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Swimming pool chemistry

Learning objectives

1 Describe how the water in swimming pools is disinfected.

2 Calculate concentration of various ions present in the water.

3 Interpret data obtained from a mass spectrometer.

4 Determine the structure of organic molecules.

Introduction

Chlorine (Cl_2) is now rarely added directly to pools in the UK because of the hazards associated with its storage and use. Other chlorinating agents are used instead.

In a typical swimming pool, sodium chlorate(I) is added to disinfect the water. The chlorate(I) ion is the conjugate base of the weak acid $HOCl$. The equilibrium constant K_a for $HOCl = 2.9 \times 10^{-8}$ mol dm^{-3} at 298 K. Both the chlorate(I) ion and the acid $HOCl$ are involved in the disinfecting.

Some data were obtained from a swimming pool in Taunton, on a particular day in September. The combined concentration of $HOCl(aq)$ was measured as 0.50 parts per million (ppm). The pH was 7.3.

Questions

Part one

1. Convert the combined concentration of $HOCl(aq)$ and $OCl^-(aq)$ from parts per million into mol dm^{-3}.

2. Calculate the concentration of $HOCl(aq)$.

Sodium hydrogen carbonate and CO_2 gas are also added to buffer the swimming pool water. The K_a value for carbonic acid (the weak acid formed when CO_2 dissolves in water) is 4.2×10^{-7} mol dm^{-3}. The 'total alkalinity' (combined concentration of all the bases present) was measured as 1.08×10^{-3} mol dm^{-3}.

3. Assuming the only bases detected in the total alkalinity test are OCl^- and HCO^{-3}, calculate the concetration of carbonic acid in the swimming pool.

4. Explain the effect on the concentration of $HOCl$ of adding extra CO_2 gas.

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Calcium chloride is also added to swimming pool water. Another calcium compound, calcium sulfate, is a slightly soluble component of the grout used in between the tiles inside the swimming pool. The solubility product (K_{sp}) of a salt is the equilibrium constant for an ionic substance in saturated solution, such that K_{sp} for a salt $M_aX_b \ = \ [M]^a[X]^b$ with the units that depend on a and b.

5. Give a general expression for the units of a solubility product of salt M_aX_b in terms of a and b.
6. K_{sp} for calcium sulfate has a value of $2.4 \ \times \ 10^{-5}\ \mathrm{mol^2\ dm^{-6}}$ at $298\ \mathrm{K}$. If the concentration of chloride ions from the $CaCl_2$ added is $0.1\ \mathrm{mol\ dm^{-3}}$, what is the concentration of the sulfate ions in the swimming pool?
7. Explain how adding calcium chloride helps to prevent grout dissolving.
8. The enthalpy change of solution for $NaCl(s)$ is $+3.9\ \mathrm{kJ\ mol^{-1}}$ and for $CaSO_4(s)$ it is $-17.8\ \mathrm{kJ\ mol^{-1}}$. Why is $CaSO_4$ only sparingly soluble and $NaCl$ very soluble?

Part 2

Sometimes organic compounds are added to swimming pool water instead of, or in addition to $HOCl$ and OCl^-. One example is trichloroisocyanuric acid. This undergoes hydrolysis to form an equilibrium with $HOCl$ and isocyanuric acid.

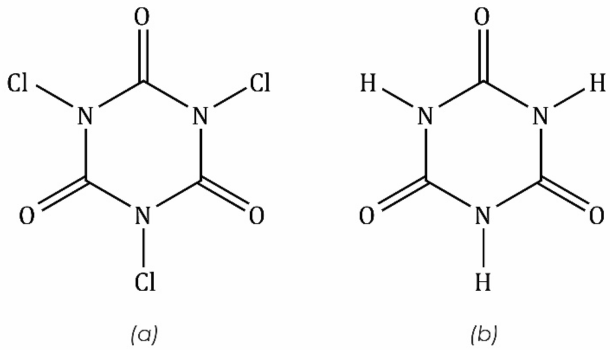

Figure 1: the structure of (a) trichloroisocyanuric acid and (b) isocyanuric acid

9. Some data from the mass spectra of trichloroisocyanuric acid are shown below. The isotopes chlorine-35 and chlorine-37 occur in the ration 3 : 1.

(a) Identify the species detected at the peaks listed in the table. Note that molecules often fragment inside mass spectrometers and there can be rearrangement of the atoms in the fragments.

Mass/charge ratio	Relative height of peak as a percentage of the most abundant peak	Species giving rise to the peak
42	17.9	NCO^+
70	100.0	and
72	12.9	
74	2.3	
77	81.4	
79	26.4	
154	18.4	
156	11.7	
158	2.0	
231	24.6	
233	23.4	
235	7.8	
237	1.0	

(b) Account for the relative heights of the peaks at mass/charge (m/c):

i. 154, 156 and 158
ii. 231, 233, 235 and 237.

(c) Use the relative heights of the peaks at m/c 231, 233, 235 and 237 to calculate the relative molecular mass of trichloroisocyanuric acid to two decimal places.

(d) It seems likely that the peak at m/c 70 is due to two species. A high resolution mass spectrometer would resolve the single peak at m/c into two separate peaks. Calculate what their relative heights would be.

10. How many peaks would you expect to see in the proton NMR spectra of isocyanuric acid?

11. Discuss whether you think that isocyanuric acid will have delocalised π system like benzene.

12. Write a balanced equation for the reaction of trichloroisocyanuric acid and water.

13. Discuss the oxidation state of the chlorine in trichloroisocyanuric acid. Electronegativity values are given below.

H 2.1	Li 1.0	Be 1.5	B	C	N	O	F
	Na 0.9	Mg 1.2	Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0

Pauling electronegativity values for some elements

Most ketones and aldehydes exist in solution as two tautomeric forms that are in dynamic equilibrium. The two tautomers (the 'keto' and 'enol' forms) interchange rapidly in the presence of H^+ ions. An example of these forms for propanone is shown below:

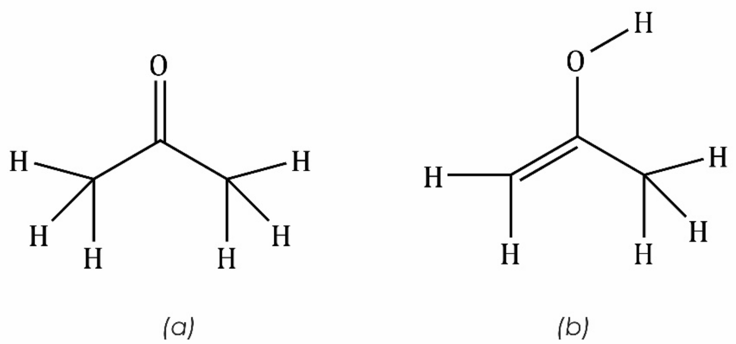

Figure 2: the structures of (a) the keto and (b) the enol – tautomers of propanone

14. Suggest a mechanism for the conversion of the keto to the enol tautomer of propanone.

15. Suggest a structure for cyanuric acid, the tautomeric form of isocyanuric acid.