Mon. Not. R. Astron. Soc. **300,** 131–134 (1998)

Precise laboratory wavelengths of the Mg I and Mg II resonance transitions at 2853, 2803 and 2796 Å

J. C. Pickering,[1⋆] A. P. Thorne[1⋆] and J. K. Webb[2⋆]
[1] *Blackett Laboratory, Imperial College, London SW7 2BZ*
[2] *School of Physics, University of New South Wales, Sydney, NSW 2052, Australia*

Accepted 1998 May 28. Received 1998 March 31

ABSTRACT

Strong ultraviolet resonance transitions are observed routinely both in the Galactic interstellar medium and in quasar absorption systems. The quality of the astronomical spectroscopic data now available demands more precise laboratory rest wavelengths. Of particular interest is the accuracy with which one can constrain space–time variations in fundamental constants using quasar spectra. A recent analysis by Webb et al. of 25 quasar spectra using Mg and Fe transitions tentatively suggests that the fine-structure constant was smaller at earlier epochs. To permit a check on this result, and to allow further more extensive investigations, we have carried out a new determination of the laboratory wavelengths of Mg I 2853 Å, Mg II 2796 Å and Mg II 2803 Å by high-resolution Fourier transform spectroscopy. Our results for Mg II 2796 Å are consistent with the value measured independently by two other groups. To our knowledge, no previous measurements of comparable precision exist for Mg I 2853 Å and Mg II 2803 Å.

Key words: atomic data – line: profiles – methods: laboratory – techniques: spectroscopic – quasars: absorption lines – ultraviolet: general.

1 INTRODUCTION

The resonance transitions of Mg I at 2853 Å and Mg II at 2796 and 2803 Å are routinely observed in the interstellar medium (ISM), both in our Galaxy and in other galaxies. High-resolution spectroscopy of bright stars in the Galaxy provides important kinematic and abundance information for gas clouds along the line of sight. Telescopes such as the *Hubble Space Telescope* provide very high quality data covering a range of ultraviolet (UV) transitions, and much has been learned about the Galactic interstellar medium (Linsky et al. 1993, 1995; Piskunov et al. 1997; Vidal-Madjar, Ferlet & Lemoine 1998).

From the ground, the same transitions, redshifted into the region above 3000 Å, can be observed in distant gas clouds which intersect the sight lines to distant quasars, providing a unique probe of physics at early epochs. Recent advances in instrument and detector technology and the availability of large-aperture telescopes (e.g. Keck, VLT, Gemini) mean that the quality of the spectra obtained is extremely high. The cloud parameters (column density, velocity, velocity dispersion parameter) are generally determined by fitting Voigt profiles to the data. If the laboratory wavelengths of all species are known precisely, the model requires a single velocity (for each gas cloud), thereby reducing the number of free parameters to a minimum and putting the tightest possible constraints on the remaining parameters. At present this cannot always be done because of the uncertainties in the laboratory data needed to provide the rest wavelengths, so each line is fitted separately (Linsky et al. 1995; Piskunov et al. 1997).

The prime motivation for this paper arose in a different context: high-resolution spectroscopy of gas clouds seen against distant quasars can provide valuable constraints on space–time variations in the fundamental 'constants' (Varshalovich & Potekhin 1995; Varshalovich, Panchuk & Ivanchik 1996; Cowie & Songaila 1995). The relative wavelength separation between transitions of alkali-type doublets depends on the value of the fine-structure constant α, so high-redshift spectroscopic observations of quasars provide tight constraints on space–time variations.

In two recent papers (Dzuba, Flambaum & Webb 1998; Webb et al. 1998) this technique has been extended, using not just a single alkali-type doublet, but different species. A substantial improvement over previous methods is achieved by combining species with low and high nuclear charge in the same analysis, taking advantage of the greater sensitivity of the latter to small changes in α. By using lines for which precise laboratory wavelengths are known, specifically Mg II 2796 Å (Drullinger, Wineland & Bergquist 1980; Nagourney & Dehmelt 1981) and up to five Fe II lines (Nave et al. 1991), an improvement in sensitivity of an order of magnitude has been made, and a tentative detection of time variation in α made.

