

国外化学经典教材系列（影印版）

10

# 气相色谱与质谱 实用指南

**Gas Chromatography and Mass Spectrometry**

A Practical Guide

**(Second Edition)**

O. David Sparkman, Zelda E. Penton, Fulton G. Kitson

原著第2版



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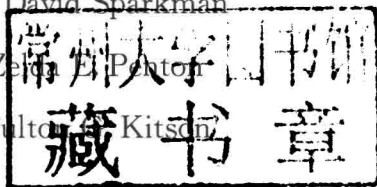
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by O. David Sparkman, Zelda E. Penton, Fulton G. Kitson

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## 导 读

近几年来,我国每年从国外进口 2000~3000 台质谱仪,价值数亿美元,其中气相色谱与质谱联用仪(GC/MS)约占一半。为了能用好这些仪器,十分需要一批掌握这一领域的广泛知识且能熟练运用各种 GC/MS 分析技巧的科技人员。只有勤奋实践和广泛读书才能成为这个领域的高层次人才。为此,需要出版各种类型的质谱书籍,供这一领域的科技人员学习之用。

《气相色谱与质谱:实用指南(原著第2版)》是气相色谱/质谱联用(GC/MS)的入门读物,对于 GC/MS 的实际工作者也是一本很实用的工具书,在 GC/MS 实际分析工作中遇到问题时,可方便地从书中查到解决问题的指导性资料。本书包含的许多资料是作者在数十年的质谱分析工作生涯中积累的实际经验,这也是本书不同于其他书的特点。本书可作为质谱领域的研究生的参考书。

本书的第1部分大约占了一半篇幅,是一些基础知识,扼要地叙述了气相色谱和质谱的基本原理、仪器构成和使用要点。对于初次涉足 GC/MS 的科技人员和研究生,读了该部分内容后,对气相色谱、质谱以及两者联用会有基本的认识。

关于气相色谱,本书着重讲述了选择合适的气相色谱的样品导入方法及其正确的操作条件。这些方面常常被分析工作者所忽视,这会导致灵敏度的损失或者样品前处理工作量的增加,例如,本书指出,在使用不分流进样时,分析工作者常常不恰当地过早打开放空阀,造成待分析物的流失,因而降低了检测灵敏度,这是常见的操作错误。书中介绍了多种可减少样品前处理工作量的实用的样品导入方法,例如固相微萃取法等,对于不同来源的样品,采用哪种样品导入方法,列出了一些建议。

为了达到良好的色谱分离效果,需要细致地选用合适的色谱柱类型和分析条件,为此,书中给出了一些选择原则,并以列表方式简明地阐述了柱长、柱内径以及固定相液膜厚度对色谱柱性能的影响,使读者一目了然。此外,适用于各类化合物的色谱分析条件,列于本书第2部分具体的化合物类型中。作者还用了相当的篇幅介绍了色谱的新进展:快速 GC,这是色谱的重要发展方向,使用该技术可大大缩短分析时间。书中讲述了实现快速色谱使用的色谱柱及操作条件,还指出能与快速色谱匹配的质谱仪,对于渴望提高工作效率的实验室工作人员,这些内容很值得一读。

本书对于质谱仪的离子化类型和  $m/z$  分析器类型做了一般性论述。在“离子化类型”一节中,要更多地关注“化学电离”和“电子捕获负离子化”这两小

节。在电子电离(EI)质谱图中常常不出现分子离子峰(即不能获得未知物的分子质量信息),因此即便是使用质谱库检索时,有相似度很高的谱图库谱图,但是由于缺少分子质量信息,仍然不能确切地鉴定未知物。化学电离是获得化合物分子质量的有效方法,以定性分析为主要工作的实验室,化学电离是不可或缺的手段。我国有许多GC/MS仪器配备了化学电离源,却没有得到充分的应用,令人惋惜。

