THE SOLAR Mg I SPECTRUM FROM ATMOS. I. IDENTIFICATION AND PRELIMINARY DISCUSSION

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ABSTRACT

As an initial step in a program to understand some puzzling aspects of the infrared solar Mg I spectrum we have examined the set of high-resolution, high signal-to-noise ratio, lines of this spectrum obtained in the 1985 ATMOS experiment on Spacelab 3. From laboratory data, supplemented by theoretical expressions, wavenumbers were obtained for the Mg I transitions lying in or near the range covered by ATMOS, namely 650 to 4800 cm⁻¹ (2.3–16 μm). Lines involving principal quantum numbers up to n = 10 are seen in the data; we describe some striking features of the Mg I spectrum and indicate some directions of interest for future analytical studies and for future flights of the experiment.

Subject headings: infrared: spectra — Sun: spectra

I. INTRODUCTION

Among the more puzzling features of the solar spectrum are the infrared emission lines first noted in FTS spectra obtained by Brault & Testerman in 1981 at the McMath Telescope on Kitt Peak. A catalog of the wavenumbers of these, and related, emission lines, along with a description of some of their characteristics, is given by Brault & Noyes (1983). These authors emphasize particularly that the two strongest lines, near 12 μm, have bright, narrow, emission cores somewhat eccentrically located in a broad background absorption. This emission displays a pronounced limb brightening, which can readily be shown to be consistent with its formation in an optically thin layer. The lines exhibit Zeeman splitting in penumbral and plage regions (they disappear in spot umbrae), and the extreme splitting opens the possibility of accurate measurements of the intrinsic magnetic field strength in the emitting region; see Deming et al. (1988). We recall that conventional magnetometers, working in the visible spectrum, yield a value only of the magnetic flux, and since the solar field is believed to be concentrated in flux tubes more or less sparsely embedded in a non-magnetic medium, any means for obtaining a direct measure of inherent field strengths is of particular interest.

Using an approximate expression for the term values, Chang & Noyes (1983) were able to associate the two strong 800 cm⁻¹ emission features with transitions between the configurations 3s7i and 3s6h (811 cm⁻¹), and 3s7h and 3s6g (818 cm⁻¹) in neutral Mg. This identification was made unassailable through the parallel association of many observed emission features with similar, weaker, transitions in the same atom.

The promise embodied in these spectral features for a new level of accuracy in solar magnetometry, together with their potential value for diagnosing the structure of the solar atmosphere, stimulated a number of workers to try to understand the characteristics of the lines. Particular emphasis was placed on the emission peaks which, at first sight, would seem a natural consequence of, and diagnostic of, the region in the solar atmosphere lying above the temperature minimum. However, straightforward calculations, e.g., by Lemke & Holweger (1989), failed to predict any emission from models of the Sun’s atmosphere such as the HSRA or the VAL model (Vernazza, Avrett, & Loeser 1981). The computed profiles were found to be wholly in absorption at all points on the disk, at least to the extent that the excitation of the atom followed LTE. Since the identification is unequivocal, and the atomic absorption coefficient cannot be in significant error (it is essentially hydrogenic for the higher l transitions) we are left with the possibility either that the excitation is not in LTE, or that the atomic model is wrong—in the sense that the amount of higher temperature material is underestimated. Indeed both assumptions may be in error. A natural possibility to consider is that the 12 μm emission features reflect thermal inhomogeneities whose presence is not significant to the intensity of the continuum radiation on whose interpretation the VAL models are based. An indication in the data that the emission feature is not centrally located in the background absorption line is not inconsistent with such an idea, although observations by Zirin & Popp (1989) suggest that any such inhomogeneities must be small in size and uniformly distributed—a conclusion supported by (unpublished) observations of Jones, Zirker, & Jeffries (1989).

