

When Porcini, Cappuccino, Golf, and Cross Sections Meet

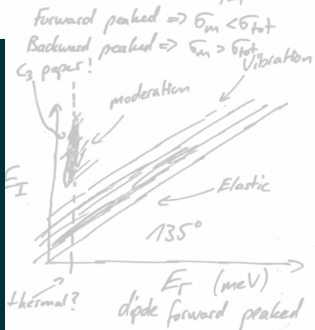
Marnik Metting van Rijn

In memoriam Stephen Biagi

DRD1

8 October 2025

Warsaw Poland



Environmental Friendly Gas Mixtures for Gaseous Tracking and Timing Detectors

Christian M. Franck

01.11.2022 – 31.10.2026

Overview

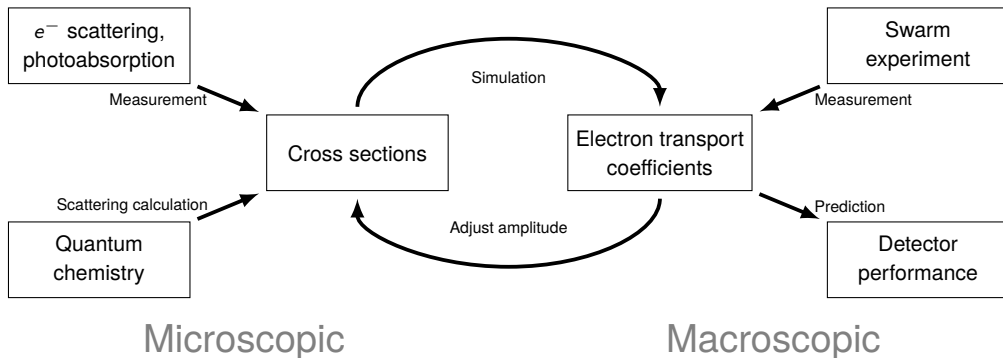
Grant number

212060

- Pulsed Townsend at ETH Zurich
- Expertise in cross sections at CERN
- 1 PhD position dedicated to extracting cross sections from alternative gases

Collaborators: Guida R, Mandelli B, Veenhof R, Verwilligen P, Franck C, Stocco D, Metting van Rijn M, and Biagi S.

Inofficially christened Zurich Project. See slide from Abbrescia M 2025 5th DRD1 
Grant number 212060 2025 Swiss National Science Foundation 



First Meeting with Stephen



Platform 14 Glasgow Central



Protective laptop sleeve



Loyal customer

Comfy Place to Study



Two Cappuccinos Later (~ 1 hour)

Cross-section evaluation 2.12.2022

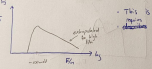
I. Vibrational degree of freedom (Dipole)

Hydrocarbons reveal vibrational excitations at around $\sim 400\text{meV}$ $\sim 500\text{meV}$
 $\rightarrow$ fluorene at $\sim 300\text{meV}$

The physics is described by Born-dipole scattering

$$Q = K \cdot \log \left[\left(1 + \sqrt{1 + \frac{E_g}{E_g}} \right) / \left(1 - \sqrt{1 + \frac{E_g}{E_g}} \right) \right] / E_g$$

$K \propto M^2$ (Matrix element squared)
 E_g (threshold energy) } two fitting parameters



• This is the dipole functional form
 • requires low E_g measurements

Find the optimal parameters values for the amplitude K and the threshold energy E_g , which yield best agreement with drift velocity measurements. Diffusion values are less important.

R137a, C₆F₆ reveal three vibrational modes. HFO1234a also three expected.

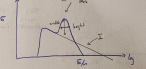
$\text{I: } 0.065\text{ eV}$	C_{60}	} Because, that vibrational modes at less than 400meV require special care, as superelastic scattering is present. no implemented in Mayhew's, uses Born-dipole with a different eqn.
$\text{II: } 0.4004\text{ eV}$	C_{60}	
$\text{III: } 0.1923\text{ eV}$	C_{60}	

Observe mixtures with $\sim 4\text{K}$ is a known gas (Argon)
 Vary the vibration amplitude to fit the measured mixtures
 Measure at low E_g

II General vibrational degree of freedom

$\sim 1-10\text{eV}$

On top of the dipole functional form, resonance is present and fitted with a gaussian



Initial guesses can be obtained from electron scattering data (Centre of Gravity the width and height of the Gaussian are the fitting parameters)

Utilize the symmetry of the molecule to exclude certain vibrational modes as for example rotational in C₆F₆.
 $\rightarrow$ quadrupole moment but often very weak.

