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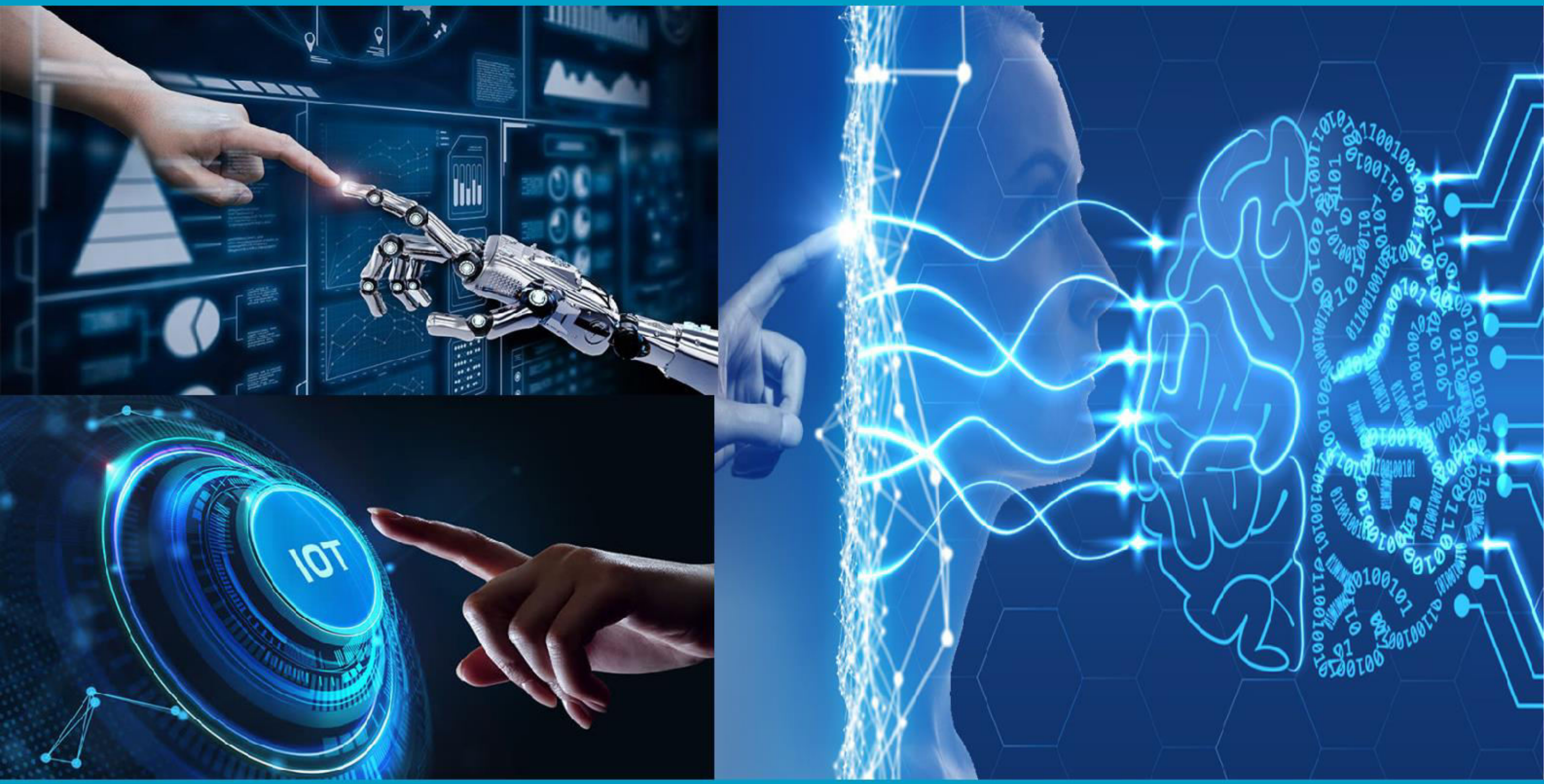

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Spectral Studies of 2 - Chloro 3 –Methyl Benzonitrile

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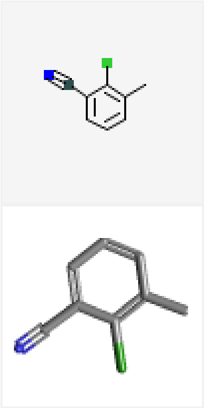
ABSTRACT: 2-Chloro-3-methylbenzonitrile

