

IAEA  
ITAMP  
July 7-9 2014  
Cambridge

Joint Workshop with IAEA on  
Uncertainty Assessment for  
Atomic and Molecular Data



1

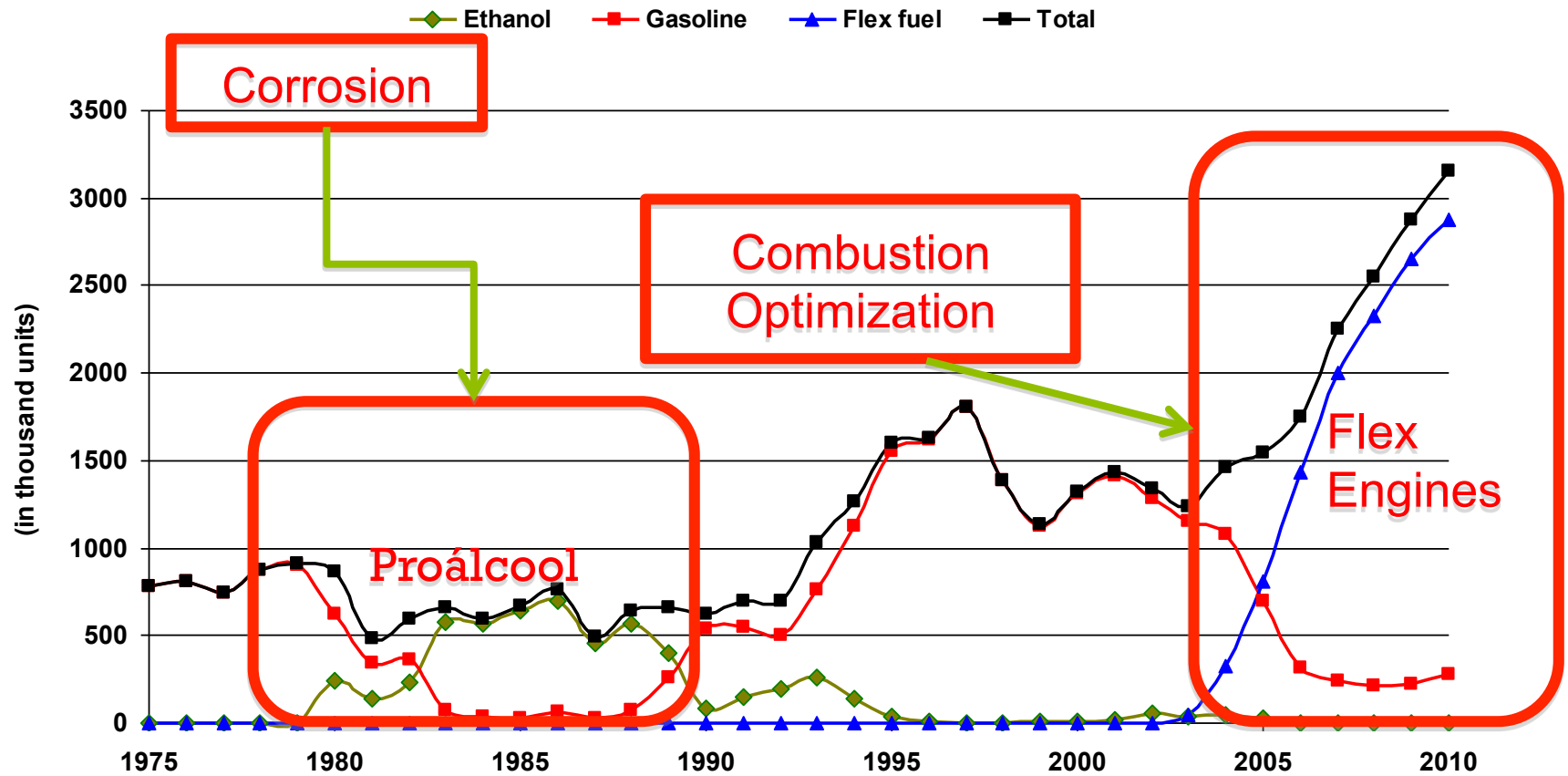
MAPLima

# Low energy electron scattering data for chemical plasma treatment of biomass

by

**Marco A. P. Lima**  
**Unicamp**

# Motivation I: large scale use of ethanol in engines



**Brazilian Sales of light fleet Vehicles (1975-2010)**

# Ethanol as Fuel: Plasma Ignition for Vehicle Engines

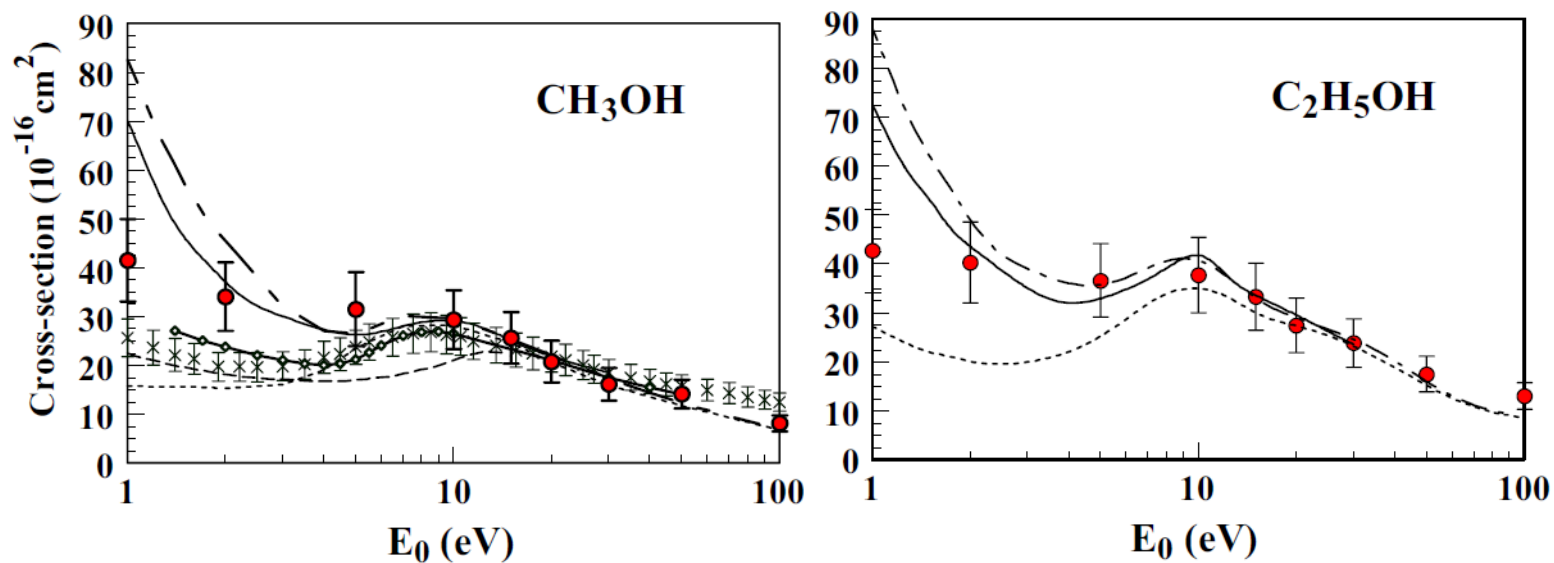


## Theoretical support for an application project working on:

- Investigation of processes occurring during the ignition of plasma and its consequences in post-discharge for an internal combustion engine;
- The proper parameters to be applied in cars that operate on "poor mixtures" reducing pollutants released into the atmosphere, especially considering the spark plug discharge.

# Low-energy electron scattering from methanol and ethanol

PHYSICAL REVIEW A 77, 042705 (2008)

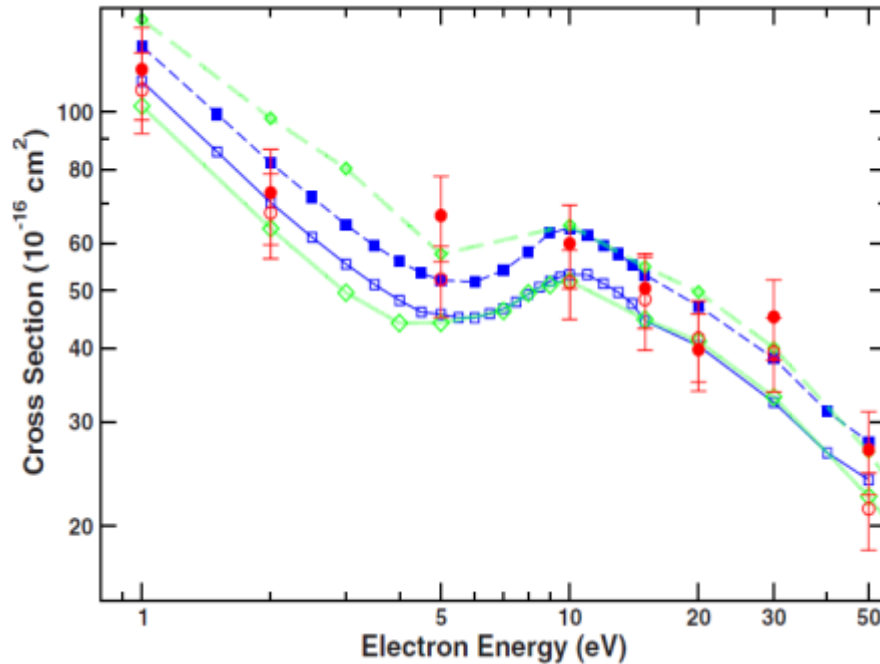


Integral elastic scattering cross sections for  $\text{CH}_3\text{OH}$ . Legend: ●: present experiment; —: SMCPP SEP; —: SMC SEP; ---- (short dashes): SMC SE which is similar to SMCPP SE; ---- (long dashes): *R*-matrix ICSs of Bouchiha *et al.* (without Born correction) [10]. × Total cross section measurements of Szymtkowski and Krzysztofowicz [24] and —◆— of Schmieder [22]. - - - - (shortdashes) are from the SMCPP SE which is similar to SMC SE.

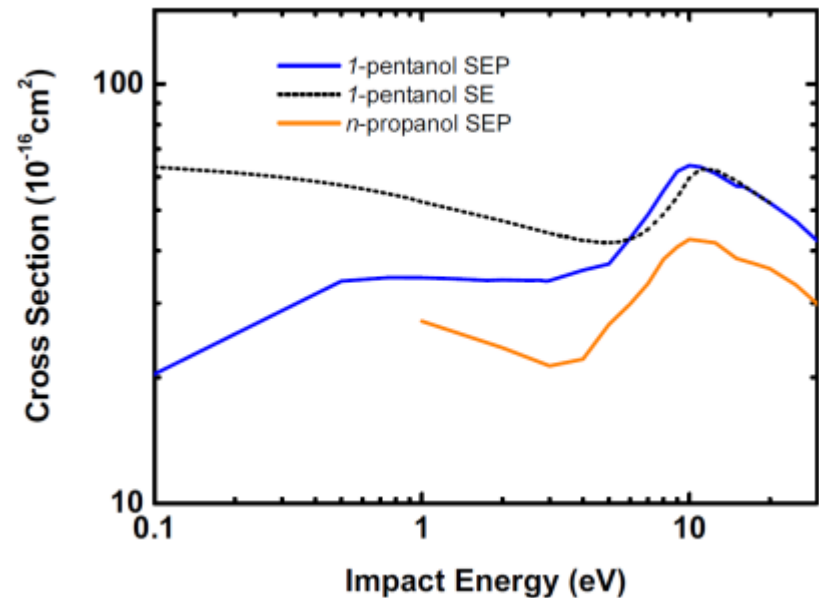
**NSF/CNPq project (experiments from Morty Khakoo's group)**

## Elastic scattering of slow electrons by *n*-propanol and *n*-butanol

PHYSICAL REVIEW A 78, 062714 (2008)



Electron scattering of slow electrons by *l*-pentanol (a drop in fuel)



Integral elastic cross sections for electron collisions with *n*-propanol and *n*-butanol. Red circles are experimental values, thin blue lines with squares results from all-electron calculations, and thick green lines with diamonds results from pseudopotential calculations. Open symbols and solid lines are propanol data; solid symbols and dashed lines are butanol data.

**NSF/CNPq project (experiments from Morty Khakoo's group)**

## Motivation II: large scale production of ethanol



**A sugarcane industry of Sugar/Ethanol/Bioelectricity**

## Motivation II: large scale production of ethanol



**Biomass: a source of energy and carbon**

## Motivation II: large scale production of ethanol



**Biomass: a source of energy and carbon**



## Motivation II: large scale production of ethanol



**First generation ethanol: crushing the cane for the juice**

## Motivation II: large scale production of ethanol



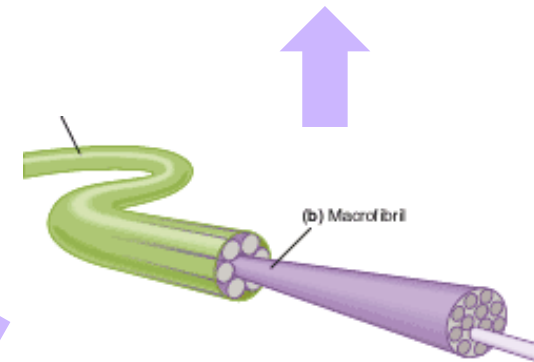
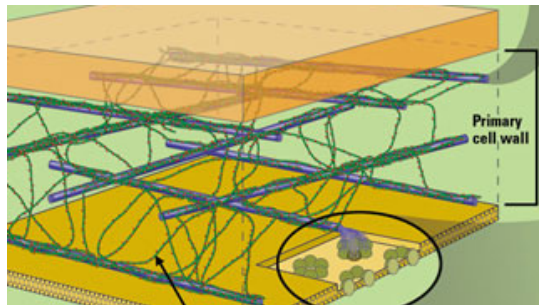
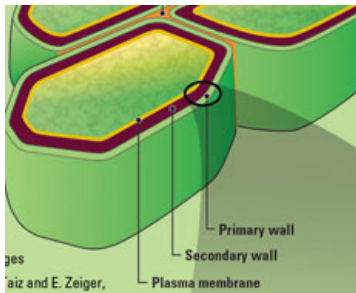
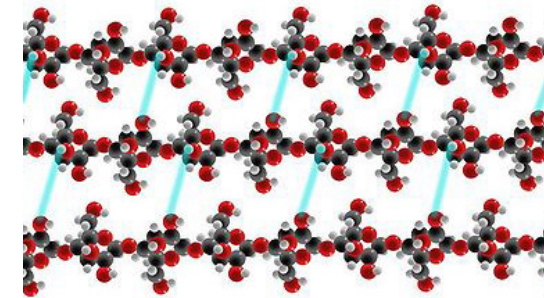
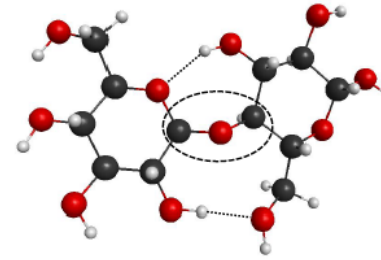
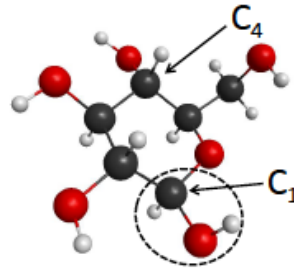
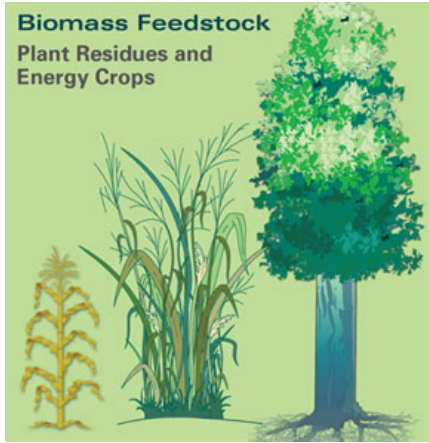
**Bagasse piles  
at the mill.**

**2nd generation  
ethanol?  
Other high value  
bioproducts?**

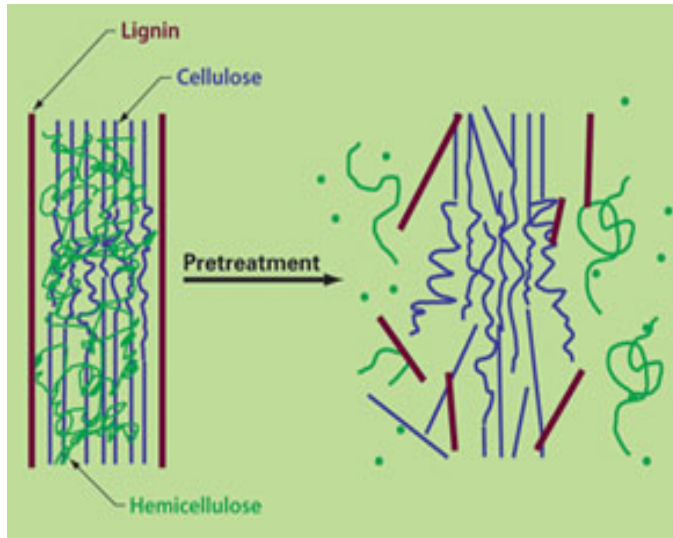


**Biomass: a source of energy and carbon**

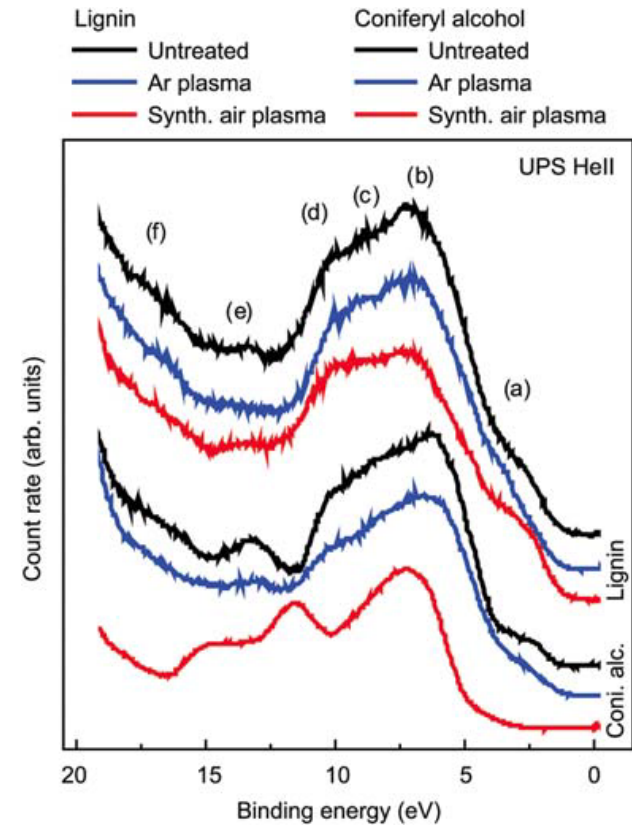
# Biomass is Made Up with Fermentable Sugars



# Lignocellulose is Resistant to Hydrolysis



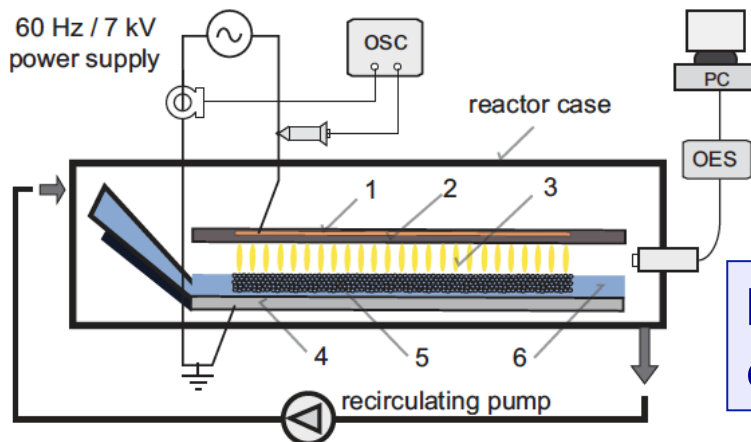
**Pretreatment: bio- and physical-chemical processes to expose the cellulose fibers**



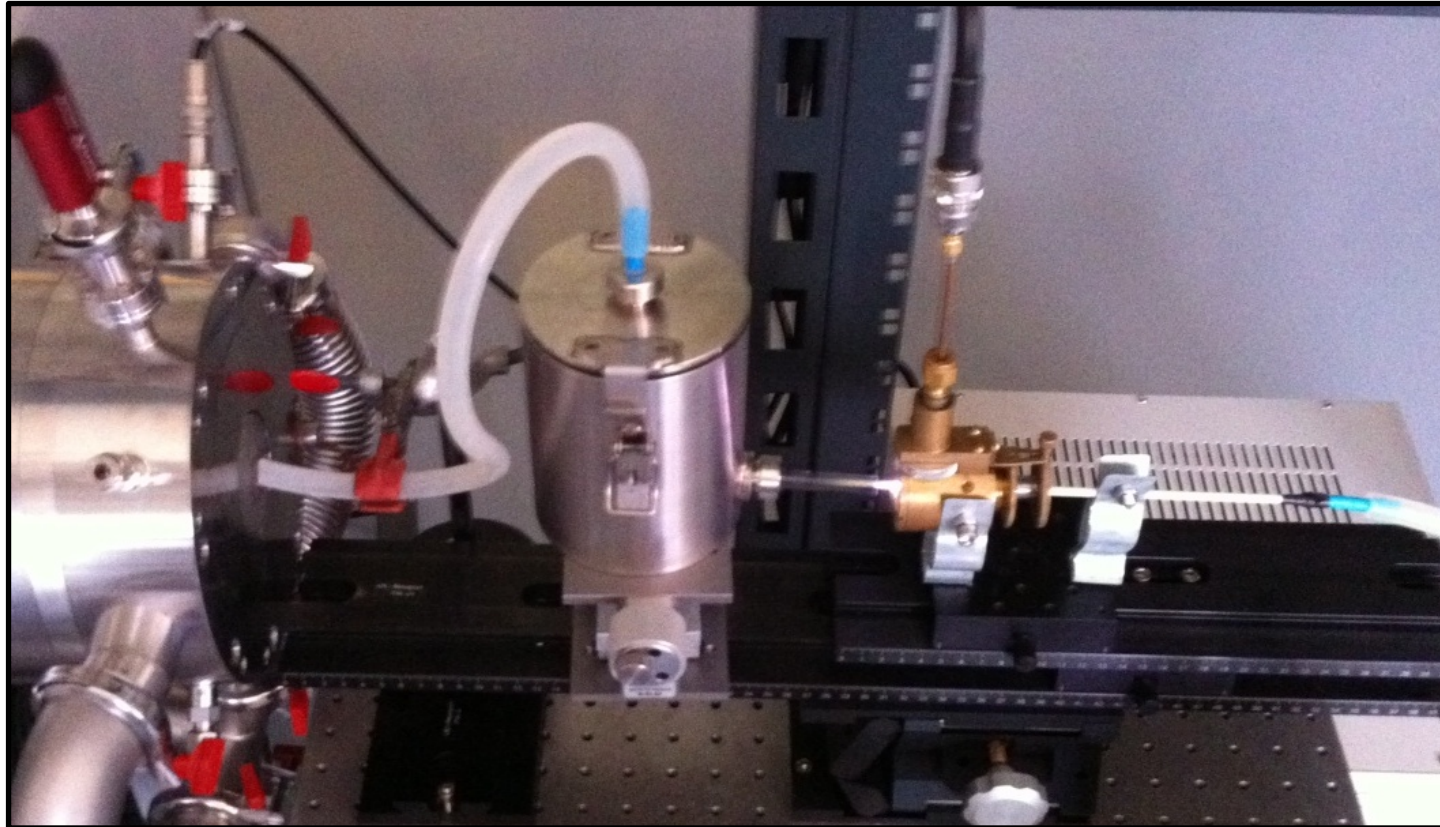
Lothar Klarhöfer<sup>1</sup>, Wolfgang Viöl<sup>2,3,\*</sup> and Wolfgang Maus-Friedrichs<sup>1</sup>

Holzforschung, Vol. 64, pp. 331–336, 2010

**Dielectric Barrier Discharge (DBD):**  
electron flux on substrate  $\sim 10^8 \text{ cm}^{-2} \text{ s}^{-1}$



# Sugarcane Bagasse Plasma Pretreatment



## Treatment conditions

- ~ 25 g of dry sugarcane bagasse (50% moisture) – milled at 500 $\mu$ m
- Gas flow Mixture: 95% Ar (1.9 SLM) and 5% O<sub>2</sub> (0.1 SML)
- $\Delta t_{\text{treatment}} = 3\text{h}$

# Biomass Chemical Analysis

Lignin concentration (%) of raw bagasse and samples related to plasma torch treatment and washing procedure by water and NaOH 1% solution at room temperature.

