Fe IX CALCULATIONS FOR THE SOLAR DYNAMICS OBSERVATORY

ADAM R. FOSTER AND PAOLA TESKA
Smithsonian Astrophysical Observatory, 60 Garden Street, Cambridge, MA 02138, USA; afoster@cfa.harvard.edu

Received 2011 July 1; accepted 2011 September 12; published 2011 October 4

ABSTRACT

New calculations of the energy levels, radiative transition rates, and collisional excitation rates of Fe IX have been carried out using the Flexible Atomic Code, paying close attention to experimentally identified levels and extending existing calculations to higher energy levels. For lower levels, R-matrix collisional excitation rates from earlier work have been used. Significant emission is predicted by these calculations in the 5f-3d transitions, which will impact analysis of Solar Dynamics Observatory Atmospheric Imaging Assembly observations using the 94 Å filter.

Key words: atomic data – Sun: UV radiation

Online-only material: color figures, machine-readable table

1. INTRODUCTION

The launch of the Solar Dynamics Observatory (SDO) allows observation of the Sun in unprecedented detail. The Atmospheric Imaging Assembly (AIA; Lemen et al. 2011) provides observation of the Sun through a variety of narrowband filters centered on individual emission lines of interest. One such filter is centered on 94 Å, and targets both the Fe xviii (93.923 Å) transition from 2s1 2p6 2p3/2 → 2s2 2p5 2p3/2 at high temperatures and the Fe x (94.012 Å) line from the 3p4 4f1 2D3/2 → 3p4 2P3/2 transition in cooler plasma. The emission from these two lines occurs in very different temperature ranges and therefore can be distinguished if the plasma temperature distribution is known (Boerner et al. 2011).

Lepson et al. (2002) observed spectra of Fe vii to Fe x using an electron beam ion trap (EBIT) and a grazing incidence spectrometer with resolution of ≈300 at 100 Å to observe lines in the 60–140 Å range. They estimated that 70% of the emission in this band was unaccounted for by the existing calculations to higher energy levels. For lower levels, R-matrix collisional excitation rates from earlier work have been used. Significant emission is predicted by these calculations in the 5f-3d transitions, which will impact analysis of Solar Dynamics Observatory Atmospheric Imaging Assembly observations using the 94 Å filter.

2. METHOD

The NIST atomic spectra database (Ralchenko et al. 2011) lists 35 observed energy levels for Fe IX, including the lowest 17 energy levels and 18 others up to the 3p5 5s1 level. Solar observations using the Hinode/EUV Imaging Spectrometer (EIS) instrument have led to the identification of four more energy levels: 3p4 3d2 3G1,2,3 and 3p4 3p1 1S0 (Young 2009).

Theoretical calculations of the Fe IX structure have been performed by several groups. The configurations included in some of these are listed in Table 1. Storey et al. (2002) performed structure calculations (Eissner et al. 1974) using the General Purpose Relativistic Atomic Structure Package (GRASP; Dyall 1989) and FAC to calculate energy levels and transition rates. They used various configuration combinations in order to match the first 17 energy levels as closely as possible, while also paying particular attention to the first 360 energy levels. They found that the effect of the CI between many of the configurations on the energy levels and subsequent oscillator strength calculations is of importance, in particular the 3s2 3p3 3d1. This was omitted during another set of calculations by Verma et al. (2006) using the cv13 (Hibbert 1975) code, and gave very different results compared to those of Aggarwal et al. (2006), and observed energy levels. The configurations listed in Table 1 are those from their best-fitting GRASP run.

The energies of Storey et al. (2002) agree with the observed energies to within 6% (the energies of the first 17 levels were set to match observed values after the structure calculation was complete), while those of Aggarwal et al. (2006) agree within the observed energies 1%–3%. The exception to this are the four levels from Young (2009), numbers 94, 95, 96, and 144 in our energy ordering. These were not identified until after the Aggarwal et al. (2006) data were created, and there is a substantial difference in both the energies and the level ordering caused by their introduction (see Figure 1).

In our FAC calculation, we have experimented with different configuration sets to obtain a good match with the observed energies in both absolute energy and energy level ordering.
and to include the higher $n$ shells from which the emission takes place. We have included the 3$s^2$3$p^5$5$f^1$ and 3$s^2$3$p^6$6$l^1$ configurations to include the higher $n$ emission which we are trying to characterize.

We have also included many other configurations for their CI effects. The coupling between configurations of the same parity can affect the energy ordering of many of the levels during the structure calculation. In this case, most of these levels do not contribute observed emission lines, and their energies are much higher than those of immediate spectroscopic interest for which there are observed lines (>200 eV), leading them to straddle the ionization energy of the ion (i.e., many of them are autoionizing).

