Benchmark calculations for electron-impact excitation of Mg^{4+}

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Synopsis In order to resolve major discrepancies between a number of previous calculations for electron impact excitation of Mg^{4+}, we carried out extensive B-Spline R-matrix calculations for this problem. In particular, we investigate the effect of the target structure description and the number of states included in the close-coupling expansion on the final results. Finally, we provide an uncertainty estimate the current predictions.

There are major discrepancies between recent B-spline R-matrix (BSR) [1] and Dirac Atomic R-matrix Code (DARC) [2] calculations regarding electron-impact excitation rates for transitions in Mg^{4+}. To identify possible reasons for these discrepancies and to estimate the accuracy of the various results, we carried out independent BSR calculations with the same 86 target states as in the previous calculations, but with a different and more accurate representation of the target structure.

We find close agreement with the previous BSR results for the majority of transitions, thereby confirming their accuracy. At the same time the differences with the DARC results are much more pronounced. The discrepancies in the final results for the collision strengths are mainly due to differences in the structure description, specifically the inclusion of correlation effects, and due to the likely occurrence of pseudoresonances in the DARC model.

To further check the convergence of the predicted collision rates, we carried out even more extensive calculations involving 316 states of Mg^{4+}. Figure 1 presents a comparison of effective collision strengths from the present BSR-86 and BSR-316 models. As expected, the corrections for the strong transitions are small and the corresponding rates are expected to be converged. The rate coefficients for all transitions between the lowest 10 levels with configurations $2s^2 2p^4$, $2s\,2p^5$, and $2p^6$ are stable against changes in the size of the CC expansion, for both strong dipole and weak intercombination transitions.

To quantify the likely uncertainties, Table 1 shows the average deviations of the BSR-86 predictions from the BSR-316 results for three electron temperatures, with relatively large ($\Upsilon \geq 1$), medium ($10^{-2} < \Upsilon < 1$), and small ($\Upsilon < 10^{-2}$) effective collision strengths. As expected, the results for the strong transitions agree well in both models, while those for the weaker transitions deviate most from each other.

Table 1. Average difference (in %) between the effective collision strengths obtained in the BSR-86 model from the results generated with BSR-316 at three electron temperatures for strong, intermediate, and weak transitions.

$T_e =$	10^4 K	10^5 K	10^6 K
$\Upsilon \geq 1$	8.4	9.3	6.0
$10^{-2} < \Upsilon < 1$	33.2	40.0	20.4
$\Upsilon < 10^{-2}$	61.8	67.6	56.3

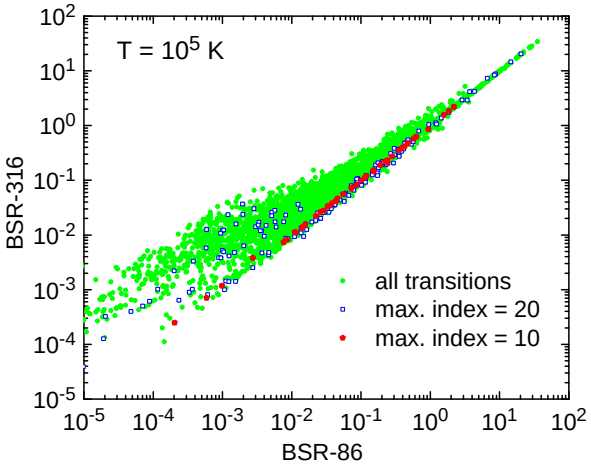

Figure 1. Comparison of effective collision strengths obtained in the present BSR-86 and BSR-316 models for an electron temperature of 10^5 K. In addition to all transitions, we illustrate the situation for the lowest 10 and 20 states, respectively.

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References

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