Astronomical Spectroscopy

An Introduction to the Atomic and Molecular

Physics of Astronomical Spectra

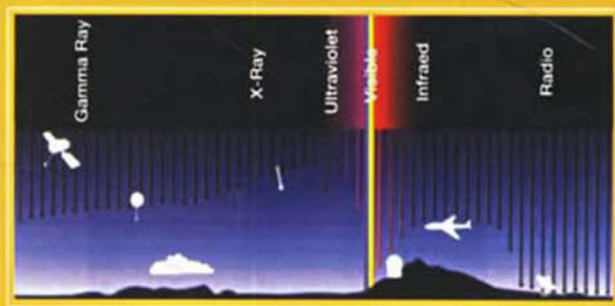# 天体光谱学

——天体光谱学的原子分子物理学导论

（英文影印版）

Jonathan Tennyson

(University College London, UK)

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〔英〕J.丁尼生　著

Jonathan Tennyson

伦敦大学学院(University College London，UCL)教授，物理和天文系主任。

1977 年获剑桥 King's College 自然科学学士学位，1980 年在导师 John Murrel 指导下，取得 Sussex 大学的理论化学(电子结构计算)博士学位。1980 年至 1982 年，以皇家学会西欧交流会员的身份赴荷兰的 Nijmegen 大学作丰富多彩的博士后研究工作。1982 年加入 Daresbury 实验室从事理论化学研究，1985 年成为终身研究员。同年到 UCL 从事理论原子物理的研究工作，并成为"Blood 讲师"。在 UCL，作者发现自己不但成了物理学家，而且成了天文学家，1991 年提升为高级讲师。1994 年成为物理学教授。1991 年至 2004 年担任原子、分子、光学、正电子课题组组长，2004 年成为物理和天文系主任，2005 年成为物理学 Massey 教授。

1989 年以访问科学家身份到访以色列的 Weizmann 科学研究所，并讲学一个学期；1995 年和 1996 年休假期间，以天体物理学家身份到美国 Harvard-Smithsonian 天文物理中心的原子和分子物理理论研究所工作 9 个月，到 Colorado 大学工作 3 个月。

作者的研究兴趣涉及小分子理论的各种专题，尤其专注于小分子的光谱计算，目前则专注于水分子的光谱，以及电子(正电子)同小分子的碰撞和碰撞过程在天文、大气科学中的应用。

内 容 简 介

人类所知的关于宇宙的几乎全部知识都是通过对来自天体的光的研究获得的。要了解这类光的信息,首先需要借助望远镜把光分解为不同的原色,同时还要知道原子分子的量子力学的详细知识,本书就是根据作者在伦敦大学学院(University College London)给学生讲授《天体光谱学》的讲稿基础上写成的。全书着重描述理解、解释天体光谱所必需的原子物理和分子物理基础知识。全书共 10 章,分别讲述天体光谱的记录、谱项的性质、原子氢、复杂原子、氦光谱、碱金属原子、星云的光谱、X 射线谱、分子结构、分子光谱等。各章都有习题,书后附有习题解答。这是近年来出版的唯一本兼顾天体物理研究和原子分子物理结构研究的教科书,不但适宜于高年级大学生和研究生用作教材,书中所列的大量文献也有利于相关专业的专家开展进一步的研究工作。

序　言

从 1998 年到 2003 年，我在伦敦大学学院（University College London, UCL）连续给三年级学生上《天体光谱学》这门课，本书就是紧接着讲稿出版的。参加听课的学生，事先已经读过量子力学的初级课程，亦即粗晓氢原子，但没有原子物理或光谱学的更多知识。本书就是在这种水平的预备知识的前提下展开的。