To keep our calculation to a reasonable size, we have included many configurations only during the structure calculation for CI purposes and omitted them from the collisional and radiative calculations: again, these are listed in Table 1.

Table 1

| Config. | S2002 | A2006 | Current | Config. | S2002 | A2006 | Current |
|---------|-------|-------|---------|---------|-------|-------|---------|
| 3$s^2$3$p^5$ | Y | Y | Y | 3$s^2$3$p^5$3$d^1$ | CI | Y | Y |
| 3$s^2$3$p^5$3$d^1$ | Y | Y | Y | 3$s^2$3$p^5$3$d^1$ | Y | Y | Y |
| 3$s^2$3$p^5$4$f^1$ | Y | Y | Y | 3$s^2$3$p^5$4$f^1$ | Y | Y | Y |
| 3$s^2$3$p^5$4$d^1$ | CI | Y | Y | 3$s^2$3$p^5$5$l^1$ | CI | Y | Y |
| 3$s^2$3$p^5$5$f^1$ | CI | Y | Y | 3$s^2$3$p^5$6$l^1$ | CI | Y | Y |
| 3$s^2$3$p^6$3$d^2$ | Y | Y | Y | 3$s^2$3$p^6$3$d^2$ | Y | Y | Y |
| 3$s^2$3$p^6$4$l^1$ | Y | Y | Y | 3$s^2$3$p^6$5$l^1$ | Y | Y | Y |
| 3$s^2$3$p^6$6$l^1$ | CI | Y | Y | 3$s^2$3$p^6$6$l^1$ | CI | Y | Y |
| 3$s^2$3$p^6$4$p^2$ | CI | Y | Y | 3$s^2$3$p^6$4$p^2$ | CI | Y | Y |

Notes. S2002 denotes the Storey et al. (2002) data while A2006 denotes Aggarwal et al. (2006). Levels marked “CI” are included only for configuration interaction purposes.

We note (see Figure 1) that our calculated energies are without exception higher than the observed values. This offset scales simply with energy, resulting in calculated levels which are 1%–2.5% larger than observed values. Since the goal of these calculations is to produce useful spectra for astrophysical analysis, we have adjusted the level energies after the structure calculation to match the observed values. For intermediate levels, the multiplier has been interpolated in energy and applied. The 3$p^55f^1$ levels of primary interest in this work are of a higher energy than any other experimentally identified levels of Fe IX. Noting the relatively uniform overestimate of the energy in the structure calculations, we have scaled the energies for all levels above the highest observed energy level by the mean of the adjustment used for experimentally identified levels, 0.9817. The observed energy levels are the 17 levels from NIST, the four levels from Young (2009), and the four levels calculated from the Lepson et al. (2002) measurements: (3$p^2_1^1_3^1_5^1$4$f^1_2$)$_2$ (E = 163.2 eV), (3$p^1_1^3_1_3^1_5^1$4$f^1_2$)$_2$ (E = 164.9 eV), (3$p^2_1^1_3^1_5^1$5$l^1$)$_2$ (E = 189.9 eV), and (3$p^1_1^3_1_3^1_5^1$5$l^1$)$_2$ (E = 189.6 eV).

Radiative rates were calculated by Aggarwal et al. (2006) based on their structure calculation. We have in this attempt to use these radiative rates, however the significant disagreements in the energy level ordering have made this problematic for most levels. We have therefore used the Aggarwal et al. (2006) values for transitions among the lowest 17 energy levels, where the ordering is definite, and the remainder have been calculated using the relativistic method within FAC.

Figure 1. Ratio of the observed and calculated energies for Fe IX levels from a variety of methods. Squares: superstructure (Storey et al. 2002); circles: GRASP (Aggarwal et al. 2006); and stars: this work. The levels with observed energy levels from Hinode observations (Young 2009) are highlighted, as is the 1%–3% difference band in which all the current results fall. The dashed line indicates the correction factor used for all higher energy levels. A description of these levels is in Table 2, with their indexes in Column 5. Only those levels with observed counterparts are included.

(A color version of this figure is available in the online journal.)

