+NaNO3+KNO3 is 62.49%.

Deliquescence calculations:

RH = 62.48%; three solids present; Ionic Strength = 0.177078 mol/mol; input H2O = 5.55087e-3 moles

RH = 64.10%; NaNO3+KNO3 sat'd; Ionic Strength = 0.178501 mol/mol; input H2O = 27.75 moles

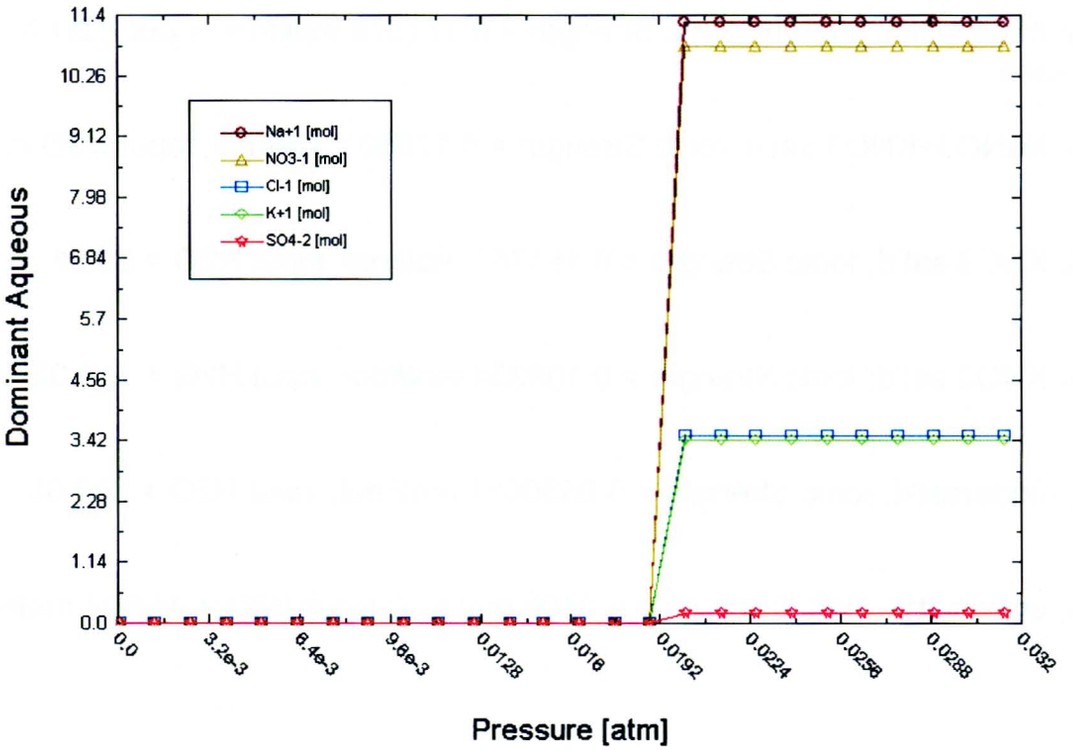
RH = 73.12%; KNO3 sat'd; Ionic Strength = 0.151761 mol/mol; input H2O = 55.51 moles

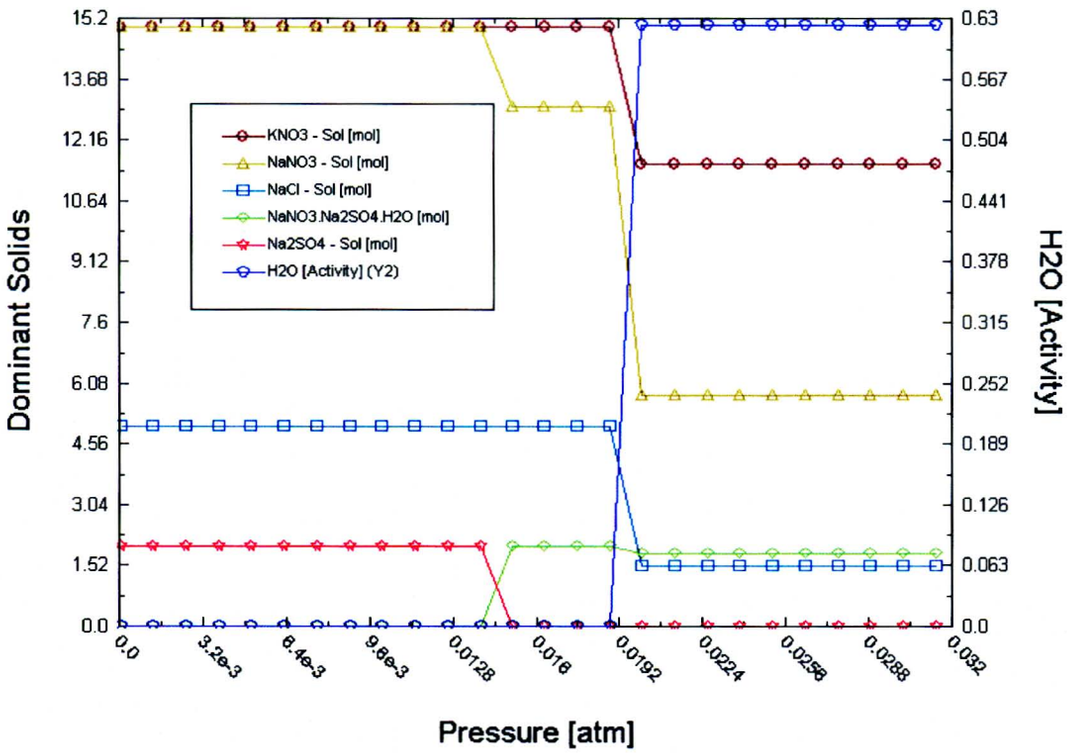
RH = 83.26%; KNO3 sat'd; Ionic Strength = 0.109334 mol/mol; input H2O = 111.02 moles

RH = 92.05%; undersat'd; Ionic Strength = 0.0530981 mol/mol; input H2O = 333.05 moles

RH = 93.70%; undersat'd; Ionic Strength = 0.0409 mol/mol; input H2O = 444.07 moles

Mixture NaCl+NaNO3+KNO3+Na2SO4





The MDRH for the NaCl+NaNO3+KNO3+Na2SO4 mixture is 62.19%. The solids present are NaCl+Na2SO4+NaNO3+KNO3. The double salt NaNO3.Na2SO4.H2O was suppressed.

Deliquescence calculation:

RH = 62.18%; four solids present (double salt suppressed); Ionic Strength = 0.180584 mol/mol; Input H2O = 5.55087e-3 moles

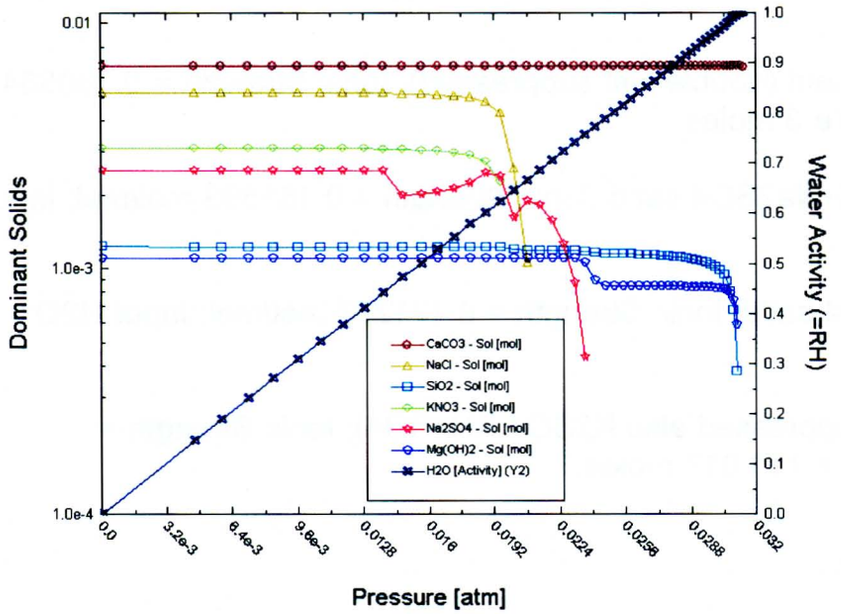
RH = 63.47%; NaNO3+KNO3+Na2SO4 sat'd; Ionic Strength = 0.181593 mol/mol; Input H2O = 27.7543 moles

RH = 69.21%; KNO3+Na2SO4 sat'd; Ionic Strength = 0.171297 mol/mol; Input H2O = 55.5087 moles

RH = 78.76%; KNO3 sat'd (suppressed also K2SO4.KNaSO4); Ionic Strength = 0.140924 mol/mol; Input H2O = 111.017 moles.

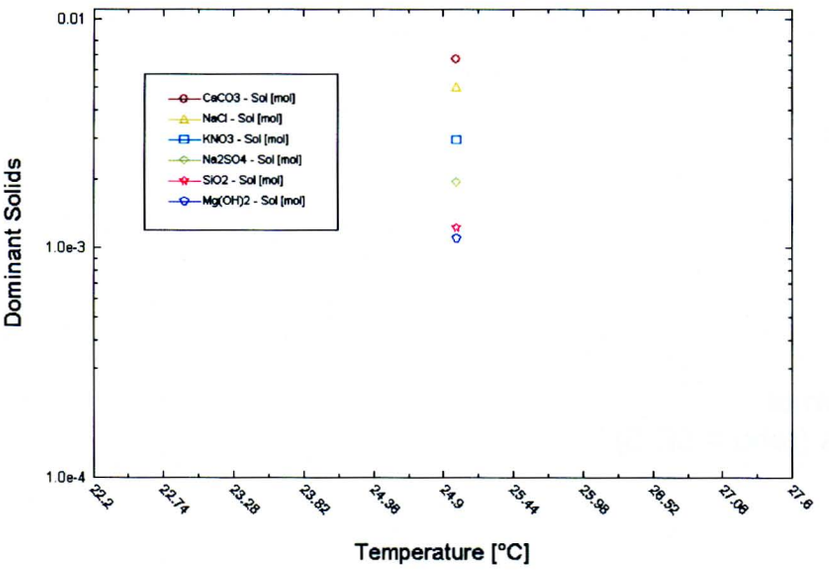
Lab Sample No. C-186098

The following figure is the result from the evaporation simulation:



To simulate deliquescence, the above solids (from the StreamAnalyzer output) were placed in a separate stream (solids only), and a water stream was used as the second stream in a mixed stream type of calculation. A single point mixed stream calculation (isothermal type) was done, specifying a water ratio value of 5E-5 (which means 5E-5 times 55.5087 moles of water was reacted with the solids. A ratio of 1E-5 did not converge.).

The following plot shows the dominant solids, which can be compared with the previous plot.


0.01
1.0e-3
1.0e-4
Dominant Solids
CaCO3 - Sol [mol]
NaCl - Sol [mol]
KNO3 - Sol [mol]
Na2SO4 - Sol [mol]
SiO2 - Sol [mol]
Mg(OH)2 - Sol [mol]
22.2
22.74
23.28
23.82
24.36
24.9
25.44
25.98
26.52
27.06
27.6
Temperature [°C]

RH = 64.43%
The saturated solids are
2Na2SO4.Na2CO3
CaCO3
KNO3
Mg(OH)2
Na2SO4
Na2SO4.NaF
NaCl
NaNO3.Na2SO4.H2O
SiO2
Ionic Strength = 0.169820 mol/mol
Input H2O = 2.77543e-3 moles (ratio = 5E-5)

RH = 64.77%
The saturated solids are
2Na2SO4.Na2CO3
CaCO3
K2SO4.KNaSO4
KNO3
Mg(OH)2
Na2SO4
Na2SO4.NaF
NaCl
SiO2
Ionic strength = 0.168318 mol/mol
Input H2O = 0.0277543 moles (ratio = 5E-4)

RH = 67.87 %
The saturated solids are
CaCO3
K2SO4.KNaSO4
Mg(OH)2
Na2SO4
Na2SO4.NaF
NaCl
SiO2
Ionic strength = 0.153632 mol/mol
Input H2O = 0.0555087 mol (ratio = 1E-3)

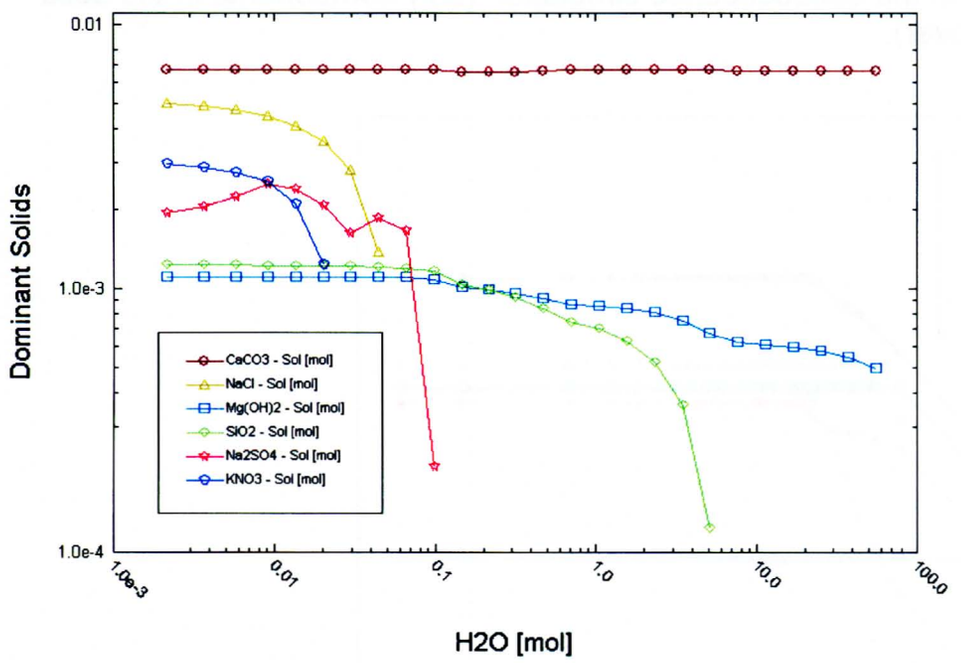
RH = 91.14%
The saturated solids are:
CaCO3
CaF2
Mg(OH)2
MgF2
SiO2

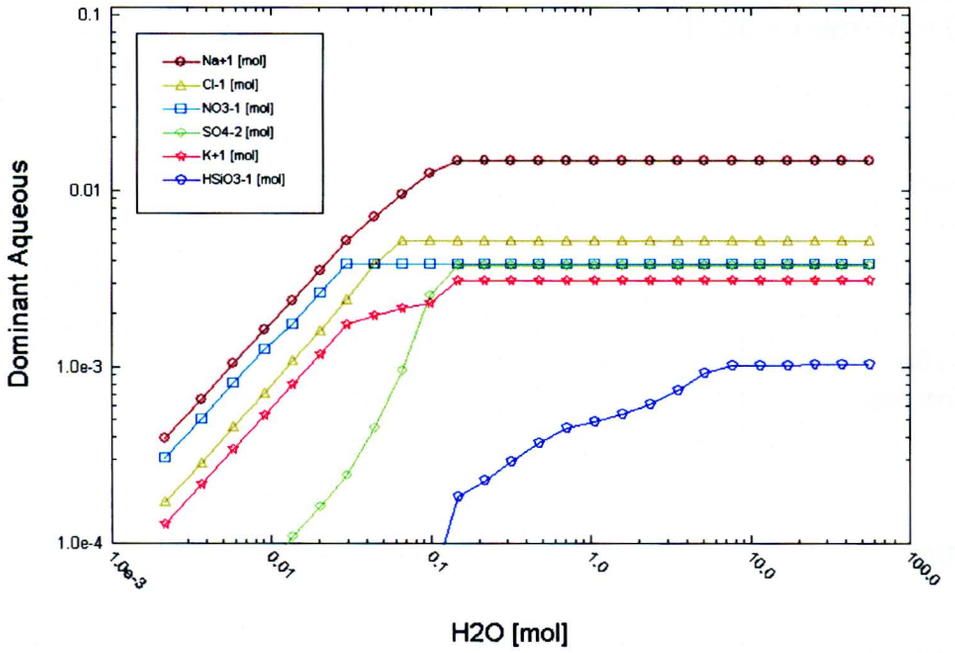
Ionic strength = 0.0710571 mol/mol
Input H2O = 0.277543 mol (ratio = 5E-3)

