

NIES-Mass Spectral Data Base for Environmental Analysis

環境分析のためのマススペクトルデータベース

March 1990

Tsuguo Mizoguchi, Akio Yasuhara, Hiroyasu Ito,

Junko Shindo and Takashi Uehiro

溝口次夫 安原昭夫 伊藤裕康

新藤純子 植弘崇嗣

THE NATIONAL INSTITUTE FOR ENVIRONMENTAL STUDIES

環境庁 国立公害研究所

PREFACE

Many synthetic toxic organic compounds can be found in the environment, e.g., in air, water, sediment, in animals and plants, and in the various components of the human diet.

Gas chromatography / mass spectrometry (GC/MS) is one of the most useful and important techniques used in the analysis of organic compounds in environmental samples. It is often very difficult to identify unknown compounds computer based in environmental samples from mass spectral data.

Both high quality reference spectra and a computer based mass spectral retrieval system are necessary to identify unknown spectra. There are several established retrieval systems used in the identification of unknown compounds e.g., the peak, Bieman, and PBM systems. A new retrieval system has been published by our group, the National Institute for Environmental Studies (NIES), to aid in the identification of unknown compounds present in environmental samples.

This data book contains reliable reference mass spectra as well as mass spectra of commonly encountered environmental pollutants.

The goal of this program is to expand the size of the mass spectral data base and to enhance the quality of the data.

It is hoped that the data book will be of value to mass spectrometrists. Contributions on any comments on the data base are welcomed.

March 1990

Tsuguo Mizoguchi

CONTENTS

1.	INTRODUCTION	I
2.	HOW TO USE THIS BOOK	II
3.	REFERENCE	IV
4.	ACKNOWLEDGEMENTS	IV
5.	MASS SPECTRAL DATA	1
6.	LIST OF COMPOUNDS	604

1. INTRODUCTION

In recent years a tremendous increase in the development and application of synthetic organic compounds has occurred. The purpose of this data book is to serve as a convenient and practical source of mass spectral reference data that can be used in research and the identification of unknown compounds in environmental samples. Reliable reference spectra are required to analyze environmental organic compounds.

During the last eight years the National Institute for Environmental Studies (NIES) and a few prefecture institutes have developed a mass spectrometry data base together with the computer software to search the data base.

This data book contains electron impact mass spectra of 1441 pure compounds. But some trimethylsilyl derivatives were measured without purification because of their unstability. All of the spectra were carefully reviewed by experienced mass spectrometrists of the NIES group before inclusion. Each spectrum was measured by GC/MS after measurement conditions has been adjusted against the standard compound, DFTPP (Decafluoro-triphenylphosphine).

All the spectra were checked and judged reliable before entry in the computer file.

All the mass spectral data are stored together with the mass spectral library search facility (NIES-MSLS) in the computer system (HITAC 280H).^{1),2)}

The system will allow retrieval of all data in magnetic tape or floppy disk form as required. This mass spectral data book was printed by a photo-offset process directly from a computer printout.