Carbonate System: H2CO3*, HCO3⁻ and CO3²⁻ Fractions at a pH

Fractions and concentrations of carbonic acid, bicarbonate and carbonate for a total carbonate concentration at a given pH, and the resulting alkalinity.

Input parameters

Unit system: SI

Parameter	Value	Unit
pH	8.0000	
Total carbonate (as carbon), mmol/L	2.0000	mmol/L
First dissociation pK (6.35 at 25 °C)	6.3500	
Second dissociation pK (10.33 at 25 °C)	10.330	
Water ion product pK (14.0 at 25 °C)	14.000	

Calculated results

Parameter	Value	Unit
Fraction as H2CO3*	2.1797	%
Fraction as HCO3⁻	97.365	%
Fraction as CO3²⁻	0.45541	%
Carbonic acid	0.043595	mmol/L
Bicarbonate	1.9473	mmol/L
Carbonate	0.009108	mmol/L
Alkalinity (as CaCO3)	98.404	mg/L

Notes for this case

• Concentration-based constants (activity coefficients taken as 1); correct pK values for temperature and ionic strength for accurate work. Alkalinity = [HCO_3^-] + 2[CO_3^{2-}] + [OH^-] − [H^+] expressed as $CaCO_3$ (50.04 g/eq).

Formula and method

$$\alpha_0 = \frac{[H^+]^2}{D}, \quad \alpha_1 = \frac{K_1[H^+]}{D}, \quad \alpha_2 = \frac{K_1 K_2}{D}, \quad D = [H^+]^2 + K_1[H^+] + K_1 K_2$$

$$Alk = C_T(\alpha_1 + 2\alpha_2) + [OH^-] - [H^+]$$

Variables

pH	pH	-
C_T	Total carbonate (as carbon), mmol/L	mol/m³
pK_1	First dissociation pK (6.35 at 25 °C)	-
pK_2	Second dissociation pK (10.33 at 25 °C)	-
pK_w	Water ion product pK (14.0 at 25 °C)	-
α_0	Fraction as H2CO3*	-
α_1	Fraction as HCO3⁻	-
α_2	Fraction as CO3²⁻	-
$[H_2CO_3^*]$	Carbonic acid	mol/m³
$[HCO_3^-]$	Bicarbonate	mol/m³

$[CO_3^{2-}]$	Carbonate	mol/m³
Alk	Alkalinity (as CaCO3)	kg/m³

Method and standards

Closed carbonate system equilibria.

Assumptions and limits

- Equilibrium; ideal (activity = concentration) unless corrected pK values are entered.

Report details

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Results are for engineering estimation. Verify critical designs against the referenced standards and your own data.

This calculator online

https://calc.firecad.com/environmental/drinking-water/carbonate-species-distribution

Open this case on calc.firecad.com →

Reopens the calculator with the inputs of this report.