CHEAQS Next Output

Program version: 0.2.1.5 (64 bits)
Print date (mm-dd-yyyy): 06-01-2022
Sample description: (not specified)

Contents

Below you will find the output of the following cation(s): H; Na; Mg; K; Ca.
Below you will find the output of the following ligand(s): (CO3); (SO4); Cl.
Both summary and details are printed.
Additional info at end consists of: General results; Precipitation; Gases; Input data for verification.

Cations

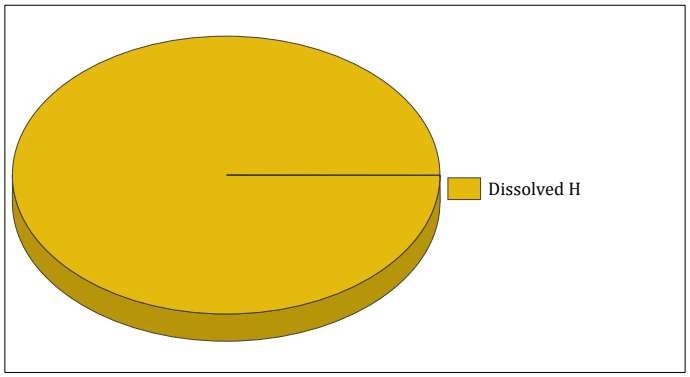
Results of: H

Summary of results

Fraction	Concentration	Unit	Percentage
Dissolved H	1.390E-003	M	100.00%
Total H	1.390E-003	M	100.00%

Details of results

Species	Concentration	Unit	Percentage	Activity	Unit	Log10(intrinsic β)	Log10(conditional β)	Literature reference
free H +	1.552E-008	M	0.00%	1.415E-008	M			
free (OH) -	7.799E-007	M	-0.06%	7.114E-007	M	13.997	13.917	NIST Database 46 Version 8.0
Na(OH) (aq)	9.693E-010	M	0.00%	9.693E-010	M	0.100	0.020	NIST Database 46 Version 8.0
Mg(OH) +	1.398E-007	M	-0.01%	1.275E-007	M	2.580	2.420	NIST Database 46 Version 8.0
Mg4(OH)4 4+	1.996E-021	M	0.00%	4.587E-022	M	16.560	16.400	NIST Database 46 Version 8.0
K(OH) (aq)	2.235E-010	M	0.00%	2.235E-010	M	0.238	0.158	NIST Database 46 Version 8.0
Ca(OH) +	1.320E-008	M	0.00%	1.204E-008	M	1.300	1.140	NIST Database 46 Version 8.0
H(CO3) -	1.292E-003	M	92.93%	1.178E-003	M	10.329	10.169	NIST Database 46 Version 8.0
H2(CO3) (aq)	3.751E-005	M	5.40%	3.751E-005	M	16.681	16.441	NIST Database 46 Version 8.0
NaH(CO3) (aq)	6.391E-007	M	0.05%	6.391E-007	M	10.029	9.789	NIST Database 46 Version 8.0
MgH(CO3) +	6.231E-006	M	0.45%	5.683E-006	M	11.339	11.020	NIST Database 46 Version 8.0
CaH(CO3) +	1.737E-005	M	1.25%	1.584E-005	M	11.529	11.210	NIST Database 46 Version 8.0
H(SO4) -	6.389E-010	M	0.00%	5.828E-010	M	1.990	1.830	NIST Database 46 Version 8.0