Samples	Soluble Lignin (%)	Insoluble Lignin (%)	Total of Lignin remaining (%)
raw bagasse	1.58 ± 0.01	20.3 ± 0.1	21.9 ± 0.1
Washed by H <sub>2</sub> O	2.4 ± 0.9	21.4 ± 0.9	23.8 ± 0.9
Washed by NaOH 1%	<b>1.3 ± 0.9</b>	<b>12.6 ± 0.9</b>	<b>13.9 ± 0.9</b>

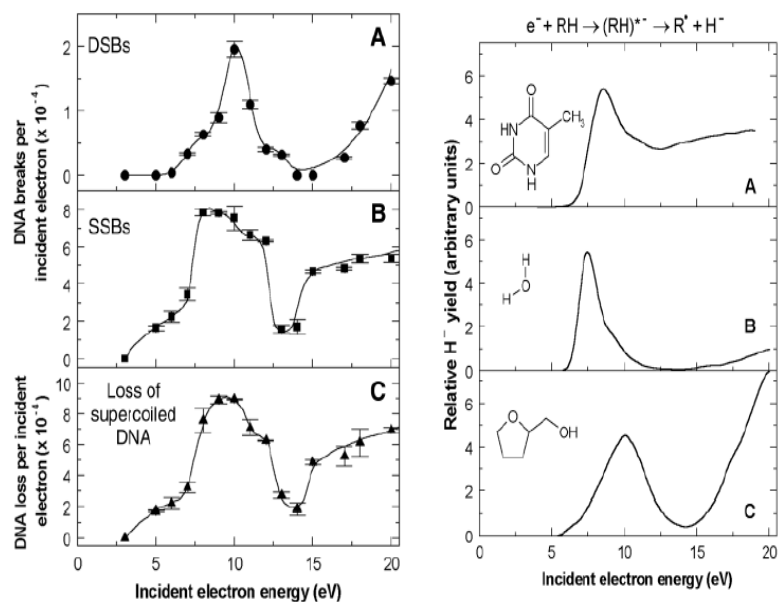
**About 40% of original lignin was removed!!!**

Jayr Amorim, Carlos Oliveira, Jorge A. Souza-Correa, Marco A. Ridenti  
Plasma Process. Polym. 2013, DOI: 10.1002/ppap.201200158

# Electron-Induced Damage to Biomolecules

## Resonant Formation of DNA Strand Breaks by Low-Energy (3 to 20 eV) Electrons

Badia Boudaïffa, Pierre Cloutier, Darel Hunting,  
Michael A. Huels,\* Léon Sanche



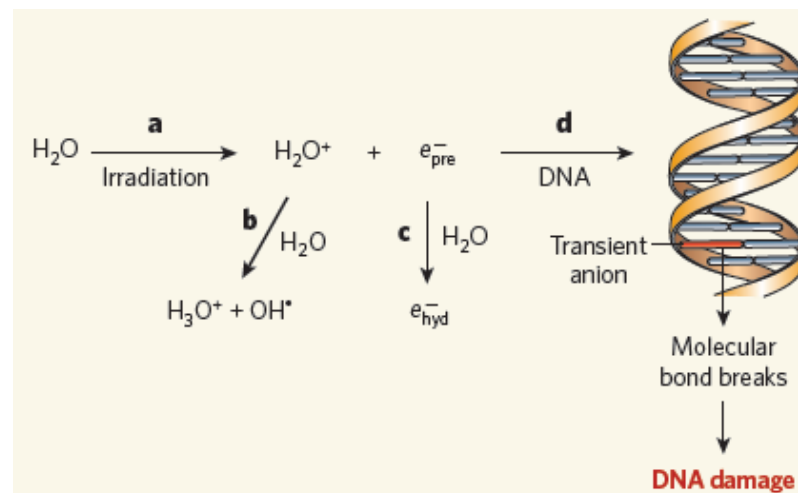
Science, **287** 1658 (2000)

### BIOLOGICAL CHEMISTRY

## Beyond radical thinking

Léon Sanche

Radiation-induced DNA damage has been attributed to hydroxyl radicals, which form when water absorbs high-energy photons or charged particles. But another product of water's radiolysis might be the real culprit.

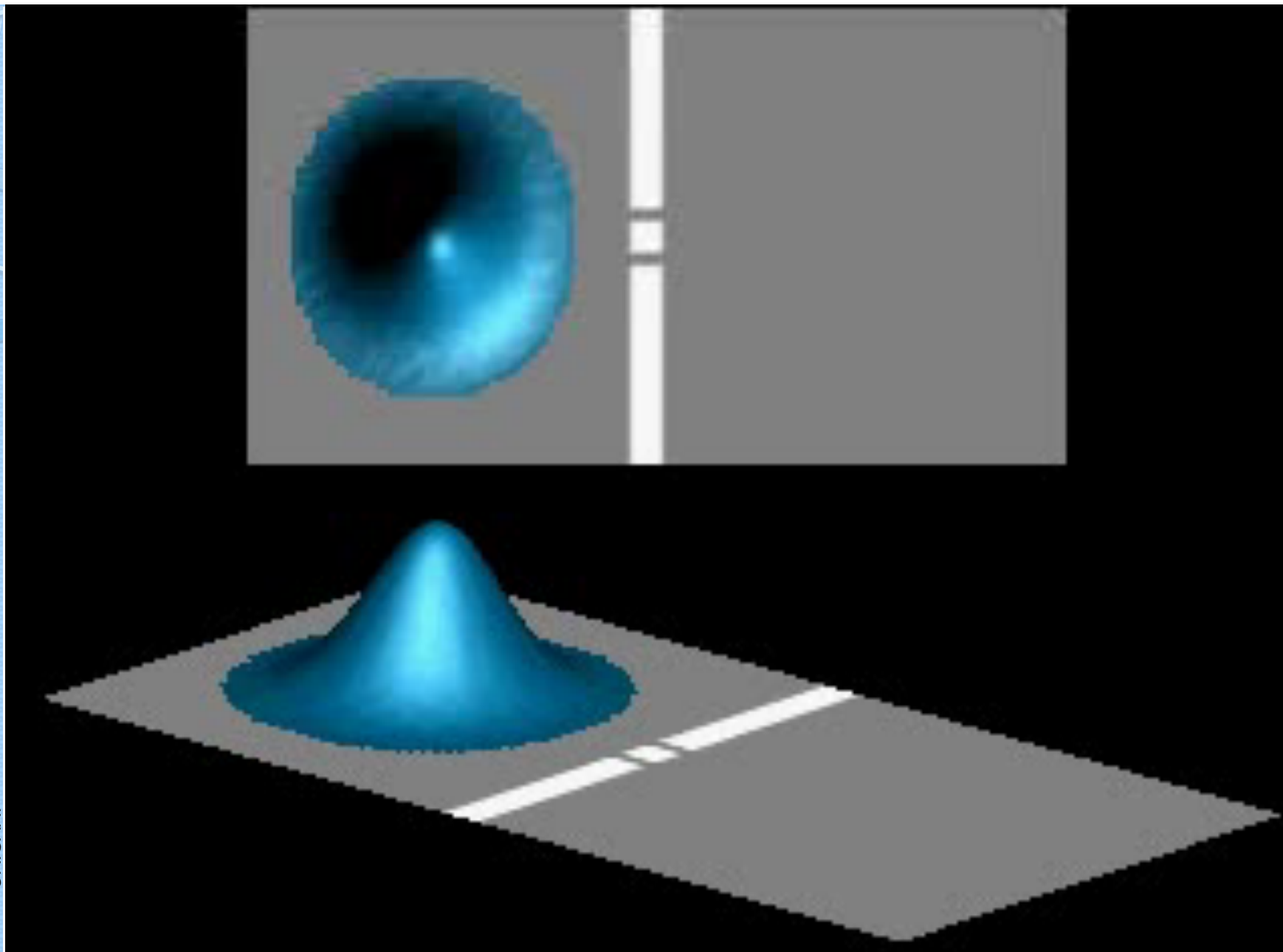


Sanche, Nature **461**, 358 (2009)

J|A|C|S  
COMMUNICATIONS

Chun-Rong Wang, Jenny Nguyen, and Qing-Bin Lu\*

J. AM. CHEM. SOC. 2009, **131**, 11320–11322



## Two slits interference

To see this animations, visit: <http://www.embd.be/quantummechanics/>



## Scattering theory

### Schrödinger equation

$$H\Psi_{\vec{k}_m}^{(\pm)}(\vec{r}_1, \dots, \vec{r}_{N+1}) = E\Psi_{\vec{k}_m}^{(\pm)}(\vec{r}_1, \dots, \vec{r}_{N+1})$$

### Asymptotic condition

$$\Psi_{\vec{k}_i}^{(\pm)}(\vec{r}_1, \dots, \vec{r}_{N+1}) \xrightarrow{r_{N+1} \rightarrow \infty} S_{\vec{k}_i} + \sum_f^{\text{open}} f_{i \rightarrow f}^B(\vec{k}_i, \vec{k}_f) \Phi_f \frac{e^{\pm i k_f r_{N+1}}}{r_{N+1}}$$

$$S_{\vec{k}_i} = \Phi_i e^{i \vec{k}_i \cdot \vec{r}_{N+1}}$$

### Differential cross section

$$\frac{d\sigma}{d\Omega}{}^{i \rightarrow f}(\vec{k}_i, \vec{k}_f) = \frac{k_f}{k_i} \left| f_{i \rightarrow f}^L(\vec{k}_i, \vec{k}_f) \right|^2$$

## Scattering theory

### Schrödinger differential equation

$$H\Psi_{\vec{k}_m}^{(\pm)} = [H_N + T_{N+1} + V]\Psi_{\vec{k}_m}^{(\pm)} = E\Psi_{\vec{k}_m}^{(\pm)}$$

### Lippmann-Schwinger integral equation

$$\Psi_{\vec{k}_m}^{(\pm)} = S_{\vec{k}_m} + G_0^{(\pm)}V\Psi_{\vec{k}_m}^{(\pm)}$$

$$S_{\vec{k}_m} = \Phi_m e^{i\vec{k}_m \cdot \vec{r}_{N+1}}$$

### Free-particle Green's function (Source of uncertainty – controllable)

$$G_0^{(\pm)} = \frac{1}{E - T_{N+1} - H_N \pm i\epsilon} = \lim_{\epsilon \rightarrow 0} \mathcal{P} \int d^3k \frac{|\Phi_m \vec{k}\rangle \langle \vec{k} \Phi_m|}{\frac{k_m^2}{2} - \frac{k^2}{2} \pm i\epsilon}$$

## Schwinger Variational Principle

(L<sup>2</sup> expansion: source of uncertainty – controllable)

The Schwinger Variational method serves to get a scattering amplitude free of first order errors for a scattering process that respect the equations

$$A^{(\pm)}|\Psi_{\mathbf{k}}^{(\pm)}\rangle = V|S_{\mathbf{k}}\rangle \text{ and } \begin{cases} f_{\mathbf{k}_f, \mathbf{k}_i} = \langle S_{\mathbf{k}_f} | V | \Psi_{\mathbf{k}_i}^{(+)} \rangle \\ f_{\mathbf{k}_f, \mathbf{k}_i} = \langle \Psi_{\mathbf{k}_f}^{(-)} | V | S_{\mathbf{k}_i} \rangle \\ f_{\mathbf{k}_f, \mathbf{k}_i} = \langle \Psi_{\mathbf{k}_f}^{(-)} | A^{(+)} | \Psi_{\mathbf{k}_i}^{(+)} \rangle \end{cases} \quad \text{and } A^{(\pm)} = V - VG_0^{(\pm)}V$$

The bilinear form of the variational principle for the scattering amplitude is

$$[f_{\mathbf{k}_f, \mathbf{k}_i}] = \langle S_{\mathbf{k}_f} | V | \Psi_{\mathbf{k}_i}^{(+)} \rangle + \langle \Psi_{\mathbf{k}_f}^{(-)} | V | S_{\mathbf{k}_i} \rangle - \langle \Psi_{\mathbf{k}_f}^{(-)} | A^{(+)} | \Psi_{\mathbf{k}_i}^{(+)} \rangle \text{ where arbitrary and}$$

$$\text{independent variations with respect to } \begin{cases} \langle \delta \Psi_{\mathbf{k}_f}^{(-)} | (V | S_{\mathbf{k}_i} \rangle - A^{(+)} | \Psi_{\mathbf{k}_i}^{(+)} \rangle \rangle = 0 \\ (\langle S_{\mathbf{k}_f} | V - \langle \Psi_{\mathbf{k}_f}^{(-)} | A^{(+)} \rangle) | \delta \Psi_{\mathbf{k}_i}^{(+)} \rangle = 0 \end{cases}$$

$$\text{lead to } \begin{cases} V | S_{\mathbf{k}_i} \rangle - A^{(+)} | \Psi_{\mathbf{k}_i}^{(+)} \rangle = 0 \Rightarrow A^{(+)} | \Psi_{\mathbf{k}_i}^{(+)} \rangle = V | S_{\mathbf{k}_i} \rangle \\ \langle S_{\mathbf{k}_f} | V - \langle \Psi_{\mathbf{k}_f}^{(-)} | A^{(+)} = 0 \Rightarrow A^{(-)} | \Psi_{\mathbf{k}_f}^{(-)} \rangle = V | S_{\mathbf{k}_f} \rangle \text{ with } A^{(+)\dagger} = A^{(-)} \end{cases}$$


$A^{(\pm)}|\Psi_{\mathbf{k}}^{(\pm)}\rangle = V|S_{\mathbf{k}}\rangle$  must be equivalent to  $H|\Psi_{\mathbf{k}}^{(\pm)}\rangle = E|\Psi_{\mathbf{k}}^{(\pm)}\rangle$  with proper boundary conditions

## Schwinger Multichannel Method for electron scattering

In this formalism the operator  $A^{(+)}$  was redefined as:

$$A^{(+)} = \frac{1}{2}(PV + VP) - VG_P^{(+)}V + \frac{1}{N+1} \left[ \hat{H} - \frac{N+1}{2}(\hat{H}P + P\hat{H}) \right]$$

where  $P \equiv \sum_{\ell=1}^{\text{open}} |\Phi_\ell\rangle\langle\Phi_\ell|$  and  $\hat{H} = E - H$

 (Channel coupling: source of uncertainty – uncontrollable)

All electrons are identical. So, an expansion of the scattering wave function must be done in a basis  $\{\chi_\mu\}$  of anti-symmetric functions (Slater determinants):

$$|\Psi_{\vec{k}_m}^{(\pm)}\rangle = \sum_{\mu} a_{\mu}^{(\pm)}(\vec{k}_m) |\chi_{\mu}\rangle \quad \text{where} \quad \{|\chi_{\mu}\rangle\} = \{a_{N+1} |\Phi_i\rangle \otimes |\varphi_j\rangle\}$$

 (N+1 wave-function expansion: source of uncertainty – controllable)

The final form of the scattering amplitude is equal to the one of the Schwinger Variational principle

$$f_{\vec{k}_i, \vec{k}_f} = -\frac{1}{2\pi} \sum_{mn} \langle S_{\vec{k}_f} | V | \chi_m \rangle (d^{-1})_{mn} \langle \chi_n | V | S_{\vec{k}_i} \rangle$$

with  $d_{mn} = \langle \chi_m | A^{(+)} | \chi_n \rangle$  and  $S_{\vec{k}_i} \equiv \Phi_i(\vec{r}_1, \dots, \vec{r}_N) e^{i\vec{k}_i \cdot \vec{r}_{N+1}}$

## Coupling level

### ➔ Elastic scattering with and without polarization effects

- ➊ Open channel Projector has only one state

$$P = |\Phi_0\rangle\langle\Phi_0|$$

➔  $\Phi_0$  is molecular target ground state obtained in Hartree-Fock approximation

(Target description: source of uncertainty – program limitation)

- ➋ Configuration space is made of

(N+1 wave-function expansion: source of uncertainty – controllable)

$$|\chi_\mu\rangle = \begin{cases} a_{N+1} |\Phi_0\rangle \otimes |\varphi_i\rangle \\ a_{N+1} |\Phi_j\rangle \otimes |\varphi_k\rangle, j \geq 2 \end{cases}$$

➔ Doublet states made of products of target triplet and singlet states by  $\varphi_k$

➔  $\Phi_j, j \geq 2$  are virtual states obtained from single excitations of the molecular target

➔  $\varphi_i$  are one-particle wave functions (square integrable molecular orbitals) used in description of the continuum

## Coupling level

➔ Inelastic scattering with and without polarization

- 1 Open channel projector contains channels of our choice (truncation means approximation)

$$P = \sum_{\ell}^{\text{open}} |\Phi_{\ell}\rangle\langle\Phi_{\ell}| \quad \Rightarrow \quad |\Phi_{\ell}\rangle \text{ are molecular target states obtained with single configuration interaction}$$

- 2 Again the configuration space is made of

$$|\chi_{\mu}\rangle = \begin{cases} \mathbf{a}_{N+1} |\Phi_0\rangle \otimes |\varphi_i\rangle \\ \mathbf{a}_{N+1} |\Phi_j\rangle \otimes |\varphi_k\rangle, j \geq 2 \end{cases} \quad \Rightarrow \quad \text{Doublet states made of products of target triplet and singlet states by } \varphi_k$$

➔ Polarization effects are included with  $j$  greater than the number of open channels

## Electron scattering by large molecules



### Pseudopotential formalism

(source of uncertainty – optional for light molecules)

[D. R. Hamann, M. Schlüter and C. Chiang, Phys. Rev. Lett. **43**, 1494 (1979)]

- 1 The pseudo-state energy is equal to the real eigenvalue for a given configuration;
- 2 The pseudopotential is equal to the real potential beyond a certain core radius  $r_c$ , and it is soft at the origin;
- 3 The normalized pseudo wave function is equal to the real one beyond the core radius  $r_c$  and it is soft and without nodes
- 4 The integrals from 0 to  $r$  of the real and pseudo functions agree for  $r > r_c$  for each valence state:

$$-\frac{1}{2} \left[ (r\Psi)^2 \frac{d}{dE} \frac{d}{dr} \ln \Psi \right]_{r>r_c} = \int_0^{r>r_c} \Psi^2 r^2 dr$$



“Norm Conservation”

## Theoretical co-authors



Eliane M. de Oliveira (posdoc)  
Alexandra Natalense  
Marco A. P. Lima



Sergio d'A. Sanchez  
Márcio H. F. Bettega



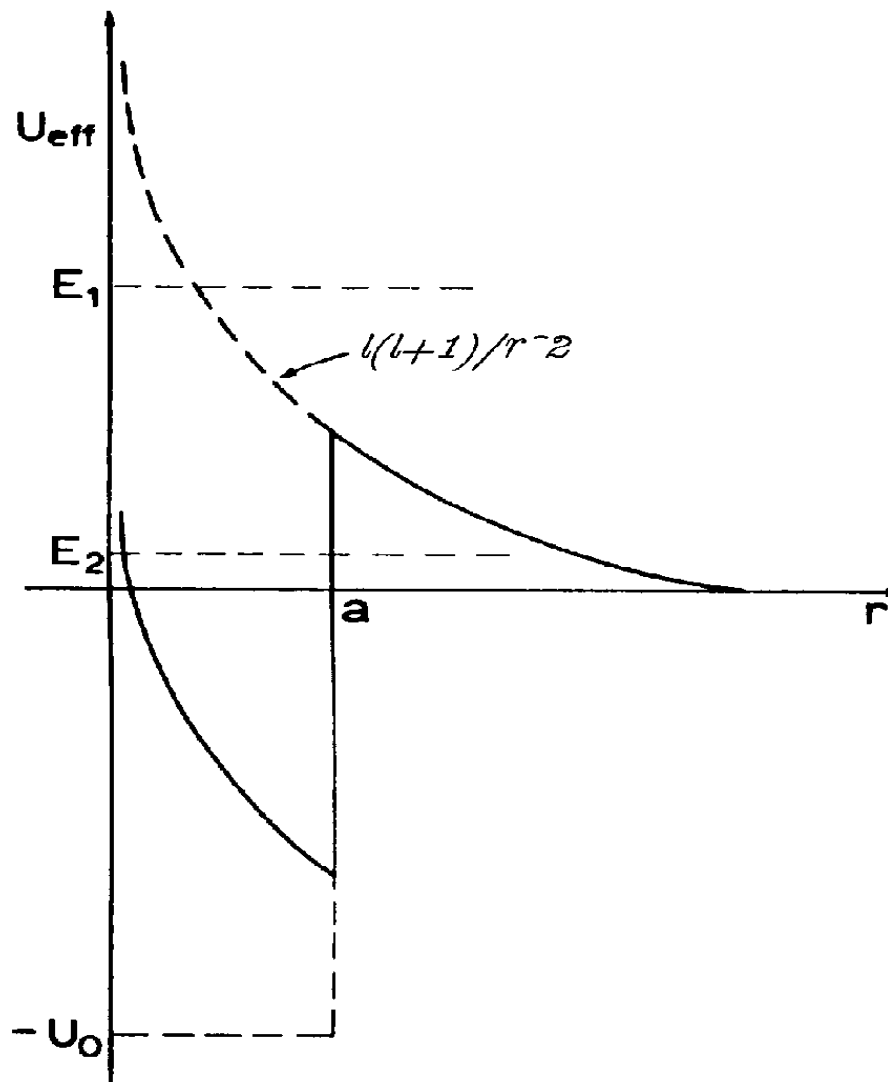
Romarly F. da Costa



Márcio T. do N. Varella (coordinator)

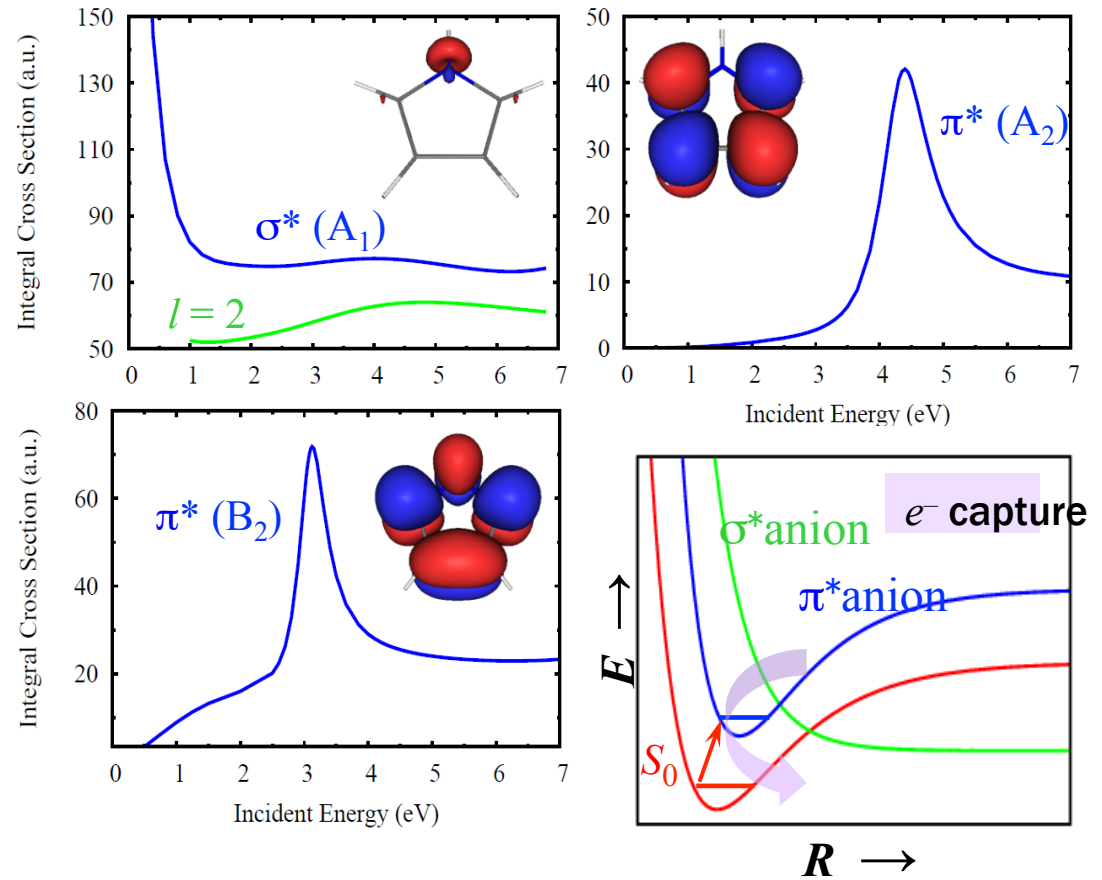
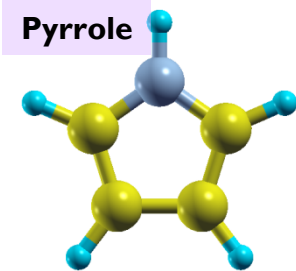


## Shape resonances are related to angular momentum traps



# Low energy elastic electron scattering from pyrrole

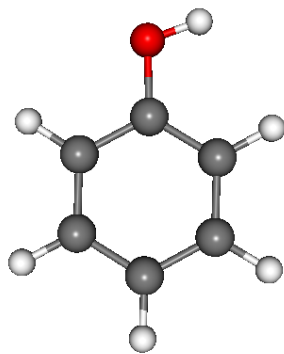
- There are  $\pi^*$  (ring) and  $\sigma^*$  (N-H) shape resonances in pyrrole. Nice prototype!



de Oliveira EM, Lima MAP, Bettega MHF, Sanchez SD, da Costa RF, and Varella MTD, J. Chem. Phys. **132**, 204301 (2010)