Such analyses are prone to various systematic effects, so the preliminary results need careful checking. One important way of

⋆ E-mail: j.pickering@ic.ac.uk (JCP); a.thorne@ic.ac.uk (APT); jkw@edwin.phys.unsw.edu.au (JKW)

reducing systematic effects is to incorporate further transitions into the analysis. The other resonance lines of magnesium, Mg I 2853 Å and Mg II 2803 Å, are of particular importance because they occur in the same part of the spectrum and thus are already available. They could not be used in the recent analysis of Webb et al. because of the lack of high-precision laboratory wavelengths.

In this paper we describe the results of an experiment to measure accurately the wavelengths of these two lines, together with that of Mg II 2796 Å to provide a consistency check against the previous measurements of this line (Drullinger et al. 1980; Nagourney & Dehmelt 1981). Unlike these last measurements, which were made on laser-cooled ions in traps with sub-Doppler resolution, the present results were obtained by Fourier transform spectrometry, with a resolution limited by the Doppler widths of the emission lines. For lines of good signal-to-noise ratio this technique is capable of a relative wavenumber accuracy of 0.001 cm^{-1}, and, by using our Fe II spectra referred to above (Nave et al. 1991) as wavenumber standards, we were able to achieve an absolute wavenumber uncertainty of 0.002 cm^{-1}.

2 EXPERIMENTAL METHOD

The wavelengths were measured by Fourier transform spectrometry (FTS), using one of the UV FT instruments at Imperial College (Thorne et al. 1987). The magnesium spectrum was excited in a hollow-cathode discharge lamp with argon at a pressure of about 1 mbar as carrier gas. A small amount of MgF_2 powder was made into a paste with distilled water and inserted in a nickel hollow cathode, giving a stable discharge after a short run-in period. The spectra of Ni I and Ni II were excited along with Mg I and Mg II, and some of the Ni I lines were used for wavelength calibration as described in the next section. The resolution used was 0.055 cm^{-1}, sufficient to resolve fully the Mg lines, which were expected to have Doppler widths of about 0.15 cm^{-1}, based on the Doppler widths of the Ni lines in the same discharge. In FTS the noise (predominantly photon noise in our case) is transformed along with the spectrum, and white noise is distributed uniformly through the spectrum. Thus every line seen by the detector contributes to the noise at every point in the spectrum, and it is disadvantageous to record lines outside the region of interest. In this case we band-limited the spectrum to approximately 3000–2400 Å by using a solar-blind photomultiplier (R166) as detector together with a UG5 filter.

A preliminary scan with a discharge current of 250 mA showed that the Mg lines were significantly self-absorbed. The spectra used for the measurements were obtained with currents of 150 mA (run A) and 100 mA (run B), each consisting of eight co-added interferograms giving a total integration time of about 30 minutes. The interferograms were transformed and phase-corrected in the usual way; the analysis is described in the next section.

3 ANALYSIS AND RESULTS

3.1 Wavenumber calibration

The wavenumber scale of an FT spectrum derives from the stabilized He–Ne laser that is used to determine the sampling intervals for the interferogram, and it is accurately linear – i.e. $\sigma_{exp} = \sigma_0(1 - \beta)$, where σ_{exp} and σ_0 are the observed and true wavenumbers respectively. The 'stretch factor' $(1 - \beta)$ results from the finite size of the interferometer entrance aperture and any possible offsets in the angle of the laser beam through the interferometer; β is of the order of the reciprocal of the resolving power. In principle a single reference line is sufficient to evaluate β. In practice a number of reference lines are used, and the mean value of $(\sigma_0 - \sigma_{exp})/\sigma$ determines β. It is *not* necessary to have the reference lines distributed through the spectrum as is the case for a grating.