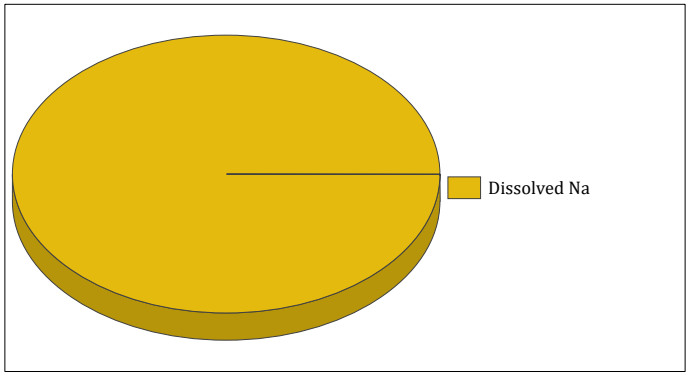
Results of: Na

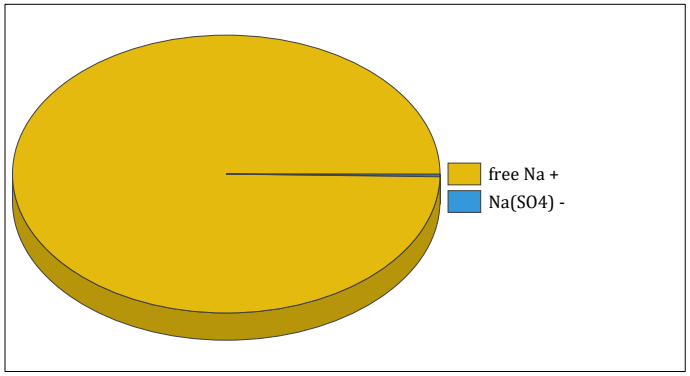
Summary of results

Fraction	Concentration	Unit	Percentage
Dissolved Na	1.190E-003	M	100.00%
Total Na	1.190E-003	M	100.00%

Details of results

Species	Concentration	Unit	Percentage	Activity	Unit	Log10(intrinsic β)	Log10(conditional β)	Literature reference
free Na +	1.187E-003	M	99.71%	1.082E-003	M			
Na(OH) (aq)	9.693E-010	M	0.00%	9.693E-010	M	0.100	0.020	NIST Database 46 Version 8.0
Na(CO3) -	8.622E-008	M	0.00%	7.865E-008	M	1.270	1.110	NIST Database 46 Version 8.0
NaH(CO3) (aq)	6.391E-007	M	0.05%	6.391E-007	M	10.029	9.789	NIST Database 46 Version 8.0
Na(SO4) -	2.747E-006	M	0.23%	2.506E-006	M	0.740	0.580	NIST Database 46 Version 8.0





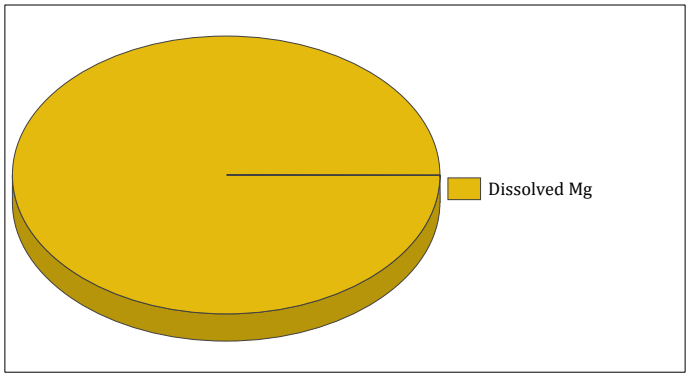
Results of: Mg

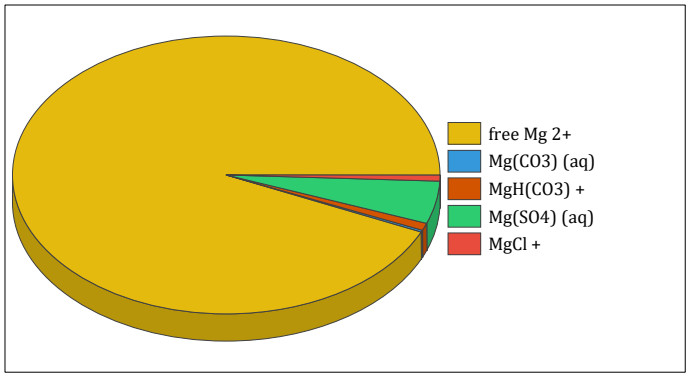
Summary of results

Fraction	Concentration	Unit	Percentage
Dissolved Mg	7.300E-004	M	100.00%
Total Mg	7.300E-004	M	100.00%

Details of results

Species	Concentration	Unit	Percentage	Activity	Unit	Log10(intrinsic β)	Log10(conditional β)	Literature reference
free Mg 2+	6.809E-004	M	93.27%	4.714E-004	M			
Mg(OH) +	1.398E-007	M	0.02%	1.275E-007	M	2.580	2.420	NIST Database 46 Version 8.0
Mg4(OH)4 4+	1.996E-021	M	0.00%	4.587E-022	M	16.560	16.400	NIST Database 46 Version 8.0
Mg(CO3) (aq)	1.530E-006	M	0.21%	1.530E-006	M	2.920	2.601	NIST Database 46 Version 8.0
MgH(CO3) +	6.231E-006	M	0.85%	5.683E-006	M	11.339	11.020	NIST Database 46 Version 8.0
Mg(SO4) (aq)	3.614E-005	M	4.95%	3.614E-005	M	2.260	1.941	NIST Database 46 Version 8.0
MgCl +	5.084E-006	M	0.70%	4.637E-006	M	0.600	0.440	NIST Database 46 Version 8.0





