

Upgrading the Atomic and Molecular Database for Astrophysics and Atmospheric Physics by Fourier Transform Spectroscopy

J. C. Pickering, R. Schermaul, G. Cox, J. Rufus, A. P. Thorne, and R. C. M. Learner
Spectroscopy Group, Blackett Laboratory, Imperial College, London, SW7 2BZ, UK
email: j.pickering@ic.ac.uk

P. L. Smith
Harvard-Smithsonian CfA, Cambridge, MA 02138, USA

Abstract

There is currently a great demand for improvements to the atomic and molecular databases for astrophysics, atmospheric physics, and theoretical physics. At Imperial College (IC), the VUV Fourier Transform (FT) Spectrometer, with its high resolving power (up to 2 million at 2000 Å), broad spectral range and unique wavelength range (down to 140 nm), is used in a continuing program to improve the accuracy and completeness of both atomic and molecular data of importance for astrophysics and atmospheric physics.

1 Atomic Spectroscopy

Until recently it was generally assumed that the atomic spectra of elements such as the transition group were well known; the existing tables of data were thought to be adequate by users such as astronomers. But now, with a new generation of telescopes equipped with spectrometers of high resolving power, the situation is very different. Many of the atomic spectra of relevance to astrophysics were last investigated back in the 1930s and 1940s using grating spectrographs and photographic plates. Accuracies of the resulting wavelengths, and line intensities estimated by eye, simply cannot meet the needs of either the astronomers, who wish, for example, to interpret the high resolution stellar spectra now accessible with the Hubble Space Telescope's (HST) spectrographs, or meet the needs of the modern atomic theorists, who with greater computing power can now carry out calculations of unprecedented sophistication. Improvements of at least an order-of-magnitude in accuracy of wavelengths and energy levels are urgently required.

Accurate transition wavelengths are of vital importance in the identification of new atomic energy levels and the correction of known energy levels. These wavelengths and energy levels are used in the identification of stellar spectral line features, and they also feed into semi-empirical calculations in atomic physics which rely heavily on experimental data of high quality. High accuracy of wavelengths, energy levels and transition probabilities, as well as knowledge of hyperfine structure and isotope shifts, is essential in generating reliable synthetic stellar spectra and in disentangling blended features and weak lines of abundant elements in astrophysical spectra of objects ranging from chemically peculiar stars to supernovae remnants. In particular, the dramatic improvements in the quality of UV stellar spectra, observed using the GHRS and STIS spectrographs of the HST, have highlighted the inadequacy of the laboratory atomic data base needed to interpret these observations, especially in the VUV region (below 2000 Å), where stellar spectral lines from doubly

and singly ionized species predominate. The IC FT spectrometer, with its unique short wavelength cut-off, is ideal for recording these spectra.

In recent years, high resolution FT visible and UV spectra of the line rich, astrophysically important neutral and singly ionized transition group elements (Fe, Ni, Cr, Co, Ti, and V) have been recorded at IC using water-cooled, hollow cathode lamps as sources. In all cases, these data have been supplemented by IR observations at the NSO *National Solar Observatory, USA*, typically out to $5\mu\text{m}$. Analyses of the spectra of Fe I, Ni I, Co I and Co II, led to improvements of at least an order of magnitude in accuracy of wavelengths and atomic energy levels and the identification of hundreds of new levels [1], [2], [3], [4], and, for Co I, the determination of hyperfine structure (hfs) constants [5]. The analyses of the spectra of Cr I, Cr II, V I and V II await completion at IC. With the FT spectrometer and suitably reliable intensity calibration, accurate branching ratios can be measured, which, when combined with lifetime measurements, yield oscillator strengths. Isotope shifts can also be observed, and the VUV platinum spectrum was recorded at IC so that accurate studies of isotope shifts could be made. A new project studying doubly ionized spectra is underway, initially beginning with Fe III, excited using a Penning discharge source.

