

CHEAQS Next output

Program version: P2016.3.

Print date (mm-dd-yyyy): 09-16-2016.

Sample description: (not specified).

Contents

Below you will find output of the following cation(s): H; Na; Mg; K; Ca.

Below you will find output of the following ligand(s): (CO₃); (SO₄); Cl.

Both summary and details are printed.

Fractions / species below 0.10% are not displayed (but free species are always displayed).

Intrinsic and conditional K's are displayed as log-10-values.

Additional info follows cations and ligands and consists of: general results; saturation solids; gases; input data.

Cations

Results of H

Summary of results

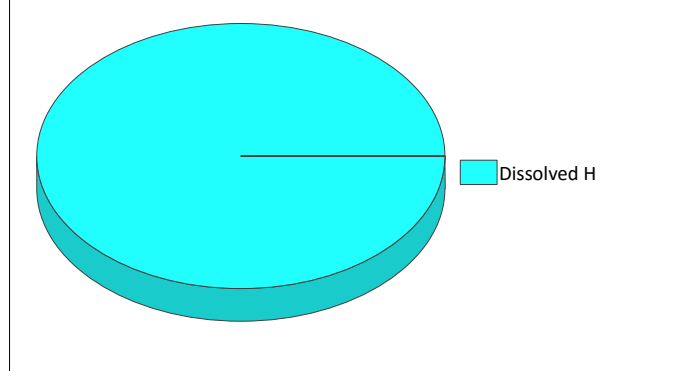
Fraction	Concentration	Unit
Dissolved H	1.753E-003	M
Total H	1.753E-003	M

Details of results

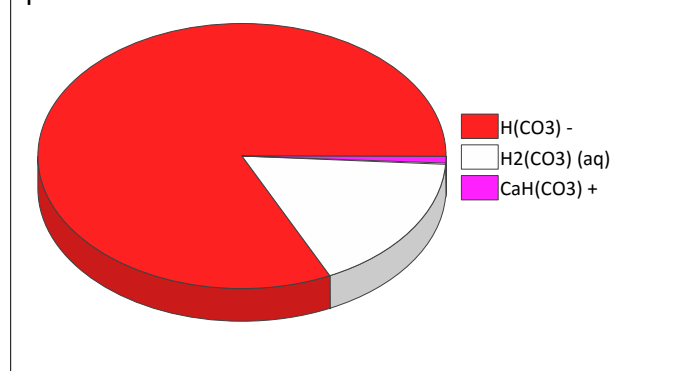
Species	Concentration	Unit	Percentage	Activity	Unit	Intrinsic K	Conditional K	Literature reference
free H +	1.089E-007	M		1.000E-007	M			
free (OH) -	1.097E-007	M		1.007E-007	M	13.997	13.923	NIST Database 46 Version 8.0
H(CO ₃) -	1.230E-003	M		1.129E-003	M	10.329	10.180	NIST Database 46 Version 8.0
H ₂ (CO ₃) (aq)	2.539E-004	M		2.539E-004	M	16.681	16.458	NIST Database 46 Version 8.0
MgH(CO ₃) +	2.366E-006	M		2.171E-006	M	11.339	11.041	NIST Database 46 Version 8.0
CaH(CO ₃) +	1.184E-005	M		1.087E-005	M	11.529	11.231	NIST Database 46 Version 8.0
Total H	1.753E-003	M						

Graphic results

Fractions



Species



Results of Na

Summary of results

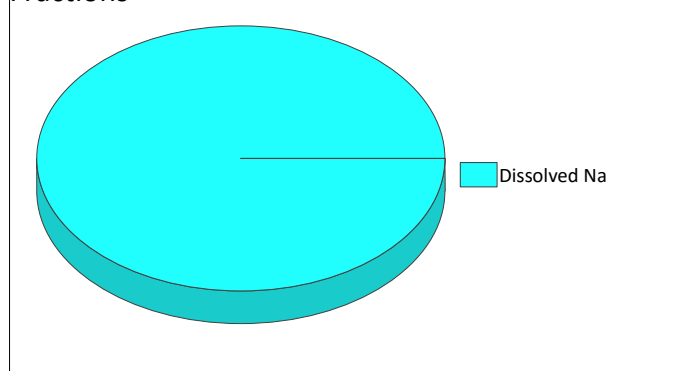
Fraction	Concentration	Unit	Percentage
Dissolved Na	1.000E-003	M	100.00%
Total Na	1.000E-003	M	100.00%

