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APPENDIX A - Microthermometry Data

Data is interpreted and discussed in Chapter 2.

Teu	Eutectic temperature / first melting temperature
Tm (aq)	Final melting temperature of ice
Tm (CO ₂)	Final melting temperature of CO ₂
Th V (CO ₂)	Homogenisation temperature of CO ₂ (L → V)
ThV	Homogenisation temperature of vapour phase
Td _{Syl}	Dissolution temperature of Sylvite daughter mineral
Td _{Hal}	Dissolution temperature of Halite daughter mineral
Td _{FPS}	Dissolution temperature of Ferropyrosmalite daughter mineral
Td _{Cal}	Dissolution temperature of Calcite daughter mineral
Td _{Ukn}	Dissolution temperature of unknown daughter mineral/s
TD	Decrepitation temperature
Th	Final homogenisation temperature

MS INCLUSIONS

DATA APPENDICES HAVE BEEN REMOVED

LVD INCLUSIONS

DATA APPENDICES HAVE BEEN REMOVED

CB INCLUSIONS

DATA APPENDICES HAVE BEEN REMOVED

CO2 INCLUSIONS

DATA APPENDICES HAVE BEEN REMOVED

40_M12: CB Inclusion

Inclusion Volume:	754 μm^3
Vapour Volume:	127.8 μm^3
Vapour Volume %:	16.95
CO ₂ : 95%	CO ₂ mass ($\times 10^{-12}\text{g}$): 103.2
N ₂ : 5%	N ₂ mass ($\times 10^{-12}\text{g}$): 5.4



Daughter Phases:

Species	Density (g/cm^3)	Volume (μm^3)	Mass ($\times 10^{-12}\text{g}$)
Halite	2.17	125.0	271.3
Sylvite	1.99	44.7	89.0
CaCO ₃	2.72	54.6	148.5
	Total	224.3	
	Daughter Vol %:	29.7	

Liquid Volume:	401.9 μm^3	Liquid Mass ($\times 10^{-12}\text{g}$):	602.9
Liquid Volume %:	62.4		(for $\rho = 1.5 \text{ g}/\text{cm}^3$)

Solute and solvent masses

		($\times 10^{-12}\text{g}$)	wt%
mass NaCl	=271.3 + (0.0062 x 602.9)	308.63	30.81
mass KCl	=89 + (0.0322 x 602.9)	126.33	12.61
mass FeCl ₂	=(0.1 x 602.9)	60.29	6.02
mass CaCO ₃	=148.5	148.51	14.83
mass H ₂ O	=(0.4134 x 602.9)	249.22	24.88
mass CO ₂	=103.2	103.20	10.30
mass N ₂	=5.4	5.43	0.54
TOTAL		1001.60	100.00

Fluid Composition:

	($\times 10^{-12}\text{g}$)		($\times 10^{-12}\text{g}$)		Molarity
mass Na ⁺	121.41	mass Cl ⁻	187.22	m Na ⁺	2.83
mass K ⁺	66.26	mass Cl ⁻	60.07	m K ⁺	0.95
mass Fe ²⁺	26.56	mass Cl ⁻	33.72	m Fe ²⁺	0.44
mass Ca ²⁺	59.47			m Ca ²⁺	2.97
		TOTAL Cl ⁻	281.02		
mass CO ₃ ⁻	89.04			m Cl ⁻	12.67
mass CO ₂	103.20			m CO ₃ ⁻	0.46
mass N ₂	5.43			m CO ₂	5.7
mass H ₂ O	2057.73			m N ₂	0.24
TOTAL	2810.11			m H ₂ O	16.16

45.77 Wt % Salts

852_1_1: MS Inclusion

Inclusion Volume: 584.95 μm^3
 Vapour Volume: 53.2 μm^3
 Vapour Volume %: 9.09



Daughter Phases:

Species	Density (g/cm^3)	Volume (μm^3)	Mass ($\times 10^{-12}\text{g}$)
Halite	2.17	296.3	643.0
Sylvite	1.99	64.0	127.4
Ferropyrosmalite	3.12	34.7	108.3
	Total	395.0	
	Daughter Vol %:	67.5	

Liquid Volume: 136.8 μm^3 **Liquid Mass ($\times 10^{-12}\text{g}$):** 205.1
Liquid Volume %: 23.38 (for $\rho = 1.5 \text{ g}/\text{cm}^3$)

Solute and solvent masses

		($\times 10^{-12}\text{g}$)	wt%
mass NaCl	=643 + (0.0062 x 205.1)	644.24	64.32
mass KCl	=127.4 + (0.0322 x 205.1)	133.97	13.38
mass FeCl ₂	=(0.1 x 205.1)	20.51	2.05
mass CaCl ₂	=(0.4482 x 205.1)	91.94	9.18
mass H ₂ O	=(0.0803 x 108.3) + (0.4134 x 205.1)	93.49	9.33
mass FeO	=(0.4908 x 108.3)	53.14	5.31
mass MnO	=(0.0471 x 108.3)	5.10	0.51
mass MgO	=(0.0038 x 108.3)	0.41	0.04
mass SiO ₂	=(0.3421 x 108.3)	37.04	3.70
Mass Cl	=(0.0404 x 108.3)	4.37	0.44
TOTAL		1084.21	108.25

Fluid Composition:

	($\times 10^{-12}\text{g}$)		($\times 10^{-12}\text{g}$)		Molarity
mass Na ⁺	253.43	mass Cl ⁻	390.82	m Na ⁺	13.27
mass K ⁺	70.26	mass Cl ⁻	63.70	m K ⁺	1.77
mass Fe ²⁺	50.34	mass Cl ⁻	11.47	m Fe ²⁺	0.86
mass Ca ²⁺	33.21	mass Cl ⁻	58.73	m Ca ²⁺	0.79
mass Mg ²⁺	0.25			m Mg ²⁺	0.01
mass Mn ²⁺	3.95			m Mn ²⁺	0.07
mass Si ⁴⁺	17.31			m Si ⁴⁺	0.58
		TOTAL Cl ⁻	529.10	m Cl ⁻	26.88
mass O	32.87			m O	1.95
mass H ₂ O	93.49			m H ₂ O	5.24
TOTAL	1084.21				

81.07 Wt % Salts

15_1_3: MS Inclusion

Inclusion Volume: 154.6 μm^3

Vapour Volume: 4.2 μm^3

Vapour Volume %: 2.72



Daughter Phases:

Species	Density (g/cm^3)	Volume (μm^3)	Mass ($\times 10^{-12}\text{g}$)
Halite	2.17	64.0	138.9
Sylvite	1.99	9.3	18.5
Ferropyrosmalite	3.12	6.8	21.1

Total
Daughter Vol %: 80.1
51.8

Liquid Volume:	70.4 μm^3	Liquid Mass ($\times 10^{-12}\text{g}$):	105.5
Liquid Volume %:	45.5		(for $\rho = 1.5 \text{ g}/\text{cm}^3$)

Solute and solvent masses

		($\times 10^{-12}\text{g}$)	wt%
mass NaCl	=138.9 + (0.0062 x 105.5)	139.53	13.93
mass KCl	=18.5 + (0.0322 x 105.5)	21.90	2.19
mass FeCl₂	=(0.1 x 105.5)	61.35	6.13
mass CaCl₂	=(0.4482 x 105.5)	47.30	4.72
mass H₂O	=(0.0803 x 21.1) + (0.4134 x 105.5)	45.32	4.52
mass FeO	=(0.4908 x 105.5)	51.79	5.17
mass MnO	=(0.0471 x 105.5)	4.97	0.50
mass MgO	=(0.0038 x 105.5)	0.40	0.04
mass SiO₂	=(0.3421 x 105.5)	36.10	3.60
Mass Cl	=(0.0404 x 105.5)	4.26	0.43
TOTAL		412.93	41.23