In this experiment we used as references some of the Ni I lines that appeared in the spectrum along with the Mg I and Mg II lines. The Ni I spectrum was recorded and analysed recently by Litzén, Brault & Thorne (1993), using FTS with a wavenumber scale calibrated from the Fe I and II lines of Nave et al. (1991). Our calibration is therefore based on these iron lines, with an absolute uncertainty of 0.001 cm^{-1} in the region of 35 000 cm^{-1}.

3.2 Line fitting

The profiles of emission lines, for both neutral and ionic species, generated in a hollow-cathode discharge are usually well described by Voigt functions with small damping factors. The line-fitting programs written for FT spectra by J. W. Brault (private communication) use an iterative least-squares procedure to evaluate the Voigt parameters. For a symmetric isolated line the uncertainty ϵ in the central wavenumber of the fitted Voigt profile is given by (Brault 1988)

$$\epsilon = W/(\sqrt{n} \times \mathrm{SNR}) \quad (1)$$

where W is the width of the line in the same units as ϵ, n is the number of independent spectral points across W, and SNR is the signal-to-noise ratio for the line. For the Ni lines used in the calibration $\epsilon \simeq 0.001$ cm^{-1}. From the widths of these lines we deduce that the Doppler widths of the Mg lines should be about 0.155 cm^{-1}.

The fitting of the Mg lines presents a rather different problem because of their isotope shifts and hyperfine structure. All components fall well within the Doppler width, so the structure is completely unresolved. Fortunately the structure has been measured in other experiments, so it is possible to simulate the composite lines and determine the wavelength shifts relative to ^{24}Mg resulting from the unresolved structure, as described below.

3.3 Simulation of the Mg I and Mg II line structure

Mg has three stable isotopes with abundance ratios $^{24}Mg:{}^{25}Mg:{}^{26}Mg = 79:10:11$. The odd isotope, ^{25}Mg, has a nuclear spin of 5/2. The Mg I resonance line at 2853 Å is an $s^2\,{}^1S_0–sp\,{}^1P_1$ transition, which has no hyperfine structure. The most recent measurements of isotope shifts in this line appear to be those of Hallstadius (1979) with a Fabry–Perot interferometer, using separated isotopes. He found 0.0243 ± 0.0004 and 0.0471 ± 0.0007 cm^{-1} for ^{25}Mg–^{24}Mg and ^{26}Mg–^{24}Mg respectively (Hallstadius 1979), in reasonable agreement with a previous accurate measurement by Kelly (1957). We have used Hallstadius's values to simulate this line, as shown in Fig. 1, using Voigt profiles for the three components with a Gaussian width of 0.14 cm^{-1} and a damping factor of 0.3, chosen to optimize the fit to the experimental line. The figure shows the synthesized line overplotted with the experimental line from run B, together with the residuals from the fit. The wavenumber of the composite line is $35\,051.277 \pm 0.001$ cm^{-1}, and the synthesis puts the ^{24}Mg component at 35 051.271 cm^{-1}, a difference of –0.006 cm^{-1}. Substituting Kelly's values for the synthesis makes a negligible difference. It was not possible to use run A for this line because of the significant self-absorption.

In both members of the Mg II resonance doublet the ^{25}Mg

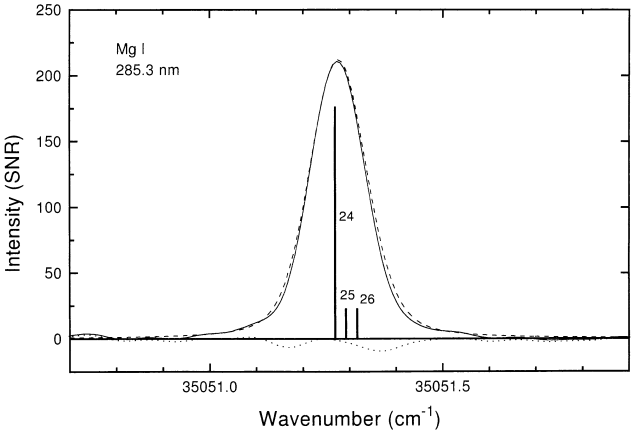

Figure 1. FT spectrum of the Mg I 2853-Å transition showing the fitted line profile (dashed line) and fit residuals (dotted line) together with the isotope components.