Details of results

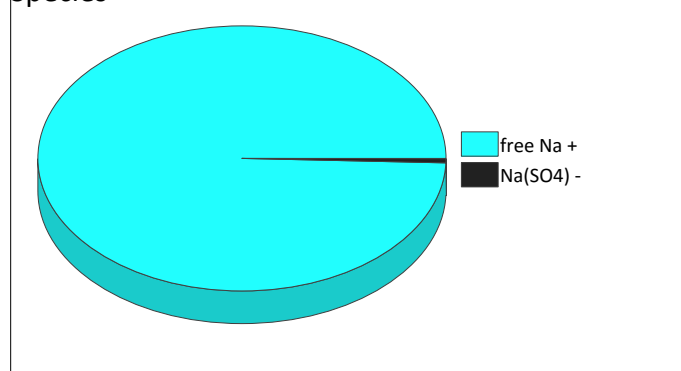
Species	Concentration	Unit	Percentage	Activity	Unit	Intrinsic K	Conditional K	Literature reference
free Na +	9.940E-004	M	99.40%	9.124E-004	M			
Na(SO4) -	5.150E-006	M	0.52%	4.727E-006	M	0.740	0.591	NIST Database 46 Version 8.0
Total Na	1.000E-003	M	100.00%					

Graphic results

Fractions



Species



Results of Mg

Summary of results

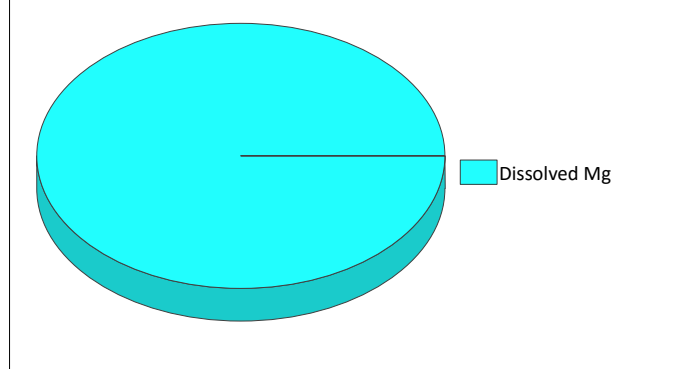
Fraction	Concentration	Unit	Percentage
Dissolved Mg	3.000E-004	M	100.00%
Total Mg	3.000E-004	M	100.00%

Details of results

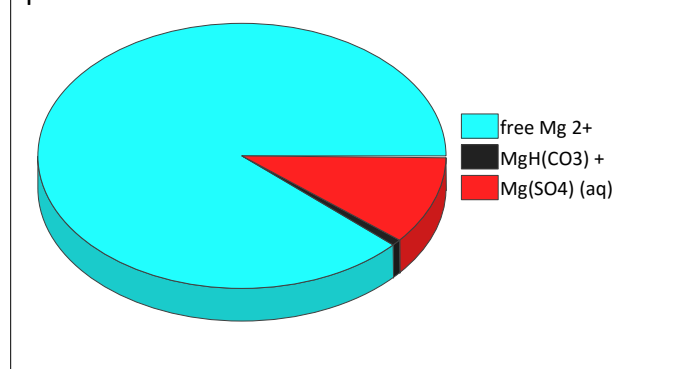
Species	Concentration	Unit	Percentage	Activity	Unit	Intrinsic K	Conditional K	Literature reference
free Mg 2+	2.648E-004	M	88.26%	1.880E-004	M			
MgH(CO ₃) +	2.366E-006	M	0.79%	2.171E-006	M	11.339	11.041	NIST Database 46 Version 8.0
Mg(SO ₄) (aq)	3.224E-005	M	10.75%	3.224E-005	M	2.260	1.962	NIST Database 46 Version 8.0
MgCl +	5.223E-007	M	0.17%	4.794E-007	M	0.600	0.451	NIST Database 46 Version 8.0
Total Mg	3.000E-004	M	100.00%					