1.1 Term Analysis

The dramatic improvement that can be achieved in the database is illustrated by the cobalt spectrum. Visible-VUV (140-600 nm) spectra recorded at IC were used together with FT IR (600-3000 nm) spectra recorded at Kitt Peak NSO. For strong transitions the wavenumber accuracy is within 1-2 mK, ($1\text{ mK} = 0.001\text{ cm}^{-1}$). In the Co I spectrum analysis [3], over 60 new energy levels were found and several hundred lines identified for the first time. Hfs splitting factors for Co I were found for over 82% of the known energy levels (see Section 1.2). For Co II, the improvement is even more dramatic; over 170 new energy levels were found, and the number of identified transitions doubled [4],[6]. The new experimental data was used in theoretical calculations to give calculated transition probabilities [7]. The vast improvements in knowledge of these spectra were not limited to the visible-VUV spectral regions, -most of the IR transitions were reported for the first time.

1.2 Measurements of Hyperfine Structure

Knowledge of hfs in iron-group elements is important not only for theoretical atomic physics but also for determinations of elemental abundances in stellar atmospheres. It has been noticeable in work reporting on stellar abundances that elements with hfs have often been neglected because of the lack of good laboratory atomic data. For the iron-group elements with odd atomic number, such as Co, the effect of hfs as a line broadening mechanism must be taken into account in abundance studies when using both curve-of-growth methods and spectrum synthesis methods. It is also important to correctly allow for any hfs in the resolution of blended lines in stellar spectra.

Although hfs has been studied for many years, the methods used, such as laser spectroscopy, atomic-beam magnetic resonance and Fabry-Perot interferometry, allowed observations of only a few selected lines, and so the hyperfine interaction constants A (magnetic dipole) and B (electric quadrupole) were known for relatively few levels. However, with the FT spectrometer, combining high resolution and a wide spectral range, thousands of lines may be observed. Co I was investigated [5] in the first use of high resolution FT spectrometry for comprehensive measurements of hfs over a wide spectral range, $3.8\mu\text{m}$ to 180 nm. Computer fits of line profiles of over 1000 Co I transitions yielded A factors for 297 energy levels with an uncertainty of between 0.2 and 3 %. For 208 of these A factors no previous measurements are known. Approximate values of the B factors were also found. Currently, studies of hfs in Co II and V II are also underway at IC.

1.3 The Measurement of Branching Ratios and Oscillator Strengths

The FT spectrometer is an ideal instrument for measuring accurate branching ratios because of its broad spectral range and smoothly varying response. Branching ratios can be reliably obtained for lines widely differing in wavelength. The limit in accuracy is determined by the uncertainty in the calibration of the VUV radiometric standard lamp, and we estimate the limit in uncertainty in relative intensities for strong lines to be about 4%. Measurements of Ti II branching ratios have been made and have yielded oscillator strengths when combined either with experimental lifetime measurements where these exist, or with calculated lifetimes. More branching ratio measurements will be made in the future depending on current interests in the astronomical community.

1.4 Doubly Ionized Spectra

The defects in the database for neutral and singly ionized species apply even more strongly for the third spectra. The accuracy of the current wavelength data is about 10 mÅ whereas wavelengths are now needed to an accuracy of 1 part in 10^7 - or 0.2 mÅ at 2000 Å. Two recent advances in laboratory techniques now make it possible to obtain vast improvements in wavelength and oscillator strength measurements of third spectra:

- i The extension of the wavelength range of the FT spectrometer into the VUV region (down to about 140 nm) with the development of a MgF₂ beamsplitter at IC [8].
- ii The development of a light source, a dc Penning discharge, that is compatible with the FT spectrometer and that excites third spectra and lines from high-lying levels of second spectra that cannot be produced in dc hollow cathode discharges. These have traditionally been excited using pulsed hollow cathode lamps and sliding sparks, but the poor "shot-to-shot" reproducibility of these sources makes them unsuitable for use with an FT spectrometer. The Penning discharge source used was originally developed as a VUV radiometric standard by Heise et al. [9].