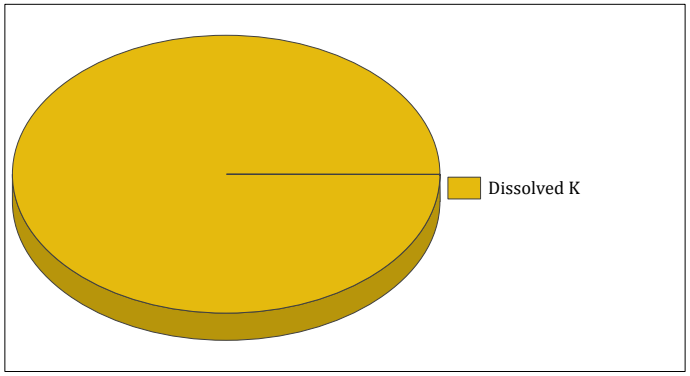
Results of: K

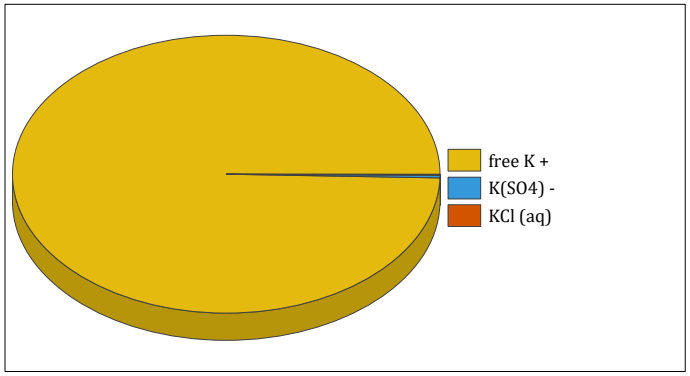
Summary of results

Fraction	Concentration	Unit	Percentage
Dissolved K	2.000E-004	M	100.00%
Total K	2.000E-004	M	100.00%

Details of results

Species	Concentration	Unit	Percentage	Activity	Unit	Log10(intrinsic β)	Log10(conditional β)	Literature reference
free K +	1.992E-004	M	99.59%	1.817E-004	M			
K(OH) (aq)	2.235E-010	M	0.00%	2.235E-010	M	0.238	0.158	NIST Database 46 Version 8.0
K(SO4) -	5.941E-007	M	0.30%	5.420E-007	M	0.850	0.690	NIST Database 46 Version 8.0
KCl (aq)	2.250E-007	M	0.11%	2.250E-007	M	-0.300	-0.380	NIST Database 46 Version 8.0





Results of: Ca

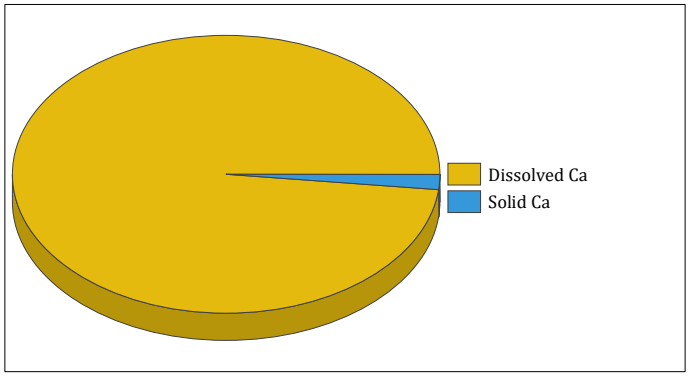
Summary of results

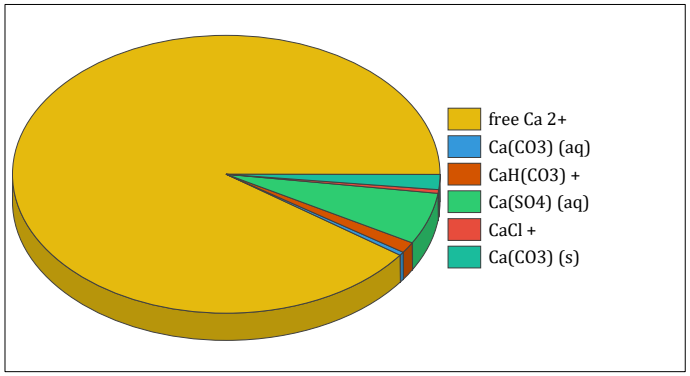
Fraction	Concentration	Unit	Percentage
Dissolved Ca	1.336E-003	M	98.25%
Solid Ca	2.384E-005	M	1.75%
Total Ca	1.360E-003	M	100.00%