Graphic results

Fractions



Species



Results of K

Summary of results

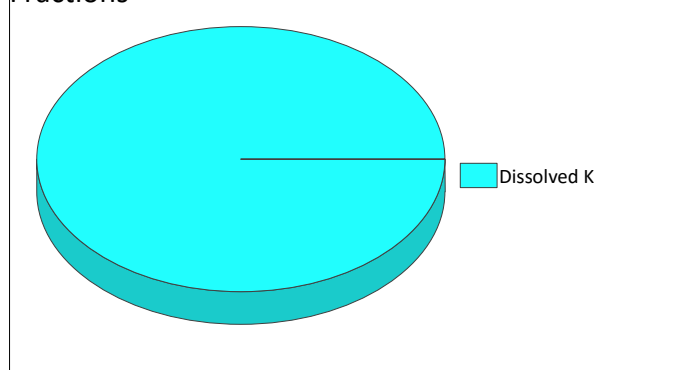
Fraction	Concentration	Unit	Percentage
Dissolved K	5.000E-004	M	100.00%
Total K	5.000E-004	M	100.00%

Details of results

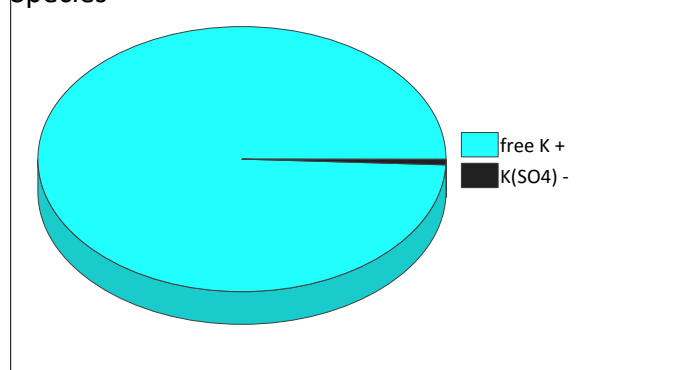
Species	Concentration	Unit	Percentage	Activity	Unit	Intrinsic K	Conditional K	Literature reference
free K +	4.965E-004	M	99.31%	4.558E-004	M			
K(SO ₄) -	3.314E-006	M	0.66%	3.042E-006	M	0.850	0.701	NIST Database 46 Version 8.0
Total K	5.000E-004	M	100.00%					

Graphic results

Fractions



Species



Results of Ca

Summary of results

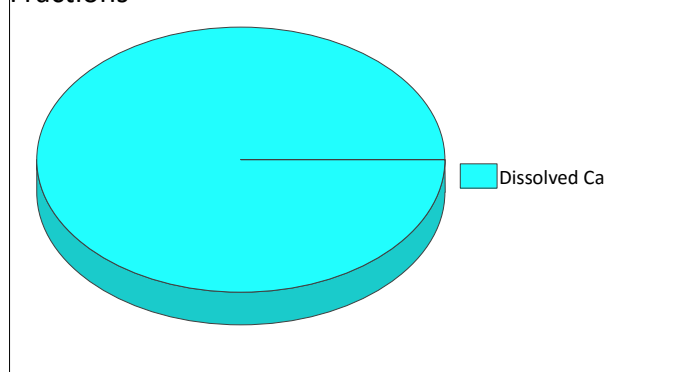
Fraction	Concentration	Unit	Percentage
Dissolved Ca	1.000E-003	M	100.00%
Total Ca	1.000E-003	M	100.00%

