The importance of using chlorination reactions

Science, Chemistry



Chlorination reactions are key processes used in industry and are also utilized in the public sector. In terms of the atomic level a chlorination reaction is any reaction or process in which chlorine, and no other element, are introduced into a molecule. These reactions must contain an active agent consisting of chlorine, be it the element chlorine or a derivative of chlorine, phosphorous oxychloride for example. Chlorination reactions are primarily used for water treatment for drinking water and to disinfect spills of microorganisms.

Chlorinations are widely popular in water treatment as they tend to be quick reactions that effectively kill many types of bacteria and fungi that can be dangerous in fluids, while having little effect on humans. The most prominent mechanism bacteria are destroyed is through the chlorine agent destabilizing the bacterial membrane by binding to reactive compounds in the membrane. This proves most effective when the chlorine is able to react with the bacterial enzymes, replacing one or more of the hydrogen atoms in the molecule with chlorine. This causes the crucial enzymatic shape to change and lose its function, leading to cell death.

In this type of process, when the chlorine comes in contact with the water it forms hypochlorous acid in the following reaction: $Cl2 + H2O \rightarrow HOCl +$ $H\neg\neg\neg\neg+ + Cl$. This is a weak acid which lends to its benefits being disastrous for bacteria while being relatively safe for humans. Hypochlorous acid being electrically neutral can penetrate the negatively charged membrane of the bacteria thus is in contact with all bacterial enzymes causing maximum damage. Not only is it safe for humans but the human immune system uses this weak acid to kill pathogens and fight infection. Chlorination reactions https://assignbuster.com/the-importance-of-using-chlorination-reactions/

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can sometimes be rather simple and just involve adding a chlorinecontaining compound to the mixture. When it comes to water treatment, usually chlorine gas is pumped directly into the water to kill the microorganisms.

Another method is adding chlorine in the form of a solid compound, calcium hypochlorite as an example. These types of agents react with water to produce free chlorine molecules. Both of these methods of chlorination are so cheap and effective that nearly all water treatment systems worldwide use one of these methods as its primary means of killing pathogens and fighting infection. Chlorination is not only useful in treatment of water. Many organochlorine compounds are vital intermediates in the synthesis of pharmaceuticals, agricultural chemicals and as functional materials. In contrast to the chlorination in water treatment, synthesising chlorine-related functional groups can prove quite difficult.

The most prominent of organochlorine intermediates used in synthesis are the allyl- and vinyl chlorides. These chlorides provide excellent intermediates in order to substitute the chlorine atom with complex side chains with relative ease. This is because chlorines, as well as the other halogens, are known to be good leaving groups. A leaving group is an atom or a group of atoms which splits from the rest of the molecule, taking the bonding pair of electrons with it. This occurs through heterolytic bond cleavage. It is this quality of organochlorines that makes synthesising these chlorides is so sought-after. In this reaction phosphorus oxychloride is used as the chlorinating agent to covert an aromatic alcohol to an organochlorine. In contrast to hypochlorous acid, when chlorine is used as part of phosphoryl chloride can be extremely harmful to humans. It is extremely toxic by inhalation and is corrosive to metals and human tissue. According to the Environmental Protection Agency, phosphorous oxychloride is an extremely hazardous material. While the phosphorous oxychloride readily releases hydrogen chloride on contact with water, the main toxicity of this chemical is not related to the HCI release. It has been found that the main mechanism of toxicity is linked with the phosphorylation of the acetylcholinesterase enzyme. When the phosphorous oxychloride is put into solution it forms phosphorodichloridic acid, an extremely powerful phosphorylating agent.

This acid then phosphorylates acetylcholinesterase's active site, inactivating the enzyme. Acetylcholinesterase controls the amount of cholinergic neurotransmitters in body. Without this active enzyme action potentials would be overproduced leading to neurotoxic effects such as pulmonary edema and can lead to death. The aromatic alcohol is a cis-4hydroxypyrimidine. This 4-hydroxypyrimidine structure can undergo tautomerisation similar to the simple keto-enol tautomerism. This means that this molecules exists in resonance with its two possible ketones forms, 4(3H)-pyrimidinone and 4(1H)-pyrimidinone.

In this form the nitrogen lone pair dissociated forming a double bond causing the carbonyl bond attack the phosphorous atom in the phosphorous oxychloride. This forms the strong oxygen-phosphorous bond. As the bond form, a chlorine atom is kicked from the phosphorous oxychloride. The phosphorous oxygen bond is very short, suggesting the presence of a double bond. This now negatively charged chlorine then proceeds to attack the original carbonyl carbon causing the oxygen to be kicked off, leading to another release of a chlorine atom from the phosphorous oxychloride structure. This chlorine atom then remove the nitrogenous hydrogen reforming the stable pyrimidine ring.

Given this reaction requires the pyrimidinone form over the hydroxypyrimidine form, the tautomeric equilibrium is extremely important to the speed of the reaction. This equilibrium is also seen in hydroxypyridine to pyridinone. In the case of a pyridine ring, data shows that the hydroxyl form is favoured. However, it had been shown that the addition of the nitrogen at the para position to the hydroxyl group, creating a pyrimidine ring, shifts the equilibrium towards the carbonyl form. This difference in tautomeric equilibrium can be attributed to a number of reasons. It was found that pyridinone rings are more aromatic than their pyrimidinone equivalent due to the higher conjugation of the alcohol and ketone functional groups interacting with the two nitrogen atoms in the pyrimidine, lowering the aromaticity.

In contrast, in pyridine rings there is only one nitrogen atom in conjugation with the keto-enol related groups. It was also found that the second nitrogen in pyrimidine rings has significant electron withdrawing effects causing the nitrogen-hydrogen bond in pyrimidinone to be a stronger bond than its pyridinone equivalent further lending to the tautomeric shift. These effects combined with suspected contributions from intramolecular hydrogen bond causes the ketonic form to be favoured for the equilibrium between cis-4-

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hydroxylpyrimidine and 4(3H)-pyrimidinone. These structures are very similar to those seen in the nitrogenous bases thymine and uracil used in nucleic acids thus also explaining their prominent form also being the ketone tautomer. Crystallisation is one of the most common methods for isolation and purification along with distillation and column chromatography.

Crystallisation is a separation process, widely used in the chemical and pharmaceutical industry. The principle of crystallizations is based on the limited solubility of a compound in a solvent at a certain temperature and pressure. By manipulating these factors, a point can be found at which the compound will crystallise out of solution while impurities and reactants stay in solution allowing for isolation of the product. Crystallisation has been used for thousands of years to produce such common household items such as sugar and salt. Despite this, many crystallisation properties are still poorly understood such as the mechanisms of nucleation and crystal growth. Given how important crystallisations are in industry such as pharmaceuticals and food where quality is crucial, there is a large interest in research into crystallisations to further improve and understand.