RH = 99.49%
The saturated solids are:
CaCO3
Mg(OH)2
MgF2
SiO2
Ionic strength = 4.00418e-3 mol/mol
Input H2O = 5.55087 moles

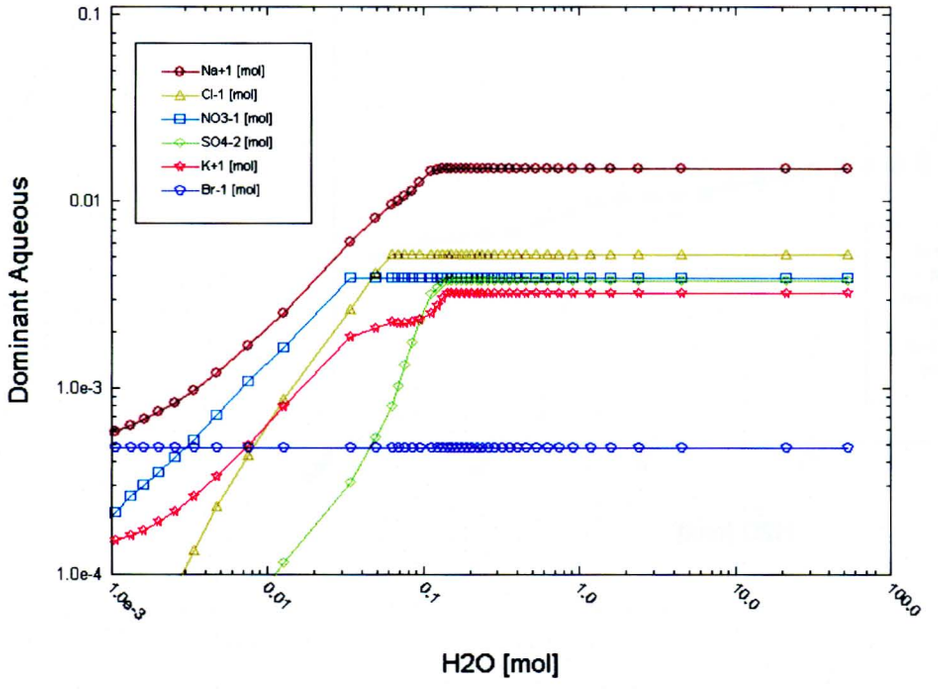
RH = 99.94%
The saturated solids are:
CaCO3
Mg(OH)2
Ionic strength = 4.15710e-4 mol/mol
Input H2O = 55.5087 moles.

The evolution of aqueous composition for **C-186098** and of the solids present are presented in the following two figures:



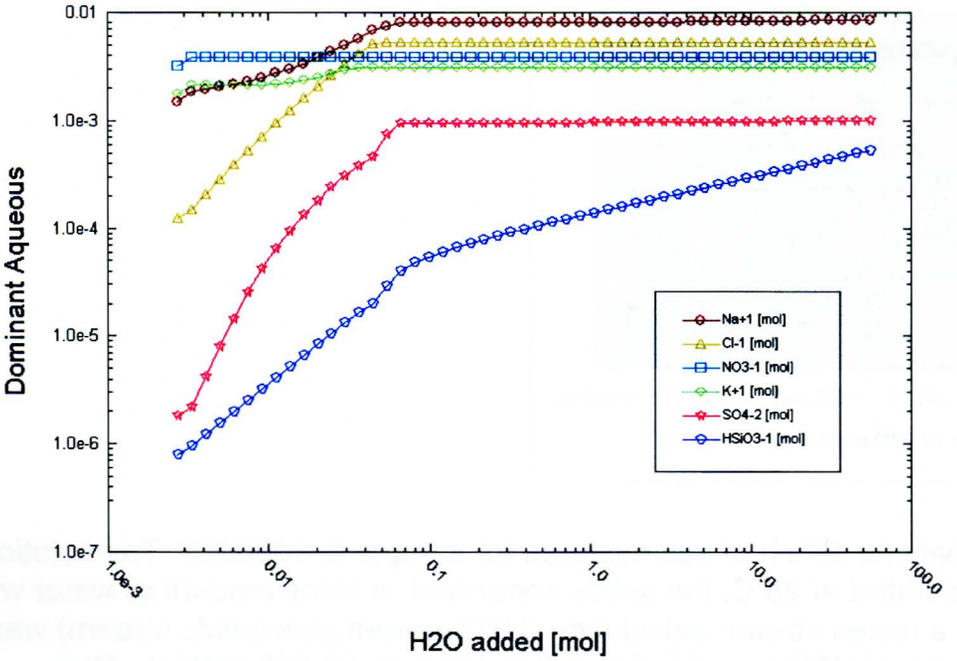


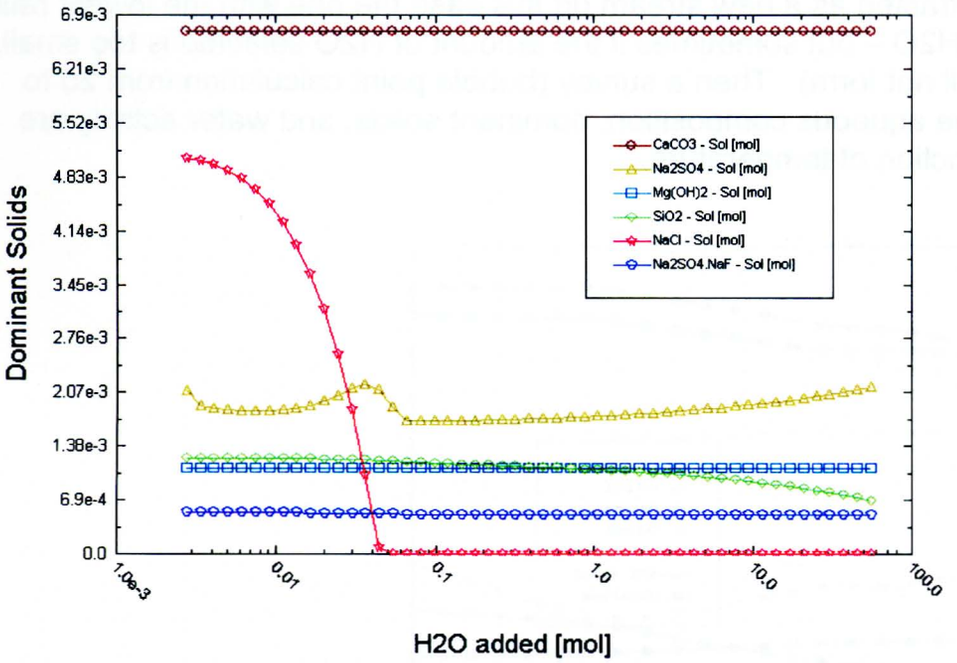
For comparison with the last figure above, below is the evolution of aqueous composition during evaporation of the initially dilute leachate water. With the exception of Br- and HSiO3-, the major ions are similar in their trends during evaporation and during deliquescence. The results cannot be the same because some components were not carried over in the deliquescence simulation (only components in the solid phases were carried over).



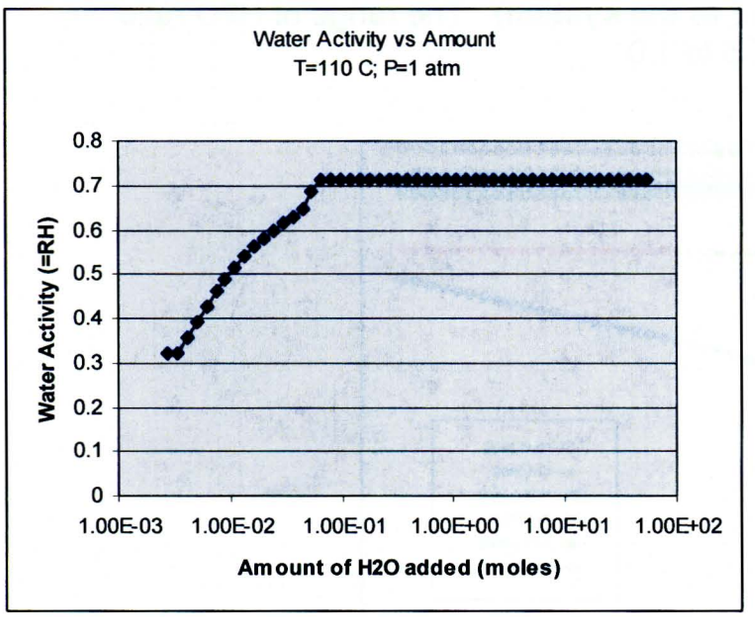
The above calculations were at 25 C.

The following figure shows the evolution of aqueous composition and solid phases as more water is added to the salt mixtures (that formed from evaporation at 25 C of C-186098) at **T=110 °C (P = 1 atm; most of the H2O went into the vapor phase; the figure X-axis is moles of H2O added to the system)**. The range of H2O ratio specified in the calculation is from 5E-5 to 1.0.

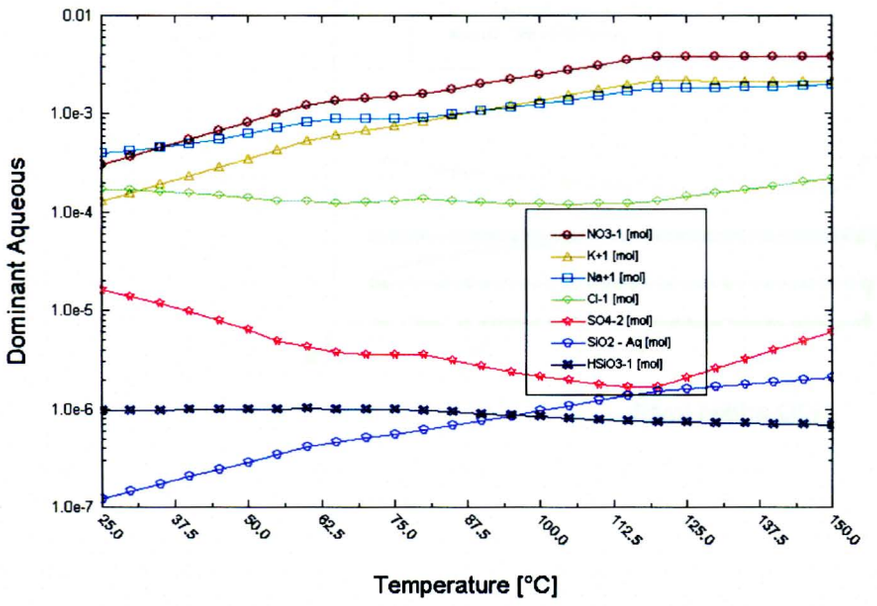


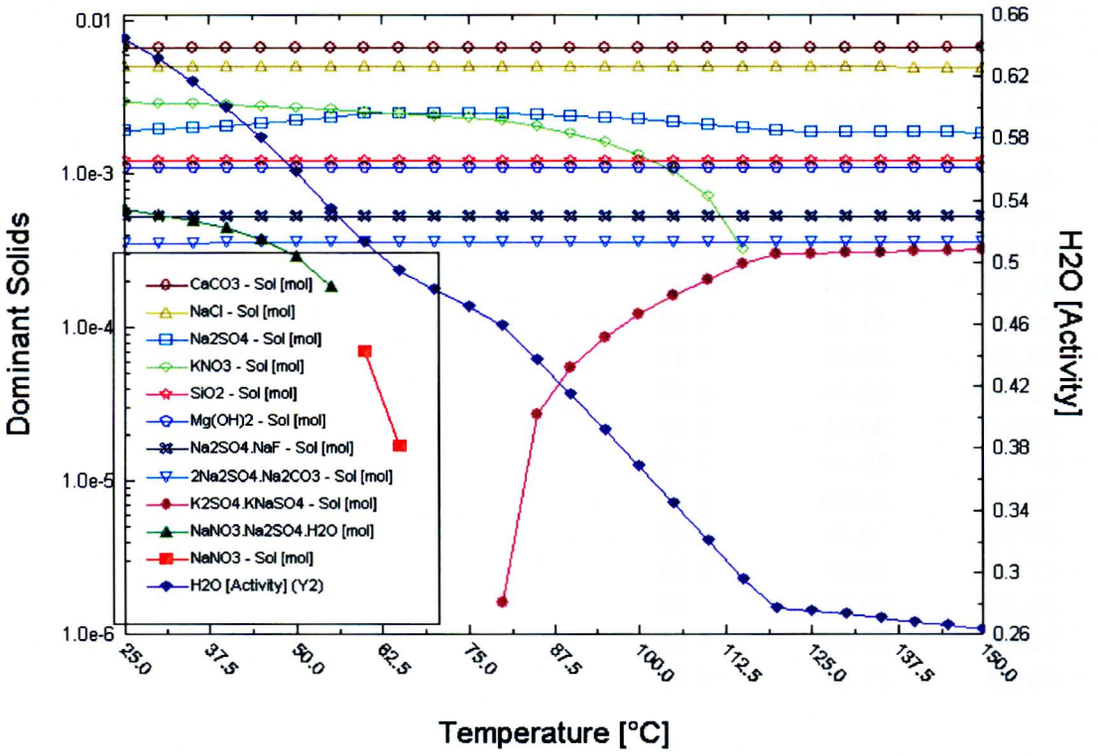


The calculated water activities (equal to RH) as a function of water amount is plotted in the following figure:



What is the water activity (or DRH) of salt mixtures for sample C-186098? The solution composition was evaporated at 25 C, the solids separated, a small amount of water was added (at 25 C), then a mixed stream calculation (H2O stream plus solids stream) was done that varied the ratio of H2O from 5E-5 to 1.0 (relative to 55.508 moles). One survey output was extracted as a new stream (in this case the one with the lowest ratio of H2O or amount of H2O – but sometimes if the amount of H2O selected is too small, an aqueous phase will not form). Then a survey (bubble point calculation from 25 to 150 C) was done. The aqueous composition, dominant solids, and water activity are plotted below as a function of temperature:





The preceding calculation for C-186098 indicates that a solid phase assemblage comprising

2Na2SO4.Na2CO3	3.57E-04	mol
CaCO3	6.69E-03	mol
KNO3	3.08E-03	mol
Mg(OH)2	1.10E-03	mol
Na2SO4	2.50E-03	mol
Na2SO4.NaF	5.26E-04	mol
NaCl	5.19E-03	mol
NaNO3	7.56E-04	mol
SiO2	1.23E-03	mol

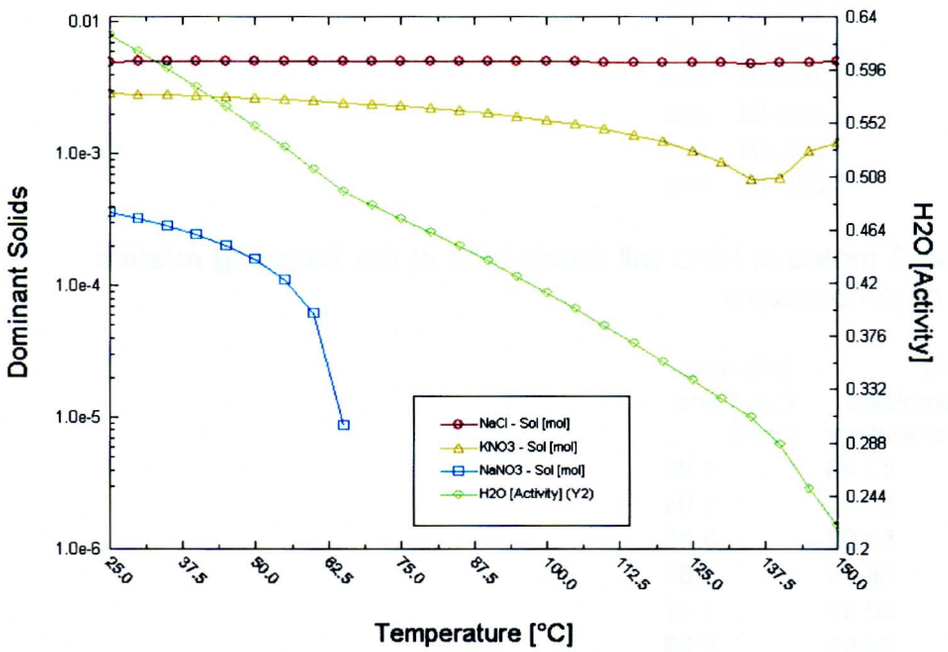
If reacted with 2.77543e-3 moles of H2O will deliquesce at the following relative humidity as a function of temperature:

Temp (C)	RH complete mineralogy	RH simplified mineralogy	Difference Col-1 and Col-2
25	64.43	62.48	1.96
30	63.16	61.12	2.04
35	61.67	59.68	2.00
40	59.97	58.16	1.81
45	58.04	56.57	1.47
50	55.86	54.91	0.95

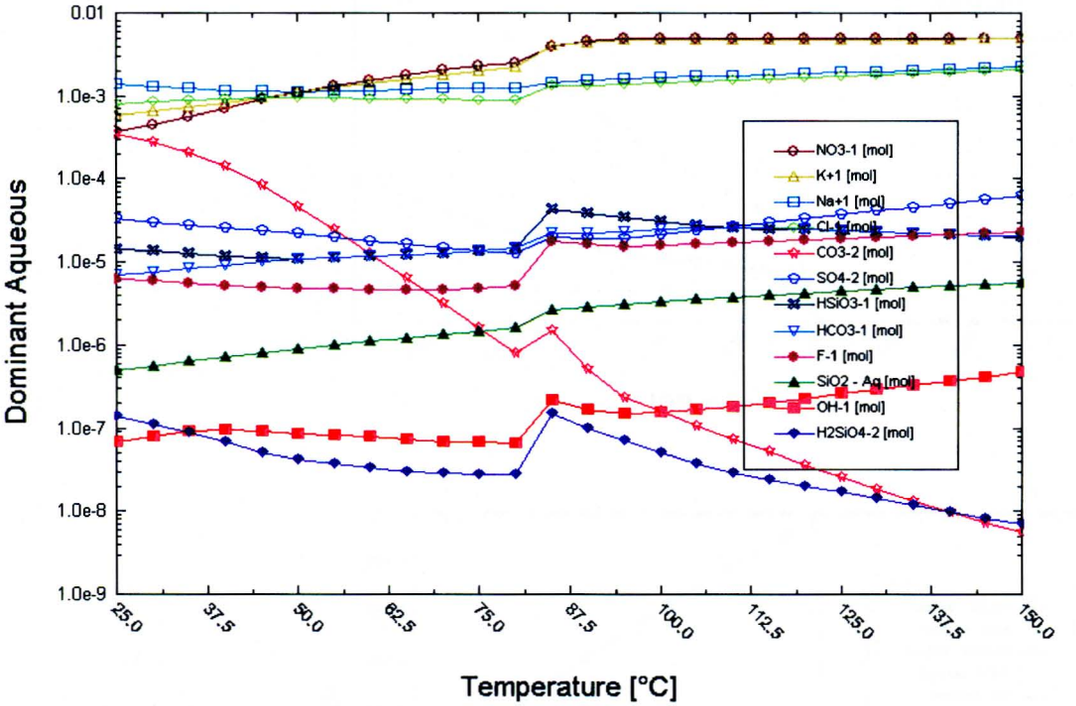
55	53.40	53.19	0.22
60	51.28	51.40	-0.13
65	49.45	49.57	-0.11
70	48.18	48.41	-0.23
75	47.12	47.34	-0.22
80	45.92	46.21	-0.28
85	43.71	45.02	-1.31
90	41.45	43.79	-2.33
95	39.15	42.51	-3.36
100	36.80	41.18	-4.38
105	34.42	39.81	-5.40
110	32.00	38.40	-6.41
115	29.54	36.96	-7.42
120	27.71	35.49	-7.78
125	27.49	33.98	-6.49
130	27.26	32.44	-5.18
135	27.02	30.87	-3.85
140	26.78	28.67	-1.89
145	26.54	25.02	1.51
150	26.30	21.92	4.37

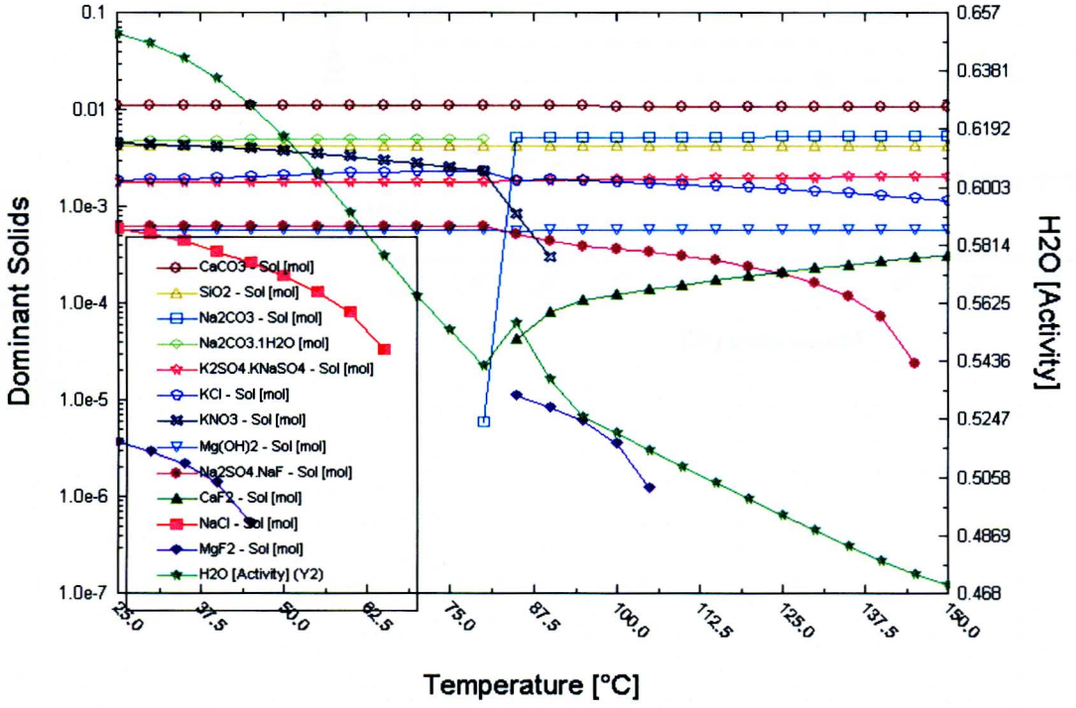
What if only the most deliquescent minerals are included in the calculation – what would be the deliquescence relative humidity as a function of temperature?

---The calculated dominant solids and the water activity (=RH) are plotted below, and the RH values as in column three of the table in the previous page. There is some difference, as expected, between the DRH of the full mineralogy and the simplified mineralogy, but the difference is acceptable for PA purposes.

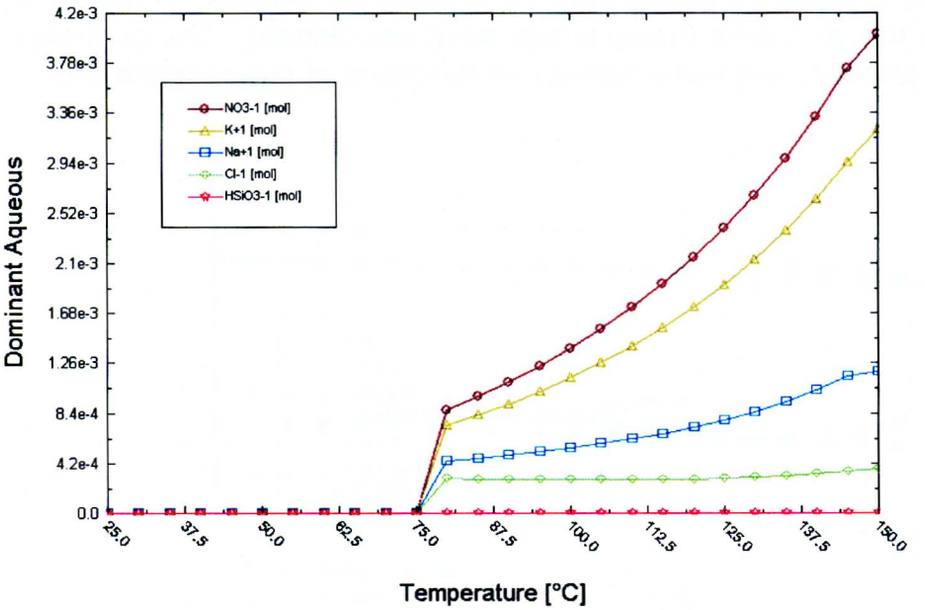


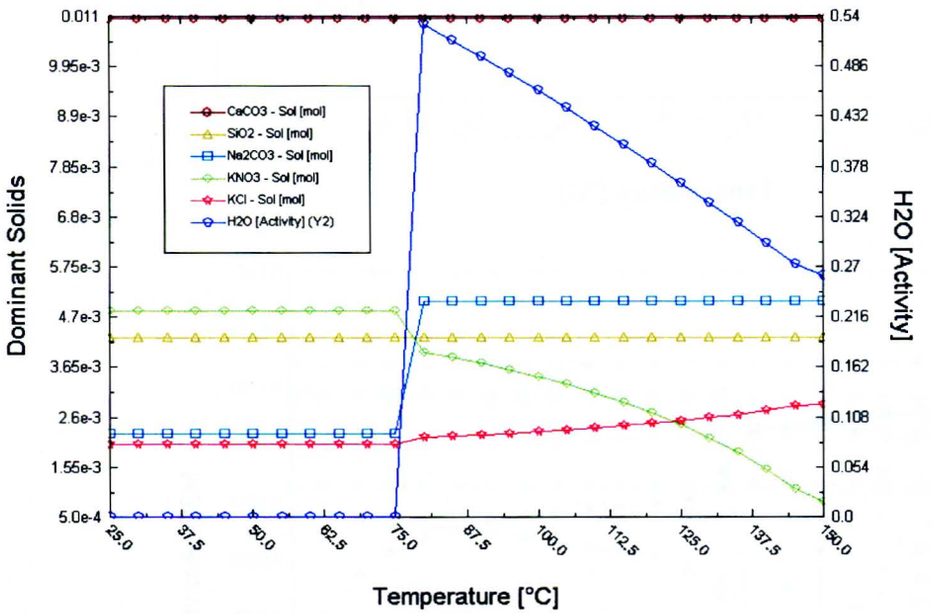
Another calculation was done for sample **C-186088** (dominant deliquescent salts are KCl, KNO3, and NaCl). In this case, the lowest ratio of H2O, when used as the input to the survey, did not produce aqueous phase from 25 to about 60 Celsius. A higher ratio of H2O was selected by trial and error (using single point calculation). The dominant aqueous ions and solid phases, and water activity as functions of temperature are shown below:



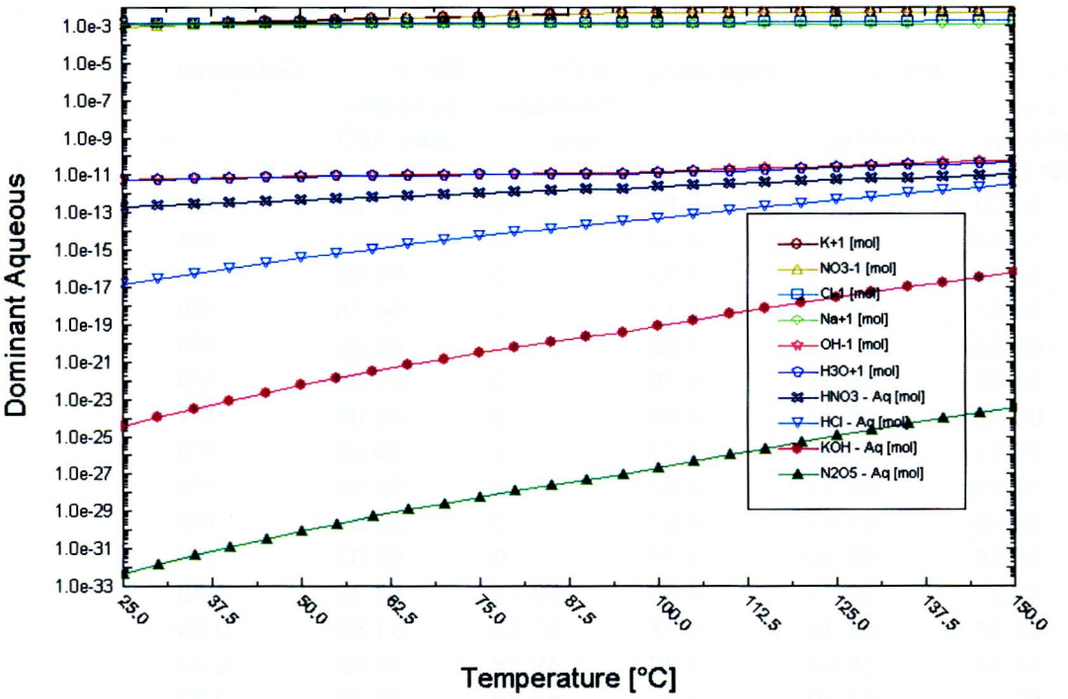


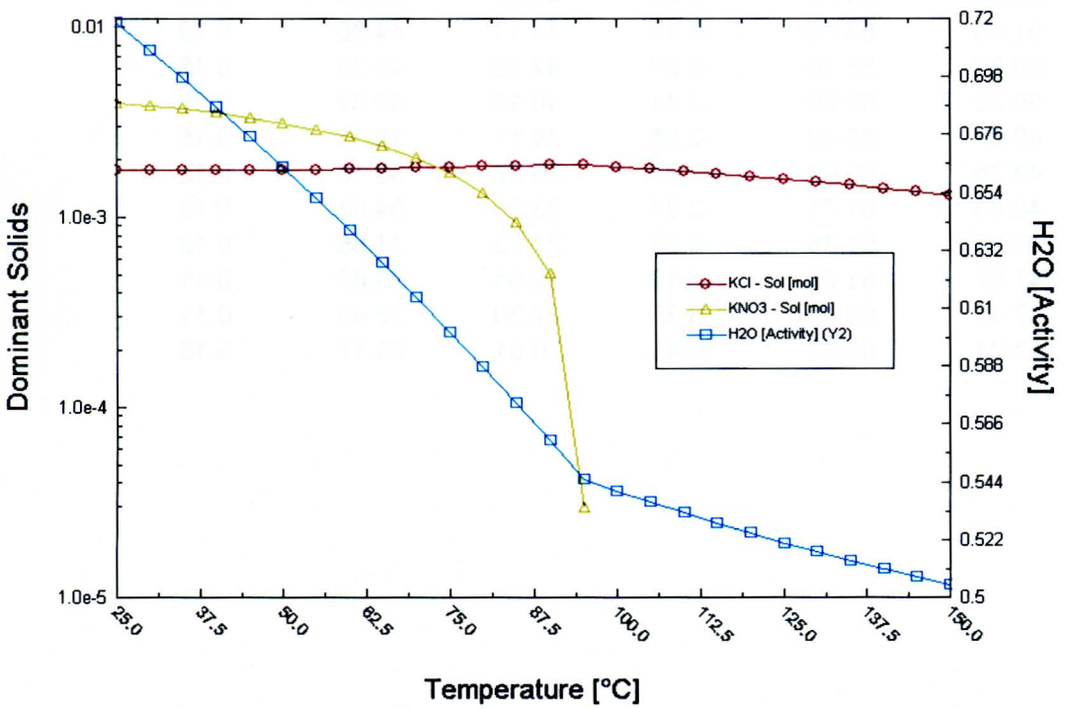
The following is the result for C-186088 using the lowest ratio of H2O:





Assuming a simplified mineralogy of deliquescent salts for sample C-186088 of KCl+KNO3+NaCl, the bubble point survey results are as follows:



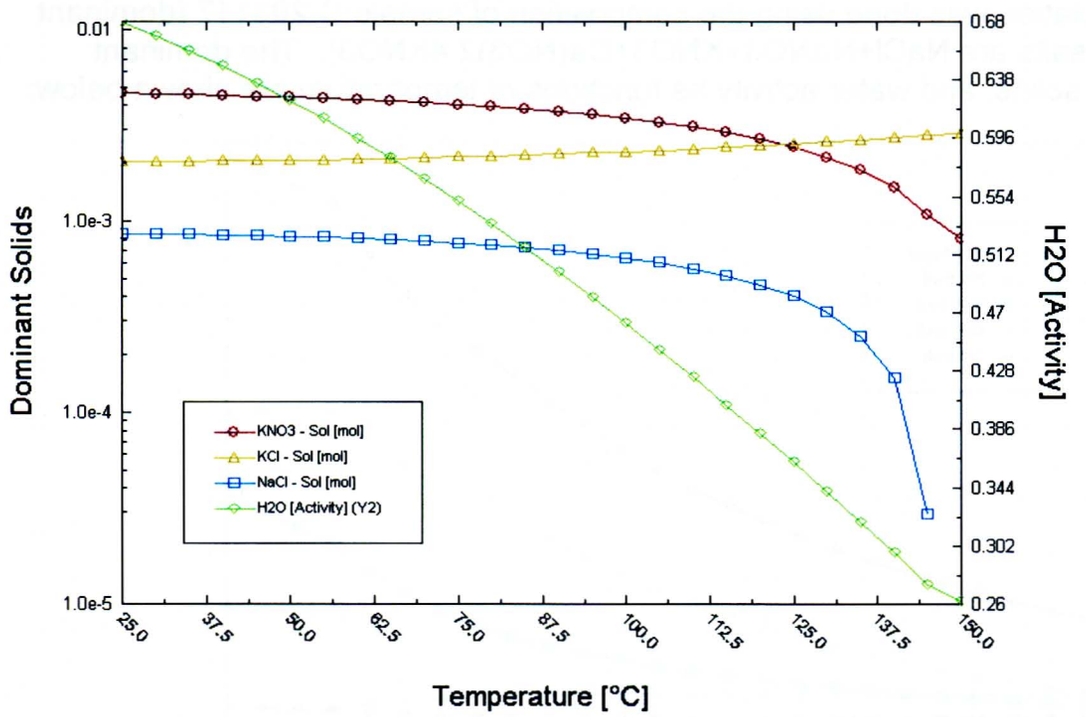


NaCl did not appear as a precipitate because the water amount was set to an amount higher than the solubility of NaCl.

The following table compares the MDRH of the complex mixture with that of the simple assemblage. The results show the simplified KCl+KNO3+NaCl assemblage approximates the complex assemblage very well where convergence in the calculations is achieved.

Temp °C	RH % Complex mineralogy; higher H2O	RH % Simplified mineralogy	Difference	RH% CompMin Least H2O	RH % Simp.Min. Less H2O	Difference
25	65.02	71.83	-6.81	0	67.93	n/a
30	64.68	70.80	-6.12	0	66.94	n/a
35	64.19	69.74	-5.55	0	65.88	n/a
40	63.54	68.65	-5.11	0	64.75	n/a
45	62.69	67.52	-4.83	0	63.56	n/a
50	61.66	66.37	-4.70	0	62.30	n/a
55	60.49	65.18	-4.69	0	60.98	n/a
60	59.19	63.96	-4.77	0	59.59	n/a
65	57.78	62.71	-4.92	0	58.14	n/a
70	56.46	61.42	-4.97	0	56.62	n/a
75	55.36	60.10	-4.74	0	55.03	n/a
80	54.21	58.75	-4.54	53.11	53.39	0.28
85	55.59	57.36	-1.78	51.43	51.69	0.26
90	53.74	55.94	-2.20	49.68	49.92	0.24
95	52.52	54.49	-1.97	47.88	48.10	0.22
100	51.99	54.00	-2.02	46.02	46.23	0.21
105	51.45	53.59	-2.14	44.11	44.30	0.19
110	50.92	53.19	-2.27	42.15	42.33	0.18
115	50.39	52.80	-2.41	40.15	40.32	0.16
120	49.87	52.43	-2.56	38.11	38.26	0.15
125	49.35	52.06	-2.71	36.02	36.16	0.14
130	48.85	51.71	-2.87	33.90	34.03	0.13
135	48.35	51.38	-3.02	31.73	31.86	0.12
140	47.87	51.05	-3.19	29.54	29.65	0.11
145	47.40	50.75	-3.35	27.30	27.40	0.11
150	47.04	50.45	-3.41	26.01	26.17	0.16

If the amount of H2O reacting with the KCl+KNO3+NaCl was decreased to 2.775E-3 from 0.0135362, the resulting solids and water activity are as follows (note that the NaCl shows up):

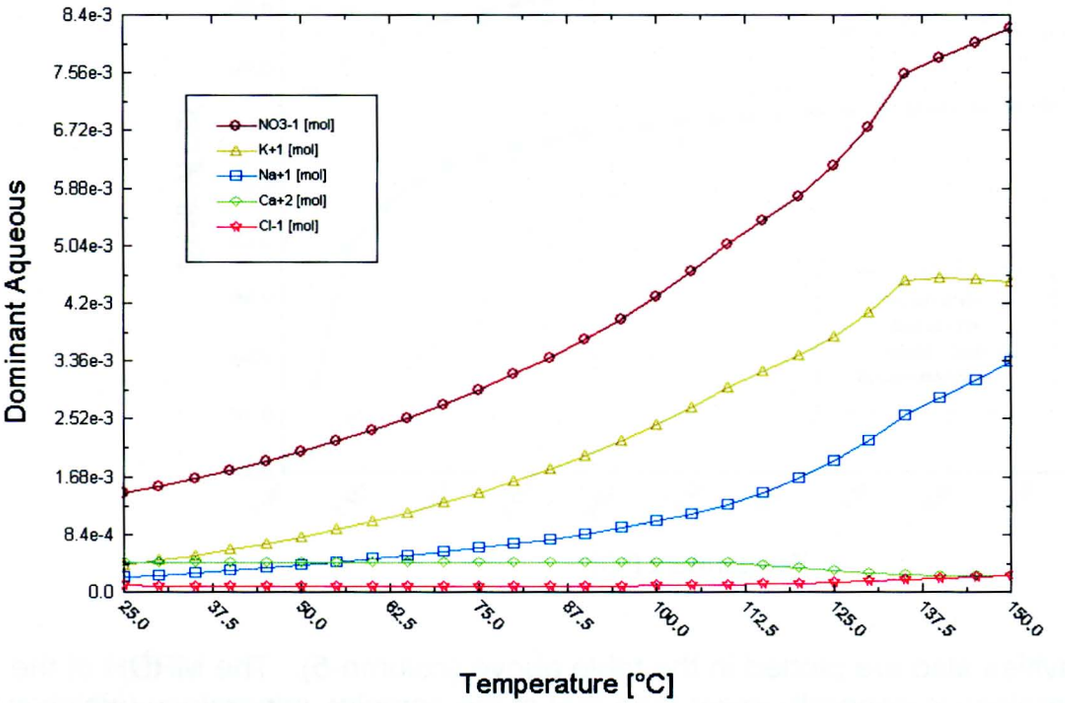


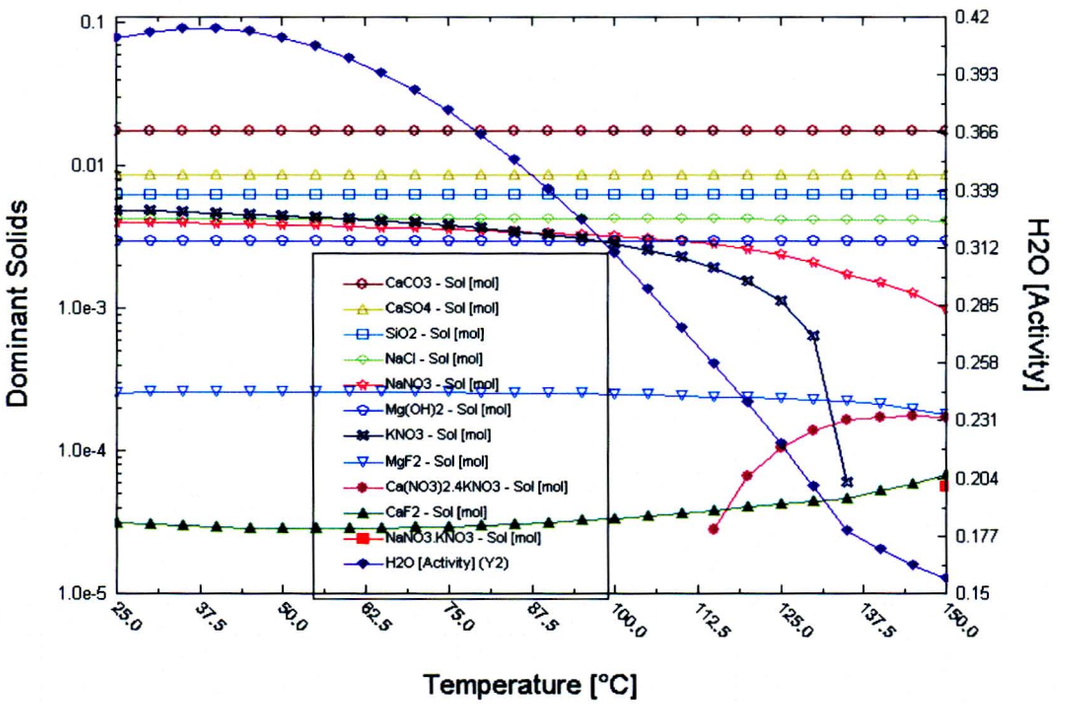
The water activities also are plotted in the table above (column-5). The MRDH of the simplified mineralogy is generally lower than that of the complex mineralogy (which is expected).

December 3, 2007

Lab sample C-203117

Another calculation was done using the composition of sample C-203117 (dominant deliquescent salts are NaCl+NaNO3+KNO3+Ca(NO3)2.4KNO3). The dominant aqueous and solids, and water activity as functions of temperature are shown below:





The following table compares the MDRH of the complex mixture with that of the simple NaCl+NaNO3+KNO3+Ca(NO3)2.4KNO3 assemblage. As shown in the table, the simplified mineralogy approximates very well the deliquescence relative humidity of the complex mixture.

Temp °C	RH% complex mineralogy	RH% simple mineralogy	Difference
25	41.03	41.67	-0.64
30	41.28	41.87	-0.59
35	41.41	41.98	-0.58
40	41.41	41.99	-0.58
45	41.28	41.87	-0.59
50	41.02	41.63	-0.61
55	40.62	41.25	-0.63
60	40.08	40.73	-0.65
65	39.40	40.07	-0.68
70	38.58	39.27	-0.70
75	37.62	38.33	-0.71
80	36.53	37.25	-0.73
85	35.30	36.04	-0.74
90	33.96	34.70	-0.74
95	32.49	33.24	-0.74
100	30.92	31.66	-0.74
105	29.24	29.97	-0.73
110	27.47	28.19	-0.72
115	25.72	26.45	-0.73
120	23.91	24.62	-0.71
125	22.00	22.70	-0.70
130	20.00	20.68	-0.68
135	17.91	18.58	-0.67
140	17.06	17.92	-0.86
145	16.32	17.22	-0.91
150	15.66	16.60	-0.94

The following table lists the concentration of dominant ions and the Cl/NO3 ratio at the deliquescence point of sample **C-203117** (dominant salts NaCl + NaNO3 + KNO3 + Ca(NO3)2.4KNO3), as a function of temperature:

Temp °C	Ca+2 molal	K+1 molal	Na+1 molal	Cl- molal	NO3- molal	Cl/NO3 ratio
25	8.67	7.85	4.13	1.79	28.81	0.062
30	8.7	9.2	4.76	1.73	30.83	0.056
35	8.71	10.68	5.43	1.68	33.04	0.051
40	8.72	12.31	6.15	1.64	35.44	0.046
45	8.73	14.1	6.92	1.6	38.03	0.042
50	8.73	16.06	7.74	1.57	40.85	0.038
55	8.73	18.21	8.62	1.54	43.89	0.035
60	8.73	20.55	9.55	1.53	47.18	0.032
65	8.73	23.11	10.54	1.52	50.74	0.03
70	8.72	25.9	11.6	1.53	54.58	0.028
75	8.71	28.94	12.74	1.54	58.75	0.026
80	8.7	32.25	13.98	1.57	63.27	0.025
85	8.69	35.85	15.34	1.6	68.19	0.024
90	8.67	39.77	16.85	1.65	73.56	0.022
95	8.65	44.04	18.53	1.72	79.45	0.022
100	8.63	48.71	20.45	1.8	85.95	0.021
105	8.6	53.84	22.65	1.91	93.17	0.02
110	8.57	59.5	25.22	2.04	101.27	0.02
115	7.97	64.16	28.67	2.22	108.09	0.021
120	7.15	68.81	32.92	2.44	115.22	0.021
125	6.34	74.29	37.99	2.69	123.95	0.022
130	5.64	81.33	44.02	3	135.4	0.022
135	5.09	90.8	51.4	3.38	150.87	0.022
140	4.81	91.35	56.35	3.74	155.68	0.024
145	4.59	91.04	61.46	4.13	159.92	0.026
150	4.47	90.14	66.72	4.58	163.94	0.028

The following table lists the dominant ions and Cl/NO3 ratio at the deliquescence point for the lab sample **C-186088** (dominant solids KCl+KNO3+NaCl):

Temp °C	K+1 molal	Na+1 molal	Cl-1 molal	NO3-1 molal	CO3-2 molal	Cl/NO3 ratio
25.00	3.69	8.57	4.93	2.33	2.21	2.12
30.00	4.08	8.15	5.28	2.84	1.78	1.86
35.00	4.60	7.77	5.61	3.56	1.33	1.57
40.00	5.29	7.47	5.89	4.58	0.90	1.29
45.00	6.16	7.31	6.07	5.85	0.54	1.04
50.00	7.16	7.30	6.14	7.26	0.30	0.85
55.00	8.22	7.40	6.13	8.73	0.16	0.70
60.00	9.34	7.58	6.09	10.25	0.08	0.59
65.00	10.54	7.81	6.02	11.85	0.04	0.51
70.00	11.83	7.99	5.94	13.45	0.02	0.44
75.00	13.23	7.98	5.84	14.97	0.01	0.39
80.00	14.76	7.98	5.75	16.60	0.01	0.35
85.00	16.50	5.98	5.55	16.42	0.01	0.34
90.00	18.24	6.38	5.52	18.63	0.00	0.30
95.00	19.26	6.67	5.62	19.85	0.00	0.28
100.00	19.35	6.82	5.84	19.85	0.00	0.29
105.00	19.43	6.98	6.08	19.85	0.00	0.31
110.00	19.50	7.17	6.32	19.85	0.00	0.32
115.00	19.56	7.37	6.56	19.85	0.00	0.33
120.00	19.61	7.60	6.81	19.85	0.00	0.34
125.00	19.66	7.83	7.07	19.85	0.00	0.36
130.00	19.71	8.09	7.34	19.85	0.00	0.37
135.00	19.75	8.36	7.62	19.85	0.00	0.38
140.00	19.80	8.65	7.92	19.85	0.00	0.40
145.00	19.84	8.95	8.22	19.85	0.00	0.41
150.00	20.01	9.11	8.50	19.85	0.00	0.43

The following lists the dominant ions and the Cl/NO3 ratio at the deliquescence point for lab sample **C-186098** (dominant solids NaCl+NaNO3+KNO3), as a function of temperature.

