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Radiative data for ions in the Mg isoelectronic sequence

ABSTRACT

A large number of energy levels, f-values and photoionisation cross sections have been calculated for ions of astrophysical interest in the Mg isoelectronic sequence. This work is part of an international collaboration which is aimed at computing stellar envelope opacities (the Opacity Project). Statistical comparisons of quantum defects, f-values and radiative lifetimes are carried out with experiment and with previous theoretical work in order to assess the accuracy of the results. We conclude that the present dataset is as accurate as those calculated using elaborate methods.

METHOD

Bound states with electronic configurations $3lnl'\ ^{1,3}L$ ($l \leq 2$, $l' \leq 4$, $n \leq 10$, $L \leq 4$) were calculated within the close-coupling formalism (Burke and Seaton 1971) for astrophysically abundant ions in the Mg sequence, namely: Mg I, Al II, Si III, S V, Ar VII, Ca IX and Fe XV. Full use was made of the recently developed Opacity Project R-matrix package described by Berrington *et al* (1987). A seven-state approximation ($3s\ ^2S$, $3p\ ^2P^0$, $3d\ ^2D$, $4s\ ^2S$, $4p\ ^2P^0$, $4d\ ^2D$, $4f\ ^2F^0$) was adopted for all target ions except Mg II where the $5s\ ^2S$ state was also included. Target representations were obtained in a similar fashion to Butler *et al* (1984) and Mendoza and Zeippen (1987), but core polarisation effects were neglected throughout. Oscillator strengths and photoionisation cross sections were calculated for all possible optically allowed transitions, and radiative lifetimes could then be easily estimated from the bound-bound data using theoretical wavelengths.

COMPARISON WITH PREVIOUS WORK

Members of the Mg sequence, particularly the neutral and lowly ionised species, have been extensively studied both theoretically and experimentally. Instead of reviewing this work, and considering the volume of data generated in the present calculation, we will attempt to assess the accuracy of the data by carrying out statistical comparisons with experiment and with representative sets of calculations which emphasise both quality and quantity.

Following Yu Yan *et al* (1987) the comparison of two datasets, for instance length/velocity f-values or theoretical/experimental quantum defects, will be carried out in terms of an average percentage difference defined as

$$\Delta = 100 \times \left[\sum_i (a_i - b_i)^2\right]^{1/2} \left[\sum_i a_i \times b_i\right]^{-1/2}$$

where a_i and b_i are corresponding values in the two sets.

Term energies

We have calculated a total of 1247 bound states, and a comparison with experimental quantum defects for 368 observed multiplets gives an average percentage difference of $\Delta = 2.4$ %. Experimental values were taken from Moore (1971), Martin and Zalubas (1979, 1980, 1983), Sugar and Corliss (1979, 1982), Joelsson *et al* (1981), Litzén and Redfors (1987) and Redfors (1988). From this comparison we have excluded 6 states with questionable experimental assignments: $3p4p\ ^1D$ and $3s7d\ ^1D$ of Si III; $3p3d\ ^1P^0$ and $3p3d\ ^1F^0$ of S V; $3s5f\ ^1F^0$ and $3s6f\ ^1F^0$ of Fe XV.

Oscillator strengths

We have computed weighted oscillator strengths, gf-values, for 17041 possible bound-bound transitions. Comparisons of gf-values in the length and velocity formulations for each ion gives $\Delta = 1.8\%$ for Mg I, increasing along the sequence up to $\Delta = 3.1\%$ in Fe XV. This is caused by the effects of series perturbers which become more conspicuous for higher Z.

In Table 1 we compare present absorption oscillator strengths with four other sets of calculations. In set MCHF we have excluded four transitions involving the strongly mixed $3p3d\ ^1P^0$ and $3s6p\ ^1P^0$ states of Si III which show fairly large f-values very different from the present ones. For similar reasons we have not included two transitions in set CIV3 involving the strongly mixed $3p4p\ ^1D$ and $3s5d\ ^1D$ states of S V; the transition $3s3p\ ^3P^0 \rightarrow 3s4s\ ^3S$ in S V is also excluded from this set since we think that the f-value given by Baluja and Hibbert (1985) has been misquoted. The agreement with set MCHF is particularly good; however, the excellent agreement with set MS is not representative of the sequence since only Mg I was considered.

Radiative lifetimes

A comparison of present radiative lifetimes (calculated

Table 1. Comparison of f-value (length formulation) average percentage differences between present results and representative sets of values calculated previously for ions in the Mg sequence. VSL: Model potential method of Victor *et al* (1976). MCHF: Multiconfiguration Hatree-Fock results of Froese Fischer (1975, 1979) and Froese Fischer and Godefroid (1982). CIV3: Configuration interaction calculations by Baluja and Hibbert (1980, 1985), Tayal and Hibbert (1984) and Tayal (1986). MS: L^2 method of Moccia and Spizzo (1988).

Set	No. Trans.	Δ (%)
VSL	615	8.3
MCHF	219	2.2
CIV3	337	4.8
MS	429	1.9

in the length formulation and theoretical wavelengths) with those given for 25 states of Mg I by Moccia and Spizzo (1988) shows an agreement well within 15%. Furthermore, the differences with the lifetimes calculated by Froese Fischer and Godefroid (1982) for 57 singlet states of the ions considered here are not larger than 20%, if one excludes the long-lived $3p^2\ ^1D$ state of Al II and the strongly mixed $3p3d\ ^1P^0$ and $3s6p\ ^1P^0$ states of Si III. The agreement could perhaps be improved if the radiative lifetimes were corrected with observed wavelengths. A comparison with measured lifetimes is not conclusive due to the wide scatter in the experimental results.

COMMENTS

This level of agreement increases our confidence in the accuracy of the present radiative data for this sequence within the context of opacity calculations. Although significant differences can always be found in computed f-values when states mix strongly or for transitions where there is a lot of cancellation, we have shown here that the present data are in general as accurate as those calculated previously for this sequence using detailed methods.

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