The first possibility, that a population anomaly exists in the higher levels of Mg in the solar atmosphere, has been considered by Lemke & Holweger (1987) through a calculation of the statistical equilibrium populations in a 38 level model of Mg. They found no inversion, but they pointed out that only a slight degree of overpopulation (a few percent) would suffice to explain the observations. A physical reason why any inversion at all should occur was not offered, however. The atomic level populations must certainly approach LTE with respect to the continuum state (Mg⁺ + e) as the energy levels come closer and closer to the continuum (given that the free states have a Boltzmann distribution), but we cannot say exactly how far from LTE any given level will be, and in what sense (inverted or not) without a detailed calculation.

Lemke and Holweger followed a common practice adopted in calculations of excitation which is simply to terminate the atomic model at some bound state and set the continuum state to begin at the formal ionization limit. This approximation is introduced to make the system of statistical equations finite; however, when, as here, the levels whose populations we are
estimating lie near the last-included level, it is clearly subject to significant error. A means must be found in excitation calculations to include the influence of transitions to and from these neglected levels before we can comment reliably on whether or not the high-lying levels are inverted or how they approach LTE with the continuum. We must also, of course, be sure that all significant processes populating and depopulating the upper levels are included. In this context we may note the suggestion by Chang (1987) that charge-exchange processes may be important in populating the high-\( n \), high-\( l \) levels. We shall return to this whole question in a later study.

The alternative possibility for accounting for the emission cores in the 12 \( \mu m \) lines—that the solar model needs the addition of hotter material with sufficient density and size to provide some (small) opacity—perhaps gains support from infrared occultation measurements obtained at the 1981 and 1988 total solar eclipses—see Lindsey et al. (1986) and Roellig et al. (1991). These occultation curves, spanning a wavelength range of 20–800 \( \mu m \), have, like the emission cores, also proved impossible to explain using the standard VAL models. The sense of the discrepancy is, again, such as to require the addition of hotter, denser, material at altitudes above the temperature minimum. We might then seek to understand both the emission cores in the Mg lines and the eclipse occultation curves in terms of an inhomogeneous model incorporating structures such as spicules, using, for example, the statistical transfer theory of Jefferies & Lindsey (1988) and Lindsey & Jefferies (1990) which was developed precisely to handle this specific problem.

In summary, we do not know why the emission peaks appear, whether from an excitation anomaly or from a deficiency in the standard model. The potential of the infrared Mg lines in solar physics, however, no less than their intrinsic interest, makes the pursuit of the question very worthwhile.

In the meantime, a new set of spectroscopic data has been published which could go far to resolving some of the above questions. This new data set has been published as a high-resolution, high-signal-to-noise ratio, spectroscopic atlas by Farmer & Norton (1989) and covers the solar spectrum from 650 to 4800 \( cm^{-1} \) (2.3 to 16 \( \mu m \)). This fine set of data was contained in the ATOMS experiment on Spacelab 3 in 1985; this paper presents a first description of the Mg \( i \) data contained in that atlas. Sections of the ATOMS data set may be compared with ground-based FTS spectra in the region 490–1250 \( cm^{-1} \) obtained by Brault & Testerman (1981), and Brault (1980) using the McMath telescope. Brault used a relatively small aperture and obtained data at a number of points across the solar disk out to \( \mu = 0.14 \). The aperture for ATOMS was about 3.5 for the higher frequencies \( \nu > 2500 \ cm^{-1} \) and double that for the longer wavelengths. The strong center-to-limb effects seen in Brault’s data make it all the more important that future ATOMS missions incorporate the ability to scan across the solar disk.

In § 2 we discuss sources for Mg \( i \) term values of the higher lying levels as a preliminary to calculating the wavelengths of the permitted lines. Sources are both theoretical and experimental; where available, we use the latter, but for most lines of interest here these do not exist and theoretical approximations are needed. These are normally accurate enough to identify the lines—indeed, their use underlay the identification of the prominent 12 \( \mu m \) emission lines in the first place. From the term values, we computed wavenumbers for all allowed transitions in the triplet and singlet series of the Mg \( i \) spectrum both for the dominant \( (l \rightarrow l - 1) \) and the weaker \( (l \rightarrow l + 1) \) series where \( l \) is the azimuthal quantum number of the upper state. Where the fine-structure splitting is resolvable at the (fraction of a mK) accuracy of the ATOMS and Brault spectra, we have also computed the wavenumber of the fine-structure lines; these are sometimes particularly well represented in the Norton-Farmer atlas.

