

## APPENDIX 2

### Percentage share of element species in water

	Points	1*	2	3	4	5	6	7	8	9	10
	Species*	%									
Ba	BaSO <sub>4</sub>	52.9	51.4	52.8	52.2	53.7	50.8	50.4	55.7	55.2	53.5
	Ba <sup>2+</sup>	46.3	47.7	46.6	47.2	45.4	48.3	48.7	43.6	44.0	45.6
	BaHCO <sub>3</sub> <sup>+</sup>	0.9	0.9	0.6	0.6	0.9	0.9	0.9	0.7	0.9	0.9
C	HCO <sub>3</sub> <sup>-</sup>	68.9	73.0	73.4	77.2	83.3	84.6	81.6	81.4	83.1	76.9
	CO <sub>2</sub>	26.9	22.9	22.6	18.9	12.2	10.0	13.2	13.8	12.1	18.8
	CaHCO <sub>3</sub> <sup>+</sup>	3.2	3.3	3.2	3.1	3.2	4.1	4.0	3.3	3.5	3.3
	MgHCO <sub>3</sub> <sup>+</sup>	0.7	0.6	0.5	0.5	0.7	0.7	0.7	0.9	0.7	0.6
Ca	Ca <sup>2+</sup>	69.5	70.8	70.3	70.8	68.7	71.2	71.6	67.4	67.6	69.2
	CaSO <sub>4</sub>	28.4	27.1	28.3	27.7	28.9	26.6	26.3	30.6	30.2	28.8
	CaHCO <sub>3</sub> <sup>+</sup>	2.0	2.1	1.4	1.4	2.2	2.1	2.1	1.8	2.1	2.0
Fe(2)	Fe <sup>2+</sup>	60.6	60.8	64.8	64.9	58.3	60.2	61.2	59.6	57.9	60.1
	FeSO <sub>4</sub>	19.9	18.6	20.9	20.3	19.7	18.0	18.0	21.7	20.7	20.0
	FeHCO <sub>3</sub> <sup>+</sup>	18.7	19.5	13.4	13.8	19.8	19.2	18.9	17.1	19.4	18.7
	FeCO <sub>3</sub>	0.7	1.0	0.7	0.9	2.1	2.5	1.8	1.5	2.0	1.2
Fe(3)	Fe(OH) <sub>2</sub> <sup>+</sup>	74.6	70.0	69.4	64.1	52.2	47.1	55.0	56.5	52.6	64.8
	Fe(OH) <sub>3</sub>	25.2	29.8	30.4	35.6	47.2	52.3	44.6	43.1	46.9	34.9
	Fe(OH) <sub>4</sub> <sup>-</sup>					0.5	0.6			0.5	
K	K <sup>+</sup>	97.4	97.6	97.5	97.6	97.3	97.6	97.7	97.1	97.1	97.4
	KSO <sub>4</sub> <sup>-</sup>	2.7	2.4	2.5	2.4	2.7	2.4	2.3	2.9	2.9	2.6
Li	Li <sup>+</sup>	97.8	98.0	97.9	98.1	97.8	98.0	98.1	97.5	97.6	97.8
	LiSO <sub>4</sub> <sup>-</sup>	2.2	2.0	2.0	1.9	2.2	1.9	1.9	2.4	2.4	2.2
Mg	Mg <sup>2+</sup>	70.0	71.3	71.0	71.6	69.4	71.8	72.2	68.2	68.3	69.9
	MgSO <sub>4</sub>	27.5	26.0	27.3	26.7	27.9	25.5	25.2	29.5	29.1	27.6
	MgHCO <sub>3</sub> <sup>+</sup>	2.5	2.6	1.7	1.7	2.7	2.6	2.5	2.2	2.6	2.5
Mn(2)	Mn <sup>2+</sup>	60.9	60.9	64.9	64.7	57.0	58.2	60.1	58.8	56.7	59.9
	MnSO <sub>4</sub>	19.8	18.5	20.7	20.0	19.0	17.2	17.4	21.1	20.0	19.7
	MnHCO <sub>3</sub> <sup>+</sup>	16.7	17.3	11.9	12.2	17.2	16.5	16.5	15.0	16.8	16.5
	MnCO <sub>3</sub>	2.4	3.2	2.3	2.9	6.7	7.9	5.8	5.0	6.5	3.9
Na	Na <sup>+</sup>	97.5	97.7	97.7	97.8	97.5	97.7	97.8	97.3	97.3	97.5
	NaSO <sub>4</sub> <sup>-</sup>	2.2	2.0	2.1	2.0	2.3	2.0	2.0	2.5	2.4	2.2
S	SO <sub>4</sub> <sup>2-</sup>	68.4	68.8	69.6	70.9	71.4	67.9	67.5	70.3	70.5	69.6
	CaSO <sub>4</sub>	26.1	26.8	26.5	25.0	23.1	27.8	27.8	23.2	24.3	25.6
	MgSO <sub>4</sub>	4.6	3.7	3.2	3.2	3.8	3.7	3.9	4.9	3.6	3.8
	NaSO <sub>4</sub> <sup>-</sup>	0.6			0.7	1.4		0.6	1.3	1.3	0.7
Sr	Sr <sup>2+</sup>	70.5	71.7	71.3	71.8	69.8	72.2	72.6	68.6	68.7	70.2
	SrSO <sub>4</sub>	27.4	26.1	27.3	26.7	27.9	25.6	25.3	29.6	29.1	27.7
	SrHCO <sub>3</sub> <sup>+</sup>	2.1	2.2	1.4	1.4	2.2	2.2	2.1	1.8	2.2	2.0
Zn	Zn <sup>2+</sup>	48.8	48.6	52.8	52.3	42.7	43.3	46.3	45.0	42.3	46.9
	ZnSO <sub>4</sub>	24.5	22.8	26.1	25.1	22.0	19.8	20.9	25.1	23.1	23.9
	ZnHCO <sub>3</sub> <sup>+</sup>	19.0	19.6	13.8	14.0	18.3	17.4	18.1	16.3	17.8	18.4
	ZnCO <sub>3</sub>	4.9	6.4	4.6	6.0	12.7	14.9	11.3	9.5	12.2	7.6
	Zn(SO <sub>4</sub> ) <sub>2</sub> <sup>2-</sup>	2.5	2.0	2.4	2.1	2.2	1.8	1.8	2.9	2.6	2.4
	Zn(CO <sub>3</sub> ) <sub>2</sub> <sup>2-</sup>					1.8	2.5	1.3	1.0	1.8	0.6

\*Numbers listed in the table represent the range of percentage share of individual speciation forms that exceeded 0.5% of total molar concentration of a given element.