CROSSECTION FOR CREATION OF H_2^- IONS IN TWO-BODY COLLISIONS

I.A.Pshenichnyuk, M.Čížek, J.Horáček

Institute of Theoretical Physics, Charles University, Prague, Czech Republic

Abstract

At present time, the fact of existence of the long-lived H_2^- ions is experimentally proved (see for ex. [3]). In spite of the fact that there are some discrepancies between the theory and the experiment [2], nonlocal resonant model (NRM) calculations, based fully on *ab initio* data successfully explain stability of such ions by their rotation with large angular momentum (J ~ 25). NRM calculations are used here to obtain the cross sections of creation of such ions in H_2+e^- and $H+H^-$ collisions. The object of present study could be formulated as follows:

To obtain the cross sections for creation of hydrogen long-lived negative ions H_2^- in H_2+e^- and $H+H^-$ collisions using NRM calculations of the cross sections for the $H_2^v+e^- \to H_2^{v'}+e^-$ and $H_2^v+e^- \to H^-+H$ processes.

$$\left[\begin{array}{l} H_2^v+e^- \to H_2^{v'}+e^- \\ H_2^v+e^- \to H^-+H \end{array}\right. \longrightarrow \left[\begin{array}{l} H_2^v+e^- \to H_2^- \\ H^-+H \to H_2^- \end{array}\right.$$

The formation of the intermediate metastable state H_2^- shows itself as narrow (~ 10^{-5} – 10^{-8} eV) peak in the cross sections for the elastic scattering, vibrational excitation and dissociative attachment. The behavior of the cross section curves close to the resonance could be described with multi-channel Fano formula (see further). This formula reduces description of a resonance to few parameters with defined physical meaning. When these parameters are determined by fitting the background term could be removed to obtain a cross section for H_2^- creation process. It also gives data about resonance lifetime (through the width Γ). The plan for the analysis of the cross sections close to the resonance will be following:

- to find resonance peak at the scattering cross section (it should present in all opened channels)
- to fit available resonance with Fano formula and determine its lifetime and amplitude
- to use properties of S-matrix to obtain data about all other possible scattering channels (for example we haven't got data about associative detachment channel)
- to extract the background and the sum through output channels to obtain the desired anion-creation cross sections

This procedure is performed for 6 resonances (J=25, 26 and 27) with the largest lifetimes (best objects for observation).

Multichannel Fano formula

Multichanel scattering matrix S(E) close to the simple pole $E=E_R-i\Gamma/2$ (which corresponds to the resonance in complex plane) could be presented as (see [4])

$$\hat{S}=\hat{B}-\frac{i\hat{C}}{E-E_R+i\Gamma/2}.$$

Matrix B here represent background (second term goes to zero while E goes to infinity), and C is a substitution matrix. Multichannel scattering amplitude is connected with S-matrix through (the thirst index denotes input channel, the second - output)

$$f_{\alpha'\alpha}=\frac{s_{\alpha'\alpha}-\delta_{\alpha'\alpha}}{2i\sqrt{p_{\alpha'}p_\alpha}},$$

where we use channel impulse concept $p_\alpha=\sqrt{2m_\alpha(E-W_\alpha)}$, E – full energy and W_α - threshold energy of the channel α. Using new notation $d_{\alpha'\alpha}=i(b_{\alpha'\alpha}-\delta_{\alpha'\alpha})$ it can be rewritten in the following form

$$f_{\alpha'\alpha}=-\frac{1}{2i\sqrt{p_{\alpha'}p_\alpha}}\left(d_{\alpha'\alpha}+\frac{c_{\alpha'\alpha}}{E-E_R+i\Gamma/2}\right).$$

This quantity is related to the scattering cross section through the well known formula from scattering theory (it is integrated through angular variables)

$$\sigma_{\alpha'\alpha}=4\pi\frac{p_{\alpha'}}{p_\alpha}\left|f_{\alpha'\alpha}\right|^2.$$