Details of results

Species	Concentration	Unit	Percentage	Activity	Unit	Log10(intrinsic β)	Log10(conditional β)	Literature reference
free Ca 2+	1.226E-003	M	90.12%	8.485E-004	M			
Ca(OH) +	1.320E-008	M	0.00%	1.204E-008	M	1.300	1.140	NIST Database 46 Version 8.0
Ca(CO3) (aq)	5.495E-006	M	0.40%	5.495E-006	M	3.220	2.901	NIST Database 46 Version 8.0
CaH(CO3) +	1.737E-005	M	1.28%	1.584E-005	M	11.529	11.210	NIST Database 46 Version 8.0
Ca(SO4) (aq)	8.190E-005	M	6.02%	8.190E-005	M	2.360	2.041	NIST Database 46 Version 8.0
CaCl +	5.774E-006	M	0.42%	5.267E-006	M	0.400	0.240	NIST Database 46 Version 8.0

Species	Concentration	Unit	Percentage	Activity	Unit	Log10(intrinsic β)	Log10(conditional β)	Literature reference
Ca(CO3) (s)	2.384E-005	M	1.75%			8.480	8.161	NIST Database 46 Version 8.0





Ligands

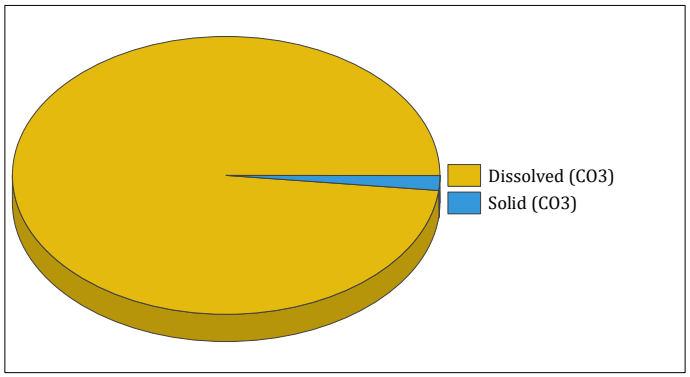
Results of: (CO3)

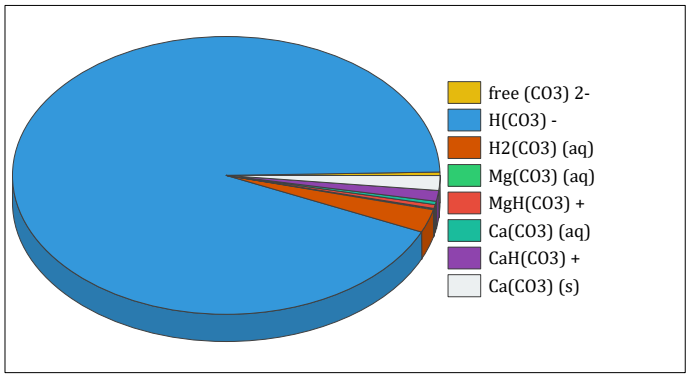
Summary of results

Fraction	Concentration	Unit	Percentage
Dissolved (CO3)	1.366E-003	M	98.28%
Solid (CO3)	2.384E-005	M	1.72%
Total (CO3)	1.390E-003	M	100.00%

Details of results

Species	Concentration	Unit	Percentage	Activity	Unit	Log10(intrinsic β)	Log10(conditional β)	Literature reference
free (CO3) 2-	5.637E-006	M	0.41%	3.902E-006	M			
H(CO3) -	1.292E-003	M	92.93%	1.178E-003	M	10.329	10.169	NIST Database 46 Version 8.0
H2(CO3) (aq)	3.751E-005	M	2.70%	3.751E-005	M	16.681	16.441	NIST Database 46 Version 8.0
Na(CO3) -	8.622E-008	M	0.00%	7.865E-008	M	1.270	1.110	NIST Database 46 Version 8.0
NaH(CO3) (aq)	6.391E-007	M	0.05%	6.391E-007	M	10.029	9.789	NIST Database 46 Version 8.0
Mg(CO3) (aq)	1.530E-006	M	0.11%	1.530E-006	M	2.920	2.601	NIST Database 46 Version 8.0
MgH(CO3) +	6.231E-006	M	0.45%	5.683E-006	M	11.339	11.020	NIST Database 46 Version 8.0
Ca(CO3) (aq)	5.495E-006	M	0.40%	5.495E-006	M	3.220	2.901	NIST Database 46 Version 8.0
CaH(CO3) +	1.737E-005	M	1.25%	1.584E-005	M	11.529	11.210	NIST Database 46 Version 8.0
Ca(CO3) (s)	2.384E-005	M	1.72%			8.480	8.161	NIST Database 46 Version 8.0