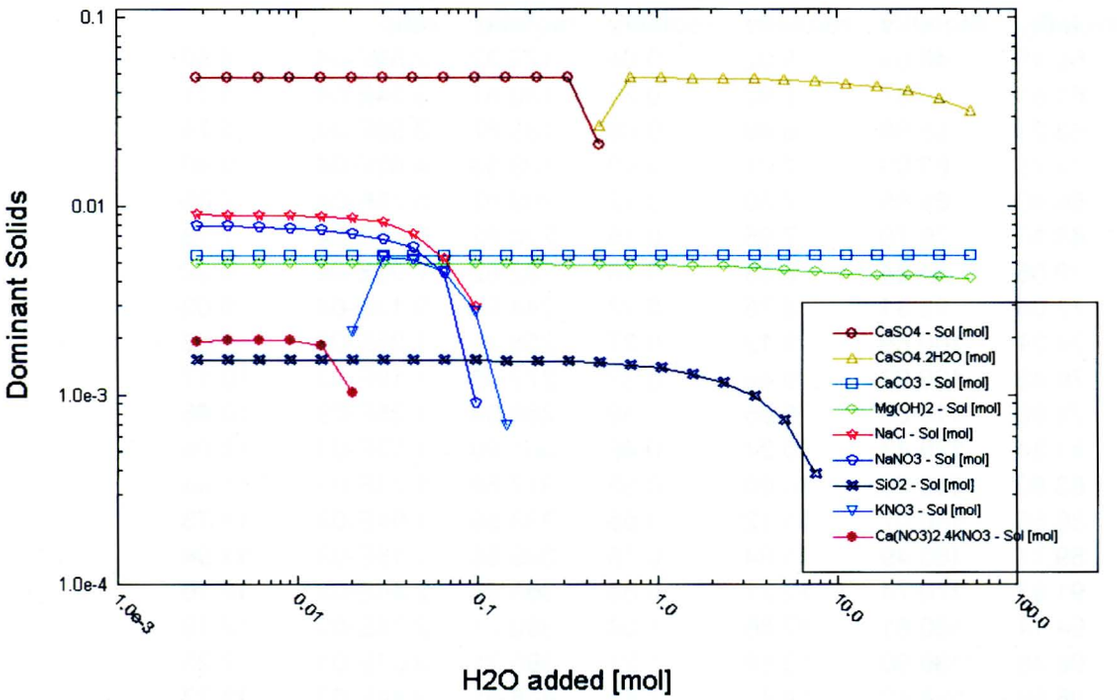
Temp °C	K+1 molal	Na+1 molal	Cl-1 molal	NO3-1 molal	Cl/NO3 ratio
25	3.25	9.97	4.32	7.66	0.563
30	3.91	10.40	4.17	9.20	0.453
35	4.69	10.98	3.96	10.99	0.360
40	5.61	11.74	3.71	13.08	0.284
45	6.66	12.68	3.42	15.49	0.221
50	7.88	13.86	3.12	18.29	0.170
55	9.28	15.33	2.79	21.55	0.130
60	10.73	16.53	2.60	24.45	0.106
65	12.23	17.47	2.50	27.02	0.092
70	13.70	17.83	2.52	28.82	0.088
75	15.21	17.93	2.62	30.33	0.086
80	16.88	18.11	2.70	32.10	0.084
85	19.08	19.53	2.60	35.84	0.073
90	21.53	21.11	2.52	39.97	0.063
95	24.28	22.90	2.47	44.58	0.055
100	27.38	24.93	2.43	49.76	0.049
105	30.91	27.26	2.42	55.63	0.044
110	34.95	29.97	2.44	62.37	0.039
115	39.63	33.15	2.49	70.20	0.035
120	43.46	35.91	2.61	76.66	0.034
125	43.32	36.30	2.85	76.66	0.037
130	43.16	36.75	3.12	76.66	0.041
135	42.97	37.25	3.40	76.65	0.044
140	42.76	37.80	3.71	76.65	0.048
145	42.55	38.39	4.05	76.65	0.053
150	42.34	39.01	4.42	76.65	0.058

The following lists the dominant ions, the Cl/NO3 ratio, and the relative humidity at the deliquescence point for lab sample **C-203120** (dominant solids NaCl + NaNO3 + Ca(NO3)2 + Ca(NO3)2.4KNO3), as a function of temperature. The calculation used 2.77543e-3 moles of H2O added to the solid phases.

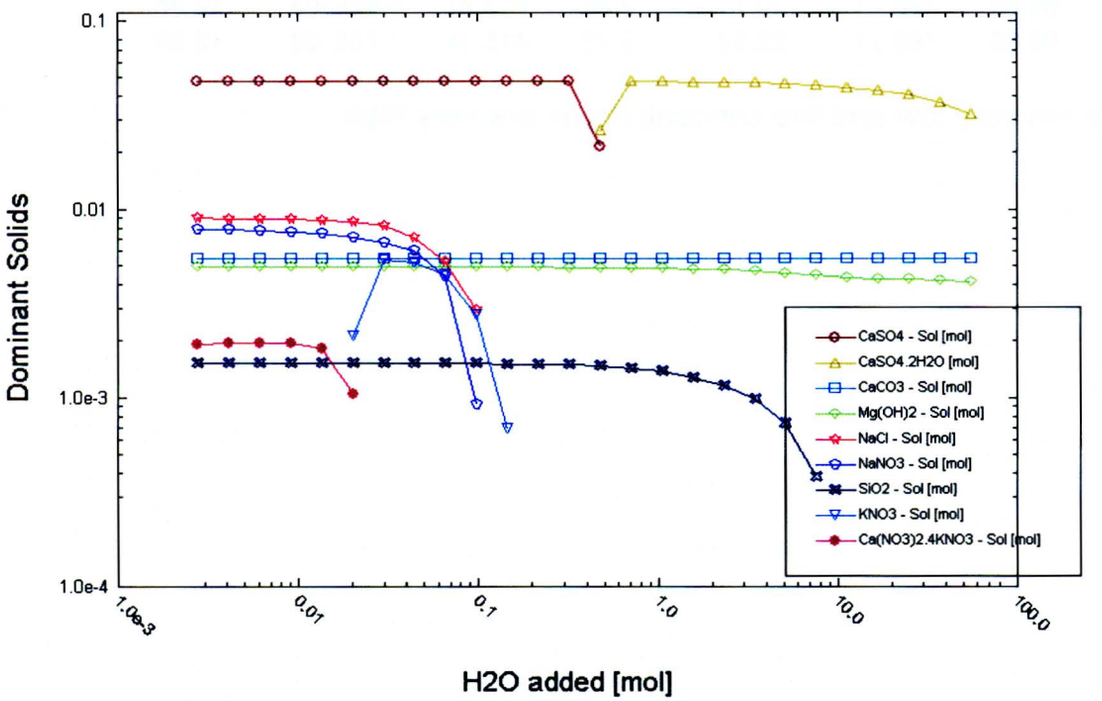
Temp °C	Ca+2 molality	K+1 molality	Na+1 molality	Cl-1 molality	NO3-1 molality	Cl/NO3 ratio	DRH%
25	60.48	46.04	5.32	0.04	172.32	2.59E-04	4.50
30	61.81	51.31	5.92	0.06	180.81	3.24E-04	5.11
35	63.23	56.99	6.49	0.08	189.87	3.98E-04	5.74
40	64.76	63.09	7.01	0.10	199.53	4.82E-04	6.40
45	66.40	69.65	7.50	0.12	209.83	5.75E-04	7.06
50	68.16	76.70	7.95	0.15	220.82	6.77E-04	7.73
55	70.05	84.24	8.36	0.18	232.52	7.90E-04	8.39
60	72.06	92.31	8.75	0.22	244.96	9.13E-04	9.02
65	74.21	100.89	9.12	0.27	258.16	1.05E-03	9.62
70	76.48	109.97	9.48	0.32	272.08	1.19E-03	10.17
75	78.86	119.50	9.85	0.39	286.69	1.35E-03	10.66
80	81.34	129.43	10.24	0.46	301.90	1.53E-03	11.08
85	83.90	139.66	10.66	0.55	317.58	1.73E-03	11.44
90	86.50	150.07	11.12	0.65	333.55	1.94E-03	11.73
95	89.11	160.49	11.64	0.76	349.58	2.18E-03	11.94
100	91.67	170.74	12.21	0.89	365.40	2.44E-03	12.10
105	94.14	180.61	12.86	1.04	380.71	2.74E-03	12.19
110	96.46	189.90	13.59	1.21	395.21	3.07E-03	12.23
115	98.59	198.42	14.42	1.41	408.61	3.44E-03	12.23
120	98.66	198.71	15.09	1.58	409.53	3.87E-03	12.38
125	98.66	198.71	15.87	1.78	410.11	4.35E-03	12.47
130	98.66	198.71	16.79	2.01	410.81	4.89E-03	12.52
135	98.66	198.71	17.88	2.26	411.65	5.49E-03	12.51
140	98.66	198.71	19.18	2.54	412.66	6.17E-03	12.46
145	98.66	198.71	20.71	2.86	413.87	6.92E-03	12.35
150	98.66	198.71	22.54	3.22	415.34	7.75E-03	12.20

The DRHs are very low and the concentrations are very high.

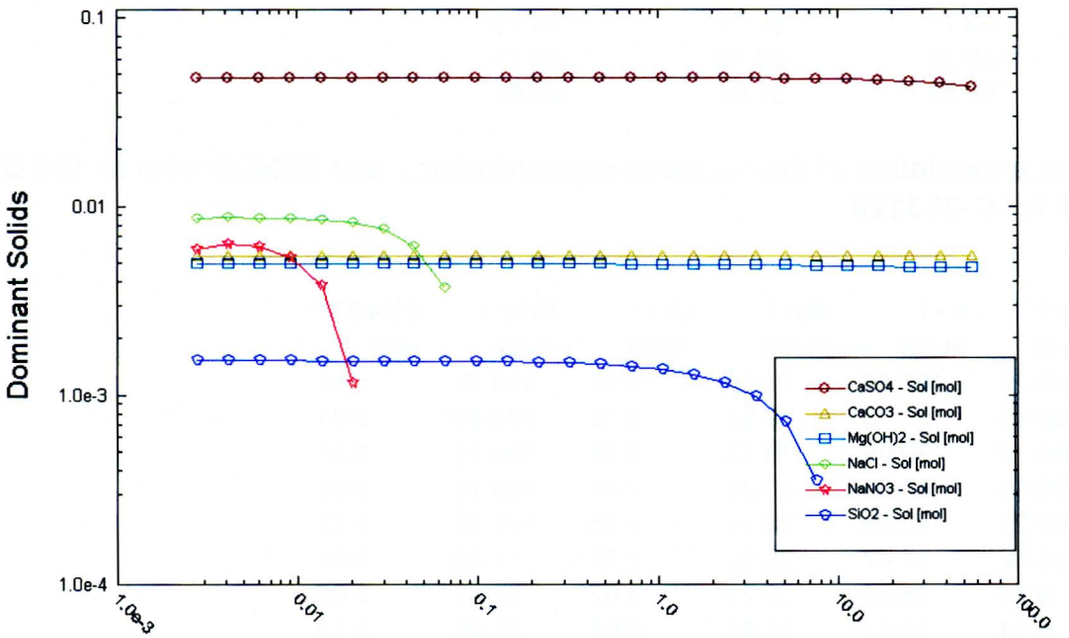
For lab sample C-203120 at 25 C, the following plots the trend in dominant solids as a function of amount of H2O added to the solid mixture. Note that the solid mixture is determined by evaporating the lab sample composition at 25 C and **the calculation type is isothermal (no H2O vapor in the output file)**. The dominant deliquescent salt mixture is NaCl + NaNO3 + Ca(NO3)2 + Ca(NO3)2.4KNO3.



The following is for **bubble point type of calculation** for **C-203120** at 25 C.



The following is for **bubble point type of calculation** for C-203120 (dominant solids NaCl + NaNO3 + Ca(NO3)2 + Ca(NO3)2.4KNO3) at 150 C. In this case, note that some salts present at 25 C no longer are present at 150 C because the solubilities are higher at the higher temperature.



The following compares the relative humidity derived from an isothermal survey at 25 C with the MDRH from bubble point calculations at 25 and 150 C for sample C-203120:

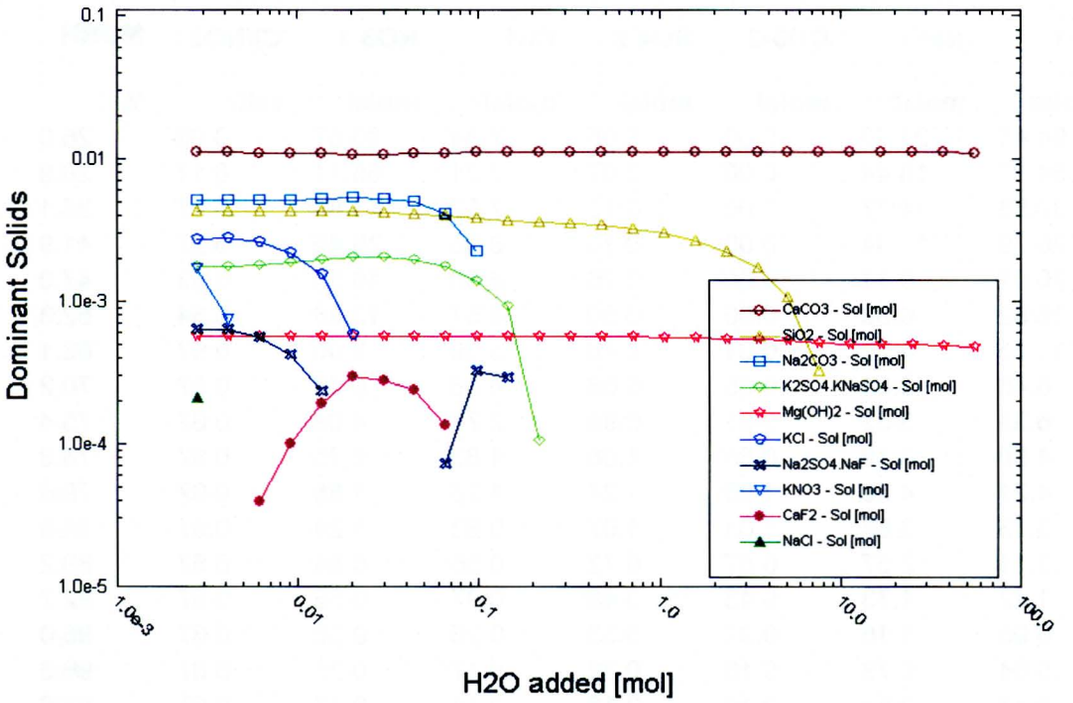
H2O added **mol**	Water Activity 25 C Isothermal	MDRH 25 C Bubble Pt	MDRH 150 C Bubble Pt
2.78E-03	4.50	4.50	12.20
4.12E-03	8.01	8.00	16.15
6.13E-03	14.16	14.16	20.35
9.11E-03	23.38	23.39	24.10
1.35E-02	33.70	33.71	26.87
2.01E-02	38.19	38.30	29.51
2.99E-02	42.02	42.03	36.10
4.44E-02	49.84	49.84	42.20
6.60E-02	55.17	55.17	47.85
9.81E-02	58.30	58.30	55.89
1.46E-01	64.87	64.88	66.73
2.17E-01	75.70	75.70	75.73
3.22E-01	83.43	83.43	82.71
4.78E-01	87.30	87.33	87.92
7.11E-01	91.07	91.07	91.71
1.06E+00	94.14	94.14	94.38
1.57E+00	96.09	96.09	96.21
2.33E+00	97.37	97.37	97.46