# Lignin Subunits

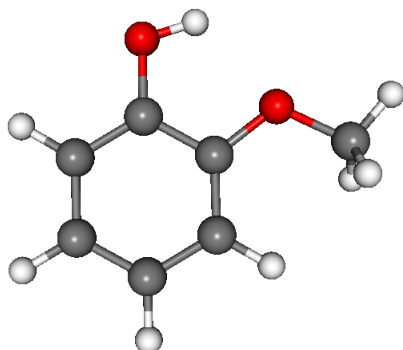
Phenol



MetOH



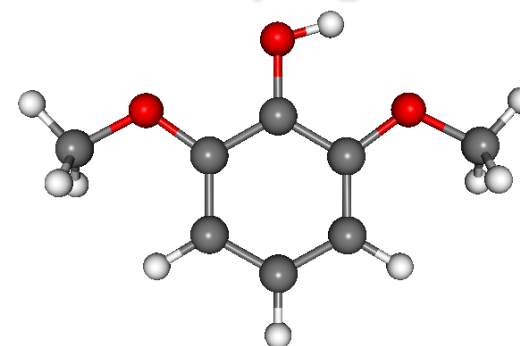
Guaiacol



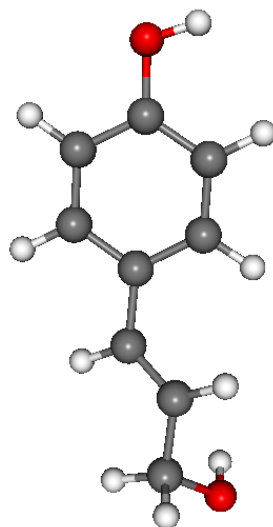
MetOH



Syringol



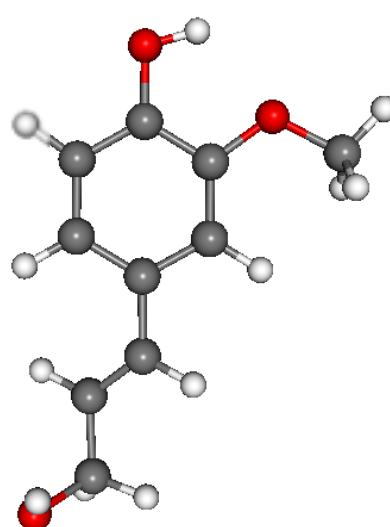
PropenylOH



**p-coumaryl alcohol**



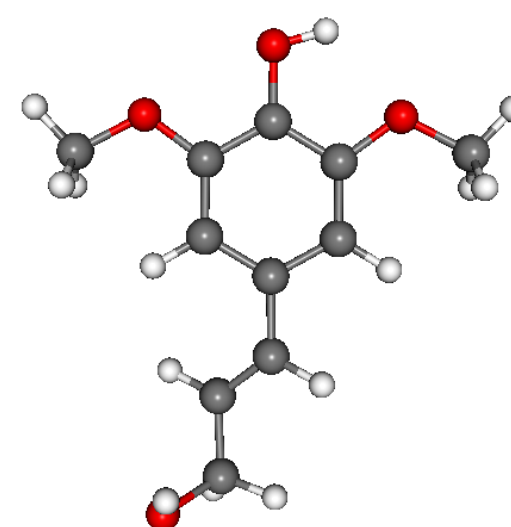
PropenylOH



**coniferyl alcohol**



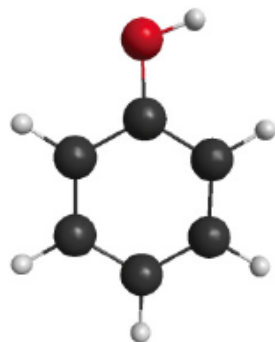
PropenylOH



**sinapyl alcohol**

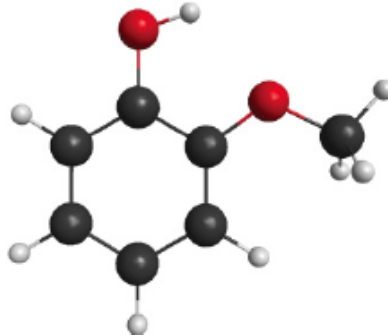
# Shape resonance spectra of lignin subunits

PHYSICAL REVIEW A 86, 020701(R) (2012)



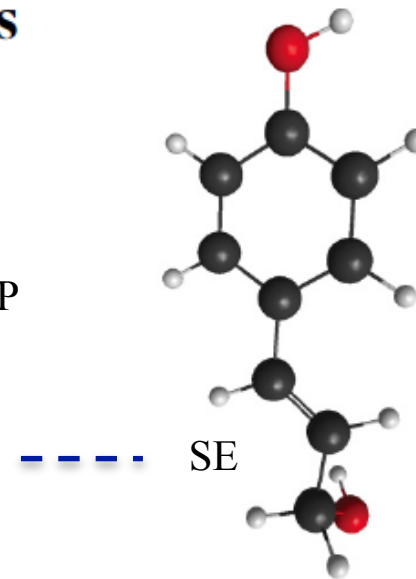
phenol

— SEP  
- - - SE



guaiacol

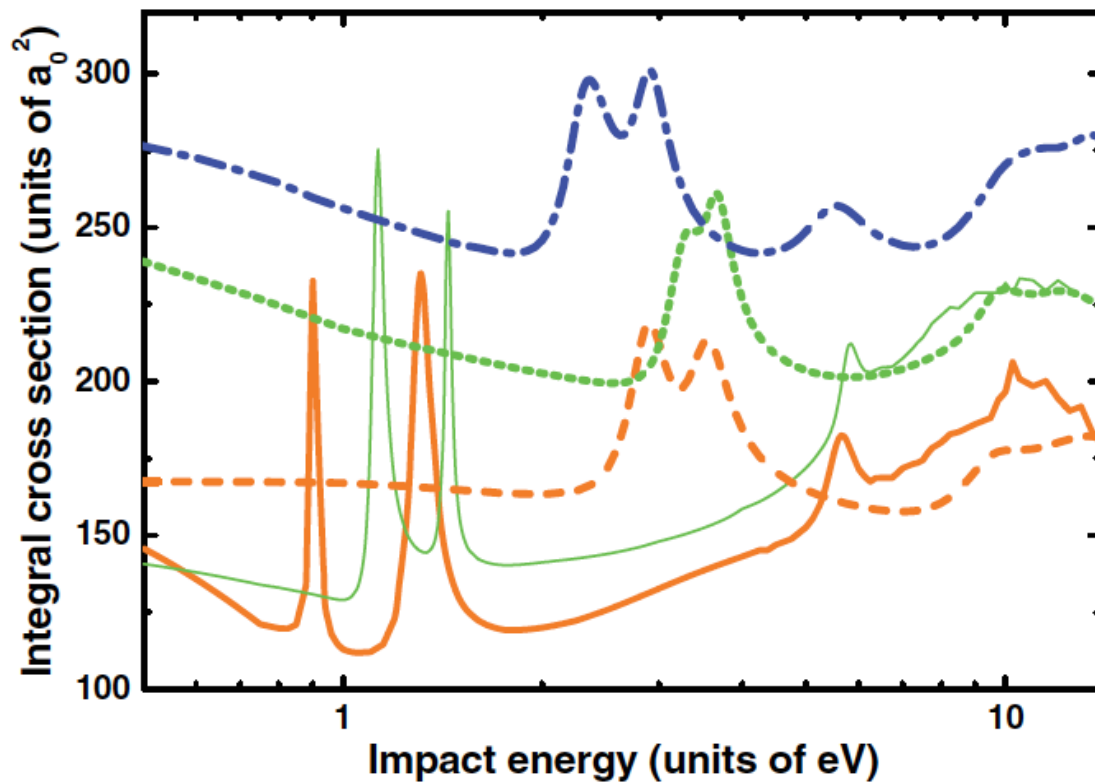
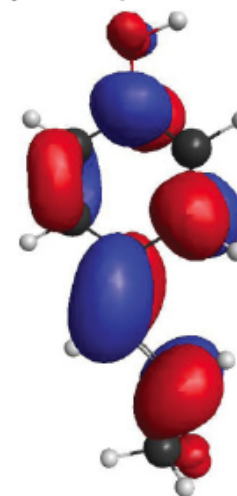
— SEP  
- - - SE

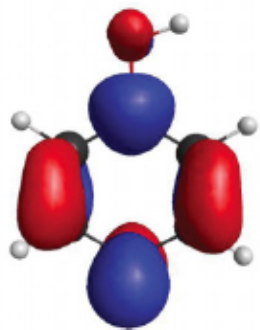


*p*-coumaryl alcohol

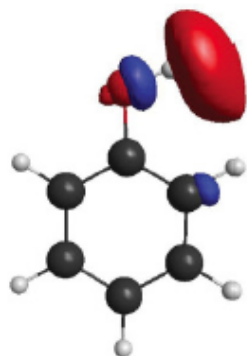
- - - SE

*p*-Cu (LUMO)



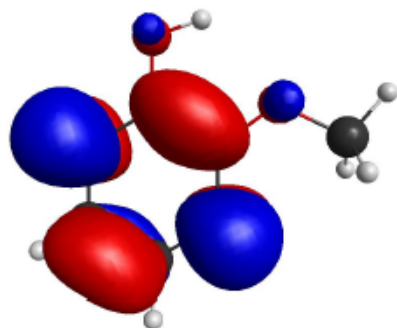


$\pi^*$  (LUMO+1)

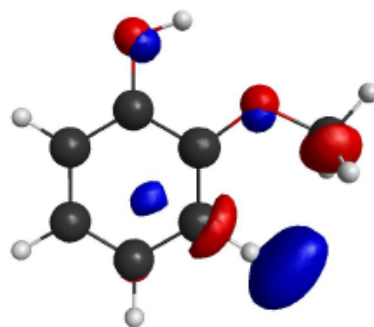


$\sigma^*$  (LUMO+2)

Phenol: Calculations, ET spectra and DEA data indicate H elimination from  $\pi^*/\sigma^*$  coupling.

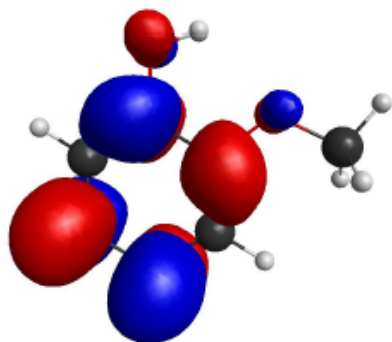


$\pi^*$  (LUMO)

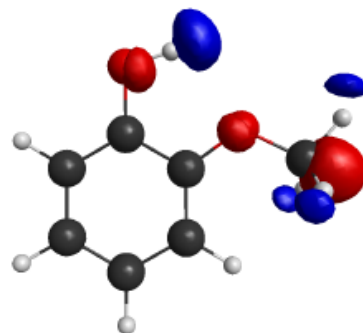


$\sigma^*$  (LUMO+2)

Guaiacol: Methoxilation is expected to give rise to other dissociation channels. H elimination should be also observed.



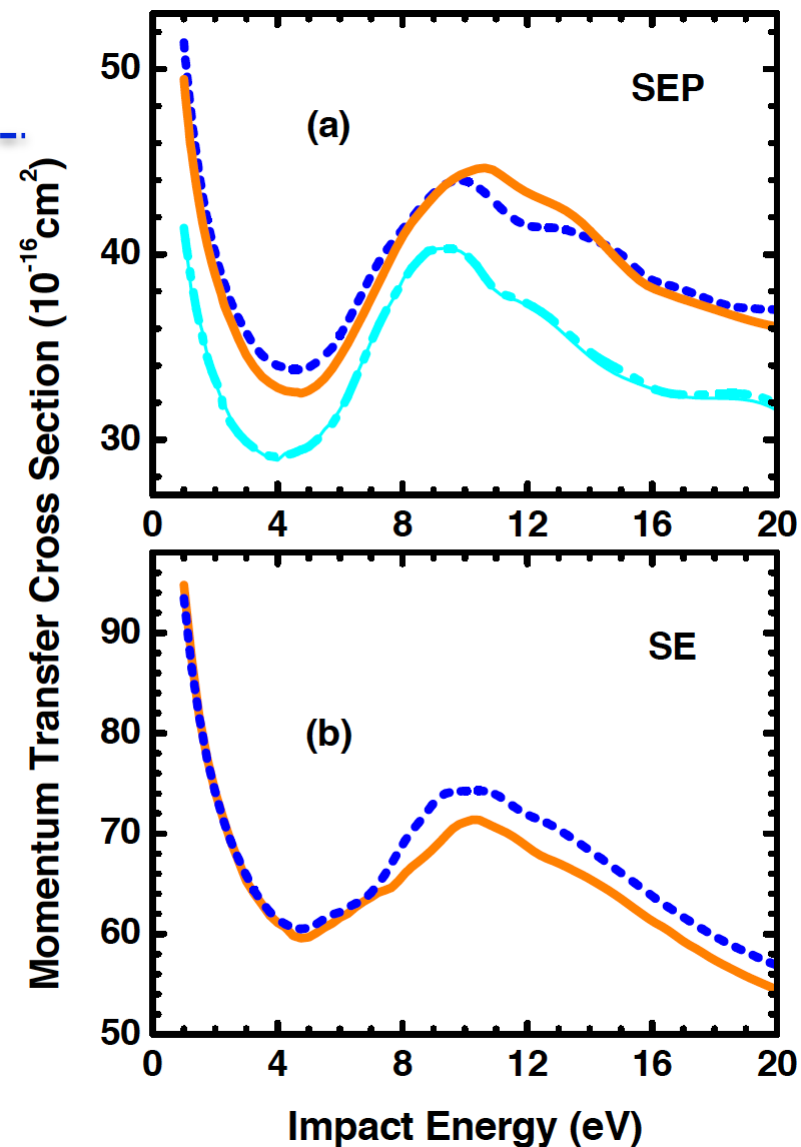
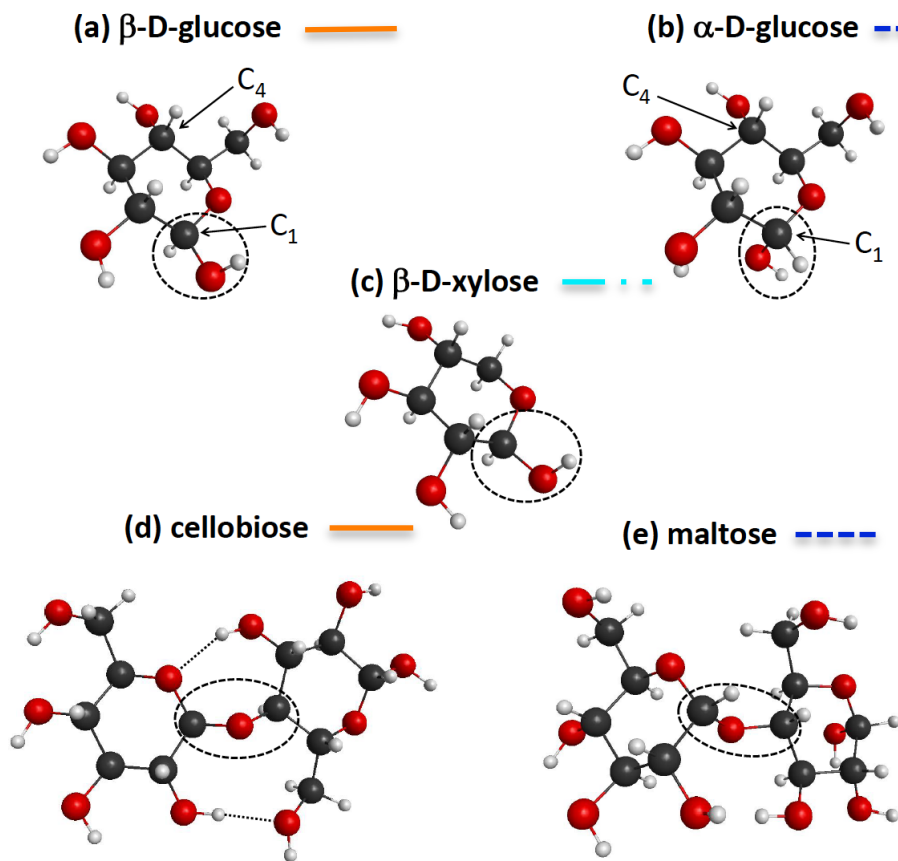
$\pi^*$  (LUMO+1)



$\sigma^*$  (LUMO+3)

# Low-energy electron scattering by cellulose and Hemicellulose components

Phys. Chem. Chem. Phys. **15**, 1682 (2013).



# Theoretical team on electron-scattering of microsolvated molecules



Sylvio Canuto (microsolvation)  
Kaline Coutinho (microsolvation)  
Márcio T. do N. Varella



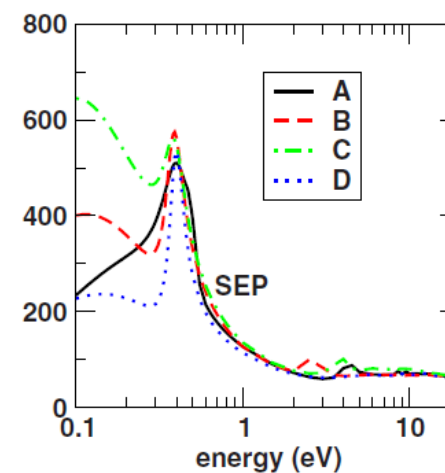
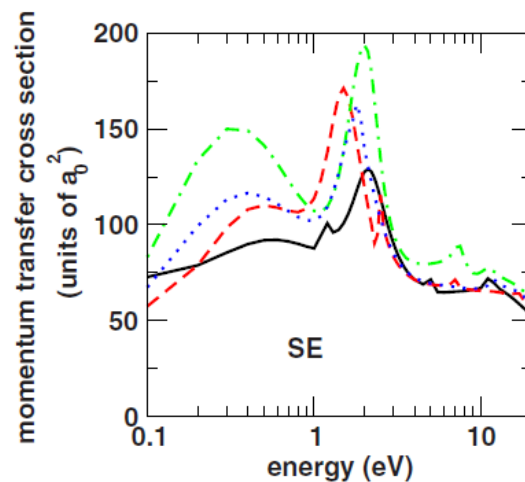
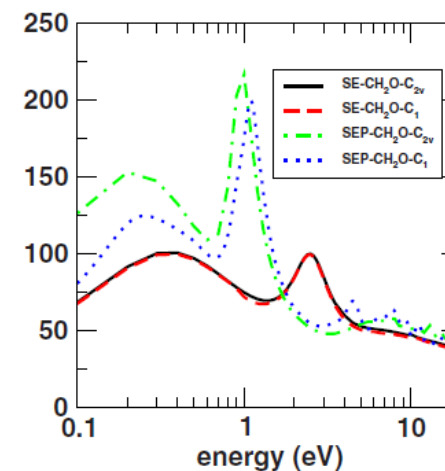
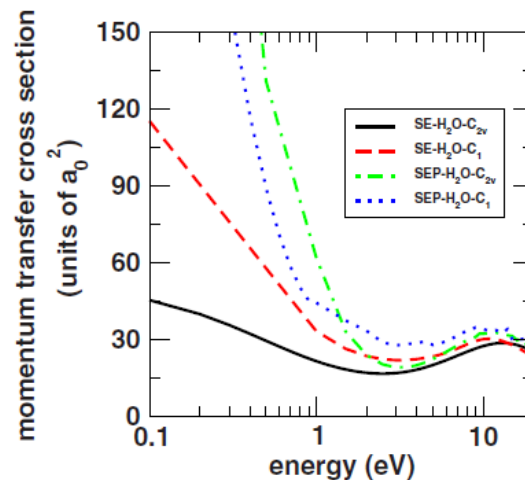
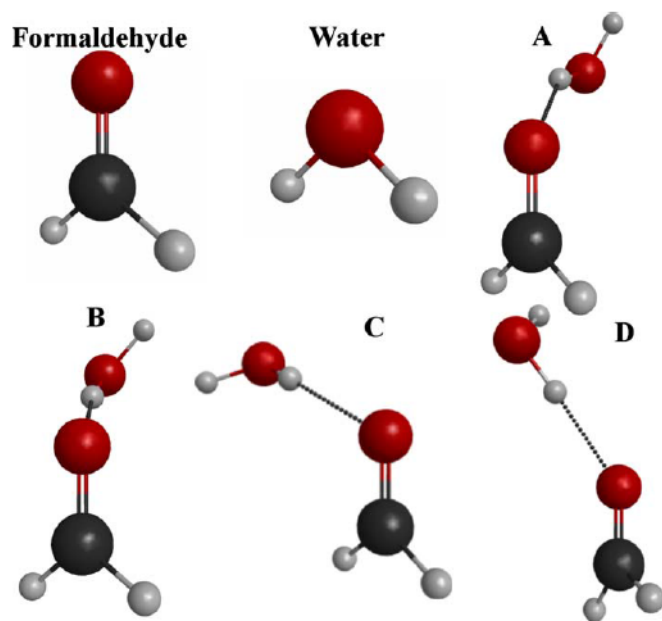
Eliane M. de Oliveira (scattering of solvated phenol)  
Marco A. P. Lima



Thiago C. Freitas (his Ph.D. Thesis)  
Márcio H. F. Bettega (coordinator)

# Electron Collisions with the CH<sub>2</sub>O-H<sub>2</sub>O complex

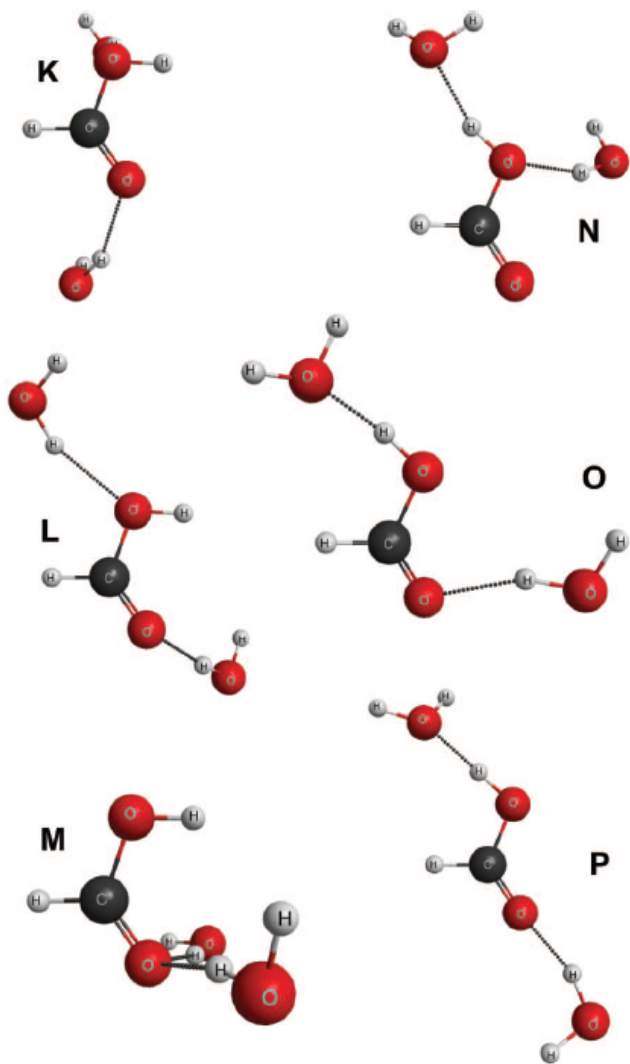
PHYSICAL REVIEW A 80, 062710 (2009)



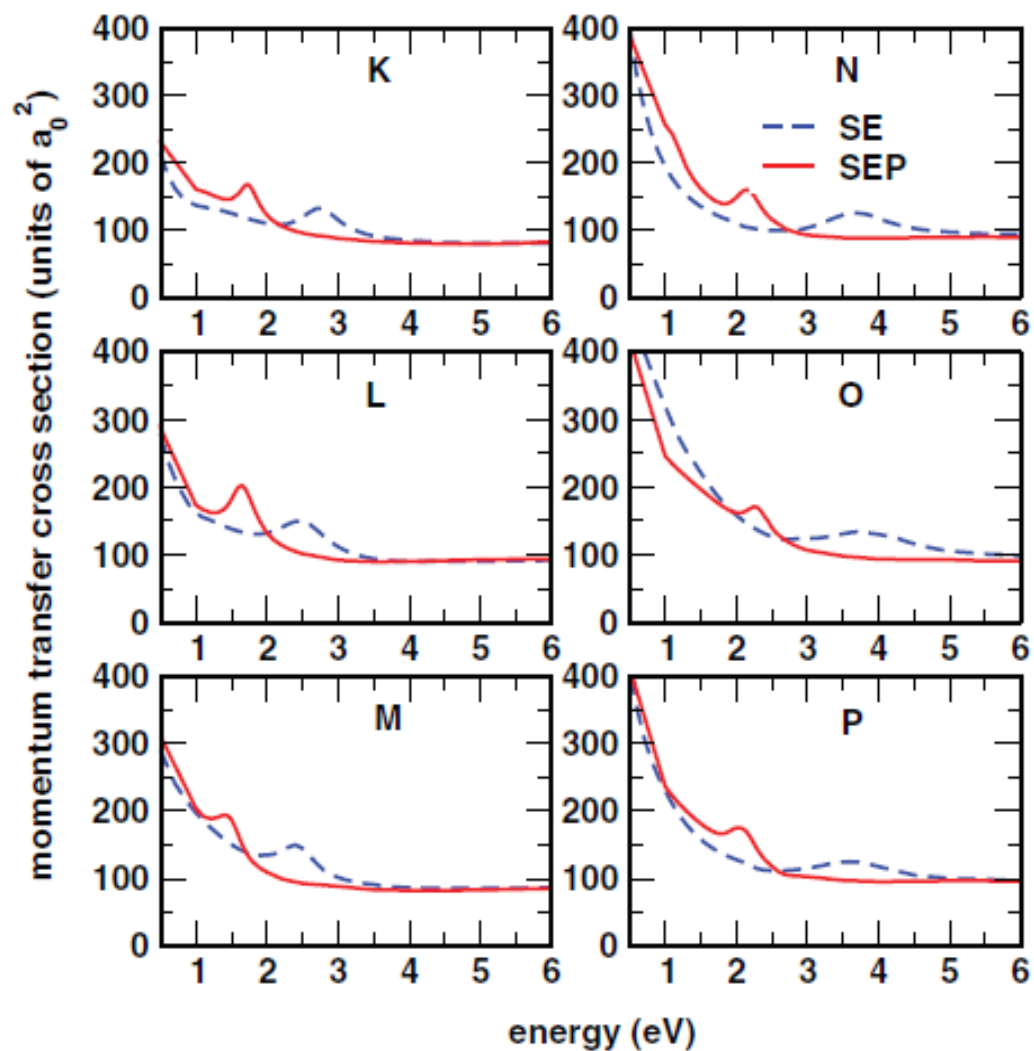


# Electron collisions with the HCOOH...(H<sub>2</sub>O)<sub>n</sub> complexes (n=1, 2) in liquid phase: The influence of microsolvation on the $\pi^*$ resonance of formic acid

THE JOURNAL OF CHEMICAL PHYSICS 138, 174307 (2013)

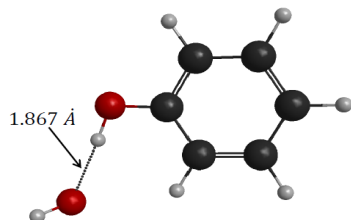


$\pi^*$  shape resonance for HCOOH at around 1.9 eV.