第1部分的第5章扼要地阐述了与质谱图解析相关的基础知识,这对于从待分析物的质谱图推导出其化学结构是十分有益的。其中,①谱图库检索,详细地介绍了NIST(National Institute of Standards and Technology,美国国家标准与技术研究院)质谱图库检索系统的功能及其使用方法。若能全面掌握该检索系统的使用操作,则可以方便、灵活地从质谱图中提取许多有用的结构信息。该检索系统是质谱图解析的强有力工具。②离子的元素组成:从未知物质谱图推导其化学结构时,若能获知离子的元素组成,则可达到事半功倍的作用。在质谱技术发展的初期,一般是用高分辨力质谱仪测定离子的准确质量数,再进而求得其可能的元素组成。本书除了对这一技术详细介绍外,还介绍了另外一种方法,即在低分辨力质谱图中,利用离子的同位素峰丰度分布,求得该离子的可能的元素组成,NIST检索系统可以进行这种计算。后一种方法提高了四极质谱仪和离子阱质谱仪的定性分析能力;使用这两种低分辨力质谱仪进行定性分析的质谱工作者很有必要掌握此方法。在此,还需指出,读者不要误解,认为低分辨力质谱仪可以替代高分辨力质谱仪。从同位素峰丰度分布,求出该离子的可能元素组成的前提是该离子峰必须是单一的成分,显然,若离子峰是重叠峰,则这一方法将导致错误结果。在这种情况下,只有用高分辨力质谱仪将重叠峰剥离开后,才能测得各离子的准确质量,进而求得其元素组成。③识别分子离子峰。本书给出一些判别原则,虽然是很短的一段叙述,但不要被忽视,读者需要记住这些原则。④色谱重叠峰的拆分。对于十分复杂的混合物,色谱往往不能将全部组分分离开,因此会出现一些色谱峰的重叠,即该色谱峰包含两个或更多的成分,与其对应的质谱图也是若干成分的质谱图的叠加,造成待分析物鉴定的困难。该书推荐了NIST开发的重叠峰自动拆分的软件AMDIS(Automated Mass Spectral Deconvolution and Identification),能方便地鉴定重叠色谱峰中包含的化合物。⑤质量色谱图。读者要很好地理解质量色谱图是怎样生成的及其应用技巧,这是提高数据分析效率的有效方法,例如,可从众多的色谱峰中迅速查找待分析目标化合物。再者,掌握了质量色谱图的应用技巧后,可以十分有效地进行重叠峰的人工拆分,若使用得当,可得到优于AMDIS的效果。⑥衍生化。气相色谱毕竟比液相色谱容易使用且分析费用较低,因此,采用衍生化与GC/MS的结合,仍

然不失为一种可以接受的分析方案。再者，特别设计的衍生化反应还可提供结构信息，因此绝不可忽视本章内容。

第2部分是各种化学类型化合物的具体分析方法，覆盖范围很广，除了醇、醛、酸、醚、酯、氨基酸、核苷等各种化学类型外，还包括常见的污染物、药物及其代谢产物、农药、塑料和其他聚合物的添加剂、溶剂及其杂质等。每一章都给出了色谱分析条件和具体的质谱图解析。这部分内容可作为手册，随时查阅。

本书的最后部分是附录，提供了许多很实用的资料。其中要着重指出的是：①用于GC/MS的衍生化方法。列举了一个很好的例子，说明经过衍生化后，待分析物的电子电离质谱图可以提供更多的结构信息。在此项附录中，同时还列出了各种官能团的衍生化试剂，并对衍生化需要用的设备和操作步骤做了简要的说明。②现有的EI质谱图库清单。这份清单十分齐全，除了通用的质谱图库外，还有专用的农药库、代谢物库、环境污染物库、毒物库等。读者可以根据工作需要去订购。③GC/MS分析报告应包含的信息。为写一份合格的GC/MS分析报告给出很好的指导，可以避免许多常见的错误。④用于GC/MS的第三方软件。列出一些可用于GC/MS数据分析的软件以及ChemDraw等用于画结构式及提供化学性质的软件。⑤有助于推导未知物结构的碎片离子。列出了众多的碎片离子的结构，根据未知物谱图中出现的碎片离子的质荷比( $m/z$ )，可以从中找到可能的化合物类型或部分结构(子结构)，有助于最终确定未知物的结构。