3.47E+00	98.21	98.21	98.29
5.15E+00	98.78	98.78	98.84
7.66E+00	99.16	99.16	99.21
1.14E+01	99.41	99.41	99.46
1.69E+01	99.59	99.59	99.63
2.51E+01	99.71	99.71	99.75
3.74E+01	99.79	99.79	99.83
5.55E+01	99.85	99.85	99.88

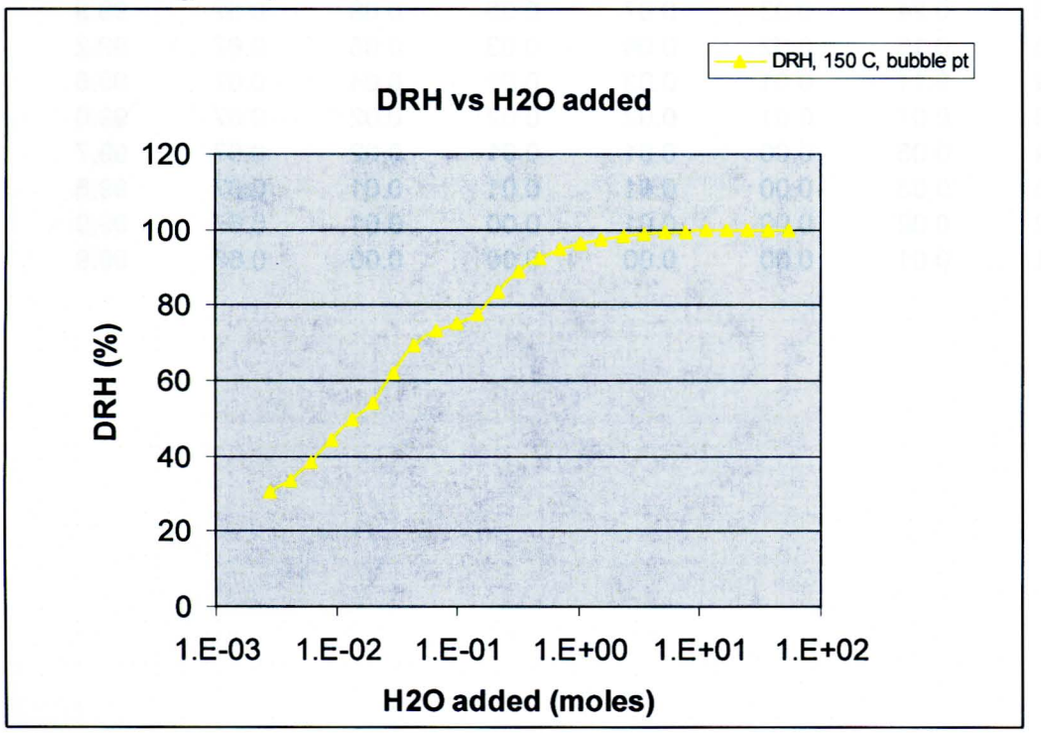
The following is a tabulation of the aqueous concentrations and Cl/NO3 ratio at 150 C vs H2O added for **C-203120**:

H2O added moles	Ca+2 molal	K+1 molal	Na+1 molal	Cl-1 molal	NO3-1 molal	Cl/NO3 ratio
2.77E-03	98.75	198.90	22.56	3.22	415.74	0.01
4.12E-03	66.46	133.86	19.83	2.72	283.89	0.01
6.12E-03	44.72	90.09	19.13	2.48	196.18	0.01
9.10E-03	30.10	60.63	20.34	2.44	138.72	0.02
1.35E-02	20.25	40.80	23.14	2.55	101.89	0.03
2.01E-02	13.62	27.47	25.09	2.79	77.03	0.04
2.98E-02	9.16	18.50	18.73	3.67	51.88	0.07
4.42E-02	6.14	12.47	14.85	4.65	34.95	0.13
6.57E-02	4.10	8.40	12.44	5.50	23.54	0.23
9.76E-02	2.76	5.65	9.69	5.03	15.85	0.32
1.45E-01	1.88	3.80	6.52	3.42	10.67	0.32
2.16E-01	1.27	2.56	4.39	2.31	7.17	0.32
3.21E-01	0.85	1.72	2.95	1.55	4.82	0.32
4.77E-01	0.57	1.16	1.98	1.04	3.24	0.32
0.709491	0.39	0.78	1.33	0.70	2.18	0.32
1.0548	0.26	0.52	0.90	0.47	1.47	0.32
1.56804	0.18	0.35	0.60	0.32	0.99	0.32
2.3309	0.12	0.24	0.41	0.21	0.66	0.32
3.46477	0.08	0.16	0.27	0.14	0.45	0.32
5.15002	0.05	0.11	0.18	0.10	0.30	0.32
7.65489	0.04	0.07	0.12	0.07	0.20	0.32
11.3774	0.02	0.05	0.08	0.04	0.14	0.32
16.9095	0.02	0.03	0.06	0.03	0.09	0.32
25.1307	0.01	0.02	0.04	0.02	0.06	0.32
37.348	0.01	0.01	0.03	0.01	0.04	0.32
5.55E+01	0.01	0.01	0.02	0.01	0.03	0.32

For lab sample **C-186088 (dominant salts KCl+KNO3+NaCl)**, a bubble point survey calculation at 150 C results in the following dominant solid phases as a function of added H2O:



The following is a plot of DRH vs H2O added:



The following is a tabulation of the aqueous composition, Cl/NO3 ratio, and MDRH at 150 C of **C-186088** (dominant salt (KCl+KNO3+NaCl) at the deliquescence point vs H2O added.

H2O moles added	K+1 molal	Na+1 molal	CO3-2 molal	SO4-2 molal	Cl-1 molal	NO3-1 molal	Cl/NO3 ratio	MDRH %
2.77E-03	64.41	23.73	0.00	0.05	7.34	80.57	0.09	26.0
4.12E-03	54.17	18.44	0.00	0.07	7.21	65.11	0.11	29.9
6.12E-03	37.53	14.27	0.00	0.12	7.57	43.81	0.17	36.1
9.10E-03	26.79	11.34	0.00	0.19	8.05	29.49	0.27	41.9
1.35E-02	20.01	9.11	0.00	0.26	8.50	19.85	0.43	47.0
2.01E-02	16.52	6.38	0.00	0.30	8.57	13.36	0.64	52.3
2.98E-02	11.75	4.72	0.01	0.48	5.99	9.00	0.67	62.1
4.42E-02	8.46	3.81	0.05	0.68	4.03	6.06	0.67	70.2
6.57E-02	6.33	3.52	0.21	0.88	2.72	4.08	0.67	75.4
9.76E-02	4.98	3.79	0.55	1.08	1.83	2.75	0.67	78.3
1.45E-01	4.21	4.39	1.05	1.27	1.23	1.85	0.67	79.6
2.16E-01	3.13	3.83	1.03	1.07	0.83	1.24	0.67	84.0
3.21E-01	2.11	2.57	0.67	0.72	0.56	0.84	0.67	89.2
4.77E-01	1.42	1.73	0.43	0.48	0.37	0.56	0.67	92.7
0.709491	0.95	1.16	0.27	0.33	0.25	0.38	0.67	95.0
1.0548	0.64	0.78	0.16	0.22	0.17	0.25	0.67	96.6
1.56804	0.43	0.53	0.10	0.15	0.11	0.17	0.67	97.6
2.3309	0.29	0.35	0.05	0.10	0.08	0.12	0.67	98.4
3.46477	0.19	0.24	0.03	0.07	0.05	0.08	0.67	98.9
5.15002	0.13	0.16	0.02	0.04	0.03	0.05	0.67	99.2
7.65489	0.09	0.11	0.01	0.03	0.02	0.04	0.67	99.5
11.3774	0.06	0.07	0.01	0.02	0.02	0.02	0.67	99.6
16.9095	0.04	0.05	0.00	0.01	0.01	0.02	0.67	99.7
25.1307	0.03	0.03	0.00	0.01	0.01	0.01	0.67	99.8
37.348	0.02	0.02	0.00	0.01	0.00	0.01	0.67	99.9
5.55E+01	0.01	0.01	0.00	0.00	0.00	0.00	0.67	99.9

The following is a tabulation of the aqueous composition, Cl/NO3 ratio, and MDRH at 150 C of **C-203117** [dominant salt NaCl+NaNO3+KNO3+Ca(NO3)2.4KNO3] at the deliquescence point vs H2O added.

H2O added moles	Ca+2 molal	K+1 molal	Na+1 molal	Cl-1 molal	NO3-1 molal	Cl/NO3 ratio	MDRH %
2.78E-03	4.47	90.14	66.72	4.58	163.95	0.03	15.66
4.12E-03	4.72	70.70	58.10	4.25	137.03	0.03	18.01
6.13E-03	2.90	47.57	41.95	4.43	93.48	0.05	23.64
9.11E-03	1.84	32.01	30.12	4.85	62.90	0.08	30.34
1.35E-02	1.22	21.54	22.41	5.36	42.33	0.13	37.34
2.01E-02	0.80	14.50	17.40	5.90	28.48	0.21	44.06
2.99E-02	0.52	9.75	14.11	6.34	19.17	0.33	50.24
4.44E-02	0.36	6.56	10.60	5.39	12.90	0.42	58.76
6.60E-02	0.25	4.42	7.13	3.64	8.68	0.42	69.15
9.81E-02	0.17	2.97	4.80	2.46	5.84	0.42	77.59
1.46E-01	0.12	2.00	3.23	1.65	3.93	0.42	84.06
2.17E-01	0.08	1.35	2.17	1.11	2.64	0.42	88.85
3.22E-01	0.06	0.91	1.46	0.75	1.78	0.42	92.31
4.78E-01	0.04	0.61	0.98	0.50	1.20	0.42	94.75
0.711061	0.03	0.41	0.66	0.34	0.81	0.42	96.44
1.05669	0.02	0.28	0.45	0.23	0.54	0.42	97.59
1.57032	0.01	0.19	0.30	0.15	0.36	0.42	98.37
2.33362	0.01	0.12	0.20	0.10	0.25	0.42	98.89
3.46794	0.01	0.08	0.14	0.07	0.17	0.42	99.24
5.15363	0.01	0.06	0.09	0.05	0.11	0.42	99.47
7.65869	0.005	0.04	0.06	0.03	0.07	0.42	99.63
11.3814	0.004	0.03	0.04	0.02	0.05	0.42	99.74
16.9136	0.003	0.02	0.03	0.01	0.03	0.42	99.81
25.135	0.002	0.01	0.02	0.01	0.02	0.42	99.87
37.3525	0.002	0.01	0.01	0.01	0.02	0.42	99.90
5.55E+01	0.002	0.01	0.01	0.004	0.01	0.42	99.93

The following is a tabulation of the aqueous composition, Cl/NO3 ratio, and MDRH at 150 C of C-186101 (dominant salt NaCl+KNO3) at the deliquescence point vs H2O added:

H2O added moles	Na+1 molal	K+1 molal	SO4-2 molal	Cl-1 molal	NO3-1 molal	Cl/NO3 molal	MDRH %
2.78E-03	22.27	20.42	0.37	5.24	36.77	0.14	39.20
4.12E-03	17.26	14.34	0.55	5.79	24.74	0.23	45.54
6.13E-03	13.87	10.52	0.72	6.33	16.65	0.38	51.06
9.11E-03	11.56	8.11	0.83	6.84	11.20	0.61	55.61
1.35E-02	9.99	6.59	0.89	7.30	7.54	0.97	59.17
2.01E-02	8.92	5.62	0.91	7.68	5.07	1.51	61.80
2.99E-02	8.36	4.57	0.87	7.80	3.41	2.29	64.21
4.44E-02	8.26	3.08	0.75	7.56	2.30	3.29	67.00
6.60E-02	6.89	2.07	1.11	5.22	1.55	3.38	74.96
9.81E-02	6.14	1.39	1.49	3.51	1.04	3.38	80.72
1.46E-01	4.15	0.94	1.02	2.36	0.70	3.38	86.96
2.17E-01	2.90	0.63	0.75	1.59	0.47	3.38	90.97
3.22E-01	1.95	0.42	0.51	1.07	0.32	3.38	93.86
4.78E-01	1.31	0.29	0.35	0.72	0.21	3.38	95.84
7.11E-01	0.88	0.19	0.23	0.48	0.14	3.38	97.18
1.06	0.59	0.13	0.16	0.33	0.10	3.38	98.08
1.57	0.40	0.09	0.10	0.22	0.06	3.38	98.69
2.33	0.27	0.06	0.07	0.15	0.04	3.38	99.10
3.47	0.18	0.04	0.05	0.10	0.03	3.38	99.38
5.15	0.122	0.027	0.032	0.067	0.020	3.38	99.56
7.66	0.082	0.018	0.021	0.045	0.013	3.38	99.70
11.38	0.055	0.012	0.014	0.030	0.009	3.38	99.79
16.91	0.037	0.008	0.010	0.020	0.006	3.38	99.86
25.14	0.025	0.005	0.006	0.014	0.004	3.38	99.90
37.35	0.017	0.004	0.004	0.009	0.003	3.38	99.93
55.51	0.011	0.002	0.003	0.006	0.002	3.38	99.95

The following is a tabulation of the aqueous composition, Cl/NO3 ratio, and MDRH at 150 C of C-203112 (dominant salt KCl+KNO3) at the deliquescence point vs H2O added. **Note that this is the only composition that resulted in high Cl to NO3 ratio and high aqueous carbonate concentration.** Lab samples C-203113 and C-203114 are similar to C-203112 and likely would give similar results. The three samples have low Cl, NO3, and SO4 concentrations (USGS data have uncertain values for these samples, as shown in the table on page 199 of this notebook). The high carbonate concentration is likely the result of the charge balancing process in which HCO3- was used to charge balance the excess cations (there was significant charge imbalance in the reported chemical analysis). Nevertheless, since sulfate, bicarbonate, and carbonate ions also are corrosion inhibitors for Alloy 22, if the ratio of chloride to total inhibitor concentration is considered, the deliquescence brines are unlikely to initiate localized corrosion of Alloy 22.