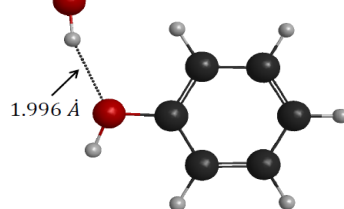


## Electron Collisions with Phenol...H<sub>2</sub>O

(proton acceptor)

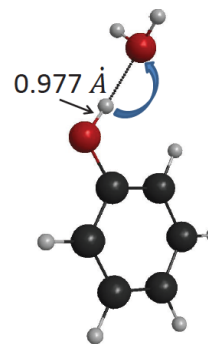


(proton donor)

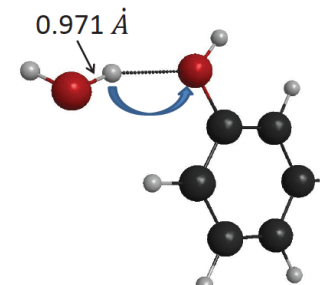


We have studied the microsolvation of Phenol using 4 complexes.

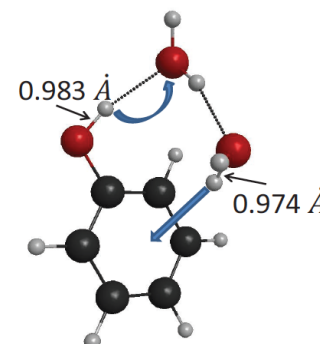
- In Complex A, the water molecule is a proton acceptor.
- In the Complex B, the water is a proton donor.
- Complexes C and D have both situations (one water molecule as acceptor and the other as proton donor).



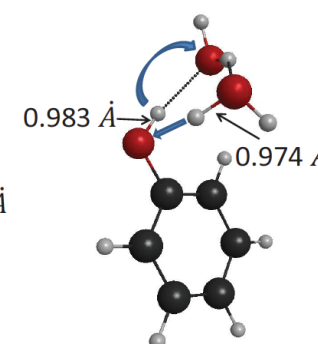
CoA



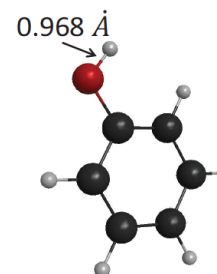
CoB



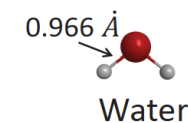
CoC



CoD

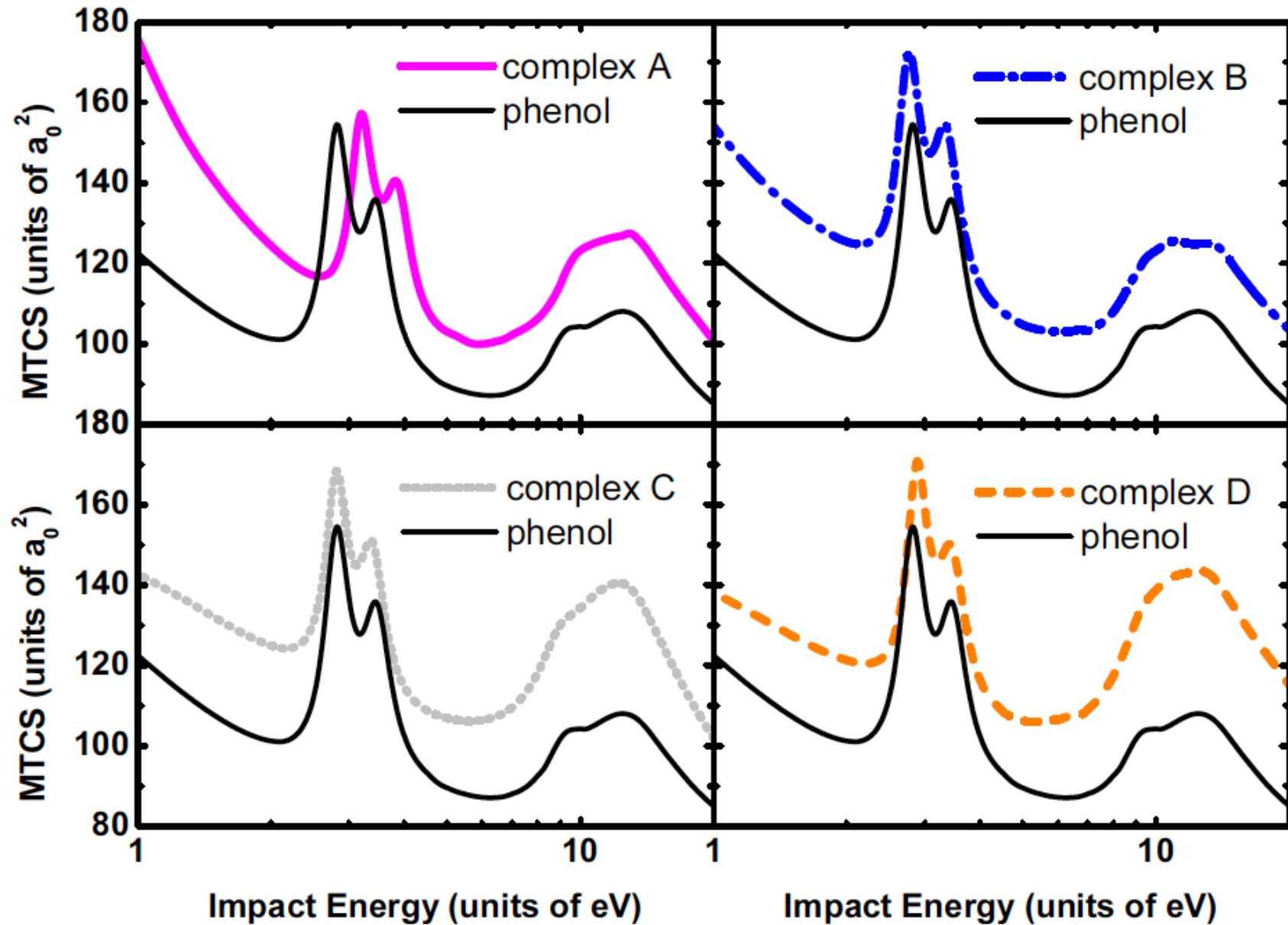


Ph



Water

# Electron Collisions with Phenol... $(H_2O)_n$ : $n=1,2$



# Electron Collisions with Phenol...H<sub>2</sub>O

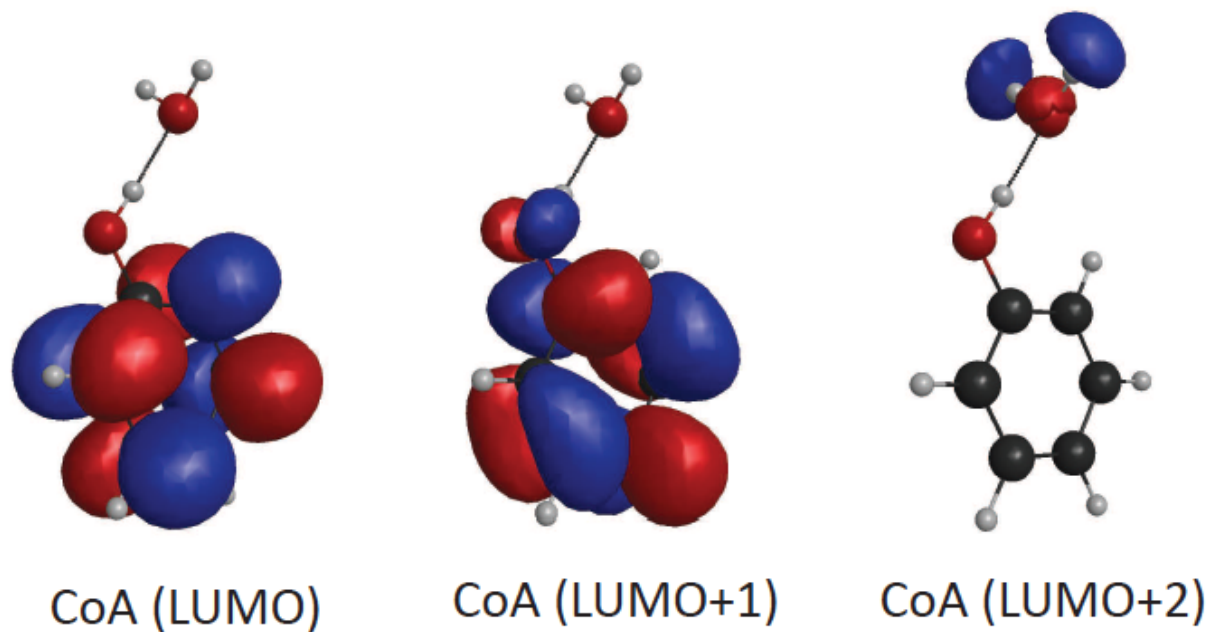


FIG. 1. (Color online) The three lowest virtual orbitals of the complex A.

# Electron Collisions with Phenol...H<sub>2</sub>O

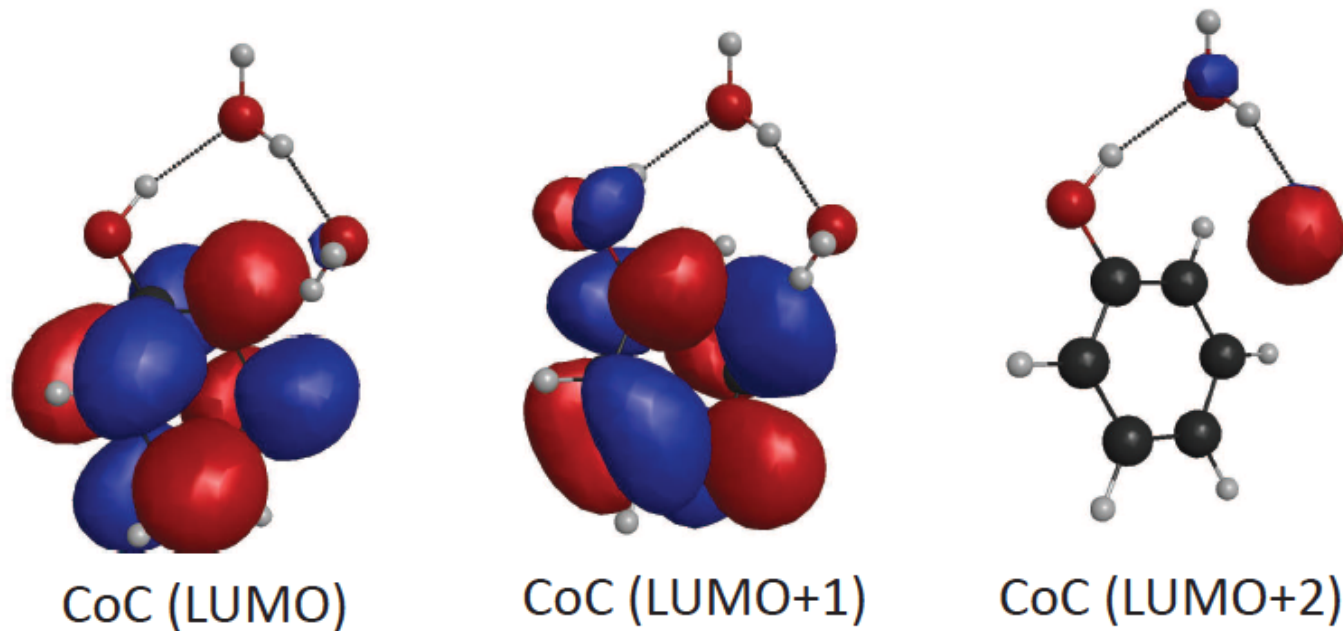
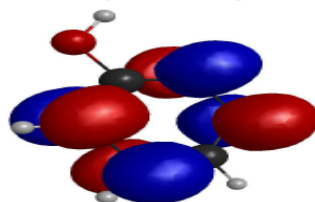


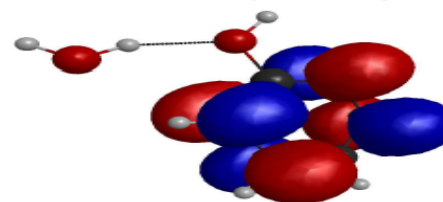
FIG. 2. (Color online) Same as in Fig. 1, but for the complex *C*.

# Electron Collisions with Phenol...H<sub>2</sub>O

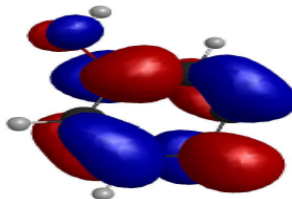
Ph (LUMO)



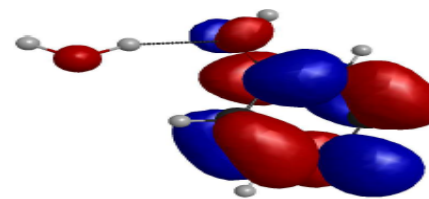
CoB (LUMO)



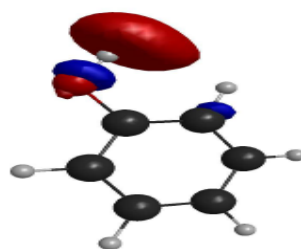
Ph (LUMO+1)



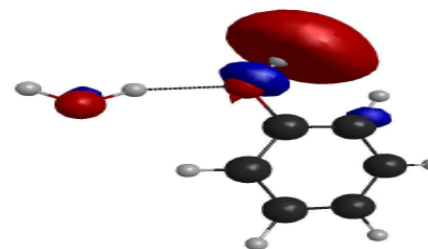
CoB (LUMO+1)



Ph (LUMO+2)



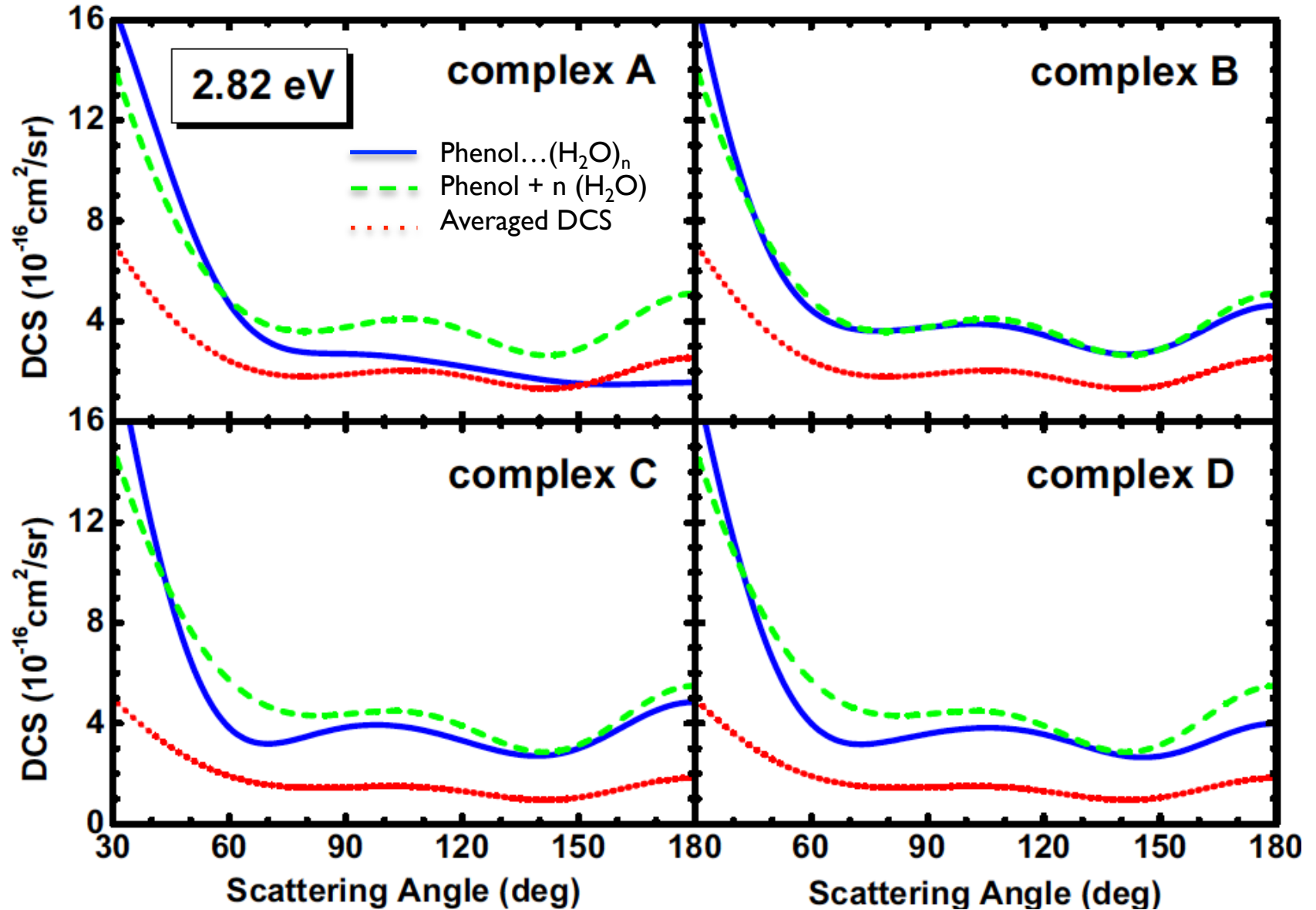
CoB (LUMO+2)



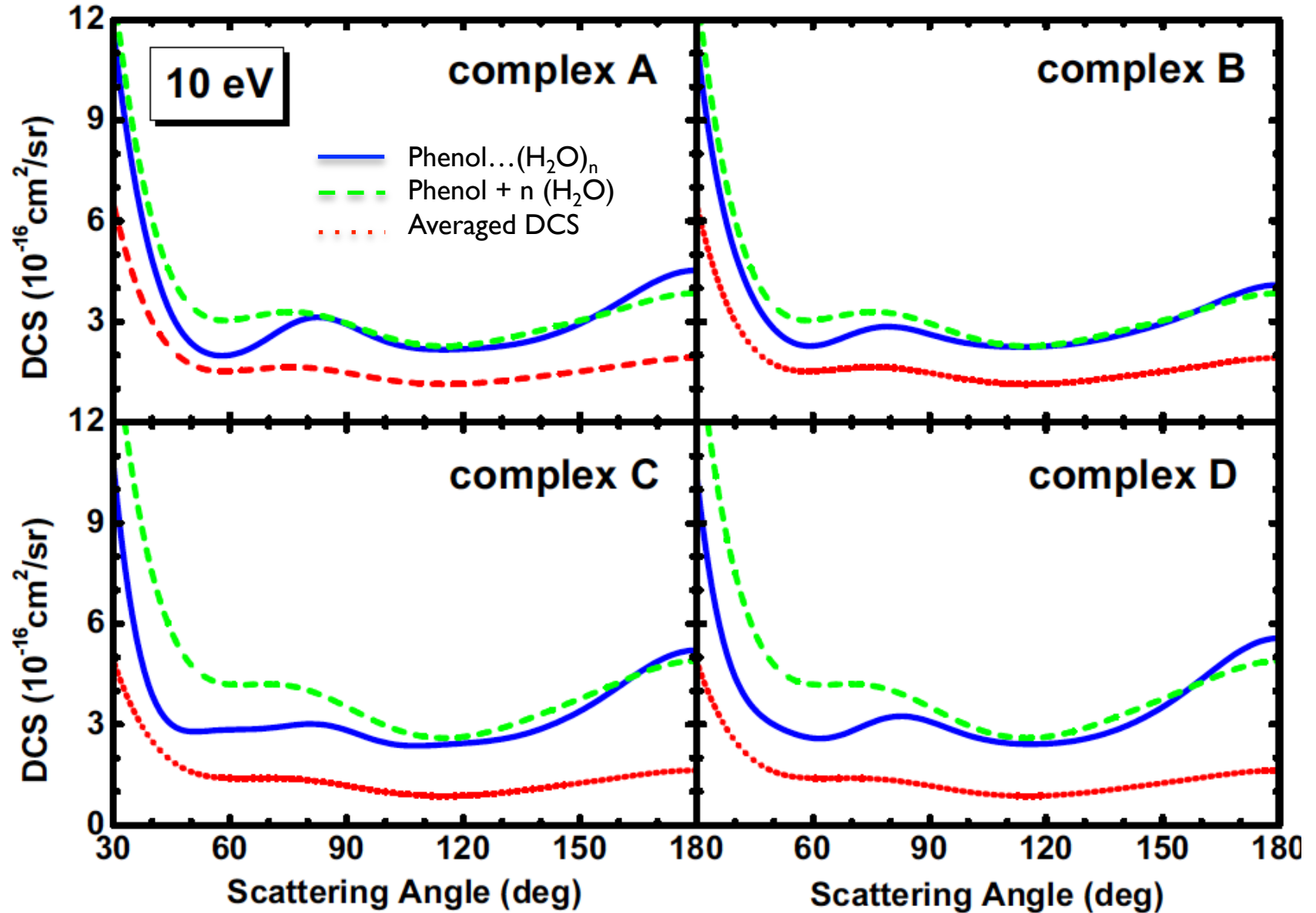
CoD (LUMO+2)