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## 前 言

本书的目的是为气相色谱/质谱 (GC/MS) 的实际工作者提供一些工具, 有助于他们进行分析操作和从分析数据中获取信息。为此, 除了提供这些工具资料外, 还介绍了最新发展的技术。本书不打算详尽讨论 GC/MS 的理论, 而是提供用气相色谱 (GC) 分离化合物并进而用质谱进行鉴定的相关资料。本书没有提供关于液相色谱/质谱 (LC/MS) 的资料。

第 1 部分: 在本书第 2 版中, GC/MS 基础知识、可用的仪器和技术 (第 1~6 章) 比第 1 版大为扩展。更多地关注可用的电子电离 (EI) 的质谱图库, 用软件及质谱数据拆分色谱共流出成分, 根据质谱峰强度用软件推导离子的元素组成。

第 2 部分: 阐述了 GC 条件、衍生化方法及若干类化合物的质谱图解析 (第 7~36 章), 删去关于填充柱的资料, 因为在现代的 GC/MS 实验室中, 这些柱已不被使用, 而是被多孔层开口管柱 (porous-layered open tubular, PLOT) 和涂壁开口管柱 (wall-coated open tubular, WCOT) 所取代。第 2 章中概述了 GC 的检测器, 这有助于使用气相色谱/质谱联用仪偶尔进行 GC 分析。在某些应用中, 用选择性 GC 检查器和质谱仪组合, 可在单次分析中获得有价值的信息。

除了通过 GC 将样品引入 GC/MS 离子源外, 也可将样品直接引入离子源, 在第 2 和 4 章中详尽阐述这些技术及其优缺点。

在本书的表格中列了许多资料, 如何进行某一具体类型样品的分析以及如何识别待分析物可从这些表中获得指导。本书应该放在分析人员的案头以及仪器的旁边。第 1 版已展示了本书是很好的工具书。第 2 版主要是扩展了文字叙述部分并保留和修改了表格中的数据, 在前一版中已显示这些数据是十分有益的。同时, 第 2 版扩展了质谱图解析的技巧。第 3 章很短, 是新加的, 涵盖了气相色谱和质谱的接口。第 5 章则更深入地阐述了质谱图的解析。第 6 章, 用 GC/MS 进行定量分析, 是完全改写的。第 3 部分的附录也扩展了, 增加了更多的有益的质谱图解析工具。在各类化合物的质谱图解析的章节中, 还可获得更多关于质谱图解析的资料 (第 2 部分, 第 7~36 章)。

在第 1 版中, 关于 GC 分析条件、衍生化方法和一些类型化合物的质谱图解析的许多资料, 是源于 Fulton G. Kitson 在 GC 和质谱领域经历 30 年职业生涯中取得的经验。这些资料多数被保留和扩展, 其表述也做了少许修改; 不是来自他的经验及由他精心组织的资料, 将不包括在这些资料中 (第 7~36 章以及若干附录)。



附录的数目由 12 增加到 17。附录中“原子质量和同位素丰度”已被扩展，可用于从同位素峰强度比值确定其元素组成。“根据同位素峰丰度比确定元素组成的步骤”是新增加的附录。附录中还增加了：选用 GC/MS 或 LC/MS；用于数据分析的第三方软件；GC/MS 数据分析报告应包含的信息；根据离子中碳的数目产生的  $X+1$  和  $X+2$  峰的相对强度的列表以及现有的 EI 质谱图库清单。其他诸如衍生化；含 Cl（或）Br 离子的同位素分布模式；用于 GC 和质谱的术语；气相色谱的条件设置、维护和故障排除的技巧，都被扩展和修改；附录中，质谱仪的维护和故障排除也同样被扩展和修改。