H2O added	Na+1	K+1	HCO3-1	SO4-2	CO3-2	Cl-1	NO3-1	Cl/NO3	Cl/(NO3+SO4 +HCO3+CO3)	MDRH
moles	molal	molal	molal	molal	molal	molal	molal	ratio	ratio	%
2.7E-03	3.21	23.24	2.37	0.03	10.50	2.41	0.02	143.41	0.19	39.80
4.0E-03	3.21	23.24	2.37	0.03	10.50	2.41	0.02	143.41	0.19	39.80
5.9E-03	3.21	23.24	2.37	0.03	10.50	2.41	0.02	143.41	0.19	39.80
8.8E-03	3.61	18.56	1.67	0.04	8.30	3.30	0.05	63.60	0.33	47.63
1.3E-02	4.34	13.29	1.22	0.10	6.41	2.84	0.16	18.24	0.36	58.12
2.0E-02	4.95	9.74	1.05	0.19	5.33	1.90	0.32	6.01	0.28	66.06
2.9E-02	4.40	6.85	0.79	0.35	3.97	1.27	0.21	6.01	0.24	75.49
4.4E-02	3.04	4.88	0.58	0.42	2.60	0.85	0.14	6.01	0.23	83.47
6.6E-02	2.04	3.27	0.43	0.28	1.69	0.57	0.10	6.01	0.23	89.00
9.8E-02	1.37	2.20	0.33	0.19	1.08	0.39	0.06	6.01	0.23	92.46
1.5E-01	0.92	1.48	0.25	0.13	0.68	0.26	0.04	6.01	0.24	94.75
2.2E-01	0.62	0.99	0.20	0.09	0.42	0.17	0.03	6.01	0.23	96.34
3.2E-01	0.42	0.67	0.16	0.06	0.26	0.12	0.02	6.01	0.24	97.44
4.8E-01	0.28	0.45	0.13	0.04	0.15	0.08	0.013	6.01	0.24	98.21
7.1E-01	0.19	0.30	0.10	0.03	0.09	0.05	0.009	6.01	0.22	98.73
1.06	0.13	0.20	0.08	0.02	0.05	0.04	0.006	6.01	0.26	99.10
1.57	0.09	0.14	0.06	0.01	0.03	0.02	0.004	6.01	0.19	99.36
2.33	0.06	0.09	0.04	0.01	0.01	0.02	0.003	6.01	0.32	99.55
3.47	0.04	0.06	0.03	0.01	0.01	0.01	0.002	6.01	0.19	99.68
5.15	0.03	0.04	0.02	3.6E-03	2.8E-03	7.3E-03	1.2E-03	6.01	0.26	99.77
7.66	0.02	0.03	0.02	2.4E-03	1.3E-03	4.9E-03	8.2E-04	6.01	0.20	99.84
11.38	0.01	0.02	0.01	1.6E-03	5.8E-04	3.3E-03	5.5E-04	6.01	0.26	99.88
16.91	7.9E-03	1.3E-02	7.5E-03	1.1E-03	2.6E-04	2.2E-03	3.7E-04	6.01	0.24	99.91
25.13	5.3E-03	8.5E-03	5.1E-03	7.3E-04	1.4E-04	1.5E-03	2.5E-04	6.01	0.24	99.94
37.35	3.6E-03	5.7E-03	3.4E-03	4.9E-04	8.5E-05	1.0E-03	1.7E-04	6.01	0.24	99.96
55.51	2.4E-03	3.9E-03	2.3E-03	3.3E-04	4.9E-05	6.8E-04	1.1E-04	6.01	0.24	99.97

The following is a tabulation of the aqueous composition, Cl/NO3 ratio, and MDRH at 150 C of C-186098 (dominant salt NaCl+NaNO3+KNO3) at the deliquescence point vs H2O added:

H2O added moles	K+1 molal	Na+1 molal	SO4-2 molal	Cl-1 molal	NO3-1 molal	Cl/NO3 ratio	MDRH %
2.77E-03	42.34	39.01	0.12	4.42	76.65	0.06	26.30
4.12E-03	28.31	28.54	0.23	4.78	51.58	0.09	33.29
6.13E-03	19.34	21.48	0.39	5.29	34.71	0.15	40.15
9.11E-03	13.67	16.74	0.58	5.84	23.36	0.25	46.38
0.014	10.10	13.53	0.74	6.38	15.72	0.41	51.75
0.020	7.85	11.35	0.84	6.88	10.58	0.65	56.16
0.030	5.71	10.21	0.84	7.05	7.12	0.99	60.23
0.044	3.85	9.24	0.86	6.49	4.79	1.35	65.18
0.066	2.59	7.59	1.23	4.37	3.22	1.35	73.40
0.098	1.74	6.72	1.59	2.94	2.17	1.35	79.17
0.146	1.17	5.18	1.29	1.98	1.46	1.35	84.62
0.216	0.79	3.76	0.96	1.33	0.98	1.35	89.00
0.322	0.53	2.53	0.65	0.90	0.66	1.35	92.47
0.478	0.36	1.70	0.43	0.60	0.44	1.35	94.85
0.711	0.24	1.15	0.29	0.41	0.30	1.35	96.49
1.06	0.16	0.77	0.20	0.27	0.20	1.35	97.61
1.57	0.11	0.52	0.13	0.18	0.14	1.35	98.36
2.33	0.07	0.35	0.09	0.12	0.09	1.35	98.88
3.47	0.05	0.23	0.06	0.08	0.06	1.35	99.22
5.15	0.03	0.16	0.04	0.06	0.04	1.35	99.47
7.66	0.02	0.11	0.03	0.04	0.03	1.35	99.64
11.38	0.02	0.07	0.02	0.03	0.02	1.35	99.75
16.91	0.010	0.048	0.012	0.017	0.013	1.35	99.83
25.13	0.007	0.032	0.008	0.011	0.008	1.35	99.88
37.35	0.005	0.022	0.006	0.008	0.006	1.35	99.92
55.51	0.003	0.015	0.004	0.005	0.004	1.35	99.94

What happens if the calculation is isothermal instead of bubble point? The following is the aqueous composition, Cl/NO3 ratio, and water activity (or RH) at 150 C as a function of amount of H2O added:

H2O mol	Cl-1 molal	K+1 molal	Na+1 molal	NO3-1 molal	Cl/NO3 ratio	RH %
2.78E-03	4.32	55.64	48.62	99.73	0.04	21.91
4.12E-03	4.32	55.60	48.60	99.66	0.04	21.92
6.13E-03	4.32	55.58	48.59	99.63	0.04	21.92
9.11E-03	4.32	55.57	48.59	99.60	0.04	21.92
0.013536	4.32	55.56	48.58	99.58	0.04	21.92
0.020116	4.32	55.55	48.58	99.55	0.04	21.92
0.029894	4.32	55.54	48.58	99.53	0.04	21.92
0.044424	4.32	55.53	48.58	99.50	0.04	21.92
0.066018	4.32	55.52	48.58	99.48	0.04	21.92
0.098107	4.32	55.51	48.58	99.45	0.04	21.92
0.145795	4.32	55.49	48.58	99.41	0.04	21.92
0.216663	4.31	55.48	48.58	99.37	0.04	21.92
0.321977	4.31	55.46	48.58	99.33	0.04	21.92
0.478483	4.31	55.44	48.58	99.28	0.04	21.92
0.711062	4.31	55.42	48.58	99.22	0.04	21.92
1.05669	4.31	55.39	48.58	99.16	0.04	21.92
1.57033	4.31	55.37	48.58	99.08	0.04	21.92
2.33363	4.30	55.33	48.58	99.00	0.04	21.92
3.46795	4.30	55.29	48.58	98.90	0.04	21.92
5.15364	4.30	55.25	48.59	98.79	0.04	21.92
7.6587	4.29	55.20	48.59	98.66	0.04	21.92
11.3814	4.29	55.15	48.59	98.52	0.04	21.92
16.9136	4.28	55.08	48.59	98.36	0.04	21.92
25.135	4.28	55.01	48.59	98.17	0.04	21.92
37.3525	4.27	54.93	48.60	97.96	0.04	21.92
55.5087	4.26	54.83	48.60	97.72	0.04	21.92

Note that the relative humidity or water activity is constant. The output (not shown) of the calculations indicate most of the water is going into the vapor phase (evaporating).

Here is a summary of the potential deliquescent salt mixture compositions resulting from evaporation of leachable components in dusts sampled by the USGS:

Lab No.	Salt mixture composition		Lab No.	Salt mixture composition
Phase I				
C-186098	NaCl+NaNO3+KNO3		C-203117	NaCl+NaNO3+KNO3+ Ca(NO3)2.4KNO3
C-186091	NaCl+NaNO3+KNO3		C-203118	NaCl+KNO3
C-186099	NaCl+NaNO3+KNO3		C-203119	NaCl+KNO3
C-186092	NaCl+NaNO3+KNO3		C-203120	NaCl+NaNO3+Ca(NO3)2+ Ca(NO3)2.4KNO3
C-186093	NaCl+NaNO3+KNO3		C-203121	NaCl+KNO3
C-186100	NaCl+NaNO3+KNO3		C-203122	NaCl+NaNO3+KNO3
C-186094	NaCl+NaNO3+KNO3		C-203123	NaCl+NaNO3+KNO3
C-186101	NaCl+KNO3		C-203124	NaCl+NaNO3+KNO3
C-186102	NaCl+KNO3		C-203125	NaCl+NaNO3+KNO3
C-186095	NaCl+NaNO3+KNO3		C-203126	NaCl+NaNO3+KNO3
C-186096	NaCl+NaNO3+KNO3		C-203127	NaCl+KNO3
C-186097	NaCl+NaNO3+KNO3		C-203128	---
C-186090	NaCl+KNO3		C-203129	---
C-186089	NaCl+NaNO3+KNO3		C-203130	NaCl+KNO3
C-186088	NaCl+KCl+KNO3		C-203131	NaCl+KNO3
C-186087	NaCl+NaNO3+KNO3		C-203132	NaCl+NaNO3+KNO3
C-186086	NaCl+NaNO3+KNO3		C-203133	NaCl+KNO3
C-186085	NaCl+NaNO3+KNO3		C-203134	NaCl+KNO3
C-186084	NaCl+NaNO3+KNO3		C-203135	NaCl+NaNO3+KNO3
C-186082	NaCl+KNO3		C-203136	NaCl+KNO3
C-186081	NaCl+KNO3		C-203137	NaCl+NaNO3+KNO3
C-186080	NaCl+KNO3		C-203138	NaCl+NaNO3+KNO3
C-186077	NaCl+NaNO3+Ca(NO3)2+ Ca(NO3)2.4KNO3		C-203139	NaCl+KNO3
			C-203140	NaCl+KNO3
			C-203141	NaCl+KNO3
Phase II			C-203142	NaCl+KNO3
C-203112	KCl+KNO3		C-203143	NaCl+KNO3
C-203113	KCl+KNO3		C-203144	NaCl+ KNO3
C-203114	KCl+KNO3		C-203145	NaCl+ KCl+KNO3
C-203115	NaCl+KNO3		C-203146	NaCl+ KCl+KNO3
C-203116	NaCl+NaNO3+KNO3		C-203147	NaCl+KNO3

These are the six potential salt assemblages and the number of USGS samples that fit into each assemblage:

NaCl+KNO3	**23**
KCl+KNO3	**3**
NaCl+KCl+KNO3	**3**
NaCl+NaNO3+KNO3	**25**
NaCl+NaNO3+Ca(NO3)2+ Ca(NO3)2.4KNO3	**2**
NaCl+NaNO3+KNO3+ Ca(NO3)2.4KNO3	**1**
Total	**57**

Lab No. C-186098 — representative of NaCl+NaNO3+KNO3 assemblage

Lab No. C-186101 — representative of NaCl+KNO3 assemblage

Lab No. C-186088 — representative of NaCl+KCl+KNO3 assemblage

Lab No. C-203112 — representative of KCl+KNO3 assemblage (had poor analytical data, see page 199 of this notebook)

Lab No. C-203117 — representative of NaCl+NaNO3+KNO3+Ca(NO3)2.4KNO3 assemblage

Lab No. C-203120 — representative of NaCl+NaNO3+Ca(NO3)2+ Ca(NO3)2.4KNO3 assemblage

Deliquescence at high temperature is likely. Calcium-bearing assemblages will have lowest MDRH. But all assemblages will have low Cl/NO3 ratios (less than 10), except for the KCl+KNO3 assemblage, which had poor analytical data and probably can be excluded from consideration. Localized corrosion of Alloy 22 is unlikely.

December 5, 2007

StreamAnalyzer Version 2.0 calculations were conducted to determine the potential concentration of aqueous carbonate species in concentrated salt mixtures in the system Na–K–Cl–NO3 at high temperatures. The carbonate concentrations are relevant to the potential stress corrosion cracking (SCC) of Alloy 22. Previous CNWRA experiments indicated that dissolved carbonate enhances the susceptibility of Alloy 22 to SCC. It is of interest to evaluate the potential for SCC of Alloy 22 in deliquescence brines at high temperatures.

Two sets of calculations were conducted. In one set, atmospheric CO2(g) was assumed to be the source of dissolved carbonate and pCO2 was set to $10^{-3.5}$ atm. In the second set, calcite was assumed to be present and also pCO2 was assumed equal to $10^{-3.5}$ atm. Single-point, bubble point calculations were done at 140 and 160 °C. The second set of calculations was done iteratively by changing the input CO2(g) moles, such that the resulting pCO2 is close to $10^{-3.5}$ atm. pCO2 is calculated from the equation:

$$pCO2(g) = P_{total} \times MoleFraction_{CO2(g)}$$

where P_{total} and $MoleFraction_{CO2(g)}$ are from the StreamAnalyzer output file (the Units Manager in the software needs to be changed to specify Mole Fraction units).

The following summarizes the output of the StreamAnalyzer calculations:

Calculation 1: pCO2 = $10^{-3.5}$ atm, T=140 °C				
Temperature = 140 C				
Pressure	0.624971	atm		
pH	5.99			
Deliq. RH	17.97%			
log pCO2	-3.502	atm		
Stream Inflows				
H2O	55.5087	mol		
NaCl	20	mol		
NaNO3	70	mol		
KNO3	100	mol		
CO2	1.90E-05	mol		
Solids Present:				
NaCl				
KNO3				
NaNO3.KNO3				
Species Output (True Species)				
	Total	Aqueous	Vapor	Solid
	mol	mol	mol	mol

H2O	55.5087	55.5087	9.99E-09	0
NaCl	16.3589	0	0	16.3589
KNO3	6.05874	0	0	6.05874
CO2	1.85E-05	1.85E-05	5.04E-12	0
HCl	3.76E-08	3.76E-08	3.02E-16	0
HNO3	3.86E-07	3.86E-07	2.97E-16	0
KOH	4.21E-17	4.21E-17	0	0
N2O5	1.40E-19	1.40E-19	1.97E-28	0
NaNO3.KNO3	15.0893	0	0	15.0893
Cl-1	3.64114	3.64114	0	0
CO3-2	2.09E-20	2.09E-20	0	0
H3O+1	7.68E-08	7.68E-08	0	0
HCO3-1	4.99E-07	**4.99E-07**	0	0
K+1	78.852	78.852	0	0
Na+1	58.5519	58.5519	0	0
NO3-1	133.763	133.763	0	0
OH-1	1.91E-09	1.91E-09	0	0

Calculation 2: pCO2 = $10^{-3.5}$ atm, T=160 °C				
Temperature = 160 C				
Pressure	0.967591	atm		
pH	6.19			
Deliq. RH	16.47%			
log pCO2	-3.506	atm		
Stream Inflows				
H2O	55.5087	mol		
NaCl	10	mol		
NaNO3	100	mol		
KNO3	90	mol		
CO2	1.10E-05	mol		
Solids Present:				
NaNO3.KNO3				
NaNO3				
NaCl				
Species Output (True Species)				
	Total	Aqueous	Vapor	Solid
	mol	mol	mol	mol
H2O	55.5087	55.5087	1.00E-08	0
NaCl	5.1961	0	0	5.1961
NaNO3	7.86735	0	0	7.86735
CO2	1.05E-05	1.05E-05	3.22E-12	0
HCl	7.25E-08	7.25E-08	3.70E-16	0
HNO3	4.28E-07	4.28E-07	4.26E-16	0
KOH	7.35E-16	7.35E-16	0	0
N2O5	7.52E-19	7.52E-19	6.97E-28	0

NaNO3.KNO3	21.4768	0	0	21.4768
Cl-1	4.8039	4.8039	0	0
CO3-2	4.39E-21	4.39E-21	0	0
H3O+1	5.08E-08	5.08E-08	0	0
HCO3-1	5.38E-07	**5.38E-07**	0	0
K+1	68.5232	68.5232	0	0
Na+1	75.4598	75.4598	0	0
NO3-1	139.179	139.179	0	0
OH-1	1.36E-08	1.36E-08	0	0

Calculation 3: Calcite saturation; $pCO2 = 10^{-3.5}$ atm, T=140 °C

Temperature = 140 C				
Pressure	0.632161	atm		
pH	9.18			
Deliq. RH	18.17%			
log pCO2	-3.503	atm		
Stream Inflows				
H2O	55.5087	mol		
NaCl	10	mol		
NaNO3	100	mol		
KNO3	90	mol		
CaCO3	1	mol		
CO2	4.05E-04	mol		
Solids Present:				
CaCO3				
NaCl				
NaNO3				
NaNO3.KNO3				
Species Output (True Species)				
	Total	Aqueous	Vapor	Solid
	mol	mol	mol	mol
H2O	55.5083	55.5083	1.00E-08	0
NaCl	6.4709	0	0	6.4709
NaNO3	29.797	0	0	29.797
CaCO3	0.999605	**7.77E-04**	0	0.998828
CO2	1.60E-05	1.60E-05	4.96E-12	0
CaCl2	4.62E-06	4.62E-06	0	0
HCl	2.34E-11	2.34E-11	1.88E-19	0
HNO3	2.48E-10	2.48E-10	1.91E-19	0
KOH	6.69E-14	6.69E-14	0	0
N2O5	5.79E-26	5.79E-26	8.13E-35	0
NaNO3.KNO3	14.5373	0	0	14.5373
Ca+2	3.88E-04	3.88E-04	0	0

CaOH+1	2.78E-06	2.78E-06	0	0
Cl-1	3.52909	3.52909	0	0
CO3-2	5.86E-14	5.86E-14	0	0
H3O+1	4.96E-11	4.96E-11	0	0
HCO3-1	7.84E-04	**7.84E-04**	0	0
K+1	75.4627	7.55E+01	0	0
Na+1	59.1948	5.92E+01	0	0
NO3-1	131.128	1.31E+02	0	0
OH-1	3.26E-06	3.26E-06	0	0

1. For Na-K-Cl-NO3 solutions in which atmospheric CO2(g) (pCO2 = 10^-3.5 atm) is the only source of dissolved carbonate, the calculated concentration of HCO3- species is ~5E-7 molal. No SCC is expected under this condition based on previous CNWRA experiments.