没有许多人的帮助，本书是根本难以完成的。首先我要感谢 Bill Somerville，是他率先开设了《天体光谱学》这门课，并且在我之前已经教了两年。他毫无私心地把他的讲稿和其他资料都交给了我。我同样应当感谢 Ceinwen Sanderson，是他帮助我把手稿长卷转成 LATEX 文本。我还对同事 Tony Lynas-Gray，Bill Somerville，Peter Storey 以及 Jeremy Yates 等表示感谢，因为他们对本书的初稿作了广泛的评说。我还要对我的研究生 Bob Barber 和 Natasha Doss 表示衷心的谢意，他们帮助我验算了全部习题并纠正了许多差错。凡是参与过有益订正的人我都表示感谢，书中遗留的任何差错都归我本人。

我同样要感谢参加《天体光谱学》听课的学生，给他们上课十分有趣，不仅仅是因为能把天体物理学的最新进展随时直接融入讲课之中，更因为 2003 级学生还对本书的内容作了许多有益的评论和建议。

有关光谱学的图书都需要好的插图来烘托，我也厚着脸皮从文献和其他图谱资料中寻找到了本书的插图。我要感谢 Xiaowei Liu，他帮我把许多出版了的图谱数字化。我的学生 Iryna Rozum，我的儿子 Matthew，尤其是 David Rage，他们帮助我完成了其他的插图。我还要对杂志社和论文的作者表示感谢，

他们毫不犹豫地答应我引用作品，尤其是允许引用其插图，在本书的插图说明中，我对每份杂志，每一个作者都一一注明并给予致谢。

最后，我还要对 UCL 的天文学家们，不管现在的还是过去的，表示衷心的感谢，因为他们耐心而毫无保留地回答了我向他们请教的很多天体物理问题。其中最突出的是 Pete Storey 和 Mike Barlow，还有午餐俱乐部的其他成员，我都不能忘怀。如果没有你们，我的天文学知识只可能停留在我来到 UCL 之前的无知的水平上。

Jonathan Tennyson
2004 年 7 月
于伦敦

CONTENTS

WHY RECORD SPECTRA OF ASTRONOMICAL OBJECTS?

'We will never know how to study by any means the chemical
composition (of stars), or their mineralogical structure'

– Auguste Comte (1835)

1.1 A Historical Introduction

In the first part of the 19th century, astronomers began to make parallax measurements which revealed for the first time how distant even the closest stars are from us. Since travel to the stars was, and still is, impossible with foreseeable technology, many scientists believed that the composition and character of the stars would forever remain a mystery. This view is pithily summarised by the quote from the positivist French philosopher Auguste Comte (1798–1857) given above.

Today, the composition of stars, and indeed of the diffuse material in the large spaces in between the stars, is well known. How did this situation come about? In fact the first steps to finding the solution to the problem had been taken even before Comte began writing.

In 1814, Joseph von Fraunhofer (1787–1826) used one of the high-quality prisms he had manufactured to diffract a beam of sunlight, taken from a slit in his shutters, onto a whitewashed wall. Besides the characteristic colours of the rainbow, which had been observed in this fashion since Newton, he saw many dark lines (see Fig. 1.1). He meticulously catalogued the exact wavelength of each dark line — which are still known today as
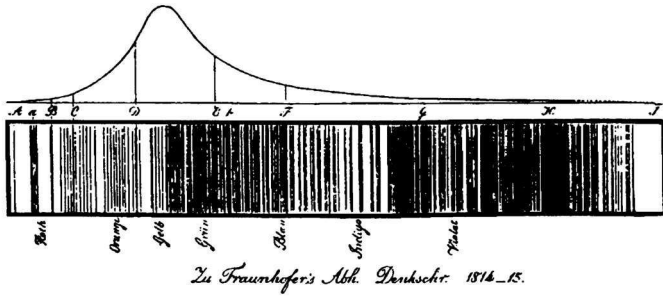
Fig. 1.1.   The solar spectrum as recorded by Fraunhofer.

Fraunhofer lines — and labelled the strongest of them with letters. Many of these labels, such as the sodium D lines (see Sec. 6.4) are still used today. Fraunhofer not only recorded the first astronomical spectrum, he recorded the first-ever high-resolution spectrum. Fraunhofer's spectrum was the first to resolve discrete line transitions.

