

Search and Retrieval of ^{13}C NMR Data

D.A. Ross

Directorate of Scientific Information Services
Research and Development Branch
Department of National Defence
Ottawa, Canada

ABSTRACT

This paper examines three aspects of ^{13}C NMR Spectroscopy and its literature: (a) the principles of nuclear magnetic resonance and its application to structural problems in chemistry; (b) experimental data for a ^{13}C NMR SDI profile covering the defence literature over a 15-year period; and (c) experience in searching the ^{13}C NMR/IR file via the STN network, on-line.

Many databases which DSIS searches are bibliographic ones; however, others, such as the ^{13}C NMR/IR file, are not. An example of a factual or numeric database, it is described in the paper.

Since most attendees are likely not familiar with NMR Spectroscopy, a brief introduction to the field is given for the non-specialist. This enables the attendee to gain an insight into the nature of searching on the ^{13}C NMR file, for organic compounds.

The retrieval of ^{13}C NMR data is described by following the development of a DSIS SDI profile, for which records were searched from the Defense Technical Information Center. A copy of the original profile is presented along with tables which describe the success of the profile in locating defence information for chemical structure determination by ^{13}C NMR Spectroscopy. Other nuclei, such as ^{31}P , ^{19}F , ^{29}Si ; and ^1H are also mentioned.

Finally, it is concluded that the information professional can indeed help the chemist in obtaining pertinent and critical NMR data by both on-line retrieval methods, and by SDI profiles.