Figure 2. Matrix calculations, producing collisional excitation rates among the lowest 140 energy levels. Further work was performed using FAC by Liang et al.
The Astrophysical Journal Letters, 740:L52 (5pp), 2011 October 20

Foster & Testa

Table 2
The List of Energy Levels Resulting from This Work

| Index | jj Symbol | $E_{\text{FAC}}$ (eV) | $E_{\text{corr}}$ (eV) | Ind Figure 1 | $E_G$ (eV) | Ind$_G$ |
|-------|-----------|----------------|----------------|-------------|--------|---------|
| 1     | $3p^33p^1(0, 0)_0$ | 0.000 | 0.000 | 0 | 0.000 | 1 |
| 2     | $3p^33p^1 3d^1(0, 1/2, 1/2)_0$ | 50.949 | 50.309 | 1 | 50.925 | 2 |
| 3     | $3p^33p^1 3d^1(0, 3/2, 3/2)_0$ | 51.264 | 50.625 | 2 | 51.242 | 3 |
| 4     | $3p^33p^1 3d^1(0, 1/2, 1/2)_1$ | 51.923 | 51.288 | 3 | 51.907 | 4 |
| 94    | $3p^33p^1 4s^1(0, 1/2, 1/2)_1$ | 120.922 | 117.850 | 17 | 121.033 | 94 |
| 95    | $3p^33p^1 3d^1 3d^1(0, 2, 1/2, 1/2)_1$ | 121.280 | 118.637 | 18 | 123.412 | 97 |
| 96    | $3p^33p^1 3d^1 3d^1(4, 3/2, 3/2)_5$ | 121.346 | 118.703 | 19 | 123.470 | 98 |
| 97    | $3p^33p^1 3d^1 3d^1(0, 2, 1/2, 1/2)_1$ | 121.461 | 118.761 | 20 | 123.521 | 99 |
| 98    | $3p^33p^1 4s^1(1, 0, 1/2)_0$ | 122.173 | 119.247 | 21 | 123.330 | 95 |
| 99    | $3p^33p^1 3d^1 3d^1(1/2, 1/2, 1/2)_3$ | 122.577 | 119.521 | 22 | 124.507 | 100 |
| 100   | $3p^33p^1 4s^1(0, 1/2, 1/2)_1$ | 122.863 | 119.715 | 23 | 122.951 | 96 |

Notes. $E_{\text{FAC}}$ refers to the original results from FAC calculations, $E_{\text{corr}}$ are the energies after correction as described in the text. For each level with an observed energy value, the index of this level in Figure 1 is given (Ind$_{\text{Fig1}}$): for these levels $E_{\text{corr}} = E_{\text{observed}}$. For comparison, the GRASP results of Aggarwal et al. (2006) are listed ($E_G$), along with the energy order from that work (Ind$_G$). A star denotes a level for which a different configuration is found between our work and Aggarwal et al. (2006).

(Also provides a table with energy levels, indices, and correction details.

(2009), although again these did not incorporate $n = 5$ configurations.

A full $R$-matrix calculation including all of the excited levels on the $n = 5$ level would be a prohibitively large calculation and is beyond the scope of this work. We have therefore used the distorted wave FAC collision code to calculate collision strengths between all of the levels of Fe $\text{xix}$ included in our structure calculations. The advantage of this approach is the fast production of results and the inclusion of large numbers of levels. The downside is the omission of low-energy resonance effects, which can be significant. We therefore use the $R$-matrix collision strengths of Storey et al. (2002) where they exist. We note that the problem of matching levels between the calculations persists. For most levels, we have matched the levels with the same electron configuration and total angular momentum, $J$, and then paired these results in energy order. For the $3p^33d^2$ and $3p^33d^3$ levels there are different numbers of levels (for the former configuration, our calculation has two more levels for each of $J = 2, 3,$ and $4$; for the latter Storey et al. 2002 have two more). We have therefore combined these two configurations, which overlap completely in energy at the higher end of the $3p^33d^2$ energies ($\approx 130$ eV).

3. RESULTS

We have taken the results of our FAC calculation, merged where appropriate with other calculations as outlined above, and used the APEC code to model the emission from an optically thin plasma with solar photospheric elemental abundances (Anders & Grevesse 1989) in collisional ionization equilibrium. We show this result in Figure 2, for $T = 10^6$ K plasma with the emission lines broadened by Gaussians with width 0.05 Å. Overplotted on this figure is the same result from the current version (2.0) of AtomDB (A. R. Foster et al. 2011, in preparation), which uses the old Fe $\text{xix}$ data. Overlaid is the effective area curve of the AIA instrument with the 94 Å filter in place, taken from Boerner et al. (2011), which can also be obtained by the routine aia_get_response.pro in the SolarSoftware package. It can be seen that there are clearly two strong lines and several weaker lines, which are also from $5f \rightarrow 3d$ transitions, within the region of interest.

The weaker lines are a significant fraction of the two main $5f-3d$ lines, with emissivities of around 10%–20% of the main lines. Their exact wavelengths are, however, unknown: the $5f-3d$ lines were already weak in the EBIT measurements, the weaker neighboring lines were not distinguished from the background. The correction applied to the $5f-3d$ lines was a further $\pm 5\%$ compared to the simple multiplication by the 0.9817 scaling factor, in opposite directions. This implies that a correction at a similar level may be required in the case of these weaker lines.

We have not further adjusted the energy levels of these weaker lines after the general initial scaling. Further experimental measurements of these lines would be valuable in estimating their effects more clearly.

In Figure 2 we have also convolved the line emissivities for all ions with the effective area of the filter at each wavelength and show the total as a function of temperature. We have done this for the AtomDB 2.0.1 model, which omits the 94 Å lines, and for an identical data set but using the new Fe $\text{xix}$ data from this work. The low temperature peak, previously due to Fe x, is significantly increased due to the strong Fe $\text{xix}$ emission as part of this work, by over a factor of two at $\log_{10}(T_e/K) = 5.8$.

In addition, further lines are positively identified in the Fe $\text{xix}$ spectrum. The lines at $134.08$ and $136.70$ Å, identified as belonging to the $3p^34f^1 \rightarrow 3p^53d^1$ transition, are clearly identifiable in the new calculations of the spectrum. Figure 3 shows the spectrum calculated using the old and new Fe $\text{xix}$ data, combined with a quiet Sun spectrum taken from the SDO Extreme Ultraviolet Variability Experiment (EVE) Multiple EUV Grating Spectrographs (MEGS). The previously unidentified lines at $134.08$ Å and $136.70$ Å are clearly observable. These wavelengths fall sufficiently far away from the $131$ Å filter transmission band that there is no discernable change in the estimated flux in this filter due to the inclusion of these lines.
The Astrophysical Journal Letters, 740:L52 (5pp), 2011 October 20

Foster & Testa

Figure 2. Left: the emissivity of Fe\textit{ix} at $T = 10^6$ K. Dotted line: from AtomDB v2.0.1; solid line: from AtomDB v2.0.1 with Fe\textit{ix} data from this work; and dashed line: the effective area of the 94 Å channel of the SDO/AIA. The AtomDB v2.0.1 data are effectively zero, and hence too small to be notable on the graph. Right: the total emissivity of elemental emission lines convolved with the effective area of the 94 Å filter. Dashed line: data from AtomDB v2.0 and solid line: data from AtomDB v2.0 including the Fe\textit{ix} data from this work.

(A color version of this figure is available in the online journal.)

Figure 3. Top: a quiet Sun spectrum taken from the SDO EVE MEGS instrument. Bottom: the spectrum calculated using AtomDB 2.0.1, with (dashed) the old Fe\textit{ix} data and (solid) the new data from this work, with all lines broadened by Gaussians with $\sigma = 0.2$ Å.

(A color version of this figure is available in the online journal.)

4. DISCUSSION

The lack of information on the Fe\textit{ix} emission in the 94 Å region has been well known since the work of Lepson et al. (2002). Testa et al. (2011) compared the existing atomic data in \textit{chianti} 6.0.1 with observations of Procyon using the \textit{Chandra} Low Energy Transmission Grating (LETG) spectrometer, which covers wavelengths up to $\sim 170$ Å. They noted in these observations a significant missing flux in the 94 Å region. Since the launch of the SDO, the lack of a collisional excitation calculation has led to several authors using creative means to account for this difference. When looking at coronal loop emission, Schmelz et al. (2011) used a scaling factor obtained by comparing the relative intensities of the known transition lines and the 5$f \rightarrow 3d$ in the spectrum observed by Lepson et al. (2002). They eventually discounted this band from their analysis due to a low count rate, so the effectiveness of this method is unknown. Aschwanden & Boerner (2011), when looking at the temperature structure of coronal loops, derived a “correction factor,” $q_{94}$, for the low temperature ($\log_{10}(T/K) \leq 6.3$) response function of the 94 Å filter, $R_{94}$, by fitting their 100 results in the other filters with $q_{94}$ a free parameter. They obtained $q_{94} = 6.7 \pm 1.7$ at temperatures around $\log_{10}(T/K) = 6.0$. The results from this work imply a much smaller correction factor, with $q_{94} \approx 2$ being the maximum value at log$_{10}(T/K) = 6.8$ and $\approx 1.25$ at log$_{10}(T/K) = 6.0$. There is significant discrepancy here: it would be an interesting exercise to investigate whether the differential emission measure (DEM) analysis of Aschwanden & Boerner (2011) can be self consistent using the new emission estimate in this filter band. It is also possible that there are further lines from different ions in the filter which have not yet been correctly handled.

It is difficult to estimate uncertainties in the results from this work due to the many overlapping sources of error. As well as the two main lines which are the focus of this work, there are many smaller lines of uncertain wavelength. Given the observed and initially calculated 5$f \rightarrow 3d$ wavelengths differ by around 0.5%, adding normally distributed random errors to these lines of $\pm 0.5$ Å gives a 10% standard deviation in the resulting Fe\textit{ix} emission in the 94 Å filter. This 10% fluctuation is then approximately a 5% effect on the total emission in the band once Fe\textit{x} is also included. Given that the estimates of uncertainty in distorted wave excitation collisions are usually not better than 20%, this is not expected to be a dominating source of error in the calculation.

For those levels which appear in both this work and the collisional calculation of Storey et al. (2002), comparison of the collision strengths for excitation from the ground state at $T = 10^6$ K between these data and our FAC results show that they vary by on average around 25%. This is a very approximate lower limit on the likely errors on the calculation of emission in the 94 Å band, since excluding cascades from the $n = 6$ shell, this is the only way to populate the 5$f$ upper levels in this model, and for these levels we are using the distorted wave, not $R$-matrix, methods.

These data have been incorporated into AtomDB, to be released fully in AtomDB v2.1.0 which is due for release later
in 2011. In the meantime, the data can be obtained from the AtomDB Web site, http://www.atomdb.org.

A.R.F. acknowledges funding from NASA ADP grant NNX09AC71G. P.T. has been supported by contract SP02H1701R from Lockheed-Martin to SAO.

REFERENCES

Aggarwal, K. M., Keenan, F. P., Kato, T., & Murakami, I. 2006, A&A, 460, 331
Anders, E., & Grevesse, N. 1989, Geochim. Cosmochim. Acta, 53, 197
Aschwanden, M. J., & Boerner, P. 2011, ApJ, 732, 81
Bar-Shalom, A., Klapisch, M., & Oreg, J. 2001, J. Quant. Spectrosc. Radiat. Transfer, 71, 169
Boerner, P., Edwards, C., Lemen, J., et al. 2011, Sol. Phys.
Dere, K. P., Landi, E., Young, P. R., et al. 2009, A&A, 498, 915
Dyall, K. G., Grant, I. P., Johnson, C. T., Parpia, F. A., & Plummer, E. P. 1989, Comput. Phys. Commun., 55, 424
Eissner, W., Jones, M., & Nussbaumer, H. 1974, Comput. Phys. Commun., 8, 270

Gh, M. F. 2003, ApJ, 582, 1241
Hibbert, A. 1975, Comput. Phys. Commun., 9, 141
Kaastra, J. S., & Mewe, R. 1993, Legacy, 3, 6
Kaastra, J. S., Mewe, R., & Nieuwenhuijzen, H. 1996, in UV and X-ray Spectroscopy of Astrophysical and Laboratory Plasmas, ed. K. Yamashita & T. Watanabe (Tokyo: Universal Academy Press), 411
Lemen, J., Title, A. M., Akin, D. J., et al. 2011, Sol. Phys.
Lepson, J. K., Beiersdorfer, P., Brown, G. V., et al. 2002, ApJ, 578, 648
Liang, G. Y., Crespo Lpez-Urrutia, J. R., Baumann, T. M., et al. 2009, ApJ, 702, 838
Mewe, R., Kaastra, J. S., & Liedahl, D. A. 1995, Legacy, 6, 16
Ralchenko, Yu., Kramida, A. E., Reader, J., & NIST ASD Team, 2011, NIST Atomic Spectra Database (version 4.1.0; National Institute of Standards and Technology, Gaithersburg, MD), http://physics.nist.gov/asd3 [2011, June 15]
Schmelz, J. T., Jenkins, B. S., Worley, B. T., et al. 2011, ApJ, 731, 49
Smith, R. K., Brickhouse, N. S., Liedahl, D. A., & Raymond, J. C. 2001, ApJ, 556, L91
Storey, P. J., Zeippen, C. J., & Le Dourneuf, M. 2002, A&A, 394, 753
Testa, P., et al. 2011, ApJ, submitted
Verma, N., Jha, A. K. S., & Mohan, M. 2006, ApJS, 164, 297
Young, P. R. 2009, ApJ, 691, L77

Foster & Testa