Fraunhofer did not know what caused the dark lines he observed. However he performed a similar experiment using light from the nearby red-star Betelgeuse and found that the pattern of dark lines he observed changed significantly. Fraunhofer concluded correctly that most of those features were somehow related to the composition of the object he was observing. In fact some of the lines were due to the Earth's atmosphere, the so-called telluric lines. For example, the features Fraunhofer marked A and B in his solar spectrum are actually due to molecular oxygen in our own atmosphere.

The first real step in understanding Fraunhofer's observations came in the middle of the 19th century with the experiments of Gustav Kirchhoff (1824–1887) and Robert Bunsen (1811–1899). These scientists studied the colour of the light emitted when metals were burnt in flames. They found that in certain cases the wavelength of the emitted light gave an exact match with the Fraunhofer lines. The sodium D lines, which give sodium street lights their characteristic orange colour, were one such example. These experiments demonstrated that the Fraunhofer lines were a direct consequence of the atomic composition of the Sun.

Any understanding of how these lines came about had to wait until the arrival of the 20th century with the revolution of scientific theory represented by quantum mechanics. The developments of quantum mechanics and spectroscopy have always been closely linked. As it is

through the study of spectra that we have learnt of many of the riches in the Universe around us, the development of astrophysics has also been closely linked to that of spectroscopy and quantum mechanics. This book aims to give an introduction to the spectroscopy of atoms and molecules that are important for astrophysics. This book is not a text on quantum mechanics, and indeed, some basic knowledge of quantum mechanics is assumed, for it is not possible to understand or interpret spectra without some understanding of quantum mechanics.

Hearnshaw (1986) gives a fascinating historical view of the relationship between astronomy, spectroscopy and the technical developments in both fields (see further reading).

1.2   What One Can Learn from Studying Spectra

Essentially all information about astronomical objects outside the solar system comes through the study of electromagnetic radiation (light) as it reaches us. This light can contain much detailed information which is only obtained by careful analysis. Generally speaking, one can classify the information obtained by observing light according to the spectral resolution; that is the degree of sensitivity to different wavelengths, used to make the observation. One can classify such observations using the following general categories.

When one looks at the night sky with the naked eye, most astronomical bodies appear white. White light is actually light that is composed of many wavelengths which are not resolved into their different colours. Monitoring white light gives the positions of objects in the night sky. It can be used to construct maps of stars and galaxies. It can also be used to plot the movements of heavenly bodies such as comets through the night sky.

If one looks carefully at some celestial objects, such as the planets Mars and Jupiter, or stars such as Betelgeuse, one can see that these objects are tinged with a certain colour. Using instruments with low resolving power, it is possible to separate the light arriving at Earth into broad band colours. Observing colours tells us something about temperatures. For example, blue stars are hotter than red ones; objects that emit X-rays, such as the solar corona, are very hot, whereas cold objects may only emit light of very long wavelengths such as radio waves.

The most detailed astrophysical information is only obtained from high-resolution studies which involve detecting the light arriving at the earth as a function of its component wavelengths. This allows detailed

spectroscopic features to be identified separately from broad band features such as colour. At the highest resolution, such studies not only yield the central wavelength of any feature, often referred to as a line, but also the shape of the feature. Such studies can yield significant extra information and this book is largely devoted to the physical basis of this information and how it can be interpreted.

To interpret an astronomical spectrum, one needs considerable knowledge of atomic and molecular physics. This knowledge usually comes from laboratory studies which provide the basic physical parameters necessary for understanding the astronomical spectrum. There is a direct relationship between these physical parameters and the astronomical information that can be obtained by observing spectra. Thus for any line observed in an astronomical spectrum, one can potentially use laboratory data to extract the following information.

The **composition** of the object being observed can be inferred by knowing which atom (or ion or molecule) produces the observed transition.

The **temperature** and other physical conditions can be deduced from assigning the actual transition being observed to precise energy levels in the atom. Transitions take place between many different states in a particular atom. Knowing which states are involved gives direct information on the degree of excitation of the system. This can be used to determine the physical conditions, such as the temperature or density of the environment local to the system.