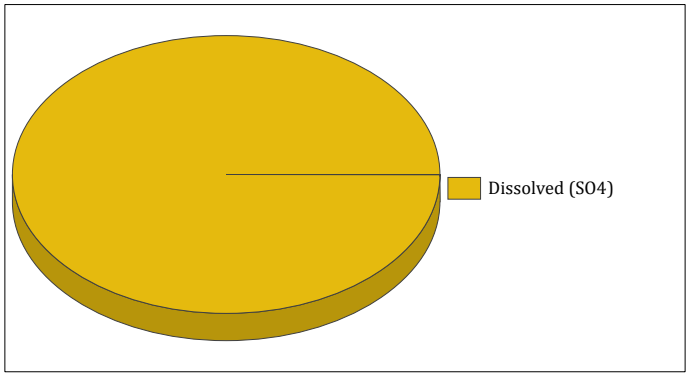
Results of: (SO4)

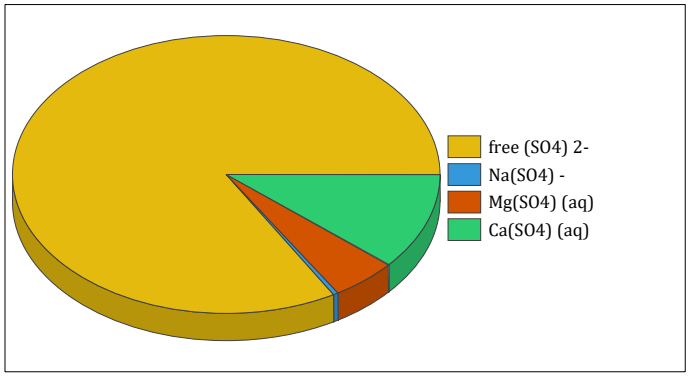
Summary of results

Fraction	Concentration	Unit	Percentage
Dissolved (SO4)	7.300E-004	M	100.00%
Total (SO4)	7.300E-004	M	100.00%

Details of results

Species	Concentration	Unit	Percentage	Activity	Unit	Log10(intrinsic β)	Log10(conditional β)	Literature reference
free (SO4) 2-	6.086E-004	M	83.37%	4.214E-004	M			
H(SO4) -	6.389E-010	M	0.00%	5.828E-010	M	1.990	1.830	NIST Database 46 Version 8.0
Na(SO4) -	2.747E-006	M	0.38%	2.506E-006	M	0.740	0.580	NIST Database 46 Version 8.0
Mg(SO4) (aq)	3.614E-005	M	4.95%	3.614E-005	M	2.260	1.941	NIST Database 46 Version 8.0
K(SO4) -	5.941E-007	M	0.08%	5.420E-007	M	0.850	0.690	NIST Database 46 Version 8.0
Ca(SO4) (aq)	8.190E-005	M	11.22%	8.190E-005	M	2.360	2.041	NIST Database 46 Version 8.0





