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SINGLE CRYSTAL AND POLYCRYSTALLINE E.P.R STUDIES OF PHOTOCHEMICAL REACTION OF THE ^{15}N LABELLED HUMULENE NITROSITE ($C_{15}H_{24}N_2O_3$)

ZIA FAROOQ KHAN*, NOOR-I-AIN NAQVI**
AND GULREZ FATIMA DURRANI**

* Dept. of Chemistry, Islamia University, Bahawalpur.
** Dept. of Chemistry, Gomal University, D.I.Khan.

ABSTRACT

E.P.R studies of red irradiated ^{15}N labelled Humulene Nitrosite has been carried out by an entirely new method. First a single crystal was irradiated by red light for about 50 to 200 hours. Various hyperfine tensors i.e., g_{xx}, g_{yy}, g_{zz} and (A^1H), A (^{15}N) were obtained theoretically using suitable computer programmes. Experimental results obtained were then matched both in single crystal and polycrystalline work. Relative sings of the Hyperfine tensors have also been calculated.

INTRODUCTION

As in earlier attempts, it was reported that the major difficulty in analyzing the E.P.R. spectra is the relative signs of the Hyperfine tensors (1,2,3,4). Infact the spectra are very complicated even at low temperatures, however a detailed experimental and theoretical studies were carried out to over come this problem. The nitroxide radical in this case, consists of one electron interacting with one proton (^1H) and on ^{15}N nucleus; therefore making the spectra very complicated (4,5,7,8,9).

The best way for extracting these tensors is to, first grow large single crystals of Humulene nitrosite and then irradiating one selected crystal with red light w.r.t. some arbitrary chosen frame of reference XYZ and obtaining useful data (10).

Using the above data we can then analyze the polycrystalline spectra using some suitable computer programme, and then calculating the theoretical spectra. (7-10).

Theoretical spectra can then be compared with experimental ones to predict the best analysis.

EXPERIMENTAL

Humulene nitrosite was prepared as described earlier (1,2) by treating Humulene with $NaNO_2$ and glacial CH_3COOH at 10°C in dark. It was recrystallized from ethanol