In § 3 we present a brief discussion of the data from ATOMS. Some perplexing behavior is noted which only adds to the challenge inherent in the 12 \( \mu m \) lines and gives some further clues to follow for the resolution of this strange spectrum.

2. TERM VALUES AND LINE OCCURRENCE

Energies for most levels associated with the \( s,p,d,f \) electrons up to \( n = 15 \) in the 3s \( nl \) configuration are given by Martin & Zalubas (1980, hereafter MZ); newer data by Biémont & Brault (1987, hereafter BB) supersedes the \( n = 4 \) and 5 triplet \( F \) levels and gives new values for the \((l = 4) \) singlet and triplet \( G \) levels for principal quantum numbers \( n = 5–8 \). We shall also need term values for azimuthal quantum numbers \( l > 4 \) and for those we use the general interpolation formula of Risberg (1965)—used by Chang & Noyes (1983)—for which the 3s \( nl \) term of neutral Mg may be written

\[
E(n, l) = E_0 - \frac{Ry}{n^2 - \alpha P(n, l)}
\]

with

\[
P(n, l) = \frac{Ry[3n^2 - l(l + 1)]}{2n^2(l - 1/2)(l + 1/2)(l + 1/2)(l + 3/2)}
\]

In these expressions \( E_0 \) is the ionization potential (61671.02 \( cm^{-1} \)); \( Ry \), the Rydberg constant for Mg (109734.81 \( cm^{-1} \)); and \( \alpha \), the dipole polarizability (in atomic units). An appropriate numerical value of \( \alpha \) may be inferred from the above interpolation formula using measured energies of the 3s \( nf \) or 3s \( ng \) configurations. A value of 33.6 gives a reasonable fit and is adopted here. Chang (1987) has developed a more accurate approximation for the term values using earlier work by Edlen (1964). However, the somewhat simpler expression (1) is quite adequate for identifying the Mg \( i \) lines in ATOMS spectra for which laboratory term values do not exist, although in applying it, its approximate nature must be kept closely in mind.

Formula (1) explicitly excludes fine-structure splitting and singlet/triplet structure. These will be negligible in the regime (of higher \( l \) values) where we shall need to apply the polarization formula; the fine-structure term values of significance to us are given by the laboratory data. An indication of the quality of equation (1) in reproducing the term values is reflected in Table 1, which compares experimental and interpolated values. This comparison shows the expected convergence between approximate and experimental data as the orbits become more and more circular. We should reiterate that approximate values are only used when experimental data are not available.

We shall not consider transitions involving values of \( n > 15 \) since the solar Mg \( i \) spectrum does not show lines that extend to such high levels. The only terms for which we lack energy values are the \( ^3P \) levels for \( n > 10 \) and the \( ^1S \) levels for \( n > 11 \). It is futile to apply the interpolation formula to such highly eccentric electron orbits. We could, no doubt, estimate the term values to adequate accuracy by extrapolation using a quantum-defect formula but we shall not have need for this data here.
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TABLE 1
COMPARISON BETWEEN EXPERIMENTAL AND CALCULATED TERM VALUES (cm⁻¹)

<table>
<thead>
<tr>
<th>Configuration</th>
<th>Term/Level</th>
<th>Energy (Experiment)</th>
<th>Energy (Calculated)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3s 4f</td>
<td>3F₁</td>
<td>54676.755 (MZ)</td>
<td>54675.43</td>
</tr>
<tr>
<td></td>
<td>3F₂</td>
<td>54676.701 (MZ)</td>
<td></td>
</tr>
<tr>
<td>3s 5g</td>
<td>1₂G</td>
<td>57262.77 (BB)</td>
<td>57262.90</td>
</tr>
<tr>
<td>3s 8f</td>
<td>1₂F</td>
<td>59953.37 (MZ)</td>
<td>59934.98</td>
</tr>
<tr>
<td>3s 9g</td>
<td>1₂F</td>
<td>60301.283 (MZ)</td>
<td>60301.00</td>
</tr>
</tbody>
</table>


We calculated the wavenumbers for the (very many) transitions formed between states with n ≤ 15—limiting ourselves to transitions permitted in LS coupling. We confine attention to transitions formed between states with n < 15—limiting ourselves to transitions permitted in LS coupling. We confine attention to transitions formed between states with n < 5.