# Electron Collisions with Phenol... $(H_2O)_n$ : search for microsolvation signatures in the DCS

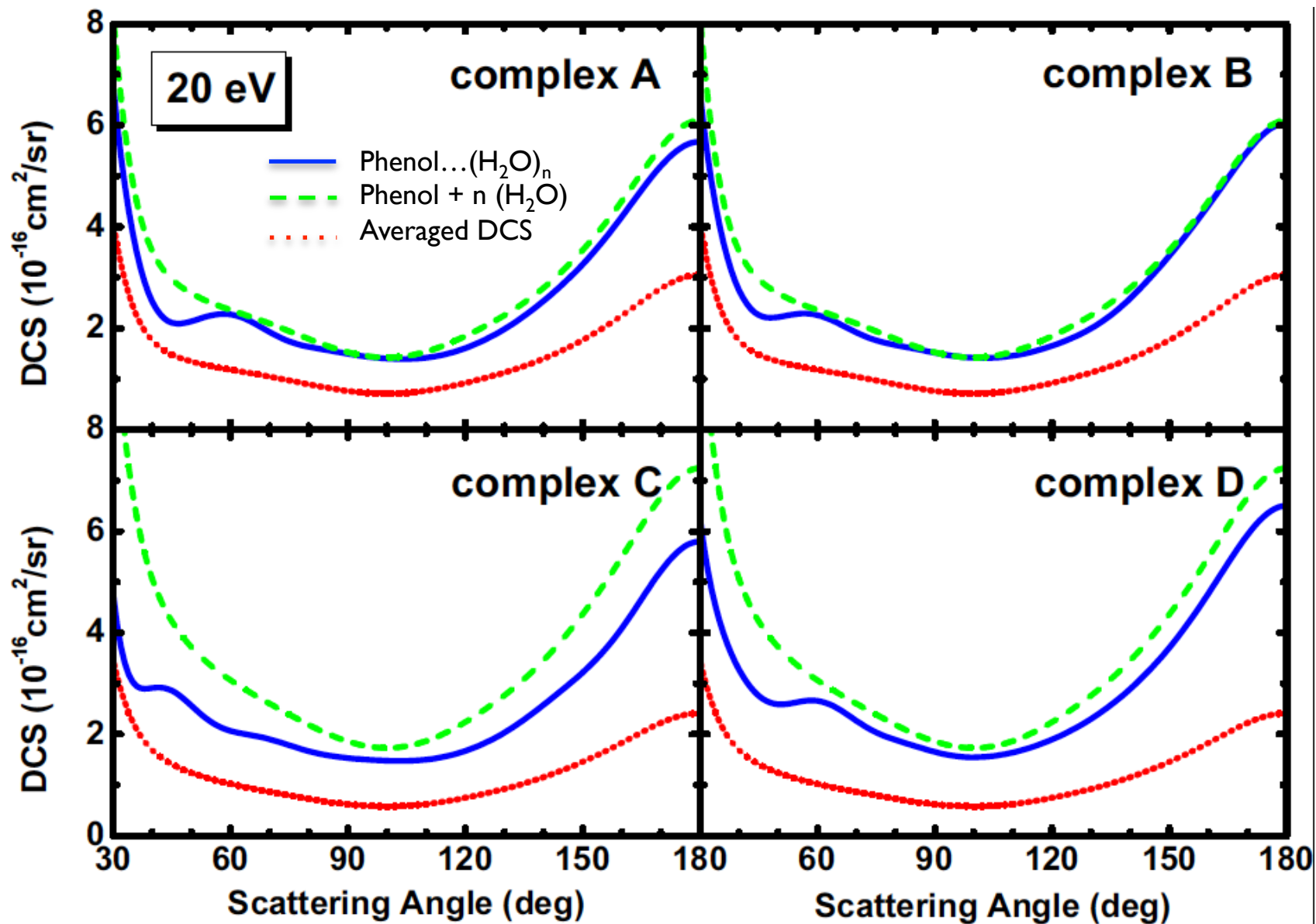


# Electron Collisions with Phenol... $(\text{H}_2\text{O})_n$ : search for microsolvation signatures in the DCS





# Electron Collisions with Phenol... $(H_2O)_n$ : search for microsolvation signatures in the DCS



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# ELECTRONIC EXCITATION

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## Theoretical co-authors



Eliane M. de Oliveira (posdoc)  
Marco A. P. Lima



Márcio H. F. Bettega

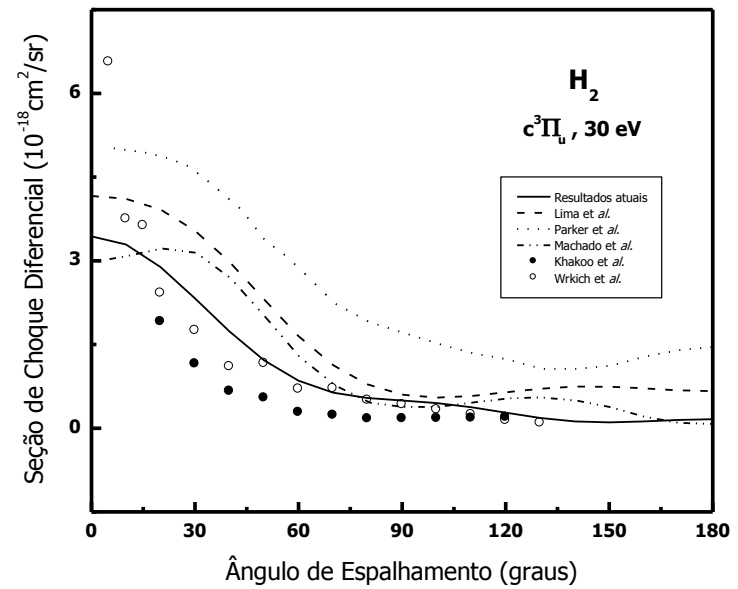
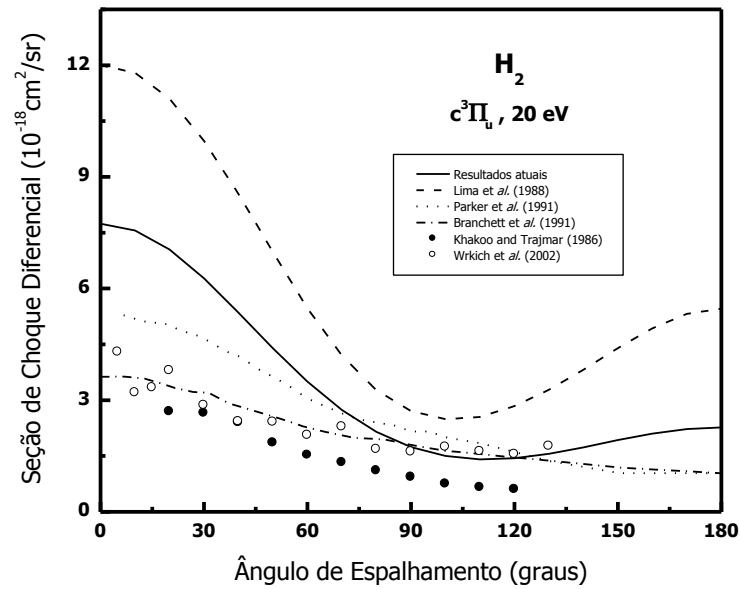
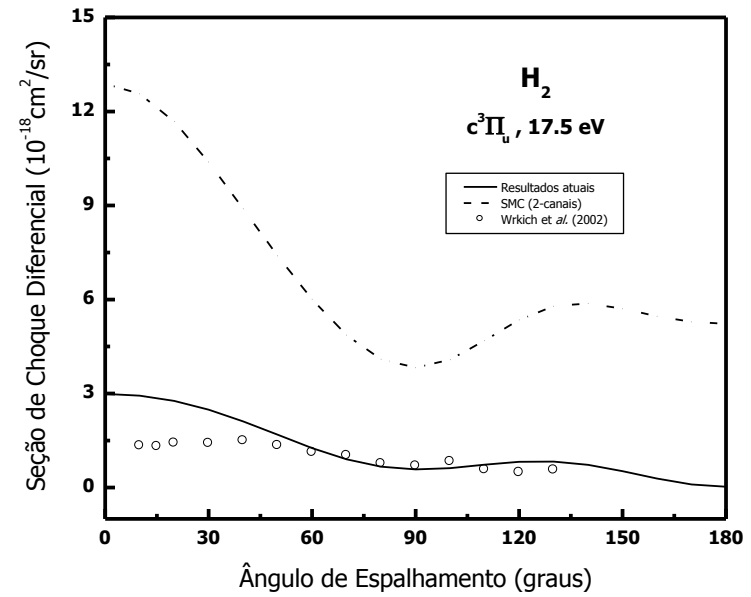
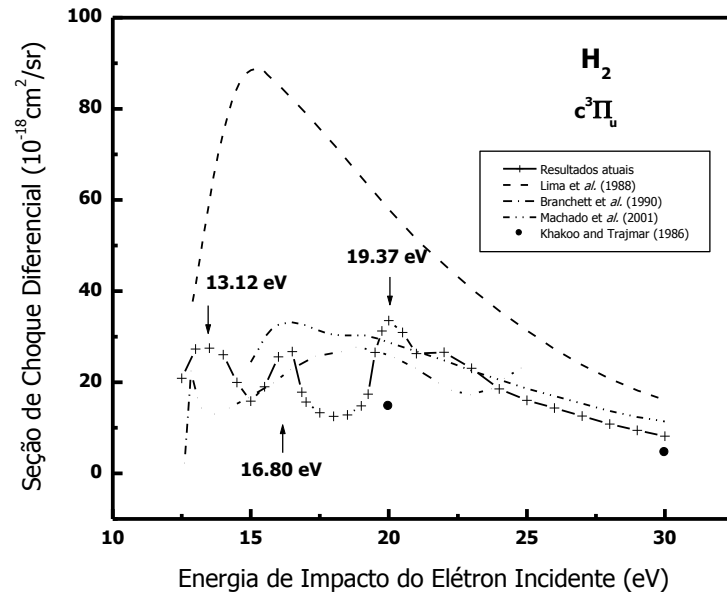


Márcio T. do N. Varella

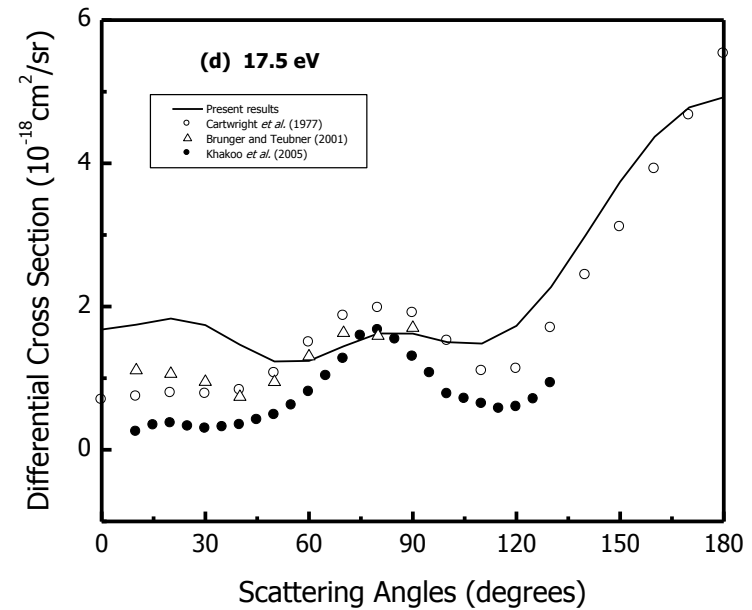
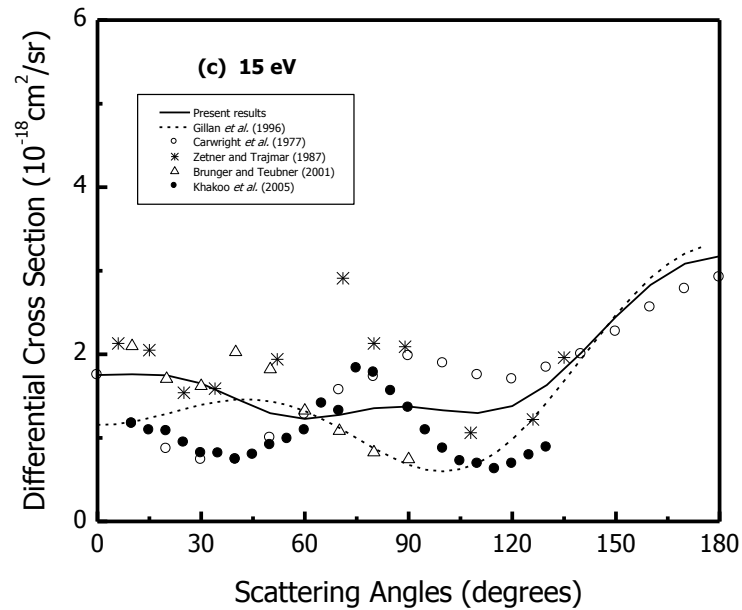
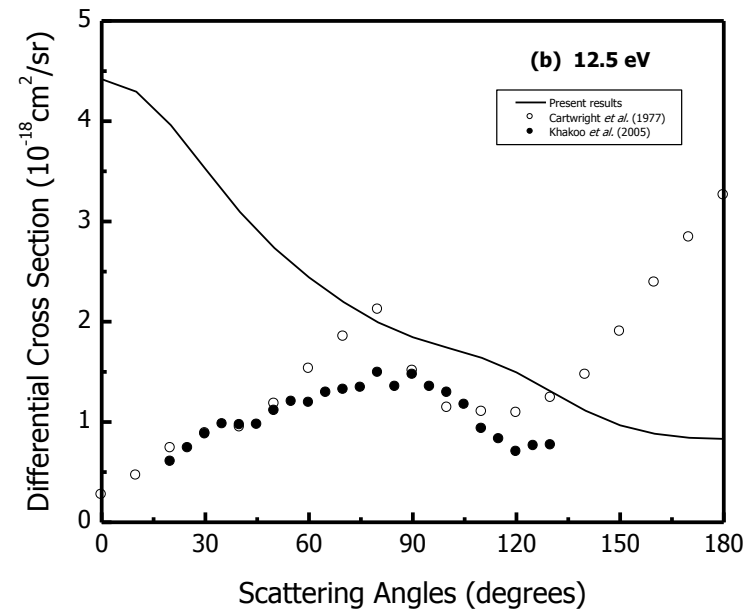
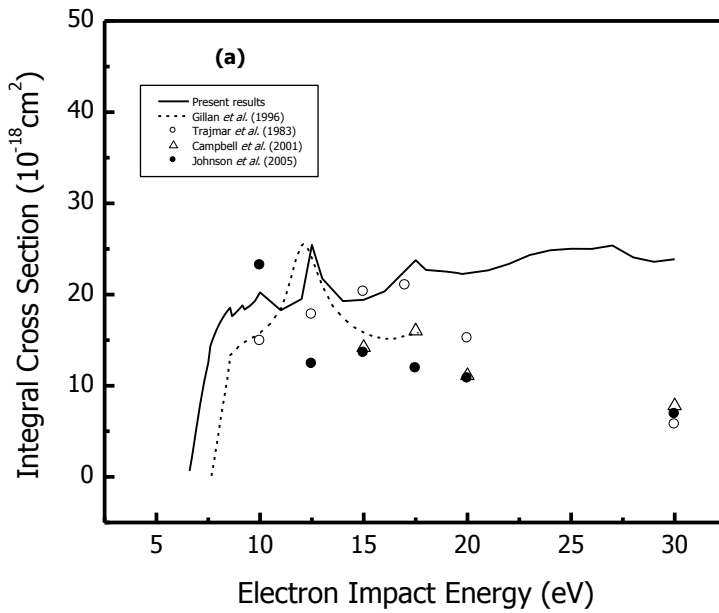


Romarly F. da Costa (coordinator)

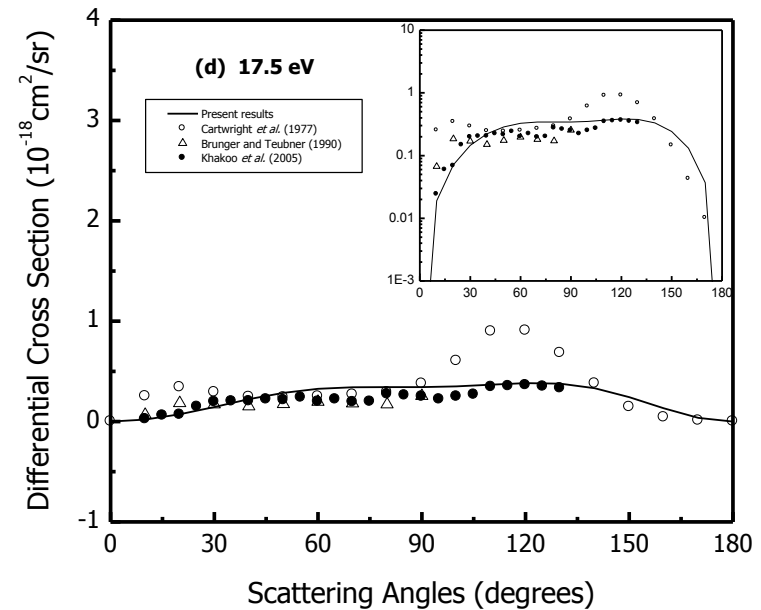
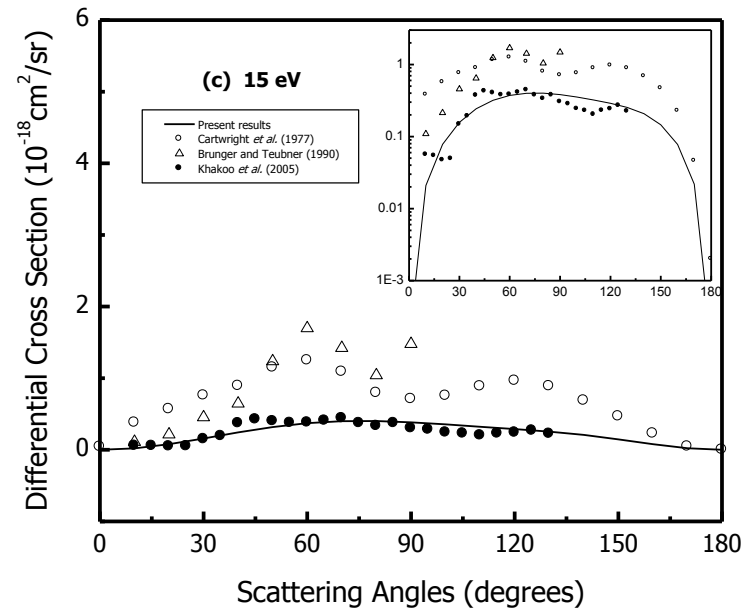
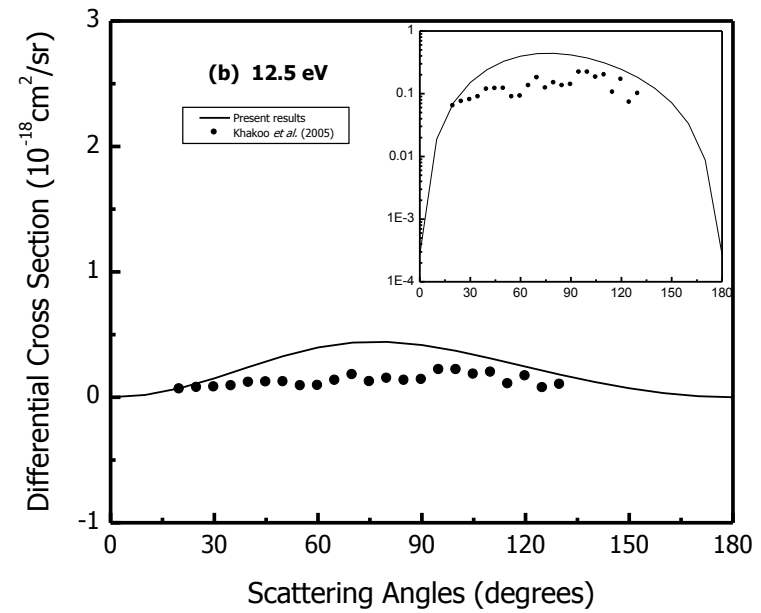
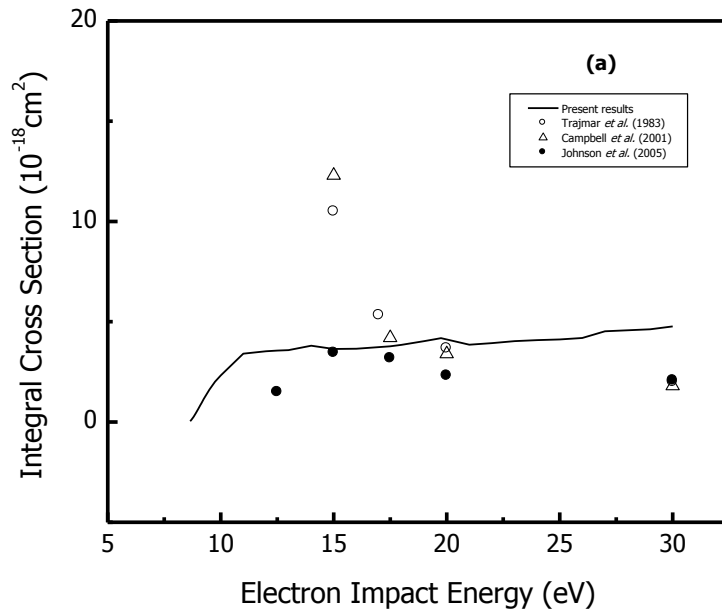
# Electronic excitation of H<sub>2</sub> by electron impact



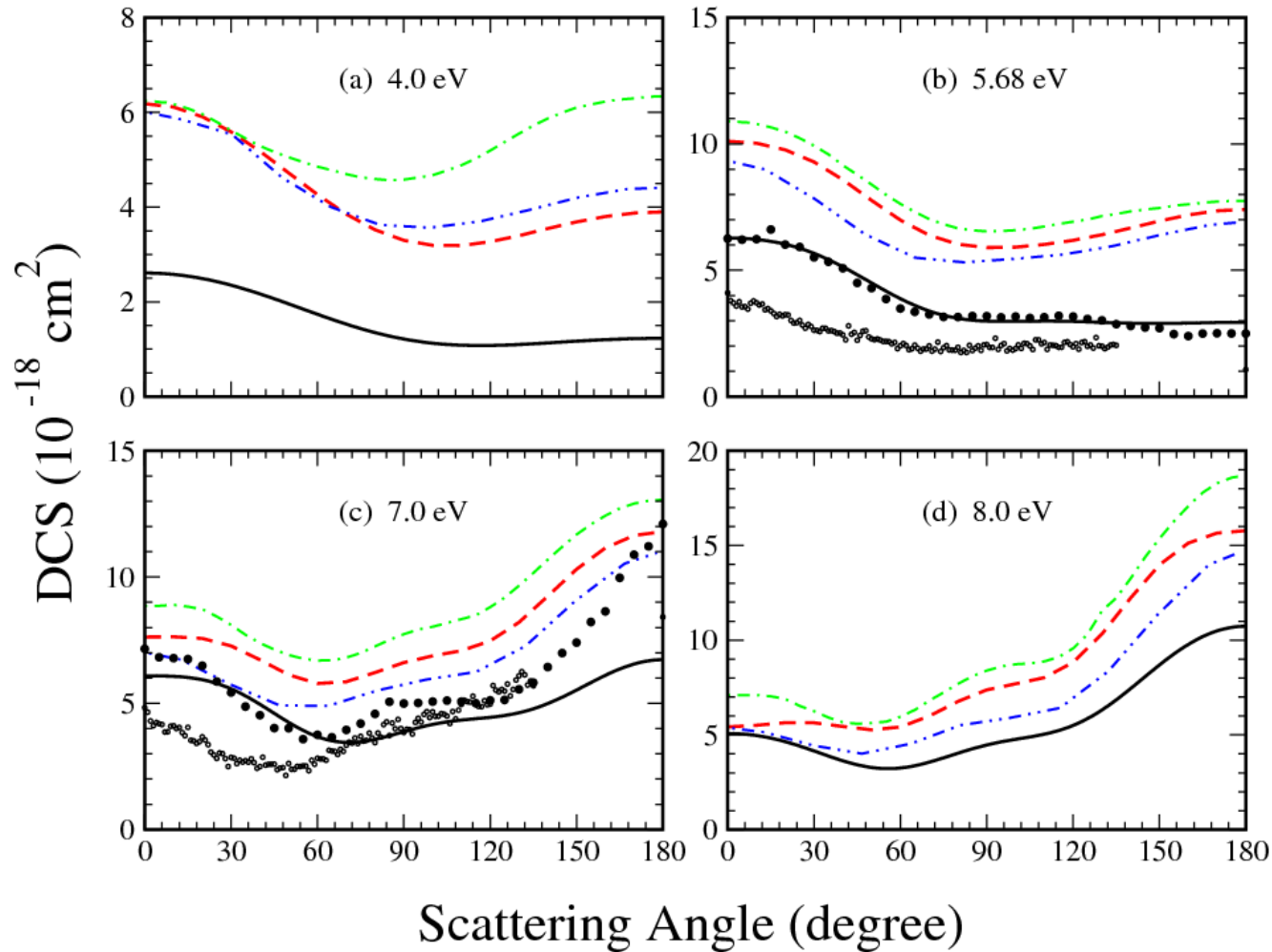
# Electronic transition $X^1\Sigma_g \rightarrow A^3\Sigma_u^+$ of $N_2$ by electron impact



