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A Method for Studying the Diffusion of Quaternary Ammonium Cations Through Polyelectrolyte Phases†

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The mobility of organic cations in polymeric phases is an important property to consider when using these materials as active ingredients in coatings. Here we describe a method for extracting such compounds from polymeric samples and how analysis of these extracts can yield insights about the diffusivity of molecules in a polymeric phase.

1 Introduction

Diffusion in polymeric phases is an important phenomenon which influences many fields. The ability to control the release of active compounds from a polymeric vehicle may be influenced by the diffusivity of these compounds, especially when strong interactions exist between the active compound and the vehicle. Particularly interesting are those cases in which these interactions can be modified to tune the diffusivity of the mobile compound.

In order to assess how different structural features assess the diffusivity of an analyte, the kinetics of analyte release must be measured. The methods used to effect this measurement are highly dependant on both the nature and quantity of the analyte of interest.

Table 1 Some typical methods used to detect different types of analyte

Analyte	Detection Method	Sensitivity
Transition metal	Flame Photometry	10-1000 ppm
	Flame AAS	1-100 ppm
	Flame AES	< 1 ppm
Organic Cations	HPLC-MS	10ppb - 10 ppm
	GC-MS	10ppb - 10 ppm
	qNMR	10 - 1000 ppm

While HPLC-MS and GC-MS are by far the most sensitive techniques for the investigation of organic compounds, much time and effort must be spent developing and optimizing analyte extraction, pre-concentration and detection methods. Alternative methods, such as flame-photometry and quantitative NMR spectroscopy require less method development but are concomitantly less sensitive. The aim of this work was to establish whether the kinetics of the ion exchange of quaternary ammonium cations could be studied using a combination of flame photometry and qNMR.

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‡ Additional footnotes to the title and authors can be included *e.g.* 'Present address:' or 'These authors contributed equally to this work' as above using the symbols: ‡, §, and ¶. Please place the appropriate symbol next to the author's name and include a `\footnotetext` entry in the the correct place in the list.

2 Ion Exchange

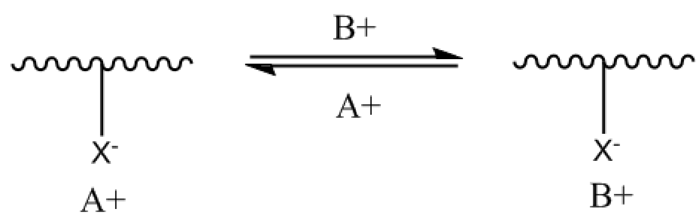

Fig. 1 Basic outline of the ion exchange equilibrium, where an incoming ion B+ can displace a resin associated ion A+

2.1 Basic Principle

Ion exchange describes the phenomenon in which an ion exchange material in some initial ionic form will, in contact with a solution containing some ion of a different type to that already contained within the resin, will take-up that ion while releasing the initial ion.

$$R\bar{A} + B^{+} \leftrightarrow R\bar{B} + A^{+} \tag{1}$$

This phenomenon is of great utility in a large number of industrially important processes; notably the preferential extraction of radioactive isotopes from the waste produced by nuclear reactors.

2.2 Ion Exchange materials

A typical ion exchange material consists of a crosslinked polymeric matrix containing acidic or basic side chains (depending upon whether cation or anion exchange is the desired behaviour of the resin). One of the most popular co-polymers used as a matrix for ion-exchange material is styrene-divinylbenzene (SDVB)(see figure 2).

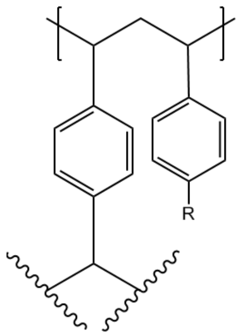

Fig. 2 The styrene-divinylbenzene co-polymer is one of the most popular skeletons for ion exchange resins. R may be any acidic or basic group, dependant upon whether cation or anion exchange functionality is desired

SDVB based resins are particularly attractive due to the ease with which polymer beads of a well controlled size distribution may be obtained. This is achieved by inverse phase suspension free radical polymerization of the monomers in water. As we shall later discuss, this size control is critical for the production of ion exchange resins which behave in a well defined and predictable manner.

3 The Kinetics of Ion Exchange

The kinetics of ion exchange are well understood, with the first pioneering studies undertaken by Hellferich at the beginning of the 20th century.

4 Equations

Equations can be typeset inline *e.g.* $y = mx + c$ or displayed with and without numbers:

$$A = \pi r^2$$

$$\frac{\gamma}{\varepsilon x} r^2 = 2r \tag{2}$$

You can also put lists into the text. You can have bulleted or numbered lists of almost any kind. The `mhchem` package can also be used so that formulae are easy to input: `\ce{H2SO4}` gives H_2SO_4.

For footnotes in the main text of the article please number the footnotes to avoid duplicate symbols. *e.g.* `\footnote[num]{your text}`. The corresponding author $*$ counts as footnote 1, ESI as footnote 2, *e.g.* if there is no ESI, please start at [num]=[2], if ESI is cited in the title please start at [num]=[3] *etc.* Please also cite the ESI within the main body of the text using †.

5 Conclusions

The conclusions section should come at the end of article. For the reference section, the style file `rsc.bst` can be used to generate the correct reference style.

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