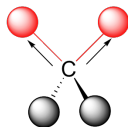
III Two body and three body attachment

- Three body is pressure dependent, whereas two body is not
- Start at low pressure to fix 2body two body attachment
- Increase pressure to obtain the three body attachment

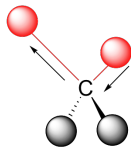
➤ Complete theory on extracting vibrational excitation cross sections.

➤ Me, first year PhD student, completely overloaded.

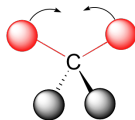
Caffeine and Vibrations



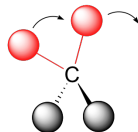
symmetric stretching



asymmetric stretching



scissoring



rocking

Vibrational Excitation in Polyatomic Molecules

$$\sigma_{\nu_0 \rightarrow \nu'} = \frac{8\pi}{3} \frac{1}{k_0^2} \log \left| \frac{k_0 + k_{\nu'}}{k_0 - k_{\nu'}} \right| \underbrace{\left| \sum_{\eta} \langle \nu' | M_{\eta}^{(1)} | \nu_0 \rangle \right|^2}_{I_{\nu' \leftarrow \nu_0}}$$

k_0	Initial electron wave vector
$k_{\nu'}$	Scattered electron wave vector
η	Irreducible representation
$M_{\eta}^{(1)}(\xi)$	Dipole moment
ξ	Nuclear configuration
I	IR absorption intensity
ω	IR frequency

In atomic units and no resonances

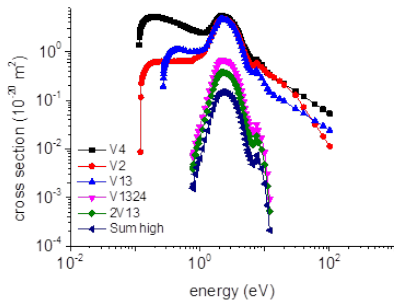
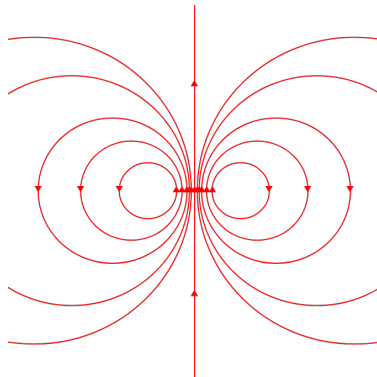


Figure: Vibrational excitations in SiH₄

- Born approximation
- Dipole approximation

Dipole Approximation



Record Harvest on the 10th September 2024



Rotational Excitation in Arbitrary Symmetry

$$\sigma_{J \rightarrow J+1} = P_J \frac{8\pi}{3k_0^2} D^2 \frac{J+1}{2J+1} \log \left| \frac{k_0 + k}{k_0 - k} \right|$$

J Total angular momentum

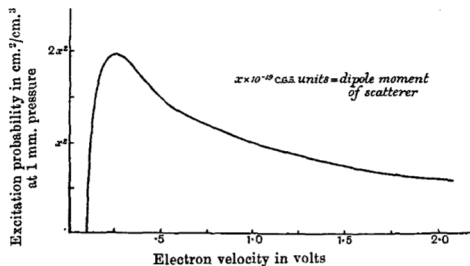
P_J Level population

k_0 Initial electron wave vector

k Scattered electron wave vector

D Static dipole moment

- Born approximation
- Dipole approximation
- Rigid rotor



In atomic units and no resonances

Combining Rotational and Elastic

Molecule	$B_{\max}$ (cm^{-1})	E_{rot} (meV)
H_2O	28	3.5
R134a	0.2	0.02
C_2F_6	0.1	0.01
C_3F_8	0.06	0.007

- Rotational spacing small
- Dipole moment is large

$$B = \frac{h}{8\pi^2 c I}$$

I moment of inertia.