2. For Na-K-Cl-NO3 solutions in which calcite (present in dusts) is the source of dissolved carbonate and in which the aqueous carbonate concentration is constrained by the atmospheric partial pressure of CO2(g) [i.e., pCO2 = 10^3-5 atm], the concentrations of the dominant aqueous carbonate species, CaCO3(aq) and HCO3-, are as follows:

CaCO3(aq) = 8E-4 or 9E-4 molal (at 140 or 160 C)

HCO3- = 8E-4 or 5E-4 molal (at 140 or 160 C)

These values are above the 1E-4 threshold value typically assumed for the occurrence of SCC.

Calculation 4: Calcite saturation; pCO2 = $10^{-3.5}$ atm, T=160 °C				
Temperature = 160 C				
Pressure	0.967561	atm		
pH	9.19			
Deliq. RH	16.47%			
log pCO2	-3.504	atm		
Stream Inflows				
H2O	55.5087	mol		
NaCl	10	mol		
NaNO3	100	mol		
KNO3	90	mol		
CaCO3	1	mol		
CO2	2.70E-04	mol		
Solids Present:				
CaCO3				
NaCl				
NaNO3				
NaNO3.KNO3				
Species Output (True Species)				
	Total	Aqueous	Vapor	Solid
	mol	mol	mol	mol
H2O	55.5084	55.5084	1.00E-08	0
NaCl	5.19601	0	0	5.19601
NaNO3	7.86783	0	0	7.86783
CaCO3	0.999722	**9.32E-04**	0	0.99879
CO2	1.05E-05	1.05E-05	3.24E-12	0
CaCl2	4.51E-06	4.51E-06	0	0
HCl	7.30E-11	7.30E-11	3.72E-19	0
HNO3	4.31E-10	4.31E-10	4.28E-19	0
KOH	7.30E-13	7.30E-13	0	0
N2O5	7.62E-25	7.62E-25	7.05E-34	0
NaNO3.KNO3	21.4748	0	0	21.4748
Ca+2	2.68E-04	2.68E-04	0	0
CaOH+1	5.37E-06	5.37E-06	0	0
Cl-1	4.80398	4.80398	0	0
CO3-2	4.36E-15	4.36E-15	0	0
H3O+1	5.11E-11	5.11E-11	0	0
HCO3-1	5.38E-04	**5.38E-04**	0	0
K+1	68.5252	68.5252	0	0
Na+1	75.4614	75.4614	0	0
NO3-1	139.183	139.183	0	0
OH-1	1.35E-05	1.35E-05	0	0

The following are the concentrations of aqueous carbonate species at the deliquescence point for lab sample C-186098 (representative of NaCl+NaNO3+KNO3 assemblage), as a function of water added to initially dry solids. The values were taken from the StreamAnalyzer output for bubble point calculations at 150 °C.

	Lab Sample C-186098		
H2O added moles	**CaCO3 - Aq molal**	**CO3-2 molal**	**HCO3-1 molal**
2.77E-03	5.80E-04	1.06E-11	1.11E-02
4.12E-03	4.58E-04	2.56E-10	1.26E-02
6.13E-03	3.80E-04	8.12E-09	1.45E-02
9.11E-03	3.29E-04	2.45E-07	1.67E-02
0.0135315	2.95E-04	5.26E-06	1.91E-02
0.0201079	2.72E-04	6.88E-05	2.16E-02
0.029881	2.53E-04	4.90E-04	2.33E-02
0.0444033	2.34E-04	2.18E-03	2.61E-02
0.0659737	2.08E-04	8.05E-03	3.70E-02
0.0980213	1.93E-04	2.17E-02	4.87E-02
0.145607	1.80E-04	6.46E-02	7.15E-02
0.216415	1.71E-04	6.08E-02	6.35E-02
0.321704	1.65E-04	3.58E-02	4.72E-02
0.478181	1.61E-04	1.98E-02	3.50E-02
0.710735	1.58E-04	1.03E-02	2.55E-02
1.05635	1.56E-04	5.04E-03	1.82E-02
1.56997	1.55E-04	2.36E-03	1.25E-02
2.33327	1.54E-04	1.07E-03	8.35E-03
3.46761	1.54E-04	4.73E-04	5.36E-03
5.1533	1.53E-04	2.60E-04	3.59E-03
7.65835	1.53E-04	1.49E-04	2.46E-03
11.3811	1.53E-04	8.44E-05	1.69E-03
16.9133	1.53E-04	4.80E-05	1.17E-03
25.1346	1.53E-04	2.75E-05	8.23E-04
37.3521	1.53E-04	1.61E-05	5.91E-04
55.5082	1.53E-04	9.72E-06	4.38E-04

The following are the concentrations of aqueous carbonate species at the deliquescence point for lab sample C-186101 (representative of NaCl+KNO3 assemblage), as a function of water added to initially dry solids. The values were taken from the StreamAnalyzer output for bubble point calculations at 150 °C.

	Lab Sample C-186101		
H2O added moles	**CaCO3 - Aq molal**	**CO3-2 molal**	**HCO3-1 molal**
2.78E-03	3.89E-04	1.54E-11	1.33E-03
4.12E-03	3.35E-04	4.74E-10	1.70E-03
6.13E-03	2.99E-04	1.08E-08	2.11E-03
9.11E-03	2.74E-04	1.53E-07	2.53E-03
1.35E-02	2.58E-04	1.26E-06	2.94E-03
2.01E-02	2.47E-04	6.21E-06	3.30E-03
2.99E-02	2.38E-04	1.92E-05	3.51E-03
0.044	2.28E-04	4.03E-05	3.54E-03
0.066	2.03E-04	9.47E-05	4.97E-03
0.098	1.89E-04	1.74E-04	6.49E-03
0.146	1.75E-04	7.82E-05	3.98E-03
0.217	1.68E-04	4.57E-05	2.90E-03
0.322	1.62E-04	4.05E-05	2.48E-03
0.478	1.59E-04	3.36E-05	1.77E-03
0.711	1.57E-04	2.65E-05	1.28E-03
1.06	1.56E-04	2.01E-05	9.27E-04
1.57	1.55E-04	1.47E-05	6.79E-04
2.33	1.54E-04	1.05E-05	5.02E-04
3.47	1.53E-04	7.32E-06	3.74E-04
5.15	1.53E-04	5.05E-06	2.81E-04
7.66	1.53E-04	3.46E-06	2.12E-04
11.4	1.53E-04	2.38E-06	1.70E-04
16.9	1.53E-04	2.21E-06	1.78E-04
25.1	1.53E-04	2.03E-06	1.83E-04
37.4	1.53E-04	1.86E-06	1.85E-04
55.5	1.53E-04	1.68E-06	1.84E-04

The following are the concentrations of aqueous carbonate species at the deliquescence point for lab sample C-186088 (representative of NaCl+KCl+KNO3 assemblage), as a function of water added to initially dry solids. The values were taken from the StreamAnalyzer output for bubble point calculations at 150 °C.

	Lab Sample C-186101		
H2O added moles	**CaCO3 - Aq molal**	**CO3-2 molal**	**HCO3-1 molal**
2.77E-03	5.86E-04	1.44E-10	5.38E-02
4.12E-03	5.11E-04	8.44E-10	6.15E-02
6.12E-03	4.23E-04	2.52E-08	6.71E-02
9.10E-03	3.64E-04	8.34E-07	7.39E-02
1.35E-02	3.24E-04	2.28E-05	8.33E-02
2.01E-02	2.91E-04	5.38E-04	1.13E-01
2.98E-02	2.46E-04	6.41E-03	1.67E-01
0.044	2.17E-04	4.75E-02	2.32E-01
0.066	2.02E-04	2.06E-01	2.87E-01
0.098	1.95E-04	5.48E-01	3.12E-01
0.145	1.92E-04	1.05E+00	3.17E-01
0.216	1.82E-04	1.03E+00	2.59E-01
0.321	1.71E-04	6.73E-01	1.95E-01
0.477	1.65E-04	4.31E-01	1.53E-01
0.709	1.61E-04	2.70E-01	1.23E-01
1.05	1.58E-04	1.64E-01	9.98E-02
1.57	1.56E-04	9.66E-02	8.09E-02
2.33	1.55E-04	5.46E-02	6.48E-02
3.46	1.54E-04	2.94E-02	5.08E-02
5.15	1.54E-04	1.51E-02	3.89E-02
7.65	1.53E-04	8.79E-03	2.75E-02
11.4	1.53E-04	5.08E-03	1.93E-02
16.9	1.53E-04	2.84E-03	1.36E-02
25.1	1.53E-04	1.54E-03	9.50E-03
37.3	1.53E-04	8.15E-04	6.61E-03
55.5	1.53E-04	4.21E-04	4.57E-03

The following are the concentrations of aqueous carbonate species at the deliquescence point for lab sample C-203117 (representative of NaCl+NaNO3+KNO3+ Ca(NO3)2.4KNO3 assemblage), as a function of water added to initially dry solids. The values were taken from the StreamAnalyzer output for bubble point calculations at 150 °C.

	Lab Sample C-203117		
H2O added moles	**CaCO3 - Aq molal**	**CO3-2 molal**	**HCO3-1 molal**
2.78E-03	9.73E-04	6.29E-20	4.33E-05
4.12E-03	8.46E-04	5.81E-20	4.14E-05
6.13E-03	6.44E-04	1.03E-18	4.07E-05
9.11E-03	5.01E-04	2.84E-17	3.83E-05
1.35E-02	4.07E-04	1.05E-15	3.41E-05
2.01E-02	3.44E-04	4.46E-14	3.12E-05
2.99E-02	3.01E-04	1.59E-12	3.06E-05
0.044424	2.59E-04	3.21E-11	3.54E-05
0.066018	2.20E-04	3.93E-10	4.49E-05
0.098107	1.97E-04	3.10E-09	5.40E-05
0.145795	1.81E-04	1.53E-08	6.18E-05
0.216662	1.72E-04	4.97E-08	6.79E-05
0.321977	1.65E-04	1.15E-07	7.18E-05
0.478482	1.61E-04	2.05E-07	7.33E-05
0.711061	1.58E-04	2.96E-07	7.19E-05
1.05669	1.56E-04	3.65E-07	6.82E-05
1.57032	1.55E-04	4.00E-07	6.27E-05
2.33362	1.54E-04	4.02E-07	5.64E-05
3.46794	1.54E-04	3.84E-07	5.01E-05
5.15363	1.53E-04	3.54E-07	4.43E-05
7.65869	1.53E-04	3.21E-07	3.93E-05
11.3814	1.53E-04	2.90E-07	3.52E-05
16.9136	1.53E-04	2.62E-07	3.36E-05
25.135	1.53E-04	2.40E-07	4.07E-05
37.3525	1.53E-04	2.23E-07	4.48E-05
55.5086	1.53E-04	2.10E-07	4.57E-05

The following are the concentrations of aqueous carbonate species at the deliquescence point for lab sample C-203120 (representative of NaCl+NaNO3+Ca(NO3)2+ Ca(NO3)2.4KNO3 assemblage), as a function of water added to initially dry solids. The values were taken from the StreamAnalyzer output for bubble point calculations at 150 °C.

	Lab Sample C-203120		
H2O added moles	**CaCO3 - Aq molal**	**CO3-2 molal**	**HCO3-1 molal**
2.78E-03	1.25E-03	3.18E-04	6.71E-12
4.12E-03	9.44E-04	2.74E-04	4.96E-12
6.13E-03	7.49E-04	2.24E-04	3.48E-12
9.11E-03	6.32E-04	1.65E-04	2.30E-12
1.35E-02	5.67E-04	1.03E-04	1.53E-12
2.01E-02	5.16E-04	5.84E-05	1.25E-12
2.99E-02	4.21E-04	3.91E-05	1.87E-12
0.044424	3.59E-04	2.25E-05	3.54E-12
0.066018	3.15E-04	1.28E-05	7.65E-12
0.098107	2.71E-04	8.68E-06	2.54E-11
0.145795	2.28E-04	7.00E-06	1.29E-10
0.216663	2.01E-04	6.03E-06	5.17E-10
0.321977	1.84E-04	5.70E-06	1.56E-09
0.478483	1.73E-04	5.91E-06	3.53E-09
0.711062	1.66E-04	6.62E-06	6.25E-09
1.05669	1.62E-04	7.82E-06	8.91E-09
1.57033	1.59E-04	9.47E-06	1.06E-08
2.33363	1.56E-04	1.15E-05	1.09E-08
3.46795	1.55E-04	1.39E-05	1.00E-08
5.15363	1.54E-04	1.67E-05	8.47E-09
7.65869	1.54E-04	1.96E-05	6.70E-09
11.3814	1.53E-04	2.12E-05	4.24E-09
16.9136	1.53E-04	2.30E-05	2.65E-09
25.135	1.53E-04	2.52E-05	1.66E-09
37.3525	1.53E-04	2.78E-05	1.05E-09
55.5086	1.53E-04	3.09E-05	6.71E-10

The following are the concentrations of aqueous carbonate species at the deliquescence point for lab sample C-203112 (representative of KCl+KNO3 assemblage; poor analytical data), as a function of water added to initially dry solids. The values were taken from the StreamAnalyzer output for bubble point calculations at 150 °C.

Lab Sample C-203120			
H2O added moles	**CaCO3 - Aq molal**	**CO3-2 molal**	**HCO3-1 molal**
2.66E-03	3.83E-04	1.05E+01	2.37E+00
3.96E-03	3.83E-04	1.05E+01	2.37E+00
5.88E-03	3.83E-04	1.05E+01	2.37E+00
8.84E-03	3.20E-04	8.30E+00	1.67E+00
0.013245	2.62E-04	6.41E+00	1.22E+00
0.019744	2.31E-04	5.33E+00	1.05E+00
0.029475	2.02E-04	3.97E+00	7.88E-01
0.043968	1.83E-04	2.60E+00	5.76E-01
0.065506	1.71E-04	1.69E+00	4.33E-01
0.097528	1.65E-04	1.08E+00	3.29E-01
0.145138	1.61E-04	6.81E-01	2.51E-01
0.215898	1.58E-04	4.23E-01	1.96E-01
0.321071	1.57E-04	2.60E-01	1.56E-01
0.477405	1.55E-04	1.55E-01	1.25E-01
0.709789	1.54E-04	8.88E-02	9.94E-02
1.05521	1.54E-04	4.88E-02	7.78E-02
1.56864	1.53E-04	2.55E-02	5.96E-02
2.33175	1.53E-04	1.27E-02	4.45E-02
3.46592	1.53E-04	6.09E-03	3.24E-02
5.15149	1.53E-04	2.82E-03	2.30E-02
7.65647	1.53E-04	1.28E-03	1.61E-02
11.3791	1.53E-04	5.76E-04	1.11E-02
16.9113	1.53E-04	2.61E-04	7.53E-03
25.1326	1.53E-04	1.44E-04	5.09E-03
37.3502	1.53E-04	8.48E-05	3.43E-03
55.5063	1.53E-04	4.95E-05	2.32E-03