# Questions

# One

Lewis structure of  $Si(OH)_4$ 

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# Step #1

Number of electrons = 4x6 + 4x1 + 1x4 = 32.

# Step #2

After 8 electrons are assigned to each oxygen, and single bonds are formed between each species all species have a full octet, (except for hydrogen which has a full valence shell consisting of two electrons)

NOTE: As silica is a period two element overfilling of the octet is possible however any additional bond formation between the oxygen and the central silicon could only increase the formal charge and so may be discounted.

# Step #3

Draw structure

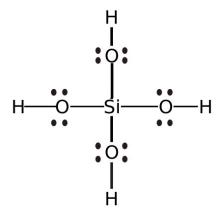


Figure 1: Silicon Hydroxide Lewis structure

# Lewis structure of $Al(OH)_4^-$

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# Step #1

Number of electrons = 4x6 + 4x1 + 1x3 + 1 = 32.

# Step #2

After 8 electrons are assigned to each oxygen, and single bonds are formed between each species all species have a full octet, (except for hydrogen which has a full valence shell consisting of two electrons). Again overfilling by creating more bonds will only increase the formal charge.

# Step #3

Draw Structure

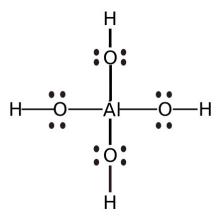


Figure 2: Aluminium Hydroxide Ion Lewis structure

Lewis Structure of  $Al(OH)_3$ 

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#### Step #1

Number of electrons = 3x6 + 3x1 + 1x3 = 32

# Step #2

After 8 electrons are assigned to each oxygen, and single bonds are formed between each species all species have a full octet, (except for hydrogen which has a full valence shell consisting of two electrons). Again overfilling by creating more bonds will only increase the formal charge.

# Step #3

Draw Structure

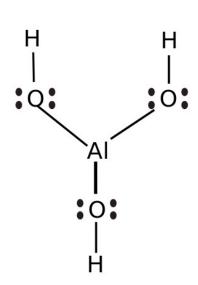


Figure 3: Aluminium Hydroxide Ion Lewis structure

# Two

(i)

# Step #1

Moles of EDTA added to EDTA standard

$$= \frac{0.914g}{372.24g.mol^{-1}} = 2.4554 \quad x \quad 10^{-3}mol$$

### Step #2

Average Titrant volume = 0.5x((4.57 - 0.04) + (5.13 - 0.10))ml = 4.78ml

# Step #3

Moles of EDTA in Titrant

$$= 2.4554 \quad x \quad 10^{-3} mol \quad x \quad \frac{4.78m}{250ml}$$
  
=  $4.6947 \quad x \quad 10^{-5} mol$ 

(ii)

# Step #1

At equivalence point of the titration all of the EDTA has reacted with calcium at the ratio of 1 mol EDTA: 1 mol calcium ions.

Hence If =  $4.6947 x 10^{-5} mol$  of calcium where added then =  $4.6947 x 10^{-5} mol$  of calcium ions where used up form the titrand.

# Step #2

As the titrand contained only 25ml of the original calcium chloride zeolite solution, It can be interpolated that 3 x 4.6947 x  $10^{-5}mol = 1.4084$  x  $10^{-4}$  of calcium ions would have been used up from the entire solution.

(iii)

#### Step #1

Moles of Calcium chloride present in the original solution.

$$= \frac{0.196g}{219.08g.mol^{-1}}$$
$$= 8.9465 \quad x \quad 10-4$$

#### Step #3

Moles of Calcium ions left in the original solution

$$= 8.9465 \quad x \quad 10^{-4} mol - 1.4084 \quad x \quad 10^{-4} mol$$
 $7.5381x \quad 10^{-4} mol$ 

(iv)

Grams of Calcium chloride left in original solution. = 7.5381x  $10^{-4}mol$  x  $40.08g.mol^{-1}$  = 3.0213 x  $10^{-2}g$ 

(v)

### Step #1

The amount of calcium ions taken up by the zeolite is equivalent to the amount fo calcium ions remaining in solution, as any calcium ions not bound would have been removed during the EDTA titration.

Hence there are 7.5381 x  $10^{-4}$  mol of Calcium ions bound by the zeolite.

(vi)

#### Step #1

Grams of Calcium ions taken up per gram of Zeolite

$$= \frac{3.0213 \times 10^{-2}g}{0.104g}$$
$$= 0.29051(g/g)$$

#### Three

This implies that zeolites may be very useful as detergents as they are capable of sequestering/removing relatively large quantities of dissolved ions from solution. (removing these ions will prevent them from resettling on whatever item is being cleaned, and increase the overall ability of the detergent to dissolve and remove unwanted deposits from the item being cleaned.)

#### Five

four acid sites are accosted with the EDTA. (one for each of the terminal carboxylic acid groups)

#### Six.

Yes. Sulphuric acid has the same activity of any normal acid catalyst, providing a ready source and sink for  $H^+$  ions, facilitating the internal structural changes necessary for ester formation.

#### Seven

Pentyl ethanol is used:

1. as a flavourant in many foods.

