Electron capture and excitation in proton collisions with Li^+ and Sn

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The results of the research, conducted under the Research Contract No. 23088 within the IAEA CRP on « Atomic and Molecular Data for Vapour Shielding in Fusion Devices », are reported. The processes considered include :

$$H^+ + Li^+(1s^2\ ^1S) \rightarrow H(nl) + Li^{2+}(1s), \quad H^+ + Li^+(1s2s\ ^{1,3}S) \rightarrow H(nl) + Li^{2+}(1s),\ n\geq 2 \quad (1)$$

$$\rightarrow H^+ + L^+(1s,nl\ ^{1,3}L) \qquad \rightarrow H^+ + L^+(1snl\ ^{1,3}L),\ n\geq 2 \quad (2)$$

$$H^+ + Sn(\ldots 5s^2 5p^2\ ^{1,3}P) \rightarrow H(nl); \quad H^+ + Sn(\ldots 5s^2 5pnl\ ^{1,3}L),\ n\geq 5 \quad (3)$$

The computational method used to calculate the cross sections of reactions (1)-(3) was the two center atomic-orbital close-coupling (TC-AOCC) method with large expansion basis sets on each of the centers. The interaction of active electron with the ion cores of Li^+ and Sn was described by spin-dependent 0ne-electron model potentials that reproduce the energies of excited states with accuracy better than 2% in the case of Li^+ states and 7% in the case of Sn states. The coupled equations for the amplitudes of the states included in the AO expansions have been solved by using the straight-line trajectory approximation for the nuclear motion. The accuracy of this approximation in the case of ion-ion reactions (1) and (2) is justified only for energies above 2.5 keV/u.

In the case of reactions (1) and (2) nl-state-selective electron capture and excitation cross sections have been calculated for all states with $n \leq 4$. In the case of reactions (3) state-selective capture cross sections have been calculated for the states with $n \leq 5$, while excitation cross sections were calculated only for the transitions from 5p to 5d, 5f, 6s-6f, 7s and 7p. The oscillator strengths and radiative transition probabilities for these transitions on Sn have also been calculated.

The energy range of calculated cross sections for reactions (1), (2) is 2.5-800keV/u, while for the processes (3) it was 1-300keV/u.