20 世纪 60 年代中期，瑞典的一家公司 LKB 推出了第一台商业 GC/MS 系统。之后，许多 GC 和 GC/MS 公司涌现出来，这些公司后来合并成为更大的公司，保留或失去他们原有的品牌标识，或者被淘汰而成为科学仪器历史的一页。20 世纪末期脱离了母公司的 Agilent Technologies（Hewlett-Packard 的非计算机/非打印机部分）于 2009 年末期兼并了 Varian Inc，它是多种科学仪器产品生产线的公司，是早期 Varian Corp 解体后剩余部分。Varian Inc 除了有真空技术、实验室光谱仪器（近-红外、紫外-可见、原子吸收和电感耦合发射光谱仪）、磁共振仪和超导磁体外，也是 GC 和 GC/MS [内离子源四极离子阱（QIT），于 1989 年从 Finnigan Corp 收购] 的主要供应商。Varian Inc 也生产用于 GC/MS 和 LC/MS 的串联四极质谱仪 MS/MS。Agilent 和 Varian 两公司的 GC 业务（仪器和耗材）以及 ICPMS 和串联四极质谱产品十分相似，欧洲经济共同体要求 Agilent 剥离这些产品才能进行收购。

Bruker 公司 [总部在 Billerica Massachusetts，是 Bruker 科学仪器部门（Bruker AXS、Bruker BioSpin、Bruker Daltonics 和 Bruker Optics）和 Bruker 能源与先进技术部门的母公司] 从 Agilent Technologies 收购了 Varian Inc 的 ICPMS、GC 和 GC/MS 串联四极质谱仪的业务。收购的 3 个产品线成为新成立的 Bruker 公司化学分析部的核心产品。可惜，剥离后不再保留 Varian 公司或产品的名称。Agilent 无需将 Varian 的内离子源 QIT GC/MS 剥离出去，Varian 是唯一提供此商业产品的公司。即便是 Agilent 恢复 QIT GC/MS 产品线（十分可能），也不再使用 Varian 的名称。贯穿本书和参考文献，关于 Varian GC、QIT 和串联四极 GC/MS 的技术还被保留。经过 Agilent 和 Bruker 的收购后，关于分析仪器的 Varian 名称，对于在近 5 年才进入这领域的实际工作者将会是陌生的，因此我们觉得需要做些解释。企业会变化，但书中资料是正确和可用的。

色谱论坛 (<http://www.chromforum.org>) 是同行相互支援的很好资源。

（王光辉 译）

## PREFACE

The purpose of this book is to provide the practitioner of gas chromatography/mass spectrometry (GC/MS) with tools that will facilitate performing analyses and extracting information from the data of those analyses. To those ends, information regarding the tools available and a treatise on the evolution of the technique are also included. This book is not intended to be a detailed text on the theory of the technique of GC/MS; it includes information only on separation of components by gas chromatography (GC) followed by identification using mass spectrometry. No information is included on liquid chromatography/mass spectrometry (LC/MS).

In *Section I. The Fundamentals on GC/MS*, the available instrumentation and techniques (Chapters 1–6) have been greatly expanded over the first edition. More attention is given to available databases of electron ionization (EI) spectra, their use, and the use of programs for deconvolution of coeluting chromatographic components using the mass spectral data as well as software that can be used to develop elemental compositions from mass spectral peaks.

In *Section II. GC Conditions, Derivatization, and Mass Spectral Interpretation of Specific Compound Types* (Chapters 7–36), information pertaining to the use of packed columns has been eliminated due to the disuse of these columns and their replacement with PLOT (porous-layered open tubular) and WCOT (wall-coated open tubular) columns in the modern GC/MS laboratory. There is an overview of GC detectors included in Chapter 2 that should be useful for those considering the use of the gas chromatograph-mass spectrometer (GC-MS) for occasional GC applications. There are also some applications from which valuable information can be obtained by combining a selective GC detector with a mass spectrometer in a single analysis.

Analytes are introduced to the ion source of the GC-MS in ways other than through a GC. These techniques are carefully detailed in Chapters 2 and 4, and their advantages and disadvantages are articulated.

A good portion of the material in this book is tabular and should be used to gain information on how to perform an analysis of a specific sample category and then in the determination of the identity of the individual analytes. This is a book that should be both on the analyst's desk and on the bench next to the instrument. The original edition did an excellent job of presenting the needed tools. This edition expands mainly on the narrative section of the original book and retains and updates those tabular data that were so helpful in the previous edition. At the same time, this edition expands on the techniques of mass spectral data interpretation. Chapter 3

is new and is relatively short because it covers the interface between the gas chromatograph and the mass spectrometer. Chapter 5 goes into more depth on the interpretation of mass spectra. Chapter 6 is a completely revised treatise on the uses of GC/MS in the area of quantitation. The information in *Section III. Appendices* has been expanded and has more helpful tools for mass spectral interpretation. Additional general mass spectral interpretation information can also be found in the chapters on Specific Compound Types (*Section II*, Chapters 7–36).