# Electronic transition $X \ ^1\Sigma_g^- \rightarrow a' \ ^1\Sigma_u^-$ of $N_2$ by electron impact

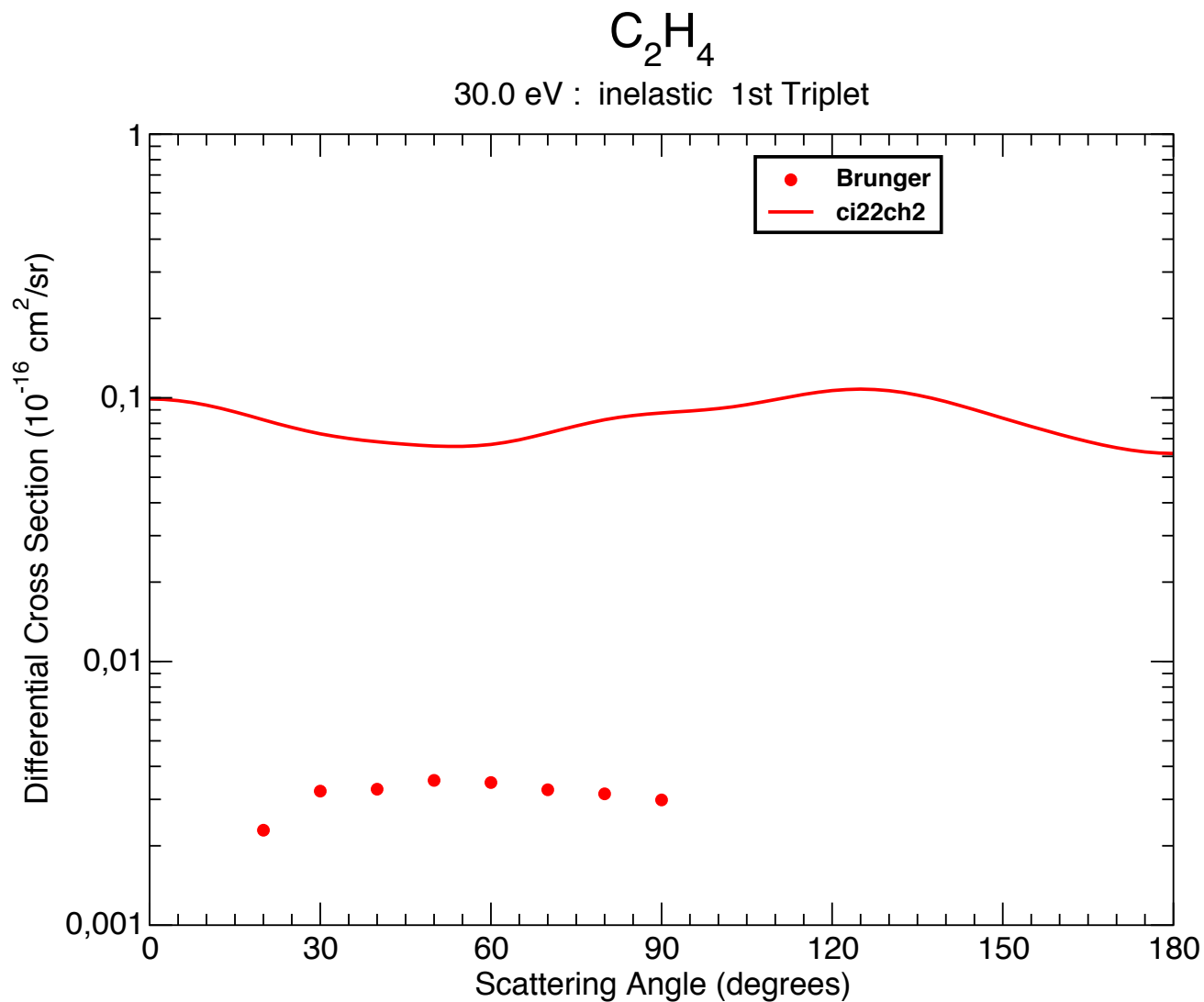


## Electronic excitation of $\tilde{a}^3B_{1u}$ state of $C_2H_4$ by electron impact



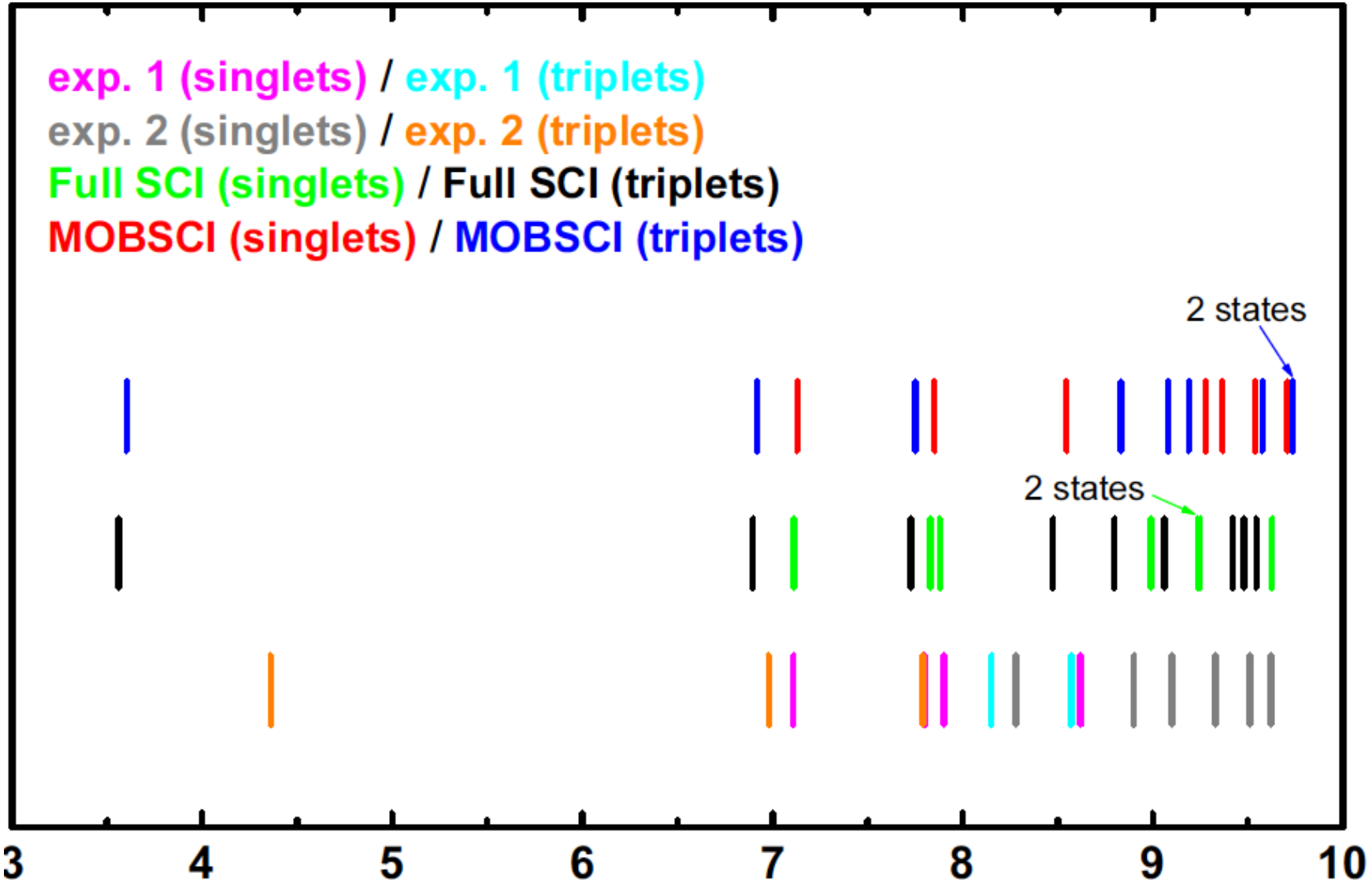
Color lines are  
Close-coupling  
Calculations  
and  
bullets are  
M.Allan's  
data

## Surprisingly, at higher energies the agreement is not good!!

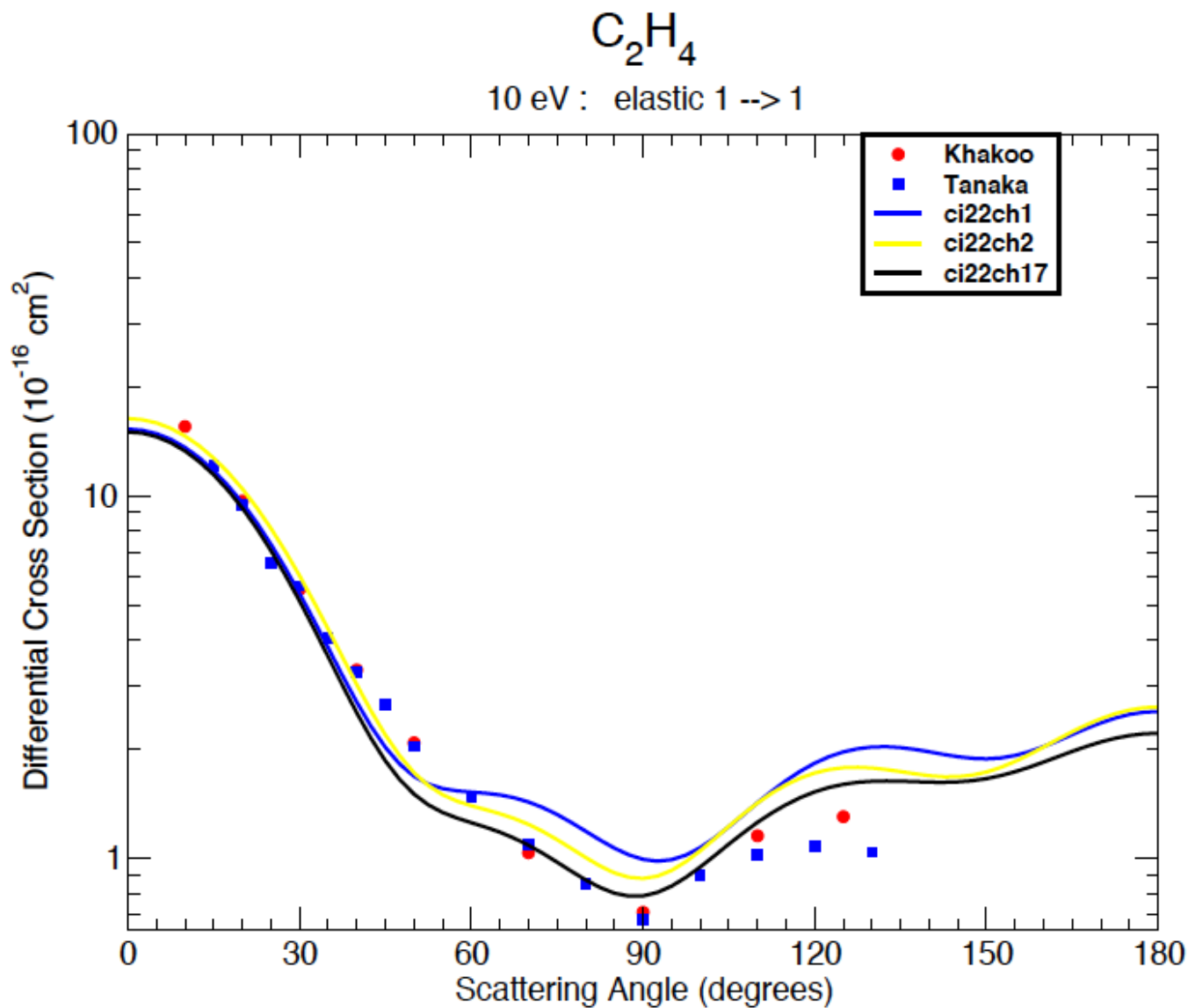




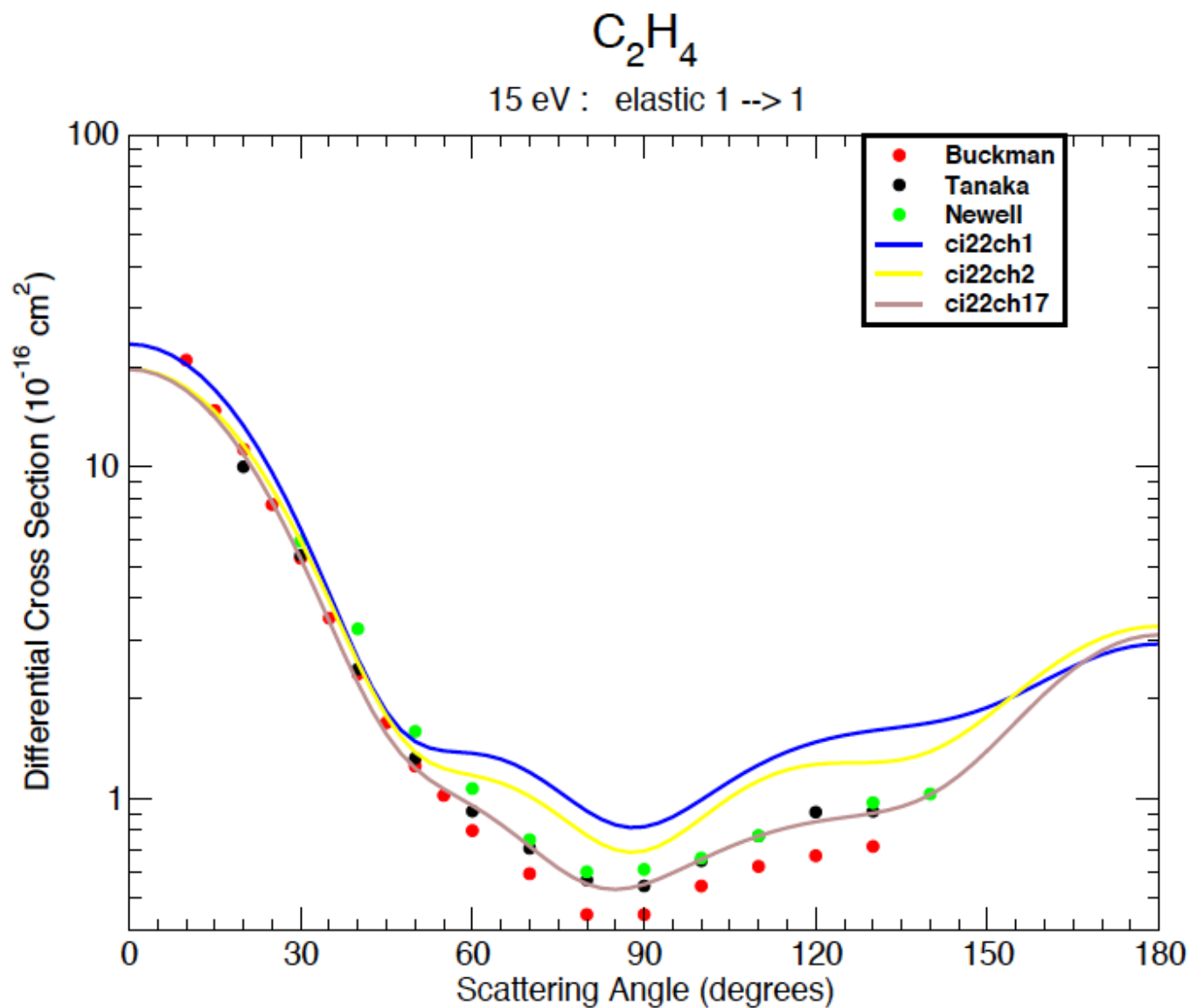
# Multichannel effects on the $e^-C_2H_4$ scattering



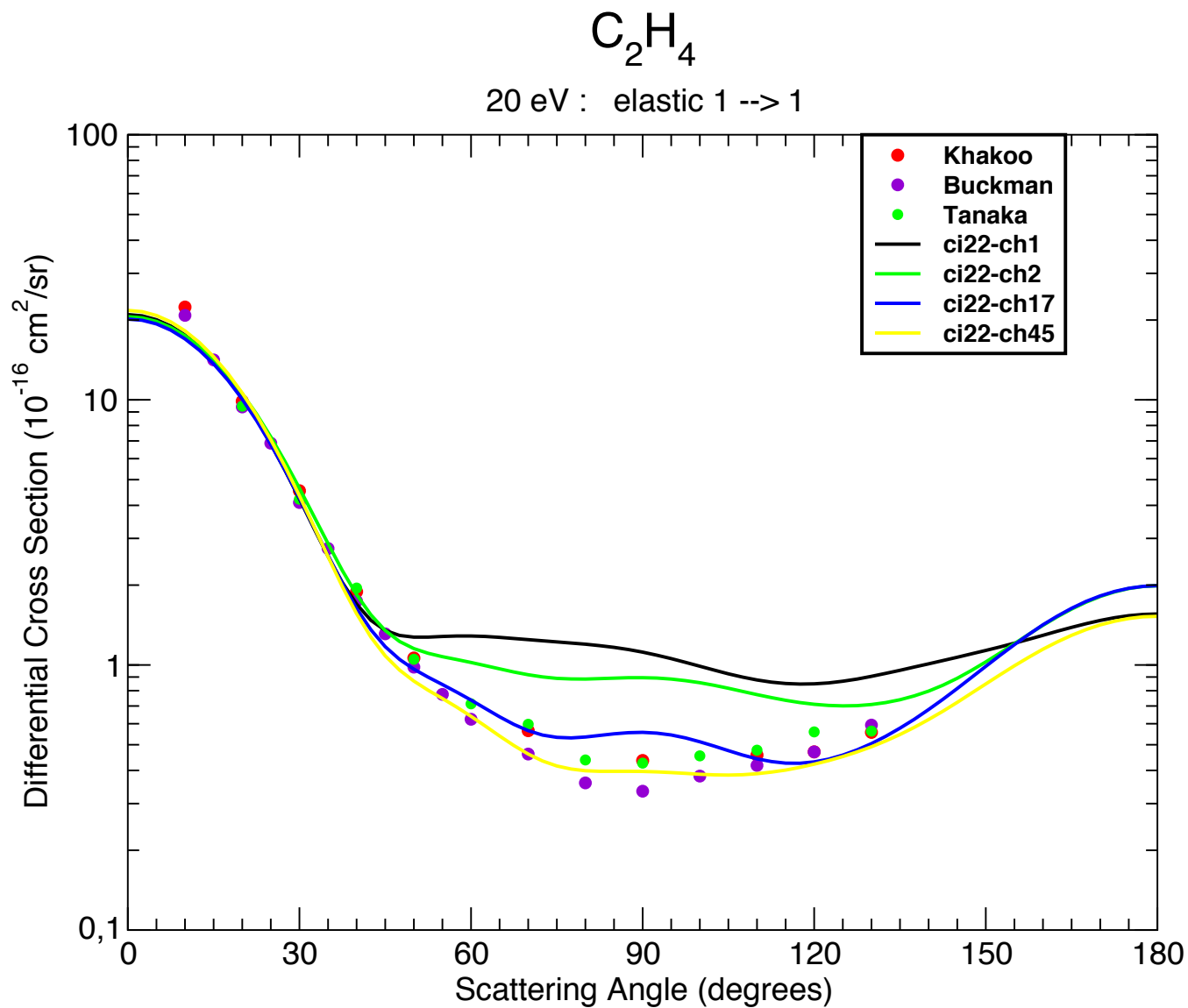
## Multichannel effects on the elastic process of $e^-C_2H_4$ scattering



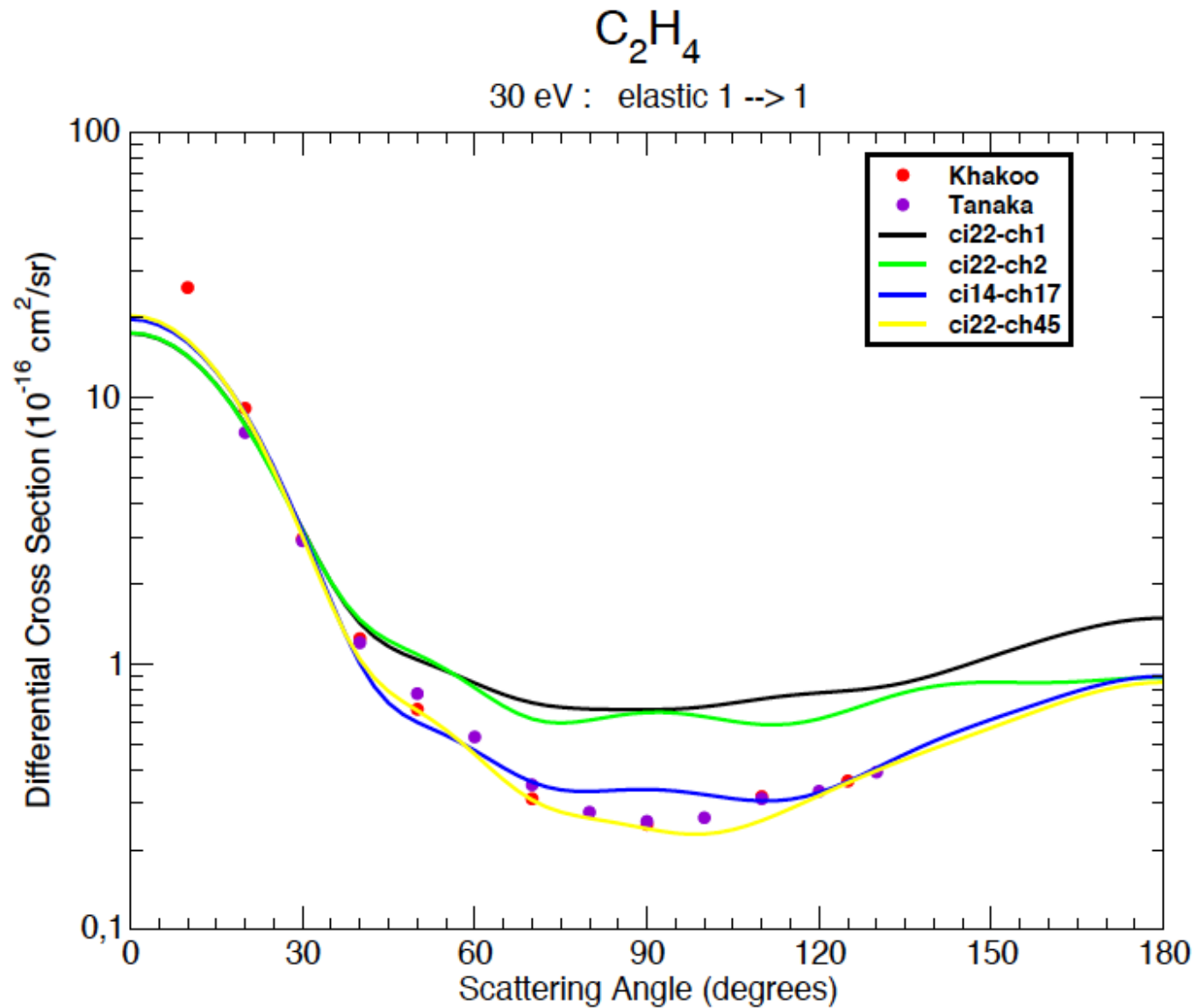
# Multichannel effects on the elastic process of e<sup>-</sup>-C<sub>2</sub>H<sub>4</sub> scattering



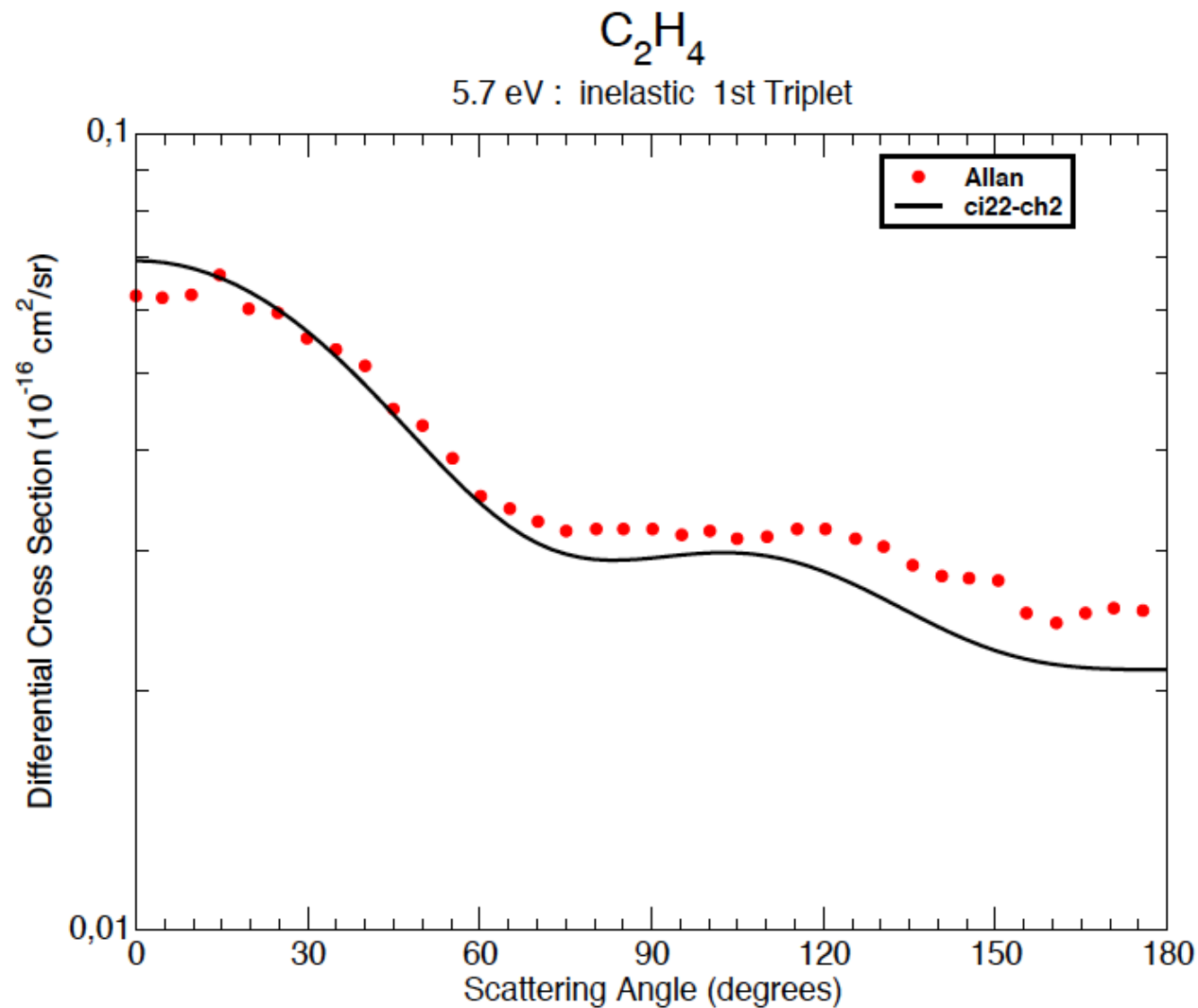
# Multichannel effects on the elastic process of e<sup>-</sup>-C<sub>2</sub>H<sub>4</sub> scattering