We also assume, that the matrix D could, in general, be imaginary $d_{\alpha'\alpha}=d^R_{\alpha'\alpha}+id^I_{\alpha'\alpha}$, while matrix C is supposed to be real in this work. The resulting formula reads

$$\sigma_{\alpha'\alpha}=\frac{\pi}{2m_\alpha E}\cdot\left(\left(d^R_{\alpha'\alpha}\right)^2+\left(d^I_{\alpha'\alpha}\right)^2+\frac{\left(c^R_{\alpha'\alpha}\right)^2+2(E-E_R)(d^R_{\alpha'\alpha}c^R_{\alpha'\alpha})-\Gamma(d^I_{\alpha'\alpha}c^R_{\alpha'\alpha})}{(E-E_R)^2+\Gamma^2/4}\right),$$

where m_α is a reduced mass in the initial channel.

Substitution matrix C is unitary and supposed to be non degenerate, i.e. it's rang is equal to 1. Together with time-inverse symmetry it leads to some important properties (see ref. [4]):

$$c_{\alpha'\alpha}=\gamma_{\alpha'}\gamma_\alpha$$
$$\sum_\alpha\left|\gamma_\alpha\right|^2=\Gamma.$$

The first one is called substitution factorization. $\Gamma_\alpha=\left|\gamma_\alpha\right|^2$ is called partial gamma of resonance for channel α. Some valuable for further conclusions could be summarized:

- Fano formula predicts for each resonance that it will appear in all opened scattering channels
- All this resonances will have the same width, but different amplitudes and Fano-shapes
- S-matrix and its substitutions matrix are symmetrical

References

[1]. M. Čížek, J. Horáček and W. Domcke, Phys. Rev. A **75**, 012507 (2007).
[2]. O. Heber, R. Golser, H. Gnaser, D. Berkovits, Y. Toker, M. Eritt, M.L. Rappaport, and D. Zajfman, Phys. Rev. A **73**, 060501 (2006).
[3]. R. Golser, H. Gnaser, W. Kutschera, A. Priller, P. Steier, A. Wallner, M. Čížek, J. Horáček, and W. Domcke, Phys. Rev. Lett. **94**, 223003 (2005).
[4]. J.R. Taylor. Scattering Theory: the Quantum Theory of Nonrelativistic Collisions. 1975