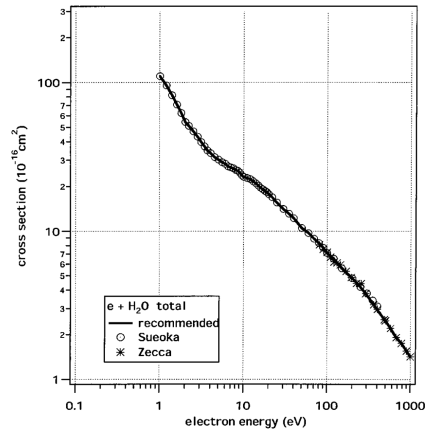
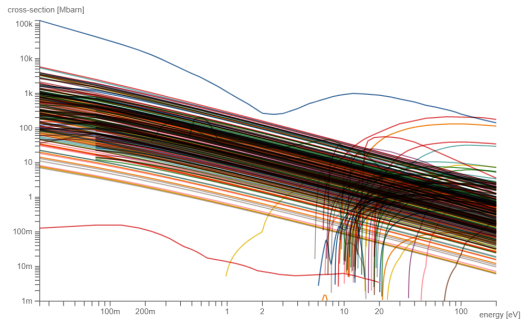


$E_{\text{rot}} \ll \langle E \rangle_{\text{avg}}$, almost hard sphere (elastic)

CCCBDB, 2022 NIST Standard Reference Database Number 101 [↗](#)
Golf.com Titleist pro v1x 2025 [↗](#)



Rotational Excitation Cross Sections in Water Vapor



Total scattering cross section

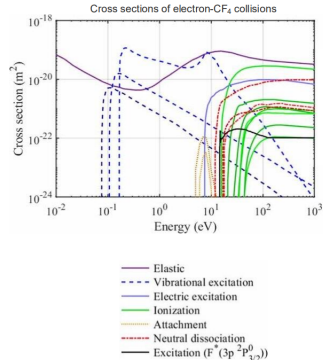
Using CF₄ to make a “fast gas”

CF₄'s vibrational modes suppress elastic electron back-scattering, enabling efficient electron propagation through the gas.

- CF₄ cross-sections are well-characterized and available in **MAGBOLTZ**.
- Monte Carlo simulations can study detector performance with lower CF₄ fractions.

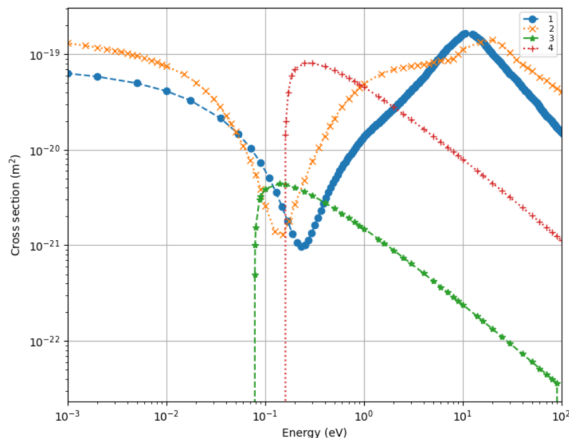
Its unique properties driving these cross-sections appear unique.

- Understanding why CF₄-based gases are fast will aid in identifying new gas candidates.
- Detector designs can be adapted for new gases.



Cross-sections plot taken from: Xiao-Kun Wang et al 2024 Plasma Sources Sci. Technol. 33 085001. 3

An Interplay of the Ramsauer Minima and Vibrations



1: Ar elastic, 2: CF₄ elastic, 3 and 4: CF₄ vibration

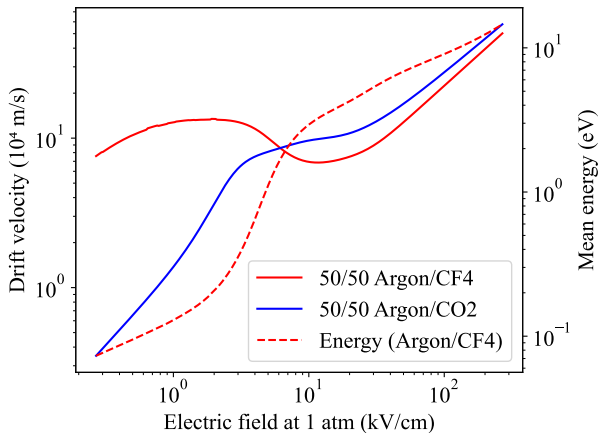
Swarms with mean energy confined to Ramsauer minima are fast.

