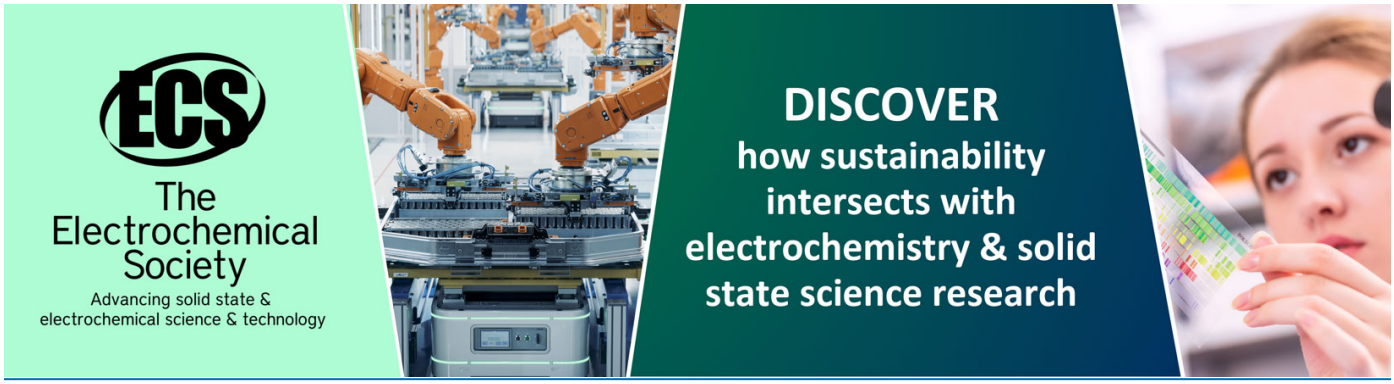
Low-energy electron scattering from methylene radicals: multichannel-coupling effects



Low-energy electron scattering from methylene radicals: multichannel-coupling effects

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Synopsis We reported elastic and excitation cross sections for electron collisions with methylene radical using R-matrix method for electron energies ranging from 0.01 to 15 eV in close-coupling (CC) approximation . We discuss the multi-channel-coupling effects on the calculated cross sections and resonances, and how the number of excited states included in the target state impacts the convergence of the elastic and the $X^3B_1 \rightarrow 1^1A_1$ and $X^3B_1 \rightarrow 1^1B_1$ excitation cross sections, especially at higher impact energy. Finally, we estimate the accuracy of the $1^1A_1$and 1^1B_1 excitation cross sections.

At low energies only the elastic channel is electronically open. With increasing the impact energy, other electronic states can be excited giving rise to the important questions: (1) how many of these states must be included in a calculation in order to predict an accurate cross section? (2) how do these multichannel effects affect the elastic cross sections and excitation cross sections? and (3) how sophisticated must the electronic states description be in order to accurately calculate the cross sections? For the purpose, we performed five different calculations within 1-state, 3-state, 15-state, 20-state, and 24-state close-coupling (CC) approximations for electron collision with methylene radical using R-matrix method [1].

Table 1. Parameters of identified e-CH_2 resonances in 24-state CC model. (in eV)

State	Type	Position	Parent state
$^2B_1$	shape	0.05	X^3B_1
$^2A_1$	shape	0.64	X^3B_1
$^2B_2$	Feshbach	7.35	1^3A_2
$^2A_1$	Feshbach	7.48	1^3A_1
$^2B_1$	Feshbach	8.63	2^3B_1

We compare elastic (integrated and differential), momentum-transfer, and excitation cross sections for e-CH_2 collision in five different CC models [2]. The results indicated that multichannel coupling has a substantial effect on the elastic and excitation cross sections and more target states are needed to include in the CC calculations in order to obtain the convergent cross section. This effect becomes even more important at higher impact energy. The obtained resonance parameters in 24-state CC model are listed in Table 1 along with the tentative assignments.

There are threshold energy differences of 0.77 eV for 1^1A_1 excited state and 0.31 eV for 1^1B_1 excited state between our calculations and experiment values from Ref. [3]. We estimate that these energy differences may introduce a 17% uncertainty in the $X^3B_1 \rightarrow 1^1A_1$ (see Fig. 1) and a 13% uncertainty for the $X^3B_1 \rightarrow 1^1B_1$ excitation cross section.

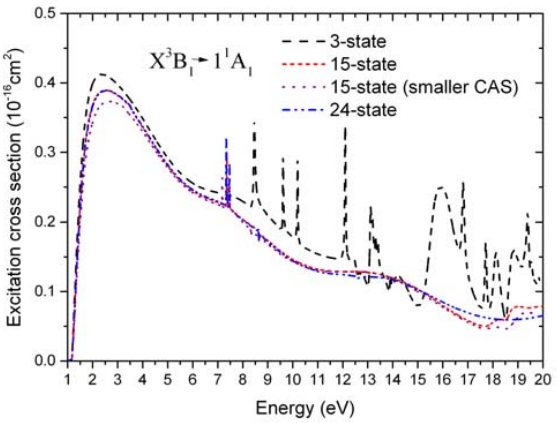

Figure 1. Excitation cross sections in 3-state, 15-state, 15-state (with a smaller CAS), 20-state, and 24-state CC models. The 15-state excitation threshold has been shifted lower by 0.28 eV.

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References

[1] Tennyson J 2010 *Phys. Rep.* **491** 29
[2] Wang K *et al* 2018 *Phys. Rev. A* **97** 012703
[3] Jensen P *et al* 1988 *J. Chem. Phys.* **89** 1327

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