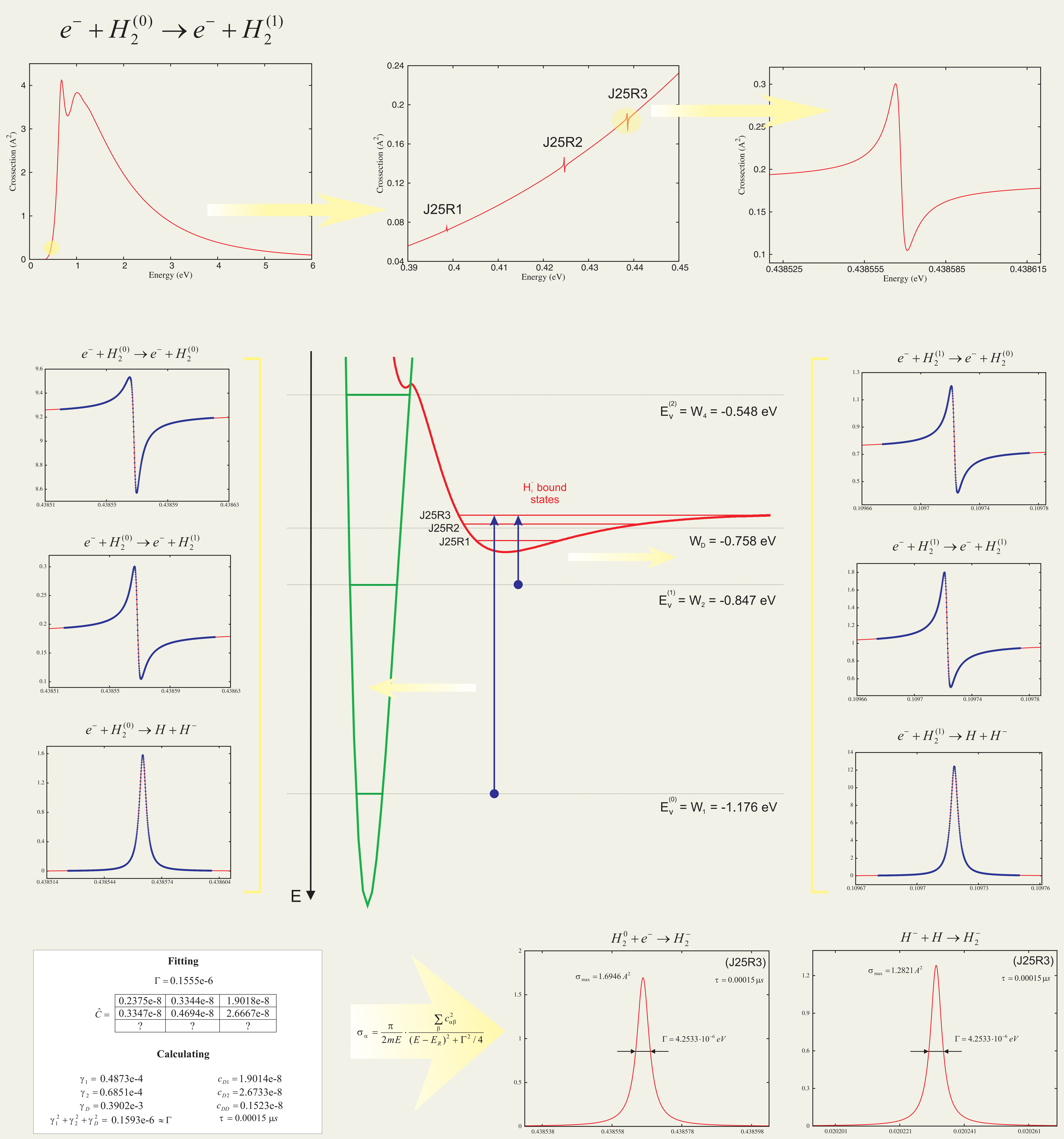
Acknowledgement

We would like to acknowledge Daniel Wolf Savin for continuously encouradgeing us to do this calculation.