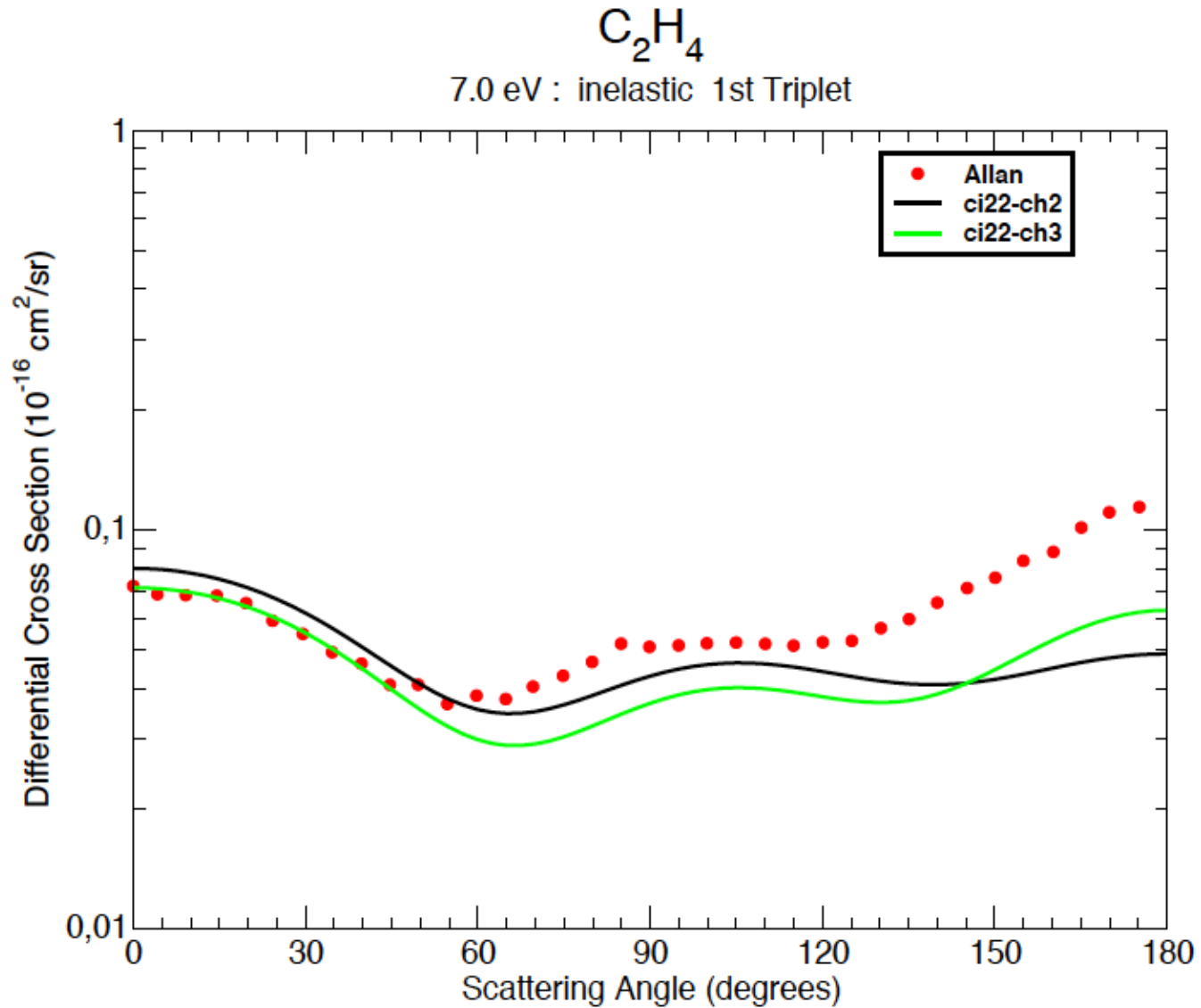
# Multichannel effects on the elastic process of e<sup>-</sup>-C<sub>2</sub>H<sub>4</sub> scattering



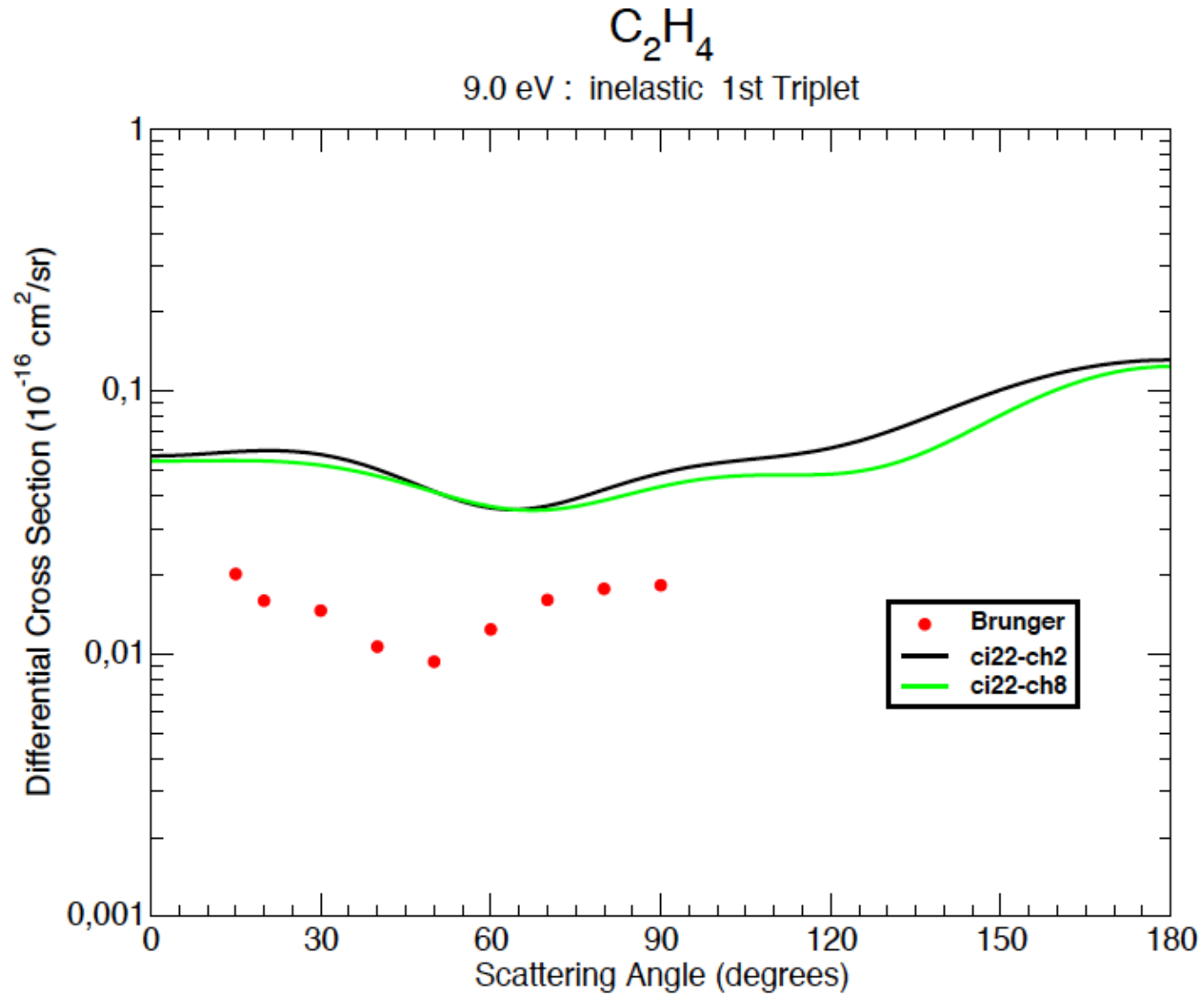
# Multichannel effects on the Electronic excitation of $\tilde{a}^3B_{1u}$ state of $C_2H_4$ by electron impact



# Multichannel effects on the Electronic excitation of $\tilde{a}^3B_{1u}$ state of $C_2H_4$ by electron impact

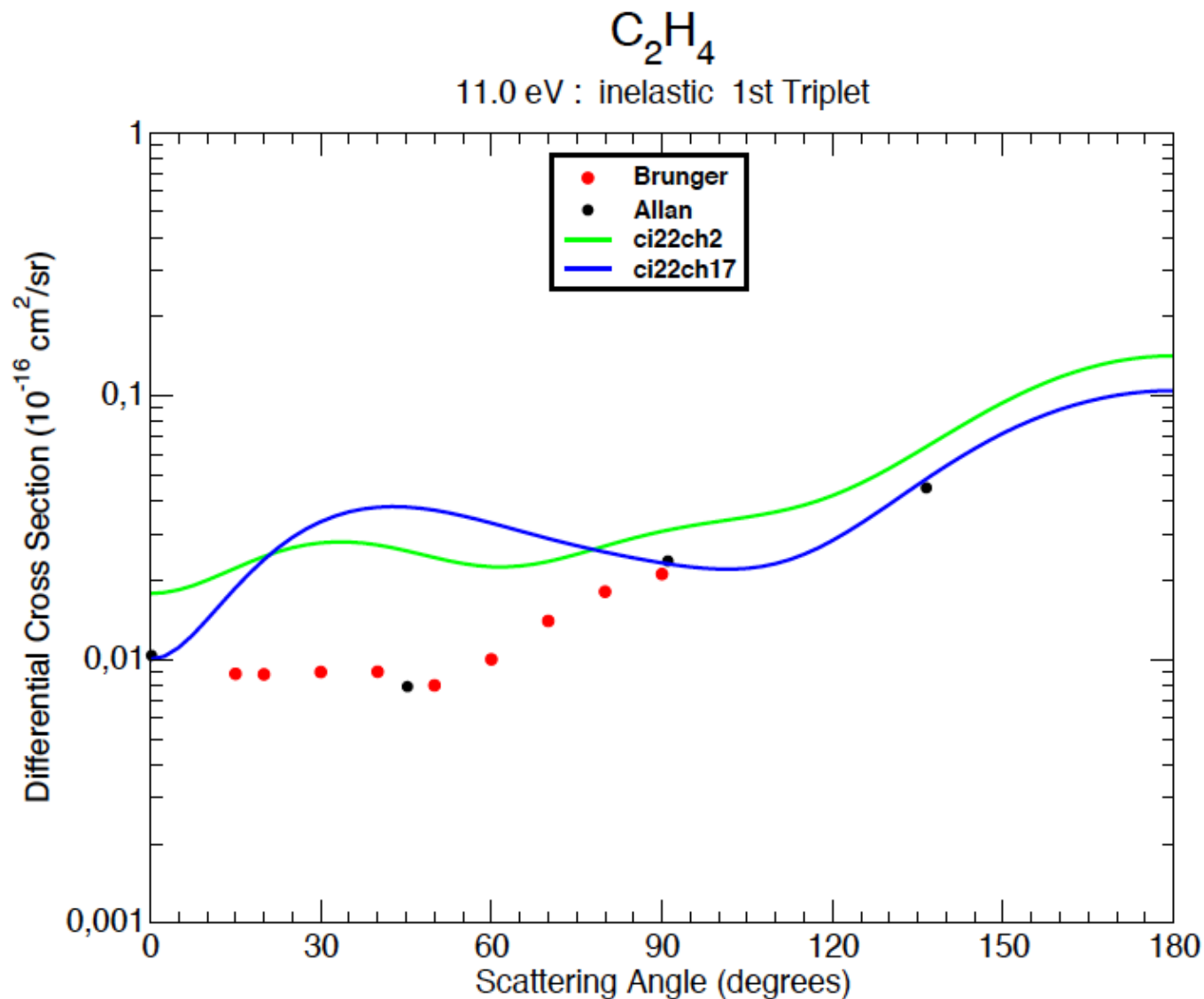


# Multichannel effects on the Electronic excitation of $\tilde{a}^3B_{1u}$ state of $C_2H_4$ by electron impact

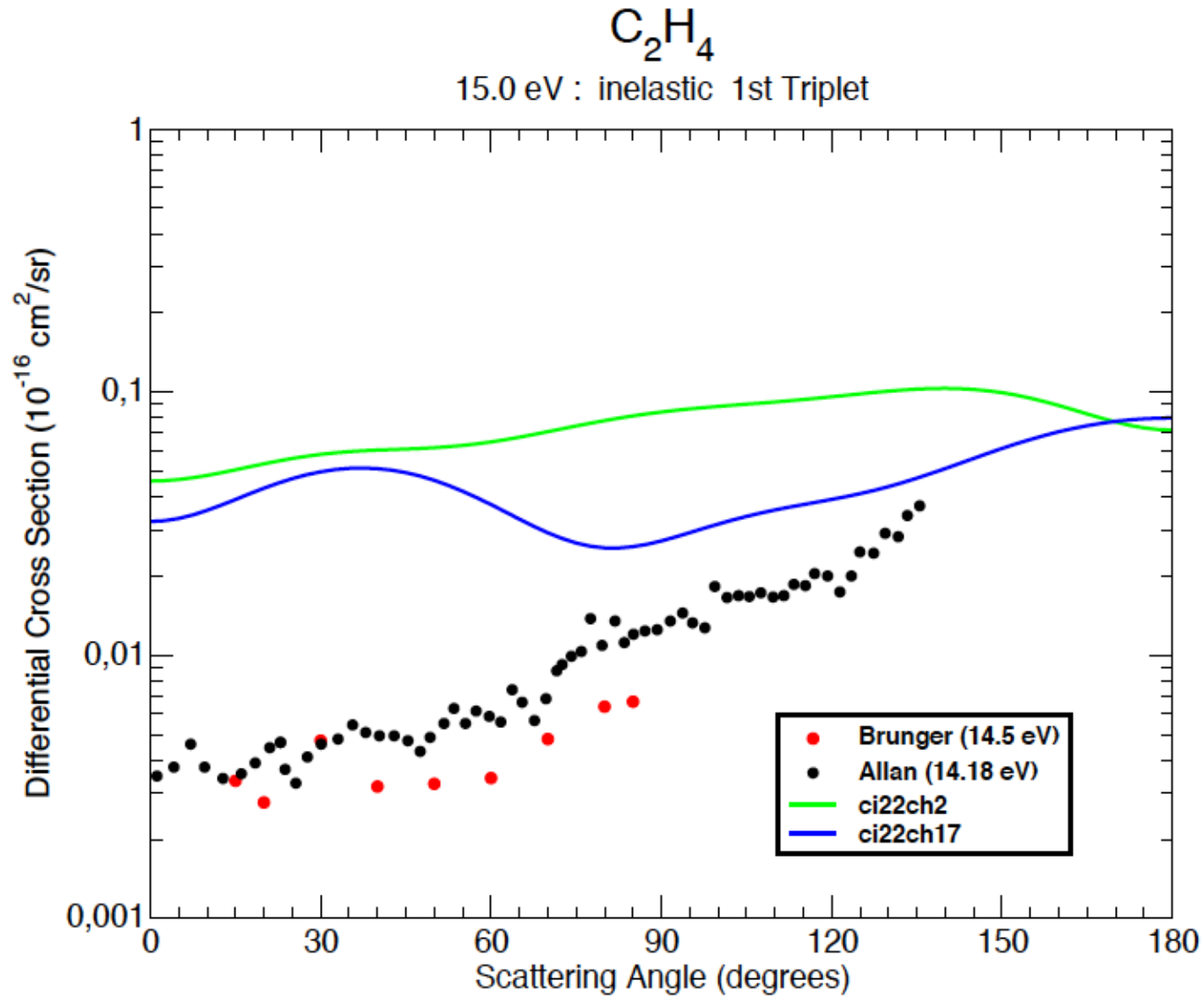




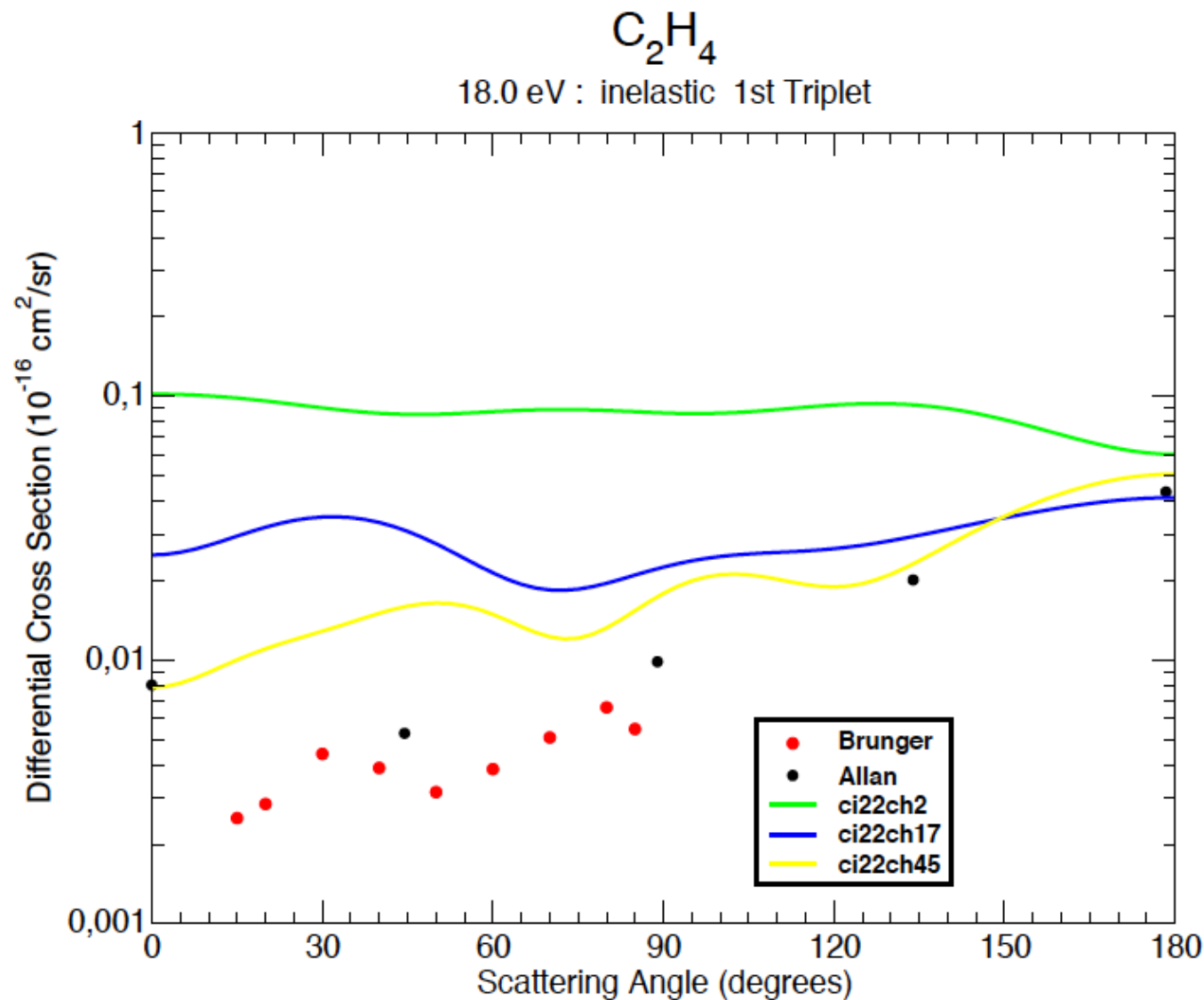
# Multichannel effects on the Electronic excitation of $\tilde{a}^3B_{1u}$ state of $C_2H_4$ by electron impact



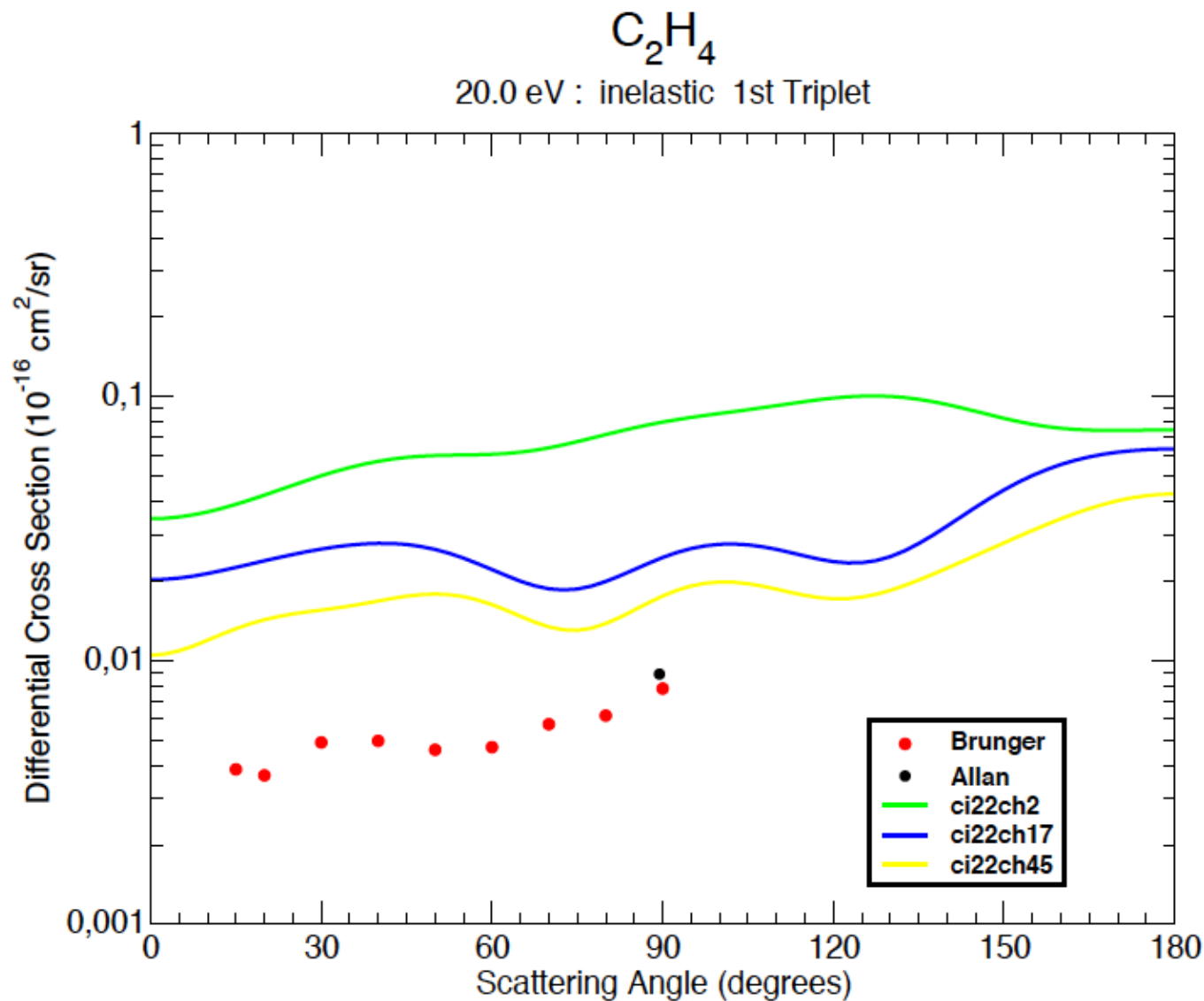
# Multichannel effects on the Electronic excitation of $\tilde{a}^3B_{1u}$ state of $C_2H_4$ by electron impact