PubChem CID	14529890
Structure	 Find Similar Structures
Molecular Formula	C_8H_6ClN
Synonyms	2-Chloro-3-methylbenzonitrile 15013-71-5 BENZONITRILE, 2-CHLORO-3-METHYL- 2-cyano-6-methylchlorobenzene SCHEMBL1344112
Molecular Weight	151.59
Chemical Structure Depiction	

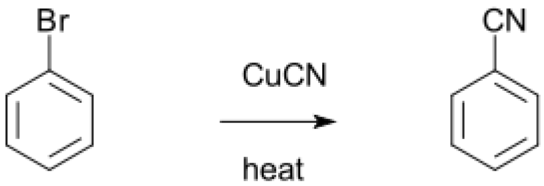
Keywords: spectral, 2-chloro, 3 methyl benzonitrile,

I. INTRODUCTION

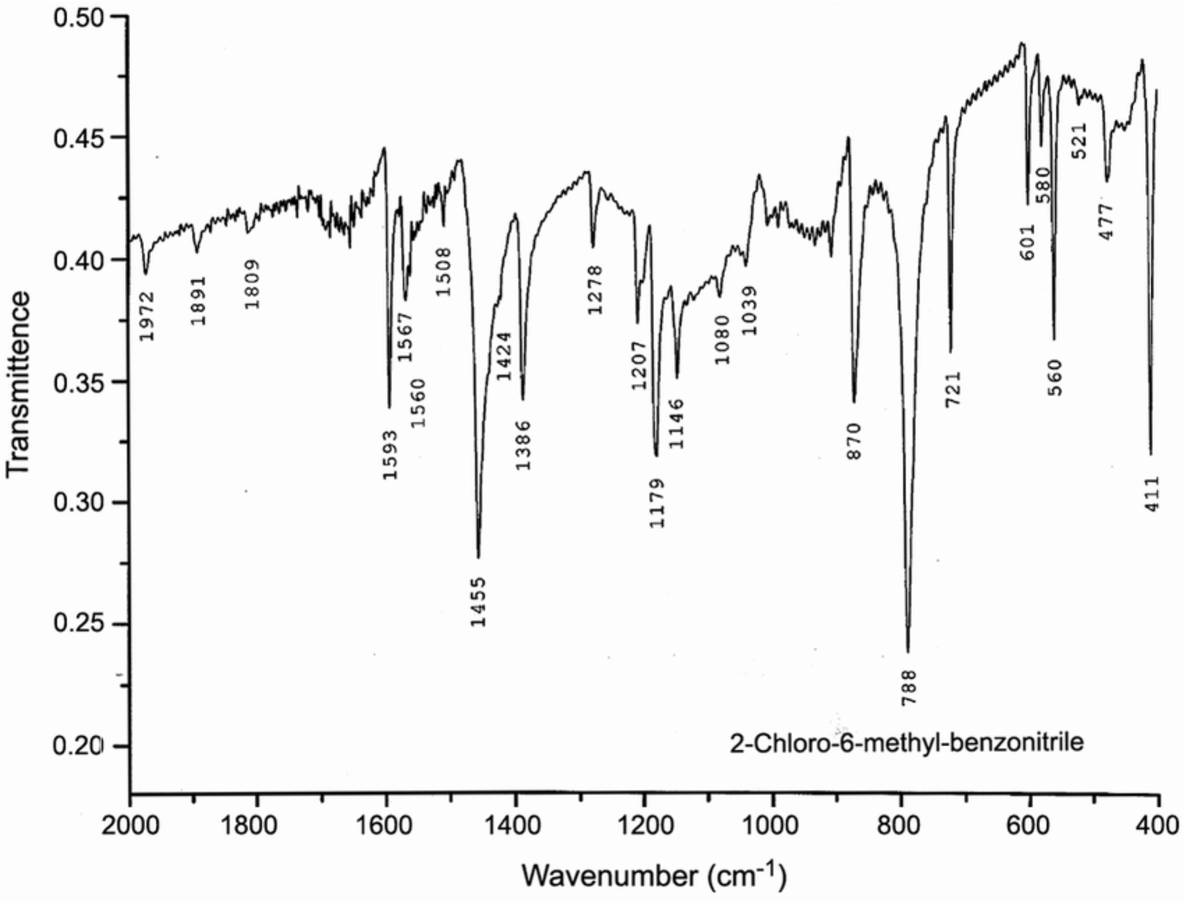
Benzonitrile is the chemical compound with the formula $C_6H_5(CN)$, abbreviated PhCN. This aromatic organic compound is a colorless liquid with a sweet bitter almond odour. It is mainly used as a precursor to the resin benzoguanamine. It is prepared by ammoxidation of toluene, that is its reaction with ammonia and oxygen (or air) at 400 to 450 °C (752 to 842 °F).[1]

$$C_6H_5CH_3 + 3/2\ O_2 + NH_3 \rightarrow C_6H_5(CN) + 3\ H_2O$$

In the laboratory it can be prepared by the dehydration of benzamide or by the Rosenmund–von Braun reaction using cuprous cyanide or NaCN/DMSO and bromobenzene.