The **abundance** of the species undergoing the transition can only be determined if the intrinsic strength of the transition being observed is known. Line strengths can be hard to determine in the laboratory. Astronomically, the strength of a transition is directly related to the number of atoms undergoing the transition under suitable conditions of optical depth (see below). Knowledge of the intensity of transitions is therefore important for determining the abundance of any species.

Motions of the species being observed relative to the earth, or indeed the whole region containing the species, lead to a shift in the wavelength of the line; this shift is known as the Doppler shift. The Doppler shift is the change in the line position from the position measured in the laboratory. This shift is given by the Doppler formula,

$$\frac{v}{c} = \frac{\Delta\lambda}{\lambda},$$

(1.1)

where v is the velocity of the source in a direction away from us, $c = 2.99792458 \times 10^8\,\text{m} \cdot \text{s}^{-1}$ is the speed of light, λ is the rest wavelength of the transition and $\Delta\lambda$ is the change in wavelength, known as the *Doppler shift*. Application of this formula requires laboratory measurement of the rest wavelength to high accuracy. Formula (1.1) is for non-relativistic motions. When an object is moving towards us, the transition is shifted to shorter wavelengths ('blue-shifted'), and when the object is moving away from us, it is shifted to longer wavelengths ('red-shifted'). It was through the monitoring of Doppler shifts of spectra of hydrogen atoms that allowed Edwin Hubble (1889–1953) to show in 1929 that our universe is uniformly expanding and so started from a single point or Big Bang.

The **pressure** or density of the environment local to the species undergoing the transitions can be monitored by observing the line profile. Such observations require particularly high resolutions. Spectral lines are broadened by collisions between species; the more frequent these collisions are, the greater the broadening. This process is called 'pressure broadening'. Lines are also broadened by the thermal motions according to the Doppler formula. Doppler broadening arises because hot species move about faster than cold ones. Both of these reveal information about the physical environment of the species being observed. However, the combined effects of pressure and temperature on the line profile can only be resolved using ultrahigh resolution observations.

Any **magnetic field** present can be monitored as certain spectral lines will be split into more than one component. Energy levels of states which possess angular momentum are split in the presence of a magnetic field. The result is that a single transition can become two or more distinct transitions. The degree of separation between these component lines depends directly on the strength of the local magnetic field. Such splittings, if observed, can therefore provide a measurement of this field.

The information obtained from such observations is the key to most astronomical knowledge. However, to interpret any astronomical spectra requires detailed information about the intrinsic properties of atomic spectra. For each atom or ion or molecule being observed, one needs to know:

(1) Its important spectral lines: these are often summarised using figures called Grotrian diagrams (see Sec. 5.4).
(2) Its energy level structure: also summarised on Grotrian diagrams.

(3) The intrinsic line strength of the transition(s) being observed.
(4) The precise rest (i.e. laboratory) wavelength of any transition observed.

Additional information is required to interpret pressure broadening of spectral lines and splitting in magnetic fields, however these topics will not be pursued in this book. Understanding and use of all this detailed spectroscopic information requires considerable knowledge of quantum mechanics.

At all wavelengths there are observed spectral lines which have yet to be identified (see for example Figs. 6.8 and 7.6). A particularly long-running current example are the diffuse interstellar bands or DIBs. This means that laboratory astrophysics, the study of astrophysical processes in the laboratory, based on either experiment or theory (or both), remains an active area of research.

Problems

Answers to problems are given at the end of the book.

1.1 While observing stars in a distant galaxy, Edwin Hubble observed discrete line emissions at 411.54 nm, 435.50 nm, 487.75 nm and 658.47 nm. There are H-atom transitions with rest wavelengths of 410.17 nm, 434.05 nm, 486.13 nm and 656.28 nm. Verify that these lines are all Doppler-shifted by the same amount. What is the speed of the distant star relative to earth? Is it moving towards us or away from us?