In Table 2 we list the calculated wavenumbers for the strongest lines in the transitions sequences n, n'; i.e., those which involve a change in azimuthal quantum number l = n' – 1 to l = n' – 2 where, again, primed and unprimed quantities refer, respectively, to the lower and upper states. We designate these as the "main" transitions.

We examined the published ATMOS and Brault atlases for the existence of spectral features at the wavenumbers given in Table 2. Results are summarized in Table 3 with the presence or absence of a line denoted by Y or N. In addition to these "main" transitions, a large number of lines from the same principal quantum numbers but with lower l values were found in the spectrum. A few such transitions are considered as examples in the following section.

3. DISCUSSION

The rich yield of Mg I lines in the ATMOS spectra demands a great deal of study to uncover its implications for solar physics. We shall illustrate some of the intriguing aspects of the data using profiles of two sequences: (a) n – 1 to n' – 1 (b) n – 2 to n' n' – 2, where n = 7, 6, 5; n' = n – 1; and the integer associated with n or n' is the azimuthal quantum number l or l'. The ATMOS data are reproduced in Figures 1 and 2; the intensity scale is in arbitrary units ranging from 0 to 1 and is normalized to a peak value in the associated ATMOS spectral range. The wavenumber scale in the figure is in cm⁻¹. The digital data base (from which Figs. 1 and 2 were prepared) uses the wavenumber scale in the reference frame of the spacecraft. Correction for its relative motion to the Sun is made from a knowledge of the circumstances of the different sets of observations which go to make up the data base. In order to compare the wavenumber calculated from equation (1), or from tabulated term values, with the observed profiles, we have corrected these calculated values back to the spacecraft reference frames; the short vertical bar in each panel of Figures 1 and 2 indicates the thus-adjusted values of the wavenumbers of the lines, or their components where these are resolved. Sets of ATMOS spectra were taken both at spacecraft sunrise and sunset. Generally we recovered both spectra from the data base and as a check corrected the wavenumbers back to the spacecraft frame for both observing aspects—this yielded consistent results, agreeing to the thickness of the vertical bar when the two spectra were lined up. We have considerable confidence, therefore, that the locations of the calculated wavenumbers in the spacecraft frame are accurately indicated in the figures.

TABLE 2
WAVENUMBERS OF MAIN TRANSITIONS IN Mg I (cm⁻¹)

<table>
<thead>
<tr>
<th>n'</th>
<th>10</th>
<th>9</th>
<th>8</th>
<th>7</th>
<th>6</th>
<th>5*</th>
<th>4*</th>
</tr>
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<tbody>
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<td>11</td>
<td>190.48</td>
<td>447.94</td>
<td>807.96</td>
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<td>1142.97</td>
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<td>9</td>
<td>...</td>
<td>...</td>
<td>360.06</td>
<td>855.51</td>
<td>1696.71</td>
<td>3052.12</td>
<td>5635.50</td>
</tr>
<tr>
<td>8</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>525.57</td>
<td>1336.66</td>
<td>2691.75</td>
<td>5274.12</td>
</tr>
<tr>
<td>7</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>811.51</td>
<td>2166.11</td>
<td>4746.79</td>
</tr>
<tr>
<td>6</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>1356.23</td>
<td>3934.05</td>
</tr>
<tr>
<td>5</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>2586.02</td>
</tr>
</tbody>
</table>

* Wavenumbers given are for the triplet transitions J, J' = 4, 3.
use the approximate formula (1). When the wavenumbers are based on experimental values, we look for closer agreement.

