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NOTES

Nature of Atrazine (2-Chloro-4-ethylamino-6-isopropylamino-*s*-triazine)-Copper Chloride Complex

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Treatment of atrazine (2-chloro-4-ethylamino-6-isopropylamino-*s*-triazine) with anhydrous copper chloride in methanol yields 1 : 1 complex. The infrared spectra and n.m.r. spectra do not suggest coordination of the nitrogen atoms of the side chain or C_3N_3 ring with the metal atom; instead a bond between the π-electrons of the C_3N_3 ring and the metal atom is indicated from the far IR spectra of this complex.

INTRODUCTION

Recently *s*-triazines have become the most important and widely used goups of herbicides[1] and have the advantage of being used as selective[2] herbicides. Among these, atrazine has found a major use in agriculture. The remarkable stability of this chain of compounds can be attributed to the electronic configuration of the heterocyclic ring, which resembles benzene though it has slightly less aromatic character than that of benzene due to the delocalization effect in combination with inductive and mesomeric effect, exerted by the substituents at C-2, C-4 and C-6. Khan *et al*[3] observed residues of atrazine and its metabolites even though the samples were taken 2–3 years after last application of the herbicide. At the same time, it was shown by field work[4] and laboratory tests[5] that the uptake of mineral nutrients is appreciably higher in atrazine treated plants than the control plants. Some strong bonding is the process which is determining the fate and behaviour of this class of herbicides. We have tried to isolate a complex of atrazine with copper chloride.

Anhydrous copper chloride was prepared by refluxing the hydrated salt with thionyl chloride for 3–4 hrs. It was washed with petroleum ether. The analytical samples of atrazine (supplied by CIBA-Geigy) and methanol (Glaxo) were used as such.

The complex was prepared as follows. The methanol solutions of copper chloride and atrazine prepared separately were made to react by refluxing for 2–3 hrs. The solution was concentrated when the crystals of the complex separated. The complex was dried under vacuum.

The methanol solution of copper chloride and atrazine is refluxed and on concentration of this solution the crystals of the complex are formed. The elemental analysis corresponds to the 1 : 1 stoichiometry. The complex gets hydrolysed when placed in the atomsphere. The specific conductance of the complex indicates it to be ionic.

The far IR spectra does not give any band in the region 450–500 cm^{-1} indicating the absence of metal-N band[6,7]. A band at 328 cm^{-1} is observed corresponding to metal-chlorine and the band at 380 cm^{-1} has been assigned to the π-bond[8] between the C_3N_3 ring and the metal atom. The band at 820 cm^{-1} is observed corresponding to C_3N_3 ring[9].

Since there is no indication of any coodination between the metal and nitrogen atom of ring or the side chain, we can infer that π-bond is formed between the C_3N_3 ring and the d-orbitals on the metal atom. This bond formed is very strong and can explain the persistence of the atrazine and its metabolites in soil and thus upsetting of micronutrient uptake by the plants.

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