2. As a solvent in paints.

# Eight

Zeolite is micro-porous, that is within its 3D chemical structure there is a regular arrangement of regular sized gaps/holes/pores,through which other molecules, if sufficiently small could pass through. molecules which are too large however, (such as molecules with a diameter greater than X in the figure below) can. Such molecules suffer size exclusion, as although they may have the correct chemical properties to react with binding sites on the interior, they are physically prevented from reaching these sites, as the are too large, and so cannot bind.

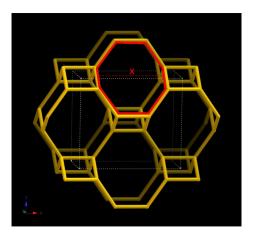


Figure 4: Zeolite Structure

# Aim

Two different experiments where performed with different aims.

The aim of experiment A was to determine the Ability of Zeolite to bind Calcium ions from solution. Both to determine how effective Zeolite could be as a cleaning/filtering agent to remove calcium impurities, and to approximate how much zeolite (by mass) would be necessary to remove calcium from a contaminated solution.

The aim of experiment B was to determine Zeolite ability to act as a Acid catalyst (in esterification.)

# Introduction

Zeolites Are complex three dimensional molecules formed from the condensation of Si(OH) 4 \$\\$ and  $Ai(OH)_4^-$  monomers. These monomers take a variety of forms including cages, chains, channels and sheets (Cejka, 2007). When these monomers bond together three dimensional structure/nets can be formed. The most striking feature of the complexes formed is the regularly sized and evenly space pores which are most commonly composed of six or eight bonded tetrahedral units, forming hexagonal or octagonal openings in the molecule respectively. (See the figure below). This regular arrangement has many potentially important chemical applications. One such application is the ability of Zeolites to act as molecular sponges/ filters soaking up particles of the correct size to fit through the microspores which binding to the interior of the molecule via a process of cation exchange. this process can be effect in removing cation contaminants from solution. (Motsi et Al 2009). Furthermore Zeolites can also act as effective inorganic acid catalyst, (provided they contain appropriate ratios of aluminium to silicon subunits). these catalyst have been demonstrated to be more effective that simple lewis or bronsted acids in catalysing important organic synthesis pathways such as the etherification of glycerol. (Aula et Al 2017) Such catalyst have the added advantage that, as the catalyst is solid state, removal and reuse if far simpler and less energetically expensive than a conventional acid catalyst.

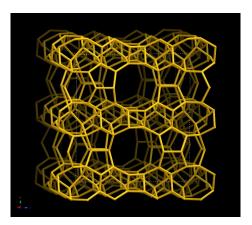


Figure 5: Zeolite Structure

# Results and discussion.

A was them mas ratio of grams of calcium taken up per gram of zeolite, calculated as = 0.291(g/g). This importance of this figure

# Material and methods

# Experiment A.

#### Preparation of standards

In the first main experiment two standard solutions where prepared, A  $\approx 0.01 M$   $CaCl_2.6H_2O$  solution and a  $\approx 0.01 M$  EDTA disodium salt solution. (The exact masses of  $CaCl_2.6H_2O$  and EDTA disodium salt can be referenced in the Data appendices.). In each case deionised water was used to make up the solution to prevent unwanted cations or other contaminants from affecting the experiment result.

#### Preparation of Analyte.

 $\approx$  of zeolite was added to 75ml of the  $CaCl_2.6H_2O$  standard solution, and mixed by means of a magnetic stirrer bar for a period of approximately five minutes. Subsequently the zeolite was removed by filtration through a gravity filter. And samples of solution where taken to serve as the analyte for titration against the EDTA di-sodium salt standard solution.

#### Titration

titration was performed in triplicate however one titration had to be discounted because of inaccuracies in identification of the endpoint. (Eriochrome black T was used as the indicator). the remaining two titration values where averaged.

#### Experiment B

#### Preparation of initial solutions.

2 solutions where prepared, solution one containing:

And solution two containing:

# **Synthesis**

both solutions where then boiled under reflux for approximately an hour.

# Work up

after cooling the solutions where rinsed several times with water to remove any remaining acid or alcohol impurities.

# **Data Appendices**

# Experiment A.

#### Materials used

Materials used in preparation

Weight of hydrated Calcium Chloride used in Solution 1

Weight of EDTA disodium salt use in Solution 2

Weight of Zeolite added to Solution 1

#### **Titration Table**

Titration of solution 2, (titrant) into solution 1 (Analyte)

Titration number

#1
#2

# Experiment B.

Description of product.

Density	Smell
Lighter than (deionised) water	Fruity aroma, reminiscent of banana, intoxicating fumes.
Lighter than (deionised) water	Intense fruity aroma, reminiscent of banana
	Lighter than (deionised) water Lighter than (deionised)

#References In-text: (Cejka, 2007)

Cejka, J. (2007). Introduction to zeolite molecular sieves. Amsterdam: Elsevier,  $\rm p.15$ 

T. Motsi, N.A. Rowson, M.J.H.Simmons, Adsorption of heavy metals from acid mine drainage by atural zeolite, International Journal of Mineral Processing, Volume 92, Issues 1–2, 2009, Pages 42-48,ISSN 0301-7516,

Aula M. Veiga, Alexandre C.L. Gomes, Cláudia O. Veloso, Cristiane A. Henriques, Acid zeolites for glycerol etherification with ethyl alcohol: Catalytic activity and catalyst properties, Applied Catalysis A: General, Volume 548, 2017, Pages 2-15,ISSN 0926-860X,