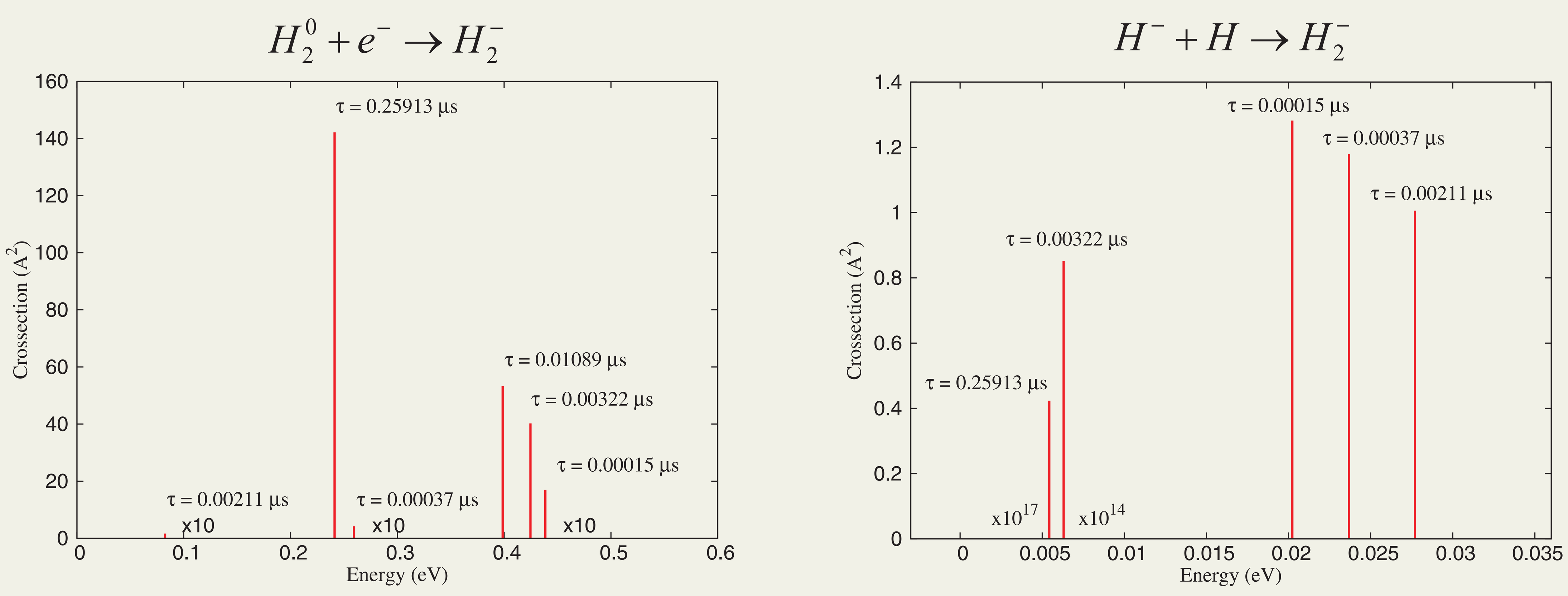
This work is supported by the Charles University Grant Agency under contract 2431/2007 and by Czech grant agency through GACR 116-13/201459

How is it works ? For one of J=25 resonances

$$e^-+H_2^{(0)}\to e^-+H_2^{(1)}$$



Results



	E_R^1, eV	$\sum c_{1i}^2$	E_R^D, eV	$\sum c_{Di}^2$	Γ, eV	lifetime, μs	γ_1^2, a.u.	γ_2^2, a.u.	γ_D^2, a.u.	$\sum\gamma_i^2$, a.u.	Γ, a.u.
J26R1	0.2412429698	0.3531e-16	0.0054318396	0.4352e-34	2.5435e-9	0.25913	0.7903e-10	-	0.9740e-28	0.7903e-10	0.9335e-10
J25R1	0.3986248137	0.1239e-13	-	-	6.0524e-8	0.01089	0.9622e-9	0.1250e-8	-	0.2230e-8	0.2221e-8
J25R2	0.4246432987	0.1143e-12	0.0063074168	0.6603e-27	2.0499e-7	0.00322	0.2725e-8	0.4809e-8	0.1550e-22	0.7533e-8	0.7523e-8
J27R1	0.0824920456	0.2122e-15	0.0277020456	0.7926e-12	0.3119e-6	0.00211	0.3168e-11	0.1183e-7	-	0.1185e-7	0.1145e-7
J26R2	0.2595030236	0.5670e-13	0.0236914072	0.2658e-10	1.8037e-6	0.00037	0.1462e-9	-	0.6849e-7	0.6861e-7	0.6620e-7
J25R3	0.4385668903	0.2140e-11	0.0202322882	0.1372e-9	4.2533e-6	0.00015	0.2375e-8	0.4694e-8	0.1523e-6	0.1593e-6	0.1561e-6

Conclusions

- we analysed the shapes of peaks in cross sections for vibrational excitation and dissociative attachment to rotationally excited molecules,
- in particular we found partial decay widths for the metastable H_2^- states to H+H$^-$ and various H_2^v+e$^-$ channels,
- and we determined the cross sections for the creation of the ions in both H+H$^-$ and H_2^v+e$^-$ collisions,
- since the parameters for different processes are not independent, the analysis can also serve as the cross check among calculations of cross sections for various processes.