Benzonitrile is a useful solvent and a versatile precursor to many derivatives. It reacts with amines to afford N-substituted benzamides after hydrolysis.[2] It is a precursor to diphenylketimine $Ph_2C=NH$ (b.p. 151 °C, 8 mm Hg) via reaction with phenylmagnesium bromide followed by methanolysis.[3]



Benzonitrile forms coordination complexes with transition metals that are both soluble in organic solvents and conveniently labile. One example is $PdCl_2(PhCN)_2$. The benzonitrile ligands are readily displaced by stronger ligands, making benzonitrile complexes useful synthetic intermediates.[4]

Benzonitrile was reported by Hermann Fehling in 1844. He found the compound as a product from the thermal dehydration of ammonium benzoate. He deduced its structure from the already known analogue reaction of ammonium formate yielding hydrogen cyanide (formonitrile). He also coined the name benzonitrile which gave the name to all the group of nitriles.[5]

In 2018, benzonitrile was reported to be detected in the interstellar medium.[6]

II. DISCUSSION

Nitriles are the organic compounds in organic chemistry which are also called Cyano Compounds. This class of organic compounds contain cyanide as the functional group with the formula $-C \equiv N$. Inorganic compounds with -CN group are called cyanides. The compound Acrylonitrile is processed in many quantities by the process of ammoxidation which depends on the oxidation state of the propylene in presence of ammonia and catalyst. This compound forms an important constituent of polymeric substances, also which includes acrylic textile fibres, synthetic rubbers as well as thermoplastic resins.[7,8]
Some compounds of nitriles are mainly manufactured by heating up carboxylic acids with the ammonia compound in presence of some catalysts. This is a process which is employed in the preparation of nitriles from oils and fats. These products are being used as the softening agents in substances such as synthetic rubbers, textiles, plastics and also in the making of amines. Nitrile compounds are also formed by the process of heating amides with the phosphorous pentoxide. They can also be reduced to primary amines by reacting lithium aluminium hydride or getting it hydrolyzed to carboxylic acids in presence of acid or base.[9,10]

The chemical and physical properties of nitriles are given below-

- Nitriles are colourless solids or liquids with unique odours.
- They have boiling points measuring between 82-118 °C.
- Nitriles exhibit strong dipole-dipole movements and also the Van der Waals forces of dispersion between the molecules.
- They also show high polarity and electronegativity.
- These are said to be highly soluble in water, and the solubility decreases as the chain length increases.

Nitrile undergoes a various set of reactions as shown below-

1. Hydrolysis- The hydrolysis of nitriles in the presence of an acid or a base produces carboxamides and carboxylic acids efficiently.[11,12]

2. Reduction- Nitriles are reduced to primary and tertiary amines by treating them with lithium aluminium hydride. The reduction process occurs in the presence of some catalysts.

3. Alkylation- The alkylation of nitrile compounds leads to the formation of nitrile anions.

The other reactions are nucleophilic addition reactions, Friedel–Crafts acylation, etc.

Nitrile finds its uses in various medical and industrial applications of which some are listed below-

- Nitriles are used in the manufacture of nitrile gloves, seals, and hoses as they exhibit resistance to chemicals.
- They are used as an antidiabetic drug which is used in the treatment of breast cancers.
- The compound of nitrile called pericyazine is used in treating opiate dependence as an antipsychotic.
- This compound is found in many plant and animal sources.
- They are utilized in the applications of oil-resistant substances and also for low-temperature uses[13,14]

They are also employed in automotive systems, hydraulic hoses and also in aircraft systems.