Fluid Composition:

	($\times 10^{-12}\text{g}$)		($\times 10^{-12}\text{g}$)		Molarity
mass Na ⁺	54.89	mass Cl ⁻	84.65	m Na ⁺	6.67
mass K ⁺	11.49	mass Cl ⁻	10.42	m K ⁺	0.73
mass Fe ²⁺	67.29	mass Cl ⁻	34.32	m Fe ²⁺	3.42
mass Ca ²⁺	17.08	mass Cl ⁻	30.21	m Ca ²⁺	1.08
mass Mg ²⁺	0.24			m Mg ²⁺	0.02
mass Mn ²⁺	3.85			m Mn ²⁺	0.17
mass Si ⁴⁺	16.87			m Si ⁴⁺	1.52
		TOTAL Cl ⁻	163.86	m Cl ⁻	18.56
mass O	32.04			m O	5.26
mass H ₂ O	45.32			m H ₂ O	6.84
TOTAL	412.93				

62.84 Wt % Salts

15_1_15: MS Inclusion

Inclusion Volume: 703.6 μm^3

Vapour Volume: 68.6 μm^3

Vapour Volume %: 9.75



Daughter Phases:

Species	Density (g/cm^3)	Volume (μm^3)	Mass ($\times 10^{-12}\text{g}$)
Halite	2.17	179.7	389.9
Sylvite	1.99	49.3	98.1
Ferropyrosmalite	3.12	65.5	204.4
	Total	294.5	
	Daughter Vol %:	41.9	

Liquid Volume:	340.5 μm^3	Liquid Mass ($\times 10^{-12}\text{g}$):	510.8
Liquid Volume %:	48.4		(for $\rho = 1.5 \text{ g}/\text{cm}^3$)

Solute and solvent masses

		($\times 10^{-12}\text{g}$)	wt%
mass NaCl	=389.9 + (0.0062 x 510.8)	393.12	39.25
mass KCl	=98.1 + (0.0322 x 510.8)	114.55	11.44
mass FeCl₂	=(0.1 x 510.8)	51.08	5.10
mass CaCl₂	=(0.4482 x 510.8)	228.92	22.86
mass H₂O	=(0.0803 x 204.4) + (0.4134 x 510.8)	227.55	22.72
mass FeO	=(0.4908 x 204.4)	250.68	25.03
mass MnO	=(0.0471 x 204.4)	24.06	2.40
mass MgO	=(0.0038 x 204.4)	1.94	0.19
mass SiO₂	=(0.3421 x 204.4)	174.73	17.44
Mass Cl	=(0.0404 x 204.4)	20.63	2.06
TOTAL		1487.25	148.49

Fluid Composition:

	($\times 10^{-12}\text{g}$)		($\times 10^{-12}\text{g}$)		Molarity
mass Na ⁺	154.64	mass Cl ⁻	238.47	M Na⁺	5.05
mass K ⁺	60.08	mass Cl ⁻	54.47	M K⁺	1.08
mass Fe ²⁺	217.36	mass Cl ⁻	28.57	M Fe²⁺	3.01
mass Ca ²⁺	82.68	mass Cl ⁻	146.24	M Ca²⁺	1.47
mass Mg ²⁺	1.17			M Mg²⁺	0.03
mass Mn ²⁺	18.63			M Mn²⁺	0.23
mass Si ⁴⁺	81.67			M Si⁴⁺	2.07
		TOTAL Cl ⁻	488.39	M Cl⁻	13.79
mass O	155.07			M O	7.28
mass H ₂ O	227.55			M H₂O	10.03
TOTAL	1487.25				

57.55 Wt % Salts

36B_51: MS Inclusion

Inclusion Volume: 1082.8 μm^3
 Vapour Volume: 67.7 μm^3
 Vapour Volume %: 6.25



Daughter Phases:

Species	Density (g/cm ³)	Volume (μm^3)	Mass ($\times 10^{-12}\text{g}$)
Halite	2.17	583.7	1266.6
Sylvite	1.99	103.5	206.0
Ferropyrosmalite	3.12	101.7	317.3
	Total	788.9	
	Daughter Vol %:	72.9	

Liquid Volume:	226.2 μm^3	Liquid Mass ($\times 10^{-12}\text{g}$):	339.3
Liquid Volume %:	20.89		(for $\rho = 1.5 \text{ g/cm}^3$)

Solute and solvent masses

		($\times 10^{-12}\text{g}$)	wt%
mass NaCl	=1266.6 + (0.0062 x 339.3)	1268.73	126.67
mass KCl	=206.0 + (0.0322 x 339.3)	216.89	21.65
mass FeCl ₂	=(0.1 x 339.3)	61.35	6.13
mass CaCl ₂	=(0.4482 x 339.3)	152.07	15.18
mass H ₂ O	=(0.0803 x 317.3) + (0.4134 x 339.3)	165.75	16.55
mass FeO	=(0.4908 x 317.3)	166.53	16.63
mass MnO	=(0.0471 x 317.3)	15.98	1.60
mass MgO	=(0.0038 x 317.3)	1.29	0.13
mass SiO ₂	=(0.3421 x 317.3)	116.07	11.59
Mass Cl	=(0.0404 x 317.3)	13.71	1.37
TOTAL		2178.37	217.49

Fluid Composition:

	($\times 10^{-12}\text{g}$)		($\times 10^{-12}\text{g}$)																							
mass Na ⁺	499.08	mass Cl ⁻	769.65	<table border="1"> <thead> <tr> <th colspan="2">Molarity</th> </tr> </thead> <tbody> <tr> <td>m Na⁺</td> <td>12.93</td> </tr> <tr> <td>m K⁺</td> <td>1.41</td> </tr> <tr> <td>m Fe²⁺</td> <td>1.36</td> </tr> <tr> <td>m Ca²⁺</td> <td>0.65</td> </tr> <tr> <td>m Mg²⁺</td> <td>0.01</td> </tr> <tr> <td>m Mn²⁺</td> <td>0.10</td> </tr> <tr> <td>m Si⁴⁺</td> <td>0.91</td> </tr> <tr> <td>m Cl⁻</td> <td>24.74</td> </tr> <tr> <td>m O</td> <td>3.10</td> </tr> <tr> <td>m H₂O</td> <td>4.57</td> </tr> </tbody> </table>	Molarity		m Na ⁺	12.93	m K ⁺	1.41	m Fe ²⁺	1.36	m Ca ²⁺	0.65	m Mg ²⁺	0.01	m Mn ²⁺	0.10	m Si ⁴⁺	0.91	m Cl ⁻	24.74	m O	3.10	m H ₂ O	4.57
Molarity																										
m Na ⁺	12.93																									
m K ⁺	1.41																									
m Fe ²⁺	1.36																									
m Ca ²⁺	0.65																									
m Mg ²⁺	0.01																									
m Mn ²⁺	0.10																									
m Si ⁴⁺	0.91																									
m Cl ⁻	24.74																									
m O	3.10																									
m H ₂ O	4.57																									
mass K ⁺	113.75	mass Cl ⁻	103.14																							
mass Fe ²⁺	156.48	mass Cl ⁻	34.32																							
mass Ca ²⁺	54.93	mass Cl ⁻	97.15																							
mass Mg ²⁺	0.78																									
mass Mn ²⁺	12.38																									
mass Si ⁴⁺	54.26																									
		TOTAL Cl ⁻	1017.96																							
mass O	103.02																									
mass H ₂ O	165.75																									
TOTAL	2178.37																									