Preliminary measurements were made at IC using this source, and results in the region 150-220 nm using iron cathodes have yielded Fe II and Fe III spectra with signal-to-noise ratios (SNRs) of several hundred for the stronger Fe III lines. The improvement in wavelength accuracy is at least an order of magnitude over the existing data. Ni III will also be recorded. Analyses of these spectra should yield dramatic improvements in accuracy of energy levels and wavelengths, as well as many new energy levels. The spectra will be intensity calibrated so that branching ratio measurements can be obtained, and these may be combined with either theoretical or experimental lifetimes to give oscillator strengths. In the future, other transition group elements will also be measured.

2 Molecular Spectroscopy

FT spectrometers are also used to record absorption spectra of species important in studies of the earth's atmosphere and other planetary atmospheres. Recent projects include:

2.1 Measurements of UV Absorption Cross Sections of SO₂

In order to avoid underestimating absorption cross sections, the sharpest features in the absorption spectrum need to be fully resolved. With support from ESA, the absorption spectrum of SO₂ was measured at high resolution using the IC FT spectrometer between 280-330 nm. These

measurements are of direct application to pollution measurements by downward-looking satellites such as GOME (*Global Ozone Monitoring Experiment*) and SCIAMACHY (*Scanning Imaging Absorption Spectrometer for Atmospheric Cartography*). Work is also in progress, in collaboration with the Harvard-Smithsonian CfA and Wellesley College, USA, on measurements of the far UV (190-220 nm) bands of SO₂. The resulting accurate absorption cross sections will enable planetary astronomers to reliably interpret SO₂ in HST spectra of the atmosphere of Io and Venus.

2.2 Measurements of VUV Absorption Cross Sections of O₂ and NO

For accurate modeling of the penetration of solar radiation into the upper atmosphere in the wavelength region 220-175 nm, computations involving O₂ and minor species, notably NO, must be carried out on a line-to-line basis. This requires both accurate wavenumbers and high resolution in order to obtain true line profiles and absolute cross sections. Good SNRs for absorption measurements require a background continuum of high photon flux, and in the VUV the best such source is synchrotron radiation. For this purpose, the IC VUV FT spectrometer was taken to the Photon Factory (KEK) in Japan, and spectra of O₂ and NO were recorded from 195-160 nm at resolution matched to the Doppler widths of about 0.12 cm⁻¹. Analysis of these spectra is in progress.

2.3 Precise Line Parameter Measurements in the Visible A Band Spectrum of O₂

The oxygen A band shows a weak absorption in a relatively empty portion of the atmospheric spectrum and is well suited for atmospheric remote sensing. Accurate O₂ data is crucially important for remote sensing of cloud-top height and coverage for satellite retrieval of atmospheric ozone, which is utilized by the GOME and the SCIAMACHY. They are also needed for the measurement of middle atmosphere ozone from O₂ A band airglow emission measurements proposed for the *High Resolution Doppler Instrument*.

The spectrum of the oxygen A band, $b^1\Sigma_g^+(v=0) \leftarrow X^3\Sigma_g^-(v=0)$, has recently been measured and analysed in order to improve the currently available data on this band. The measurements were carried out at the Rutherford Appleton Laboratory (UK) using a high-resolution Bruker FT spectrometer, together with a long pathlength multireflection absorption cell. Spectra were recorded at two different temperatures, various O₂ pressures, and absorption pathlengths in order to retrieve information on temperature and pressure dependent effects. Spectra recorded using the FT spectrometer at the NSO were also included in the analysis. Precise line intensities with an accuracy of approximately 0.3 % and pressure-broadening coefficients (accuracy approx. 2-3 %) were retrieved including their temperature dependence. This data enabled us to determine the A band transition moment and the Einstein transition probability with standard errors of approximately 0.1 %. The spectra were of sufficient quality that the line intensities, broadening coefficients, and the transition probability for the corresponding band in the isotopomer ¹⁶O¹⁸O could be determined.

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