- Rotational spacing small $B \rightarrow 0$
- Weak coupling to electron $D = 0$
- s -wave scattering, $\delta_0 = n\pi$ (Ramsauer minima)

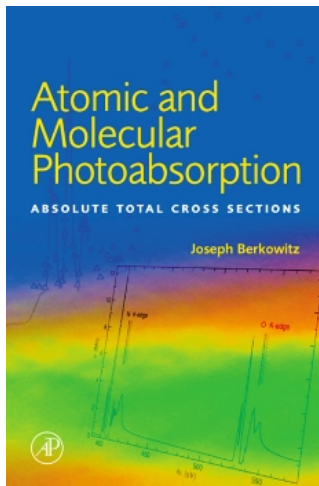
$D = 0 \not\Rightarrow$ Deep minima. Necessary but not sufficient, counterexample (CCl₄)

Bordage, M *CF₄ Bordage database* [↗](#)
Biagi, S *Ar Magboltz* [↗](#)
Plot generated on LXCat [↗](#)

Higher Mean Energy $\neq$ Higher Drift Velocity



'Always Hide the Covers of Physics Textbooks'



Ionization Impact Collision Cross Section

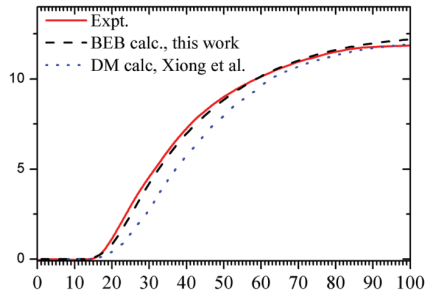


Figure: Cross section in Å² as function of incident electron energy in eV. (CF₃)₂CFCN

Ranković, Milos, et al. *Physical Chemistry Chemical Physics* **21.30** (2019): 16451-16458.

Kim, Yong-Ki, and M. Eugene Rudd. *Physical Review A* **50.5** (1994): 3954.

Mott

Electron-Electron collision

Bethe

$\sigma \sim (\log E)/E$ for $E \rightarrow \infty$

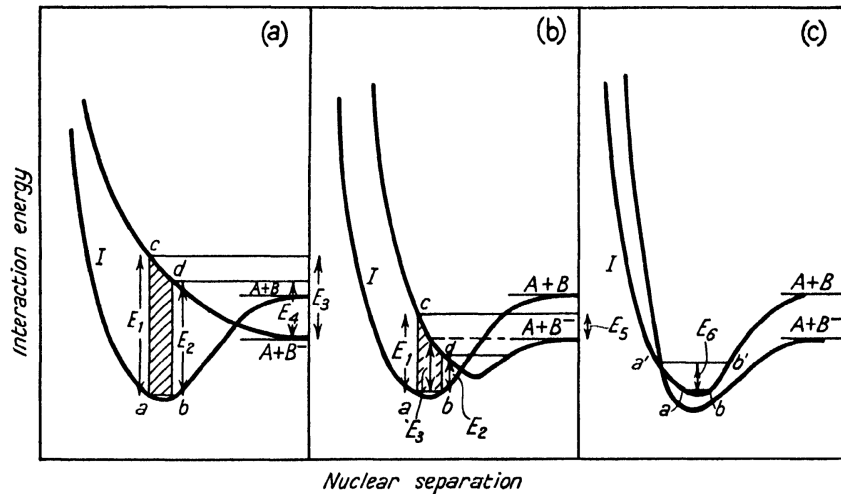
Binary-Encounter-Bethe theory (BEB) combines

$$\sigma_{\text{BEB}}(t, u) = \frac{S}{t + u + 1} \left[\frac{\log t}{2} \left(1 - \frac{1}{t^2} \right) + 1 - \frac{1}{t} - \frac{\log t}{t + 1} \right]$$

$$t = E/B, \quad u = U/B, \quad S = 4\pi a_0^2 N R_y^2 / B^2,$$

E	Electron energy
R_y	Rydberg energy
N	electrons in subshell (qt. nr. l)
B	Binding energy
U	$\langle p^2 \rangle / 2m_e$ in subshell

Resonances in Vibrations and Attachment Are Related



Massey and Burhop 1952 *The International series of monographs on physics* Oxford, Clarendon press p. 225

Finishing Steve's Last Work