Details of results

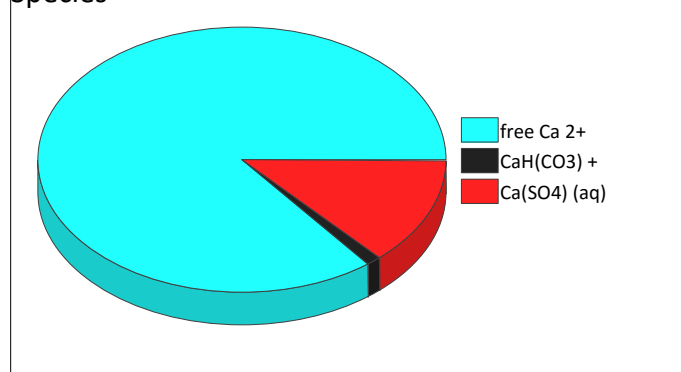
Species	Concentration	Unit	Percentage	Activity	Unit	Intrinsic K	Conditional K	Literature reference
free Ca 2+	8.554E-004	M	85.54%	6.072E-004	M			
CaH(CO ₃) +	1.184E-005	M	1.18%	1.087E-005	M	11.529	11.231	NIST Database 46 Version 8.0
Ca(SO ₄) (aq)	1.311E-004	M	13.11%	1.311E-004	M	2.360	2.062	NIST Database 46 Version 8.0
CaCl +	1.065E-006	M	0.11%	9.772E-007	M	0.400	0.251	NIST Database 46 Version 8.0
Total Ca	1.000E-003	M	100.00%					

Graphic results

Fractions



Species



Ligands

Results of (CO₃)

Summary of results

Fraction	Concentration	Unit	Percentage
Dissolved (CO ₃)	1.500E-003	M	100.00%
Total (CO ₃)	1.500E-003	M	100.00%

Details of results

Species	Concentration	Unit	Percentage	Activity	Unit	Intrinsic K	Conditional K	Literature reference
free (CO ₃) 2-	7.457E-007	M	0.05%	5.293E-007	M			
H(CO ₃) -	1.230E-003	M	82.00%	1.129E-003	M	10.329	10.180	NIST Database 46 Version 8.0

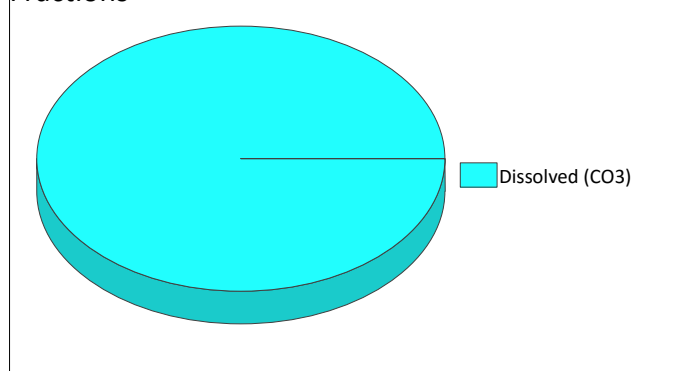
(continued on page 5)

(continued from page 4)

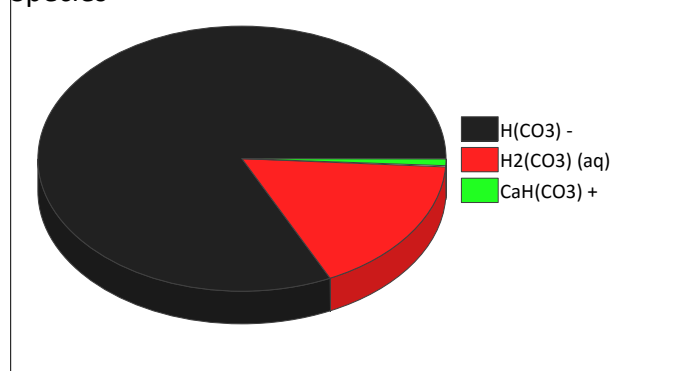
Species	Concentration	Unit	Percentage	Activity	Unit	Intrinsic K	Conditional K	Literature reference
H ₂ (CO ₃) (aq)	2.539E-004	M	16.93%	2.539E-004	M	16.681	16.458	NIST Database 46 Version 8.0
MgH(CO ₃) +	2.366E-006	M	0.16%	2.171E-006	M	11.339	11.041	NIST Database 46 Version 8.0
CaH(CO ₃) +	1.184E-005	M	0.79%	1.087E-005	M	11.529	11.231	NIST Database 46 Version 8.0
Total (CO ₃)	1.500E-003	M	100.00%					