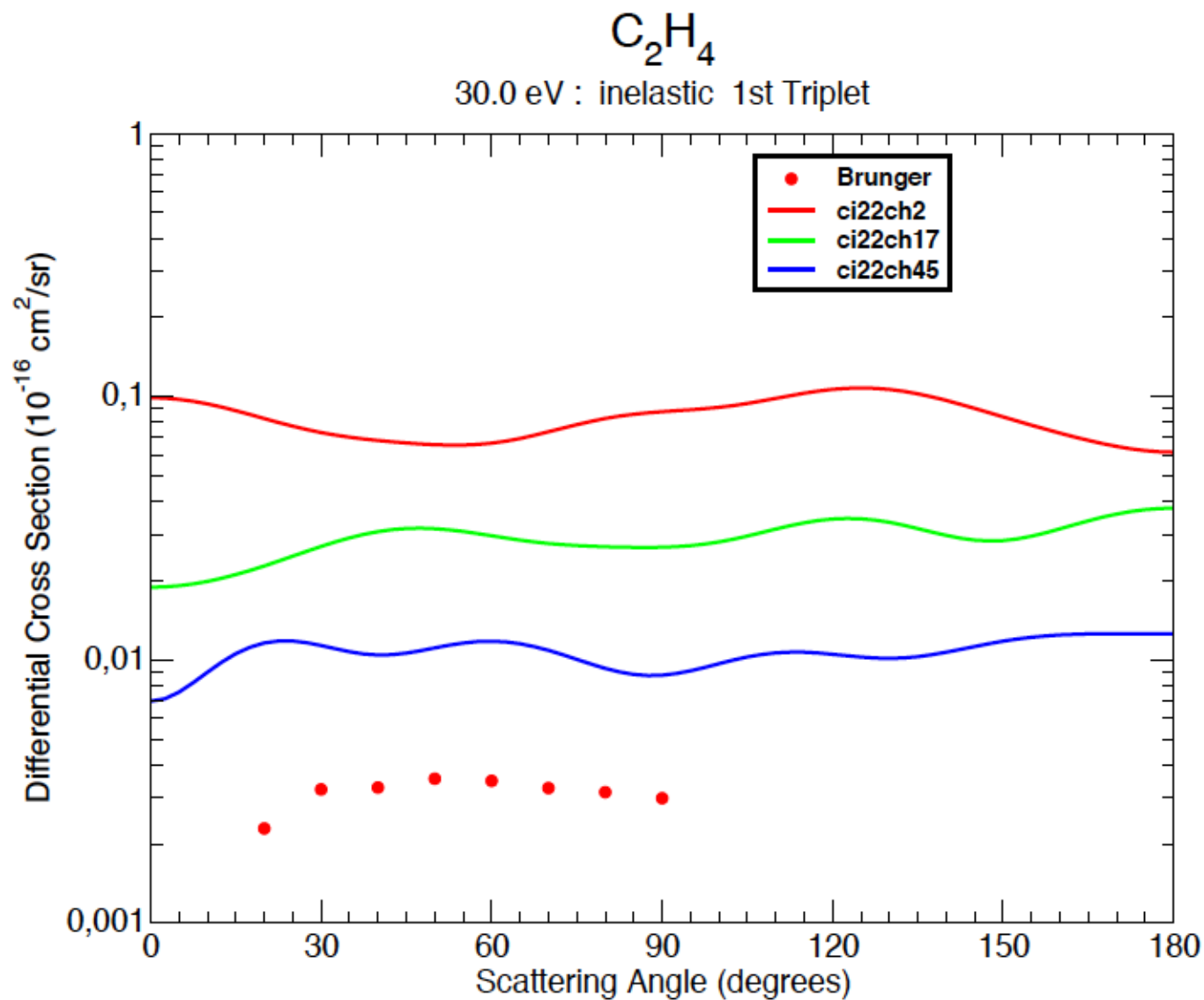
# Multichannel effects on the Electronic excitation of $\tilde{a}^3B_{1u}$ state of $C_2H_4$ by electron impact



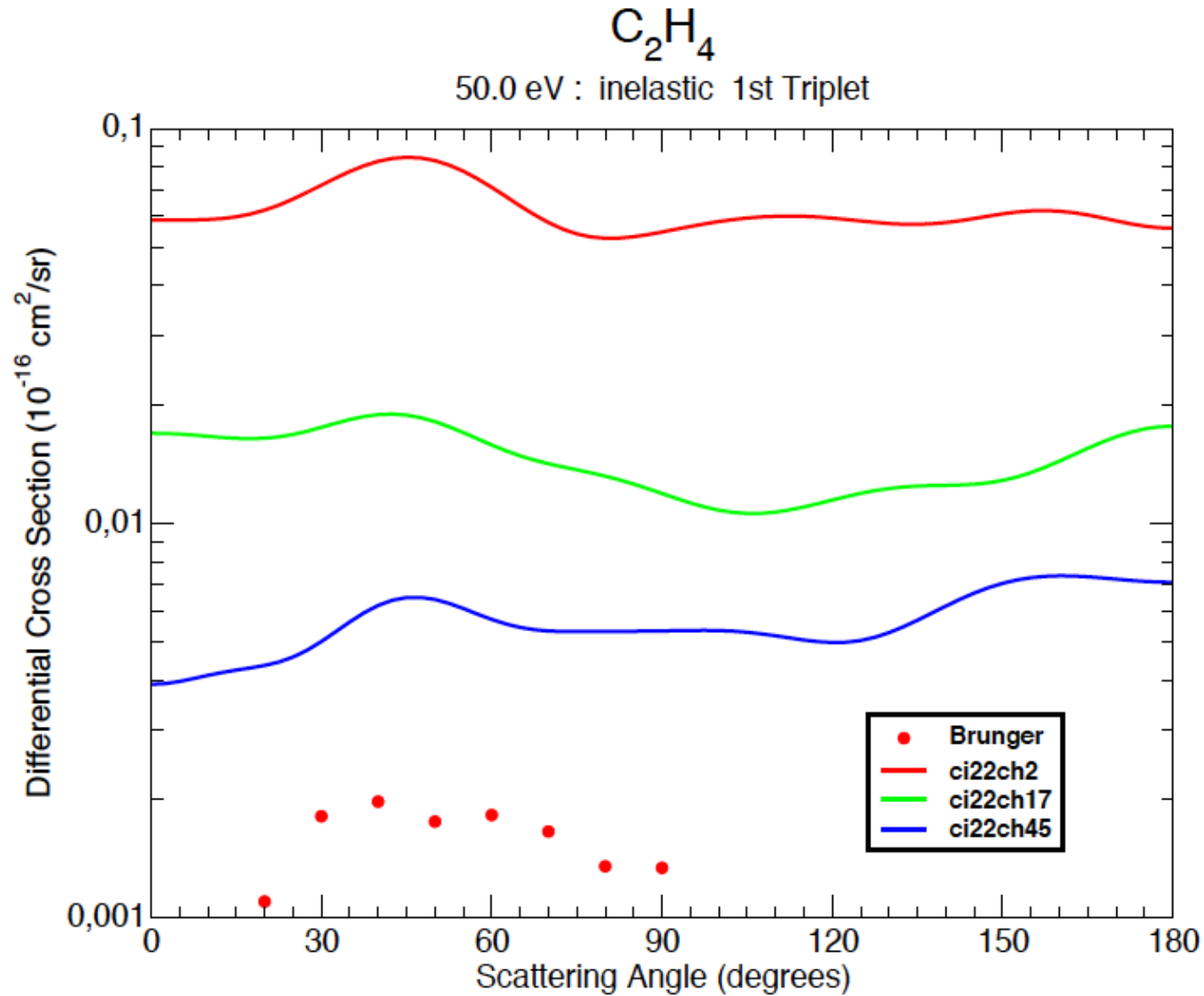
# Multichannel effects on the Electronic excitation of $\tilde{a}^3B_{1u}$ state of $C_2H_4$ by electron impact



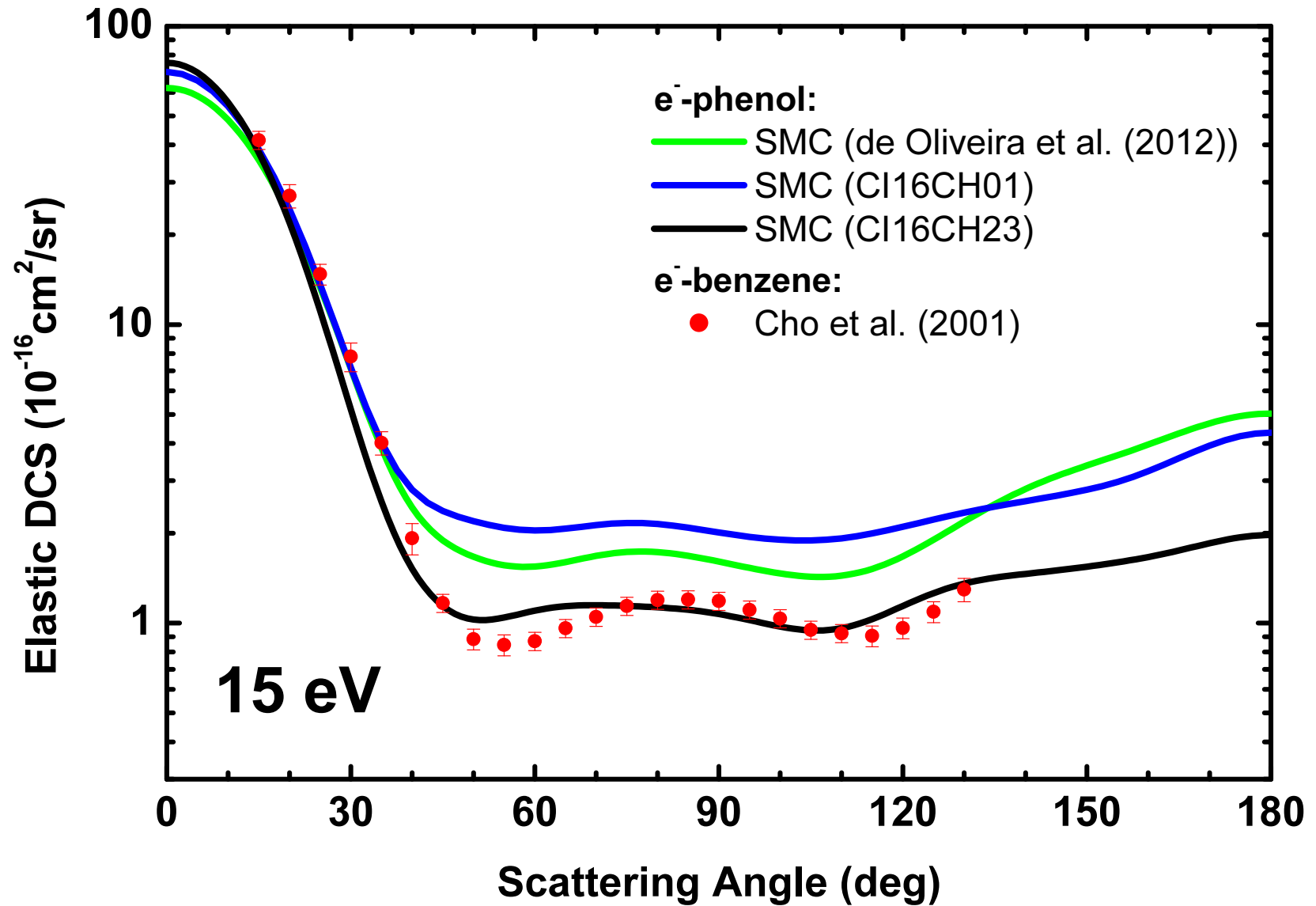
# Multichannel effects on the Electronic excitation of $\tilde{a}^3B_{1u}$ state of $C_2H_4$ by electron impact



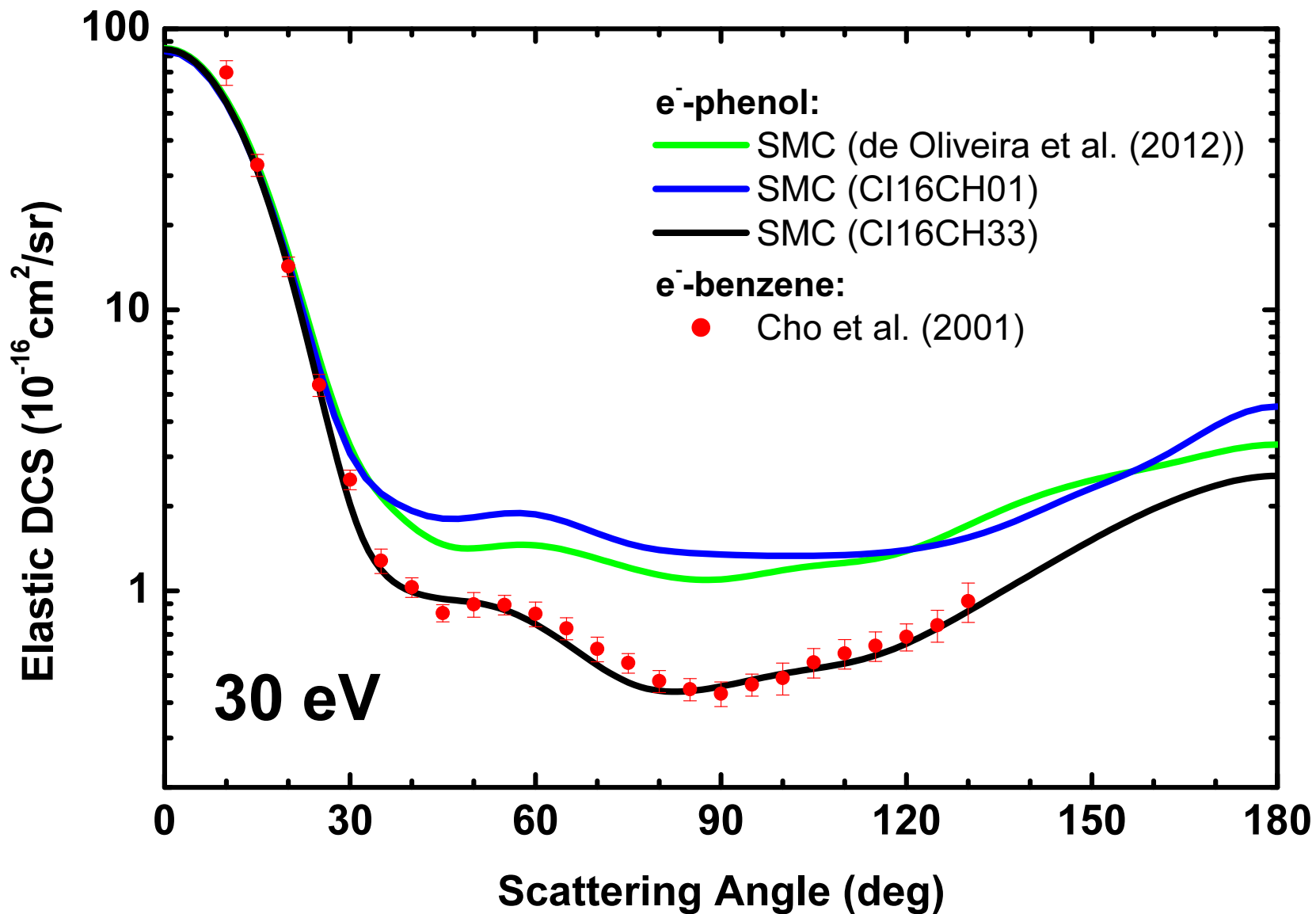
# Multichannel effects on the Electronic excitation of $\tilde{a}^3B_{1u}$ state of $C_2H_4$ by electron impact



## Back to Phenol

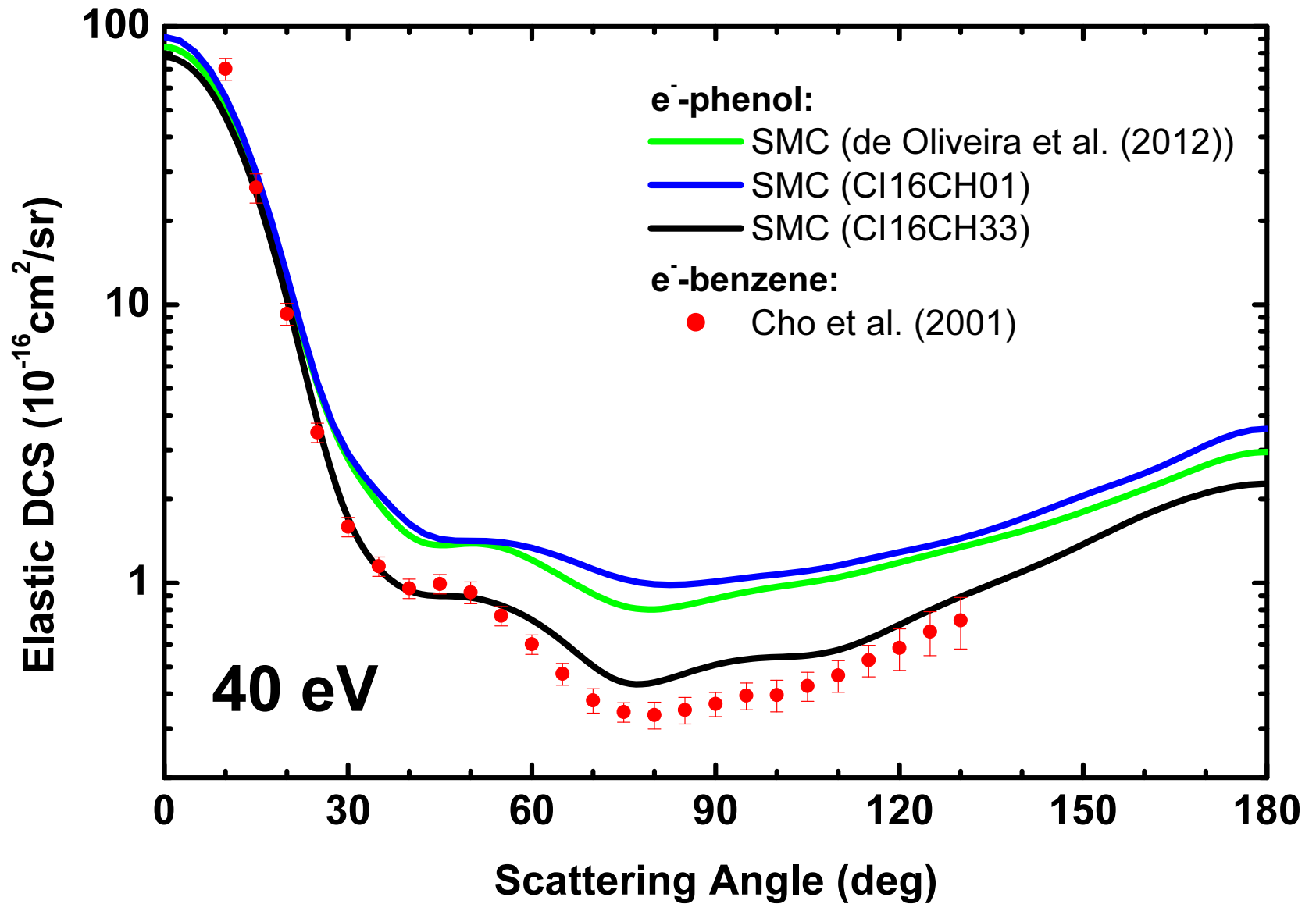


## Back to Phenol

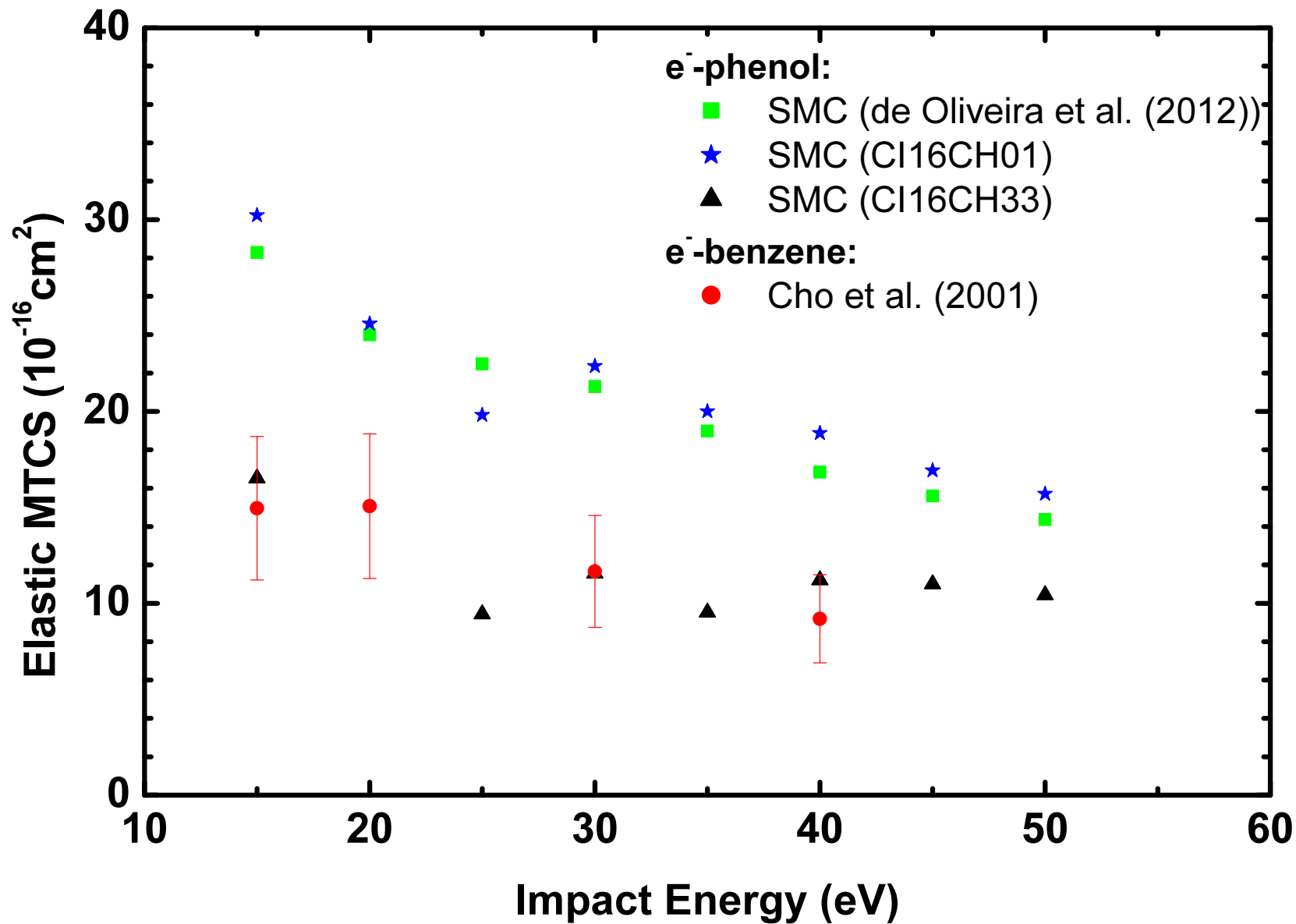




## Back to Phenol

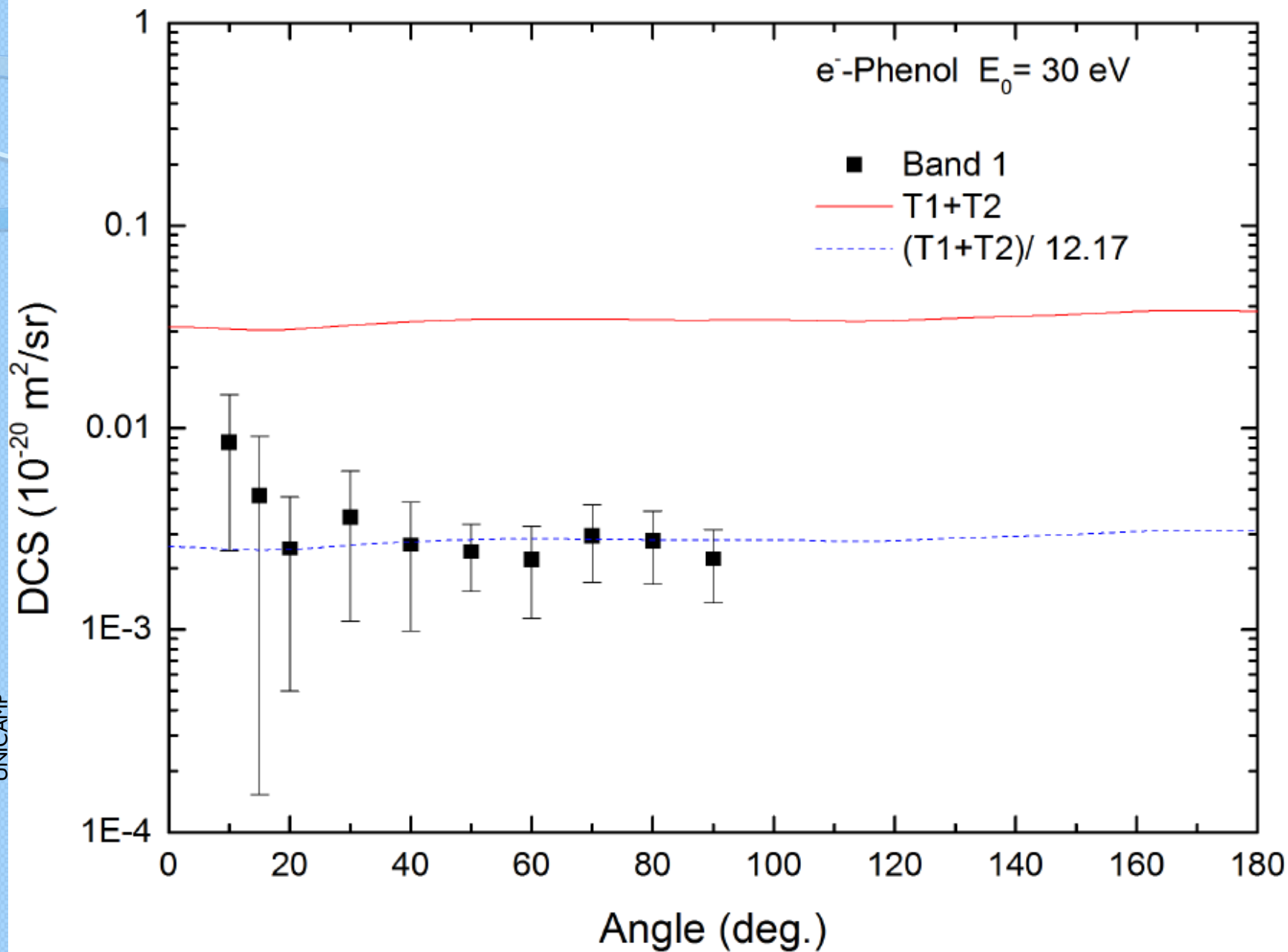


## Back to Phenol



## Back to Phenol

(very fresh data from Michael Brunger/Cristina Lopes collaboration)



# Thank you very much for your attention

A copy of this presentation is at

<http://www.ifi.unicamp.br/~maplima/maplima-IFGW.pdf>