Short-term scientific mission Scientific report

COST Action Number: CM0601

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Host's Name and Institution: Jiri Horacek, Institute of Theoretical Physics, Charles

University

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From 01/12/2008 to 20/12/2008 I have visited group of Prof. Jiri Horacek at Charles University, Prague. I have worked on the modification of the nonlocal resonance model for HCI-electron collisions. New unpublished ab-initio electron scattering calculations of eigenphase sums by Winstead and McKoy were used for construction of the model. Additionally, a different parametrization was used in the current model when compared with the older one (commonly designated as the DMHC model).

The results of the new model agree with the experimental data much better than the results of the DMHC model. Table 1 shows comparison of the integrated dissociative electron attachment (DEA) cross sections with the experimental data from Fribourg.

Additionally, the new model agrees better with the DEA temperature dependence experimental data, as can be seen from figure 1, and gives good description of the structures in the vibrational excitation spectra.

Common publication of the results obtained during the STSM is anticipated.

	New model	DMHC model	Exp.
$\sigma(\mathrm{HCl})~(\mathrm{\mathring{A}^2eV})$	6.14×10^{-2}	14.90×10^{-2}	6.85×10^{-2}
$\sigma(\mathrm{DCl})~(\mathrm{\mathring{A}^2eV})$	0.28×10^{-2}	1.25×10^{-2}	0.45×10^{-2}

Table 1 Integrated DEA cross sections for HCl and DCl

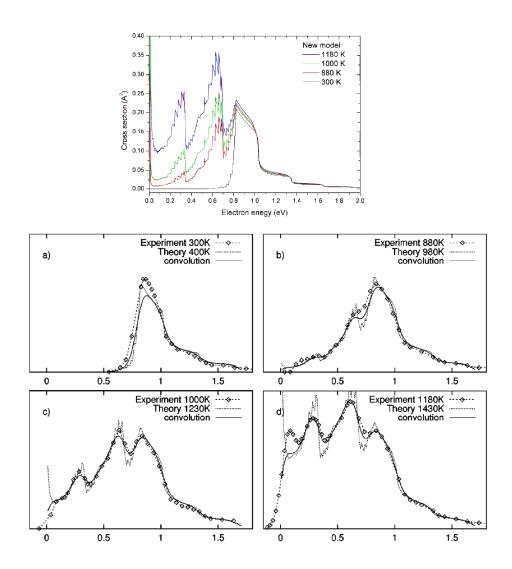


Figure 1 Temperature dependence of the DEA cross section for HCl. Top: New model, Bottom four: DMHC model and experimental data