Graphic results

Fractions



Species

Results of (SO₄)

Summary of results

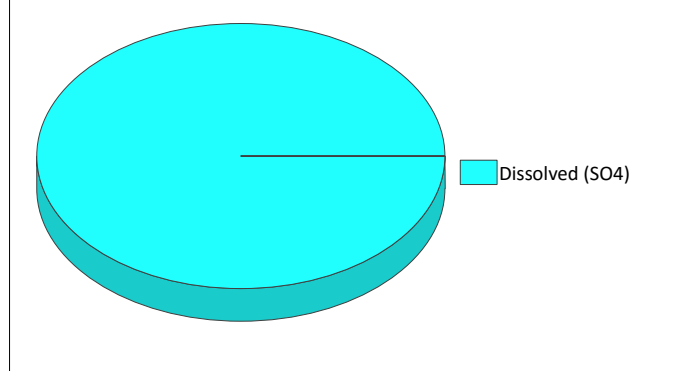
Fraction	Concentration	Unit	Percentage
Dissolved (SO ₄)	1.500E-003	M	100.00%
Total (SO ₄)	1.500E-003	M	100.00%

Details of results

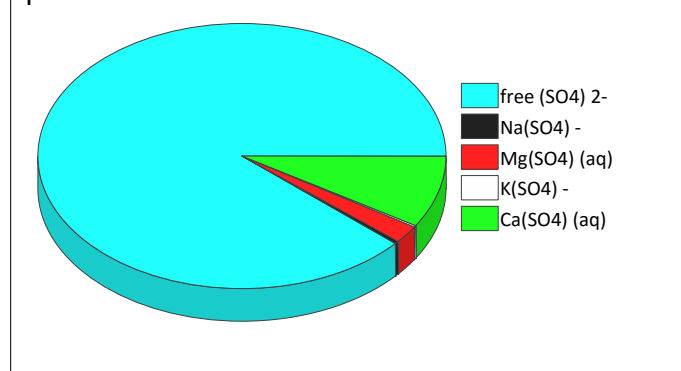
Species	Concentration	Unit	Percentage	Activity	Unit	Intrinsic K	Conditional K	Literature reference
free (SO ₄) ²⁻	1.328E-003	M	88.54%	9.428E-004	M			
Na(SO ₄) ⁻	5.150E-006	M	0.34%	4.727E-006	M	0.740	0.591	NIST Database 46 Version 8.0
Mg(SO ₄) (aq)	3.224E-005	M	2.15%	3.224E-005	M	2.260	1.962	NIST Database 46 Version 8.0
K(SO ₄) ⁻	3.314E-006	M	0.22%	3.042E-006	M	0.850	0.701	NIST Database 46 Version 8.0
Ca(SO ₄) (aq)	1.311E-004	M	8.74%	1.311E-004	M	2.360	2.062	NIST Database 46 Version 8.0
Total (SO ₄)	1.500E-003	M	100.00%					

Graphic results

Fractions



Species



Results of Cl

Summary of results

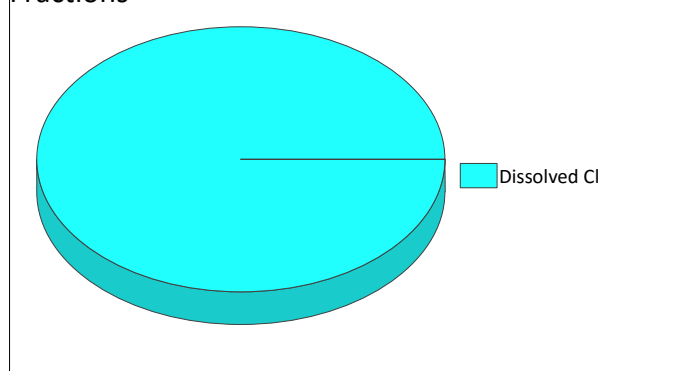
Fraction	Concentration	Unit	Percentage
Dissolved Cl	7.000E-004	M	100.00%
Total Cl	7.000E-004	M	100.00%

