

Comment on a paper by M.A. Bautista “Atomic data from the Iron Project. XVI. Photoionization cross sections and oscillator strengths for Fe V”

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Abstract. Recently, Bautista (1996) reported new calculations of photoionization cross sections for Fe V, and compared them with the earlier results of Reilman & Manson (1979) and Verner et al. (1993). Bautista claimed that beyond 10 Ry the new cross sections “converge well toward the results by Reilman and Manson”, whereas “the calculations by Verner et al. still underestimate the cross section by almost factor of two”. We show that Bautista erroneously compared the total (summed over shells) cross sections from Reilman & Manson with the partial 3*d*-shell cross sections from Verner et al. Actually, the total cross sections from Verner et al. and Reilman & Manson agree within 3% at all energies.

Key words: atomic data – atomic processes

In a recent paper, Bautista (1996) presented new R-matrix calculations of photoionization cross sections for Fe V, and compared them with the Hartree-Slater data of Reilman & Manson (1979, hereafter RM) and Hartree-Dirac-Slater data of Verner et al. (1993, hereafter VYBT). In his paper, Bautista wrote:

“Beyond 10 Ry the present cross sections converge well toward the results by Reilman and Manson as might be expected since the electron correlation effects get weaker with increasing energy. However, the calculations by Verner et al. still underestimate the cross section by almost factor of two. The low values of the photoionization cross section from Verner et al. with respect to those by Reilman and Manson are not understood since both of these calculations are based on a similar approximation.”

The reason of this “disagreement” is very simple. RM published the tables of total (summed over shells) cross sections. VYBT presented analytic fits to the partial cross

sections for separate shells. Bautista erroneously compared the total cross section from RM with the partial 3*d*-shell cross section from VYBT. The total cross sections from VYBT and RM agree within relative error $\delta < 3\%$ at all photon energies E . To illustrate that, we present (Table 1) the photoionization cross sections of Fe V calculated with the VYBT analytic fits for the first 10 entries of the RM table. Note that the 3*d*-shell ionization threshold of Fe V is 73.03 eV (5.37 Ry), the 3*p*-shell threshold 128.8 eV (9.47 Ry), and the 3*s*-shell threshold 163.3 eV (12.0 Ry) (see VYBT).

Table 1. Photoionization cross section σ [Mb] of Fe V

E, eV	VYBT			Total	RM	δ , %
	3 <i>d</i>	3 <i>p</i>	3 <i>s</i>		Total	
80	5.341	0	0	5.341	5.350	0.2
90	4.788	0	0	4.788	4.779	0.2
100	4.190	0	0	4.190	4.204	0.3
130	2.694	1.073	0	3.767	3.855	2.3
160	1.750	1.121	0	2.871	2.919	1.6
190	1.176	1.043	0.271	2.490	2.531	1.6
210	0.920	0.968	0.244	2.132	2.165	1.5
240	0.653	0.851	0.210	1.714	1.736	1.3
270	0.478	0.742	0.182	1.402	1.416	1.0
300	0.358	0.647	0.158	1.163	1.172	0.8

References

- Bautista M.A., 1996, A&AS 119, 105
 Reilman R.F., Manson S.T., 1979, ApJS 40, 815 (RM)
 Verner D.A., Yakovlev D.G., Band I.M., Trzhaskovskaya M.B., 1993, Atomic Data Nucl. Data Tables 55, 233 (VYBT)

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