84.06 Wt % Salts

APPENDIX C - Laser Raman Data

Methodology is detailed in Chapter 2, section 2.3.2

Data is discussed in and interpreted in Chapter 2, section 2.4.3

DATA APPENDICES HAVE BEEN REMOVED

APPENDIX D - NOBLE GAS AND HALOGEN DATA

Methodology is detailed in Chapter 3, section 3.2

Data is discussed and interpreted in Chapter 3, section 3.4

DATA APPENDICES HAVE BEEN REMOVED

APPENDIX E - PIXE DATA

DATA APPENDICES HAVE BEEN REMOVED

APPENDIX F - LA-ICP-MS DATA

Methodology is detailed in Chapter 4, section 4.2.2

Data is discussed in and interpreted in Chapter 4, sections 4.3 & 4.4

DATA APPENDICES HAVE BEEN REMOVED

APPENDIX G - HCh control file algorithms

Model results are presented and discussed in Chapter 5.

Symbol	Variable
T	Current temperature (°C)
P	Current pressure (bars)
I	Current step number
N	Current wave number
[1]	Input composition (1 = first, 2 = second, etc)
[A]	Bulk composition of aqueous phase in system from current wave, previous step
[S]	Bulk composition of solid phase in system from current wave, previous step
[*]	Current total system bulk composition (all phases)

[1] = rock
[2] = fluid1
[3] = fluid2

Unless otherwise specified all models are isothermal and isobaric at 600 °C and 3000 bars.

Basic Model Algorithms (after Cleverley and Oliver, 2005)

▪ *Fluid Mixing model - rock buffered (Figure 5.1A)*

Initial Step:

$$[*] = [2] + (0.1*[1])$$

General Step:

$$[*] = ([2]*(i/50)) + ([3]*(1-(i/50))) + (0.1*[1])$$

Stop when: i=50

▪ *Batch Reaction model for variable fluid rock ratios (Figure 5.1B)*

Initial Step:

$$[*] = [1] + ([2]*10^{-6})$$

General Step:

$$[*] = [1] + ([2]*(10^{i-6}))$$

Stop when: i=10

▪ *Fluid Mixing model - Isobaric Cooling (Figure 5.1C)*

Step Series 0, Initial Step:

$$T = 600$$

$$P = 3000$$

$$[*] = [1] + (0.1*[2])$$

Step Series 0, General Step:

$T=600$
 $P=3000$
 $[*] = ([1]*(i/50)) + ([3]*(1-(i/50))) + (0.1*[2])$
 Stop when: $i=50$
 Step Series N, Initial Step
 $T = T-(10*N)$
 $P = 3000$
 $[*] = [1] + (0.1*[2])$
 Step Series N, General Step
 $T = T-(10*N)$
 $P = 3000$
 $[*] = ([1]*(i/50)) + ([3]*(1-(i/50))) + (0.1*[2])$
 Stop when: $N=30$

- ***Flow-through model (Figure 5.1D)***

Initial Step:
 $[*] = [2]$
 General Step:
 $[*] = [A] + ([1]*(0.015*i))$
 Stop when: $i=20$

- ***Flush model (Figure 5.1E)***

Initial Step:
 $[*] = [1]$
 General Step:
 $[*] = [S] + (0.1*[2])$
 Stop when $i=20$

Specific fluid mixing models (Section 5.4.3.1)

- ***Model 1 (Figure 5.6)***

Initial Step:
 $T=400$
 $P=2000$
 $[*] = [2] + [3]$
 General Step:
 $T=400$
 $P=2000$
 $[*] = [A] + (0.1*[1])$
 Stop when: $i=20$

- ***Model 2 (Figure 5.7)***

Initial Step:
 $T=400$
 $P=2000$

$[*] = [2] + [3]$
General Step:
T=400
P=2000
 $[*] = [A] + (0.1*[1]) + ([3]*(i/20))$
Stop when: i=20

▪ **Model 3 (Figure 5.8)**

Initial Step:
T=400
P=2000
 $[*] = [1] + [2]$
General Step:
T=400
P=2000
 $[*] = [S] + [A] + ([3]*(i/20))$
Stop when: i=20

DATA APPENDICES HAVE BEEN REMOVED