Details of results

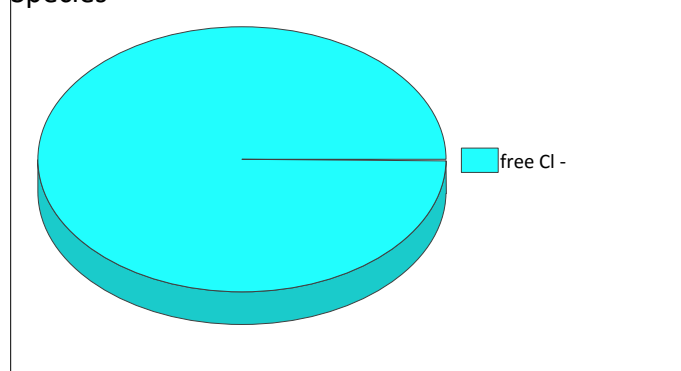
Species	Concentration	Unit	Percentage	Activity	Unit	Intrinsic K	Conditional K	Literature reference
free Cl -	6.980E-004	M	99.71%	6.407E-004	M			
CaCl +	1.065E-006	M	0.15%	9.772E-007	M	0.400	0.251	NIST Database 46 Version 8.0
Total Cl	7.000E-004	M	100.00%					

Graphic results

Fractions



Species



Other information

General results

Number of iterations:	10
Ionic strength:	6.620E-003 M
Charge of positive ions:	3.747E-003 eq
Charge of negative ions:	4.594E-003 eq
Charge difference:	-8.475E-004 eq
Charge ratio:	8.155E-001

Saturation solids

Information about saturation solids

Name	'Concentration'	Unit	Saturation index	Status	Intrinsic K	Conditional K	Literature reference
NaCl (s)	0.000E+000	M	-7.783	undersaturated	-1.550	-1.624	NIST Database 46 Version 8.0
CaMg(CO ₃) ₂ (s)	0.000E+000	M	-2.795	undersaturated	16.700	16.105	Stumm & Morgan
Mg(OH) ₂ (s)	0.000E+000	M	-6.620	undersaturated	11.100	10.877	NIST Database 46 Version 8.0
Mg(CO ₃) (s)	0.000E+000	M	-2.542	undersaturated	7.460	7.162	NIST Database 46 Version 8.0
Mg ₄ (CO ₃) ₃ (OH) ₂ (H ₂ O) ₃ (s)	0.000E+000	M	-18.227	undersaturated	29.500	28.384	Stumm & Morgan
KCl (s)	0.000E+000	M	-7.435	undersaturated	-0.900	-0.974	NIST Database 46 Version 8.0
Ca(OH) ₂ (s)	0.000E+000	M	-11.921	undersaturated	5.290	5.067	NIST Database 46 Version 8.0
Ca(CO ₃) (s)	0.000E+000	M	-1.013	undersaturated	8.480	8.182	NIST Database 46 Version 8.0
Ca(SO ₄)(H ₂ O) ₂ (s)	0.000E+000	M	-1.632	undersaturated	4.610	4.312	NIST Database 46 Version 8.0

Gases

For 1 ligand ((CO₃)²⁻), a corresponding gas pressure (CO₂ (g)) could be calculated.

Name	Partial pressure	Unit	[Free ligand]	Unit	Intrinsic K	Conditional K	Literature reference
CO ₂ (g) / (CO ₃) ²⁻	7.425E-003	atm	7.456E-007	M	18.147	17.924	NIST Database 46 Version 8.0

Input data

Input data for verification

pH:	fixed
Ionic strength:	calculated
Included:	precipitation equilibria
H	1.000E-007 M free activity
Na	1.000E-003 M total concentration
Mg	3.000E-004 M total concentration
K	5.000E-004 M total concentration

(continued on page 8)

(continued from page 7)

Ca	1.000E-003	M	total concentration
(CO3)	1.500E-003	M	total concentration
(SO4)	1.500E-003	M	total concentration
Cl	7.000E-004	M	total concentration