component is split by hyperfine structure, which is predominantly that of the common $^2S_{1/2}$ level. Drullinger et al. (1980), in the measurement of the 2796-Å line referred to above, used a Doppler-free laser technique in which the isotopes were well separated. They determined the isotope shift between the two even isotopes to be 0.102 ± 0.003 cm^{-1}. Only one component of the ^{25}Mg hyperfine structure was present because of the optical pumping in their experiment; however, it is generally accepted that volume isotope shifts are negligible for nuclei as light as Mg, so that the centre of gravity of the ^{25}Mg pattern can be found from the mass shift ratios. Hence they were able to deduce a value of -0.0203 ± 0.0017 cm^{-1} for the hyperfine splitting constant of the lower state, in fair agreement with earlier work. They estimated the splitting constant of the $^2P_{3/2}$ to be -0.0006 cm^{-1}, which is negligibly small for our purpose. We have used these numbers to simulate the composite 2796-Å line of Mg II. Fig. 2 shows the experimental data from run B together with the synthesized line in the same way as Fig. 1; in this case the parameters for the best fit were a Gaussian width of 0.165 cm^{-1} and a damping factor of 0.65. The wavenumber of the composite line is 35 760.846 cm^{-1}, and the wavenumber for ^{24}Mg obtained from the synthesis is 35 760.834 cm^{-1}, a shift of -0.012 cm^{-1}. The results from run A for both this line and the 2803-Å line are discussed below.

In synthesizing the 2803-Å line of Mg II, we have assumed that

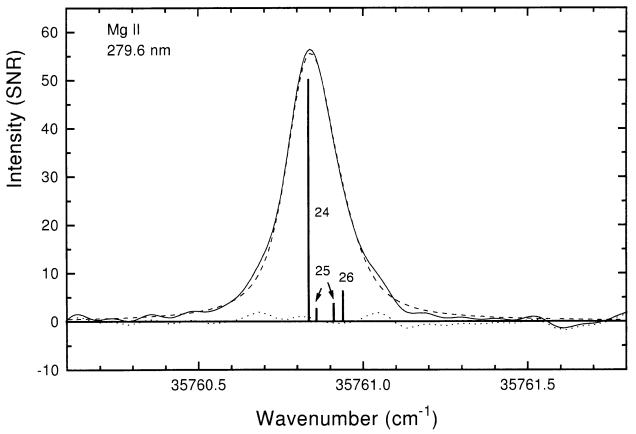

Figure 2. FT spectrum of the Mg II 2796-Å transition showing the fitted line profile (dashed line) and fit residuals (dotted line) together with the isotope components.

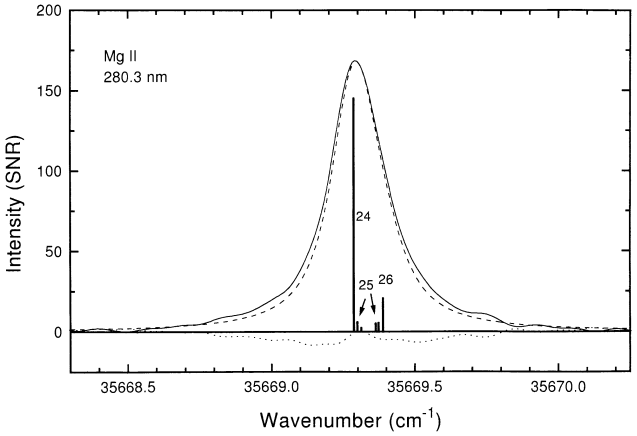

Figure 3. FT spectrum of the Mg II 2803-Å transition showing the fitted line profile (dashed line) and fit residuals (dotted line) together with the isotope and hyperfine structure components.

the specific mass shift, which constitutes 40 per cent of the measured shift in the 2796-Å line, contributes the same fraction to the $^2P_{3/2}$ and $^2P_{1/2}$ levels, a reasonable assumption for an ion with one valence electron. The two levels are sufficiently close in energy that the difference in mass shifts should then be negligible, and the two lines should have the same isotope structure. As the hyperfine splitting constant for $^2P_{1/2}$ is, according to theory, a factor of 5 larger than for $^2P_{3/2}$, we have included the splitting of this level in the synthesis, although it makes a very small difference to the result. For run B the best-fitting Voigt parameters are similar to those for the other Mg II line, and we find 35 669.298 cm^{-1} for the composite line and 35 669.285 cm^{-1} for the ^{24}Mg component, a shift of -0.0126 cm^{-1}.

In fitting the observed profiles of the two Mg II lines from run A, it was necessary to use a larger damping factor (0.8 to 0.9) to match the pronounced line wings in this spectrum, and even then the fit is not so good as for run B, as can be seen in Fig. 3. This shape is not an instrumental artefact, since the Ni lines are unaffected. We believe the most likely cause is resonance broadening as a result of the larger number density of Mg^+ ions in this run. As resonance broadening is not accompanied by line shifts, we do not expect the position of the line to be affected, and the calculated position of ^{24}Mg relative to the wavenumber of the composite line is almost independent of the Voigt parameters used for the fit. The wavenumbers found from run A are 0.002 cm^{-1} greater for λ2796 and 0.001 cm^{-1} greater for λ2803 than those for run B, differences that are within the uncertainties given by equation (1).

Table 1 sets out our final values for all three lines, together with the values from Morton's compilation (Morton 1991). We have given run A and run B equal weights in determining our values for the two Mg II lines, on the grounds that the signal-to-noise ratios for run A are better by a factor of about 5 but the fit is more convincing for run B.

Table 1. Wavenumbers of the Mg resonance lines. 'Morton' refers to Morton (1991) – see below for comment. 'Composite' is the position of our fitted line and '^{24}Mg' is the wavenumber found from the synthesis for that isotope. The last two columns give respectively the difference between columns 3 and 4, and the uncertainty in the absolute wavenumber in column 3.

Line	Morton	Composite	^{24}Mg	Difference	Uncertainty
Mg I 2853 Å	35051.264	35051.277	35051.271	0.006	0.001
Mg II 2796 Å	35760.877	35760.848	35760.835	0.013	0.002
Mg II 2803 Å	35669.304	35669.298	35669.286	0.012	0.002

Although column 2 gives Morton's values, the most accurate absolute measurements for comparison are those of Drullinger et al. (1980) and Nagourney & Dehmelt (1981) on Mg II 2796 Å, using laser-cooled ions in a radio frequency (RF) trap. They find for ^{24}Mg respectively 35 760.834 ± 0.004 and 35 760.830 ± 0.005 cm^{-1}. As their absolute wavenumbers derive from I_2 standards, whereas ours derive from ^{86}Kr via a set of Ar II lines used to calibrate our iron spectra, we consider the agreement – to 0.001 and 0.005 cm^{-1} respectively – to be remarkably and gratifyingly close.

Morton's values in the table have been given to eight digits because the vacuum wavelengths in his compilation are given to four decimal places of Å corresponding to three decimal places of cm^{-1} (Morton 1991). However, his data for magnesium are taken from the earlier compilation of Martin & Zalubas (1980), who mention that the estimated errors are 'in general less than 0.02 cm^{-1}' for Mg I, while for Mg II they give the values only to 0.01 cm^{-1}. The last digit in Morton's values does not therefore appear to be meaningful. This is borne out by the original papers from which Martin & Zalubas took their data: G. Risberg (1965) claimed that the Mg I lines 'may be correct to 0.01 cm^{-1} or better', while P. Risberg (1955) estimated the uncertainty for the Mg II lines to be about 0.02 cm^{-1}. This is a good example of the need to beware that the dates of recent compilations do not mask the age and uncertainty of earlier measurements. The present results agree with those of the two Risberg papers within their stated accuracy.

4 CONCLUSION

Motivated by recent advances in spectroscopy of high-redshift gas clouds, we have made precise measurements of Mg I and Mg II transitions which are frequently observed in quasar spectra. The importance of the additional new Mg I 2853 Å, Mg II 2796 Å and Mg II 2803 Å laboratory wavelengths, in the context of searches for space–time variation of the fine-structure constant α, is that they can now be incorporated into analyses similar to that of Webb et al., enabling a reduction of systematic effects caused by absorption-line blending (random or systematic).

Time variation in isotopic composition is an important consideration for observations at high redshift. Columns 3 and 4 of Table 1 represent respectively terrestial abundances and only ^{24}Mg. If, for example, ^{26}Mg were the predominant isotope, the rest wavelengths would be shifted with respect to column 4 by +0.047 cm^{-1} for the Mg I line and +0.102 cm^{-1} for the Mg II lines. Such an effect would mimic a variation in α.

This consideration underlines the necessity for further measurements similar to those described in this paper, to derive precise laboratory measurements of other species detected in high-redshift gas clouds. Analyses can then be implemented which involve (for example) independent pairs of different species. In this way one may in principle unambiguously disentangle isotopic changes from time- or space-varying α.

REFERENCES

Brault J. W., 1988, Mikrochim. Acta (Wien 1987 II), 215
Cowie L. L., Songaila A., 1995, ApJ, 453, 596
Drullinger R. E., Wineland D. J., Bergquist J. C., 1980, Appl. Phys. 22, 365
Dzuba V., Flambaum V. V., Webb J. K., 1998 Phys. Rev. Lett., submitted (astro-ph/9802029)
Hallstadius L., 1979, Z. Phys. A, 291, 203
Kelly F. M., 1957, Can. J. Phys., 35, 1220
Linsky J. L. et al., 1993, ApJ, 402, 694
Linsky J. L., Diplas A., Wood B. E., Brown A., Ayres T. R., Savage B. D., 1995, ApJ, 451, 335
Litzén U., Brault J. W., Thorne A. P., 1993, Phys. Scr., 47, 628
Martin W. C., Zalubas R., 1980, J. Phys. Chem. Ref. Data, 9, 1
Morton D. C., 1991, ApJ, 77, Supp. Ser., 119
Nagourney W., Dehmelt H. G., 1981, Bull. Am. Phys. Soc., 26, 805
Nave G., Learner R. C. M., Thorne A. P., Harris C. J., 1991, J. Opt. Soc. Am. B, 8, 2028
Piskunov N., Wood B. E., Linsky J. L., Dempsey R. C., Ayres T. R., 1997, ApJ, 474, 315
Risberg G., 1965, Ark. Fys., 28, 381
Risberg P., 1955, Ark. Fys., 9, 483
Thorne A. P., Harris C. J., Wynne-Jones I., Learner R. C. M., Cox G, 1987, J. Phys. E, 20, 54
Varshalovich D. A., Potekhin A. Y., 1995, Space Sci. Rev., 74, 259
Varshalovich D. A., Panchuk V. E., Ivanchik A. V., 1996, Astron. Lett., 22, 6
Vidal-Madjar A., Ferlet R., Lemoine M., 1998, PASP, 143, 3
Webb J. K., Flambaum V. V., Churchill C. W., Drinkwater M. J., Barrow J. D., 1998, Phys. Rev. Lett., submitted (astro-ph/9803165)

This paper has been typeset from a TEX/LATEX file prepared by the author.