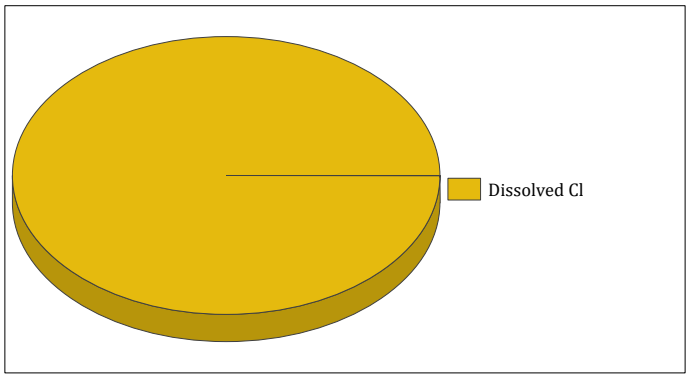
Results of: Cl

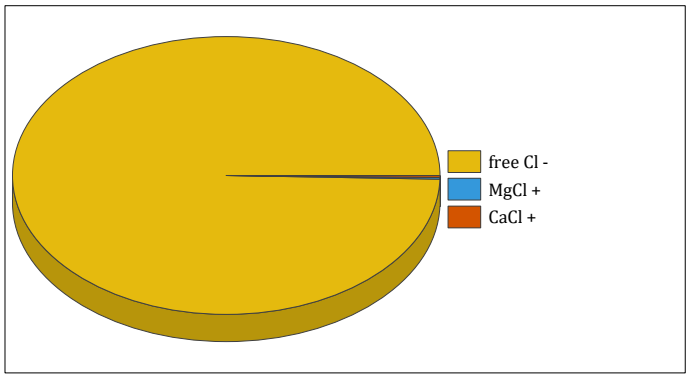
Summary of results

Fraction	Concentration	Unit	Percentage
Dissolved Cl	2.720E-003	M	100.00%
Total Cl	2.720E-003	M	100.00%

Details of results

Species	Concentration	Unit	Percentage	Activity	Unit	Log10(intrinsic β)	Log10(conditional β)	Literature reference
free Cl -	2.709E-003	M	99.59%	2.471E-003	M			
MgCl +	5.084E-006	M	0.19%	4.637E-006	M	0.600	0.440	NIST Database 46 Version 8.0
KCl (aq)	2.250E-007	M	0.00%	2.250E-007	M	-0.300	-0.380	NIST Database 46 Version 8.0
CaCl +	5.774E-006	M	0.21%	5.267E-006	M	0.400	0.240	NIST Database 46 Version 8.0





Other info

General results

Number of iterations:	33	
Ionic strength:	7.754E-003	M
Charge of positive ions:	5.233E-003	eq
Charge of negative ions:	5.233E-003	eq
Charge difference:	-2.125E-011	eq
Charge ratio:	1.000E+000	

Precipitation

Precipitation was included. See results below.

Name	'Concentration'	Unit	Saturation index	Status	Log10(intrinsic β)	Log10(conditional β)	Literature reference
Mg(OH)2 (s)	0.000E+000	M	-4.522	undersaturated	11.100	10.860	NIST Database 46 Version 8.0
Ca(OH)2 (s)	0.000E+000	M	-10.077	undersaturated	5.290	5.050	NIST Database 46 Version 8.0
CaMg(CO3)2 (s)	0.000E+000	M	-0.515	undersaturated	16.700	16.061	Stumm & Morgan
Mg(CO3) (s)	0.000E+000	M	-1.275	undersaturated	7.460	7.141	NIST Database 46 Version 8.0
Mg4(CO3)3(OH)2(H2O)3 (s)	0.000E+000	M	-12.328	undersaturated	29.500	28.302	Stumm & Morgan
Ca(CO3) (s)	2.384E-005	M	0.000	in equilibrium	8.480	8.161	NIST Database 46 Version 8.0
Ca(SO4)(H2O)2 (s)	0.000E+000	M	-1.837	undersaturated	4.610	4.291	NIST Database 46 Version 8.0
NaCl (s)	0.000E+000	M	-7.123	undersaturated	-1.550	-1.630	NIST Database 46 Version 8.0
KCl (s)	0.000E+000	M	-7.248	undersaturated	-0.900	-0.980	NIST Database 46 Version 8.0

Gases

[Free ligand] for (CO3) 2- corresponds with displayed gas pressures. See table below for details.

Gas / Ligand	Partial pressure	Unit	[Free ligand]	Unit	Log10(intrinsic β)	Log10(conditional β)	Literature reference
CO2 (g) / (CO3) 2-	1.097E-003	atm	5.637E-006	M	18.147	17.907	NIST Database 46 Version 8.0

Input data for verification

Input data for verification

Description:	(not specified)		
pH:	calculated		
Ionic strength:	calculated		
Ionic strength model:	Davies		
Convergence criterion:	1.000E-004		
Temperature:	25	°C	
Temperature correction:	no correction		
Adjusting charge balance:	not applied		
Included:	precipitation		
H	1.390E-003	M	total concentration
Na	1.190E-003	M	total concentration
Mg	7.300E-004	M	total concentration
K	2.000E-004	M	total concentration
Ca	1.360E-003	M	total concentration
(CO3)	1.390E-003	M	total concentration

(SO4)	7.300E-004	M	total concentration
Cl	2.720E-003	M	total concentration