To make full use of the ATMOS data, we need accurate values for the line frequencies. For example, we need these to assess the existence and magnitude of any systematic flows in the regions where the lines are found. Similarly, the Rydberg levels involved in many of these lines are well known to be very sensitive to perturbing fields, whether fixed or statistical in nature, and the assessment of any such effects demands very accurate term values. Again, the emission features of the 12 µm lines are asymmetrically located in the broad absorption trough (see Figs. 1a and 2a). If this is due to a differential Doppler displacement, then we must ask which component is moving with respect to the Sun. Or is this, instead, a pressure shift, and if so what are the implications of that? In many cases, we see lines whose features could be in absorption or emission (see Figs. 1c and 2c), and an unequivocal resolution of that issue is clearly critical to efforts to understand the excitation of the atom. To answer such questions, we need term values, or direct measurements of line frequencies, to accuracies of a few mK at the worst—recall that, at 1000 cm\(^{-1}\) a line will show 10\(^{-3}\) cm\(^{-1}\) Doppler shift for a 300 m s\(^{-1}\) line-of-sight velocity.

To achieve such accuracy, we can certainly not rely on the approximate "polarization" formulae. For Mg i, the available laboratory data are found in the MZ and BB tables and, most recently, in direct frequency measurements of a number of the infrared lines of interest here by Lemoine, Demuyuck, & Destombes (1988) and Lemoine et al. (1990). The latter paper gives a critical comparison of their measurements with the predicted values from MZ and BB and shows that the former tabulation sometimes contains errors large enough to result in calculated IR frequencies which are off by several times 0.01 cm\(^{-1}\). This is understandable since the MZ values come almost entirely from diffraction-grating spectra, whereas the BB frequencies are from the far higher FTS accuracy attained by J. Brault at Kitt Peak. Consistent with this, the frequencies measured by Lemoine et al. agree extremely well\(^2\) with those calculated by combinations of wavenumbers of the (higher frequency) lines measured by Biémont & Brault (1987). Lemoine et al. (1990) have given close attention to the triplet and singlet fine structure of the 6F and 7F terms; their superior data allow them to resolve the fine structure unambiguously. This is important for our purpose since many solar Mg i lines involve transitions to and from these levels.

Figure 1c shows the observed 5G-4F complex, both triplet and singlet lines. Here the term values are well established from laboratory data to an accuracy of about 1 mK. Reading to the right along the wavenumber scale, the first three fine-structure components, indicated by short vertical bars, are dominated by the \(J,J' = 5,4; 4,3; 3,2\) transitions among the triplet levels. The separated, narrower absorption line is the singlet transition. We note that the calculated wavenumbers match quite well with identifiable spectral features. Particularly notable is the tendency of the predicted triplet lines to coincide with weak core emission features in the background strong absorption line. The singlet line, however, shows no trace of emission.

The progression in shape of the spectral lines in Figure 1 present its own set of problems. The change between the lines is dramatic both in the emission and absorption components, particularly between the 6H-5G and 5G-4F lines in Figures 1b

\(^2\) Except that measurements of the 6F-7G spectrum in the earlier (1988) publication by Lemoine et al. were later found to be in error due to an instrumental problem.
and 1c. Whatever the emission mechanism may be, it appears to be strongly selective of the 6H over the 5G level—the more so since the Einstein A-value for 6H–5G is smaller than that of the 5G–4F transition. The relationship between the 6H and 7I levels requires detailed study. Certainly, it is hard to glean much evidence for a thermal origin of the emission component in such data. The expected strong growth of (photospheric) opacity is evidenced in the increasing strength of the absorption line as we move down the line sequence—no doubt this would be extended into the 4F–3D multiplet if its profile were available. The next higher transition in the sequence (8K–7I) lies at 525 cm$^{-1}$. This line is obscured in Brault's data and lies just outside the long-wavelength limit of ATMOS—although a later line in this series (8H–7G at 530.98 cm$^{-1}$) is present in Brault's atlas where it is in emission in the limb spectrum. Coverage of this line (with its associated lines of smaller $J, F$ values) would be a valuable objective for a future ATMOS flight.