Much of the material contained in the *GC Conditions, Derivatization, and Mass Spectral Interpretation of Specific Compound Types* section of the first edition was from Fulton G. Kitson's personal experiences in his 30-year career in GC and mass spectrometry. Much of this material has been retained, expanded, and its presentation somewhat modified; however, the existence of this material and the presentation style would not exist if it had not been from his experiences and efforts to organize it (Chapters 7–36 and several of the appendices).

The number of appendices has been increased from 12 to 17. The appendix on "Atomic Masses and Isotope Abundances" has been expanded to provide tools to aid in the determination of an elemental composition from isotope peak intensity ratios. An appendix with examples on "Steps to Follow in the Determination of an Elemental Composition Based on Isotope Peak Intensity Ratios" has been added. Appendices on whether to use GC/MS or LC/MS; third-party software for use in data analysis; a list of information required in reporting GC/MS data; X+1 and X+2 peak relative intensities based on the number of atoms of carbon in an ion; and a list of available EI mass spectral databases have been added. Others such as the ones on derivatization; isotope peak patterns for ions with Cl and/or Br; terms used in GC and in mass spectrometry; and tips on setting up, maintaining, and troubleshooting a gas chromatograph have all been expanded and updated as has the appendix on maintenance and troubleshooting problems in the mass spectrometer.

Since the first commercial GC/MS system was introduced in the mid-1960s by the Swedish company LKB, a number of GC and GC/MS companies have emerged only to be merged into larger companies, acquire and lose their brand identity, or just fade into the pages of scientific instrument history. In late 2009, Agilent Technologies (the noncomputer/nonprinter part of Hewlett–Packard), which was spun off in the last part of the 20th century, announced that it was acquiring Varian, Inc., which itself was a scientific multiproduct-line company that was part of an earlier breakup of Varian, Corp. In addition to vacuum technology, laboratory spectroscopy instruments (near-IR, UV-vis, atomic absorption, and inductively coupled emission spectroscopy), nuclear magnetic resonance spectroscopy, and superconducting magnets, Varian was a major provider of GC and GC/MS instruments (with the internal ionization quadrupole ion trap

(QIT) technology acquired from the then Finnigan Corp. in 1989). Varian also was a manufacturer of tandem quadrupole MS/MS instruments used in GC/MS and LC/MS. The GC business (instruments and supplies) and the ICPMS and tandem quadrupole products of the two companies were considered to be too similar, and the European Economic Community (EEC) requested that Agilent divest itself of these areas before the acquisition could go forward.

Bruker Corporation (headquartered in Billerica, Massachusetts, and the publicly traded parent company of Bruker Scientific Instruments Division (Bruker AXS, Bruker BioSpin, Bruker Daltonics, and Bruker Optics) and Bruker Energy & Supercon Technologies Division) acquired ICPMS instruments, laboratory GC instruments, and GC/MS tandem quadrupole instruments businesses of Varian from Agilent Technologies. The three acquired product lines will form the core offerings in a newly established Bruker Chemical Analysis Division. Unfortunately, this divestiture will not retain the Varian company or product name. Agilent was not required to divest itself of the Varian internal ionization QIT GC/MS technology, and Varian is the only company currently offering such an instrument commercially. Even if Agilent continues the QIT GC/MS product line (which is very likely), the Varian name will no longer be used. Throughout this book, reference is made to Varian GC, QIT, and tandem quadrupole GC/MS technology. Because of these Agilent and Bruker acquisitions, the name Varian, with respect to analytical instrumentation, will be a total unknown to practitioners entering the field in 5 years. This is why we felt this explanation was necessary. The industry will change, but the information in the book will still be valid and usable.

A very good source for peer support regarding GC and GC/MS is the Chromatography Forum at <http://www.chromforum.org>.



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