III. RESULTS

Benzonitrile is a stable compound to pyrolysis, and its decomposition starts above 550°C with a very low decomposition rate. A study performed in a flow reactor on N_2 saturated with benzonitrile [8] in the temperature range 550–600°C showed that the main pyrolysis products of this compound are HCN, benzene, monocyanodiphenyls, dicyanodiphenyls, and dicyanobenzenes as well as char. The reaction takes place by a radicalic mechanism, starting with the following initiation reaction:
H5C6−CN→H4C6•−CN+H•

The position of the hydrogen atom where the cleavage takes place is not preferential because pyrolysis generates a mixture of monocyanodiphenyls, dicyanodiphenyls, and dicyanobenzenes (e.g., 2-cyano, 3-cyano, and 4-cyanobiphenyl). The presence of dicyanobenzene in the pyrolyzate indicates that free CN$^{\bullet}$ radicals are likely to be formed in the reaction. Kinetic parameters for the reactions of benzonitrile [15,16] decomposition are reported in the literature [8], with the formation of different compounds having different reaction orders. The pyrolyzate at 575°C obtained for 30 min contact time contains about 5.9 mole % HCN, 4.9 mole % dicyanobenzenes, 3.0 mole % benzene, 1.2% monocyanobiphenyls, and the other compounds at lower levels.

Benzonitriles and phenoxy acids are widely applied as salts or esters, but they are hydrolyzed to their respective phenols or acids in the matrix. Extraction of residues from soil and water is commonly performed at acidic pH with organic solvents of medium polarity. Initially, the extraction of these herbicides from vegetable matter was done with aqueous solutions at basic pH, followed by extraction with organic solvents.At present, different techniques such as SPME for aqueous samples, UAE for soil and MAE or PLE for plant samples are often used. QuEChERS is also used for the extraction of acidic herbicides from soil and plant samples after alkaline hydrolysis with sodium hydroxide·[17,18]

A clean-up step after extraction is required in most cases to allow the determination of herbicides at trace levels. Among the clean-up techniques used, the liquid–liquid partition at basic pH has been employed, but the most common procedure is solid-phase extraction (SPE) with cartridges or columns using sorbents of different characteristics depending on the selected herbicides. Sorbents such as Florisil, silica, alumina and C_{18} are used for the determination of benzonitrile and phenoxyacid herbicides. The use of graphitized carbon black (GCB) is adequate for the removal of non-polar and oxygen-containing compounds due to hydrophobic, electronic and ion-exchange interactions. The combination of GCB and aminopropyl adsorbent is effective to remove pigments and organic acids from wheat and soil samples.

Analysis of these compounds in air is carried out by trapping herbicides in ethylene glycol or in various adsorbents, like polyurethane or amberlite resins.

Derivatization of phenoxy acids, before GC determination, is necessary to make them volatile. Various alkyl, silyl or pentafluorobenzyl derivatives are obtained with this aim. Methyl esters have been commonly prepared for the determination of phenoxy acids and the reagents most often used were diazomethane and boron trifluoride-methanol. Extraction followed by derivatization into methyl esters was also performed with sulfuric acid and methanol. A simultaneous MAE and derivatization procedure is used for the determination of chlorophenoxy acid herbicides in soil, providing shorter derivatization time and reduction of artifacts formation. Benzonitriles can be determined directly by GC, but the sensitivity and reproducibility achieved are poor. Various derivatives overcome these problems and diazomethane and heptafluorobutyric anhydride were the reagents most often employed·[19,20]

In the last years, new methods for analysis of acidic herbicides in environmental samples are used. Injection port derivatization following ion-pair hollow fiber liquid- phase microextraction has been developed for the determination of acid herbicides in water samples.

Initially, the determination of herbicides was widely carried out by GC with ECD, if the compound had halogen substituents or halogenated derivatives were obtained. MS detection has the advantage of being more selective and requiring less clean-up of extracts.The use of MS provides a level of confirmation not available with conventional detectors. Nowadays, MS/MS has gained popularity in environmental analysis due to its versatility, selectivity and specificity.

IV. CONCLUSIONS

Benzonitriles and phenoxy acids are widely applied as salts or esters, but they are hydrolysed to their respective phenols or acids in the matrix. Extraction of residues from soil and water is commonly performed at acidic pH with organic solvents of medium polarity. The extraction of these herbicides from vegetable matter is often done with aqueous solutions at basic pH, followed by extraction with organic solvents·[20]

Purification of extracts is required in most cases and this step is accomplished by liquid–liquid partition at basic pH or by chromatography on silica columns.

Analysis of these compounds in air is carried out by trapping herbicides in ethylene glycol or in various adsorbents, like polyurethane or amberlite resins.

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