Finally, why do the triplets appear to be in emission in Figure 1c while the singlet is in absorption? This is most probably to be interpreted in terms of the relative optical thickness, but again a more detailed study is needed to clarify this question. Still higher S/N in the core of this line would help to reassure us of the reality of the triplet emission as would observations towards the solar limb.

Figures 2a, 2b, and 2c invite comments which are related, though by no means equivalent. The first member of this set, 7H–6G, shows emission which is weaker than its counterpart of Figure 1a—as one might expect. The absorption shape appears, superficially, to be much the same; the calculated term value for 7H seems to be about 0.02 cm$^{-1}$ too high. A rough measurement suggests that the emission features are less eccentrically located in the absorption than for the 7I–6H line of Figures 1a or 1b. Whereas the emission component grew in strength in the latter sequence, here it decreases greatly, becoming fragmented among the fine-structure lines and appearing only as vestigial emission in the bottom of a deep absorption line. The term values for the transition 6G–5F, shown in Figure 2b, are from laboratory data and the wave-numbers accurately established. That the triplets are indeed in emission is clearly indicated from the coincidence of the calculated frequencies with the emission features. The singlet component of this transition is centered on an absorption feature with what appears to be a blended emission feature to the higher frequency side. The profile of the transition is similar in general appearance to that of Figure 1c (5G–4F) and lends some confidence to the association, there, of weak emission with the triplet lines. Figure 2c is different again; here, as for Figure 2b, we have laboratory term values to rely on in calculating wavenumbers. This figure, which shows only the triplet lines (the singlet is at 4069 cm$^{-1}$), reveals lines wholly in absorption; there is no trace of emission at the predicted line positions, which lie close to the absorption minima.

Whatever the underlying reason for the behavior exhibited in this particular selection of the Mg i infrared lines, it is both unique and confusing. Some highly unusual emission mechanism is at work or an excitation anomaly of an unaccounted kind must be operating to give such very different profiles for the 6H–5G lines than for 6G–5F; and to account for the marked difference between the triplet behavior in the 5G–4F as against 5F–4D multiplets. The emission characteristics seen here are confined to the triplet transitions—though one would surely not expect this to be a general characteristic.

Perhaps the transition from the strong emission of Figures 2a to 2h, or 1b to 1c, is just associated with the breakdown of the degeneracy in the fine-structure levels and between the two multiplicities, with an associated broadening of the line and reduction of the equivalent opacity in each component. That, too, needs to be examined as one more piece in this puzzle.

Finally in this brief survey, consider the set of transitions 7G–6F which lie near 848 cm$^{-1}$ and whose spectrum is shown in Figure 3. The experimental data of Lemoine et al. (1990) (see their Fig. 1) exhibit four resolved lines (three triplet and one singlet) grouped in two pairs, each member of which is separated by about 0.01 cm$^{-1}$, whereas the solar spectra of ATMOS (like the ground-based data of Brault & Noyes) show either two lines in emission or three in absorption depending on how one interprets the structures in the bottom of the line. Since all the levels of the 7G term have a common energy in the BB tables, while the 6$^3$F levels have a common energy in MZ (with the 6$^1$F being listed as 0.031 cm$^{-1}$ lower), we predicted only two spectral features separated by 0.03 cm$^{-1}$. Neither of these falls clearly on either an emission or an absorption feature. The better data of Lemoine et al. (1990) showed the MZ energy values to be in error and show unequivocally that in the rest frame of the Sun, the two features observed by ATMOS are to be interpreted as emission peaks.

More observations would be extremely helpful in understanding the complexities of this spectrum. Of particular importance would be center-to-limb measurements whose profound limb brightening should cast some light on many of the questions raised here and, together with the observed intensities, should allow an assessment of the relative excitation of these upper states of Mg i. Such observations must clearly be regarded as having the highest priority for any future ATMOS observations of the Sun.

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