

LETTER TO THE EDITOR

Reply to “Comment on ‘Calculations of energies of intrashell doubly excited states of beryllium-like ions’ ”

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Abstract. The energy positions of $1s^23l3l'$ resonances of C^{2+} , O^{4+} and Ne^{6+} ions are recalculated using two-electron basis functions constructed from eigenstates of the one-electron model Hamiltonian. The results are in good agreement with the new calculations of Macias *et al* and Bachau *et al*.

In a recent paper, Chen and Lin (1989) calculated the resonance energies of $1s^23l3l'$ states of C^{2+} , N^{3+} , O^{4+} and Ne^{6+} ions. For some of the lower states, it was pointed out that their results were in disagreement with the previous results of Martin *et al* (1988). In the letter by Bachau *et al* (1990), the discrepancy was attributed to the use of two-electron basis functions built from hydrogenic orbitals adopted by Chen and Lin (1989). It was argued that to project out the open channels appropriately the two-electron basis functions should be constructed from the eigenstates of the one-electron model Hamiltonian.

We have recalculated the energies of these states using two-electron basis functions constructed from the eigenstates of the one-electron Hamiltonian. The results for the two lowest $1s^23l3l' \ ^1S^e$ and $1s^23l3l' \ ^3P^o$ states are shown in table 1, together with the

Table 1. Comparison of the present results with the calculations of Macias *et al* (1989), Chen and Lin (1989) and Martin *et al* (1988) for the energies of $1s^23l3l'$ states of Be-like C, O and Ne ions. The binding energies are given in eV (1 au = 27.2116 eV).

	States	a	b	c	d	e
C^{2+}	(2,0) $^1S^e$	47.37	47.40	47.48	47.74	47.08
	(0,0) $^1S^e$	41.92	41.98	41.86 ^f	41.82	41.91
	(2,0) $^3P^o$	45.98	45.85	45.95	46.12	45.84
	(0,0) $^3P^o$	40.90	41.18	41.10	40.84	41.18
	(2,0) $^1S^e$	107.95			108.33	107.54
O^{4+}	(0,0) $^1S^e$	99.18			99.00	99.18
	(2,0) $^3P^o$	105.73			105.82	105.53
	(0,0) $^3P^o$	97.67			97.58	97.96
	(2,0) $^1S^e$	193.09	192.74	192.70	193.16	192.28
Ne^{6+}	(0,0) $^1S^e$	180.78	180.74	180.50	180.46	180.45
	(2,0) $^3P^o$	189.78	189.48	189.62	189.81	189.53
	(0,0) $^3P^o$	178.58	178.98	178.82	178.70	178.99

^a Present results.

^b Macias *et al* (1989), using the pseudopotential-Feshbach approach.

^c Macias *et al* (1989), using the conventional-Feshbach approach.

^d Chen and Lin (1989).

^e Martin *et al* (1988).

^f This state was listed at 41.96 eV in Bachau *et al* (1990).

newer calculations of Macias *et al* (1989) and Bachau *et al* (1989) and the older ones of Chen and Lin (1989) and Martin *et al* (1988). We first note that the present results are in good agreement with the newer ones of Macias *et al* (1989) and Bachau *et al* (1989). The early larger discrepancy between Chen and Lin (1989) and Martin *et al* (1988) is partly due to the lack of convergence in the results of Martin *et al* (1988). Comparing the difference between the present results and the early ones by us shows that the use of two-electron basis functions constructed from eigenstates of the one-electron model Hamiltonian only has an effect for lower- Z ions such as C^{2+} . For the higher Z ions our previous results remain essentially unchanged.

References

- Bachau H, Galan P, Martin F, Riera A and Yáñez M 1989 *At. Data Nucl. Data Tables* submitted
Bachau H, Galan P, Martin F, Riera A and Yáñez M 1990 *J. Phys. B: At. Mol. Opt. Phys.* **23** L83
Chen Z and Lin C D 1989 *J. Phys. B: At. Mol. Opt. Phys.* **22** 2875
Macias A, Mó O, Riera A, Yáñez M, Bachau H, Galan P and Martin F 1989 *J. Physique Coll.* **C1** 99
Martin F, Mó O, Riera A and Yáñez M 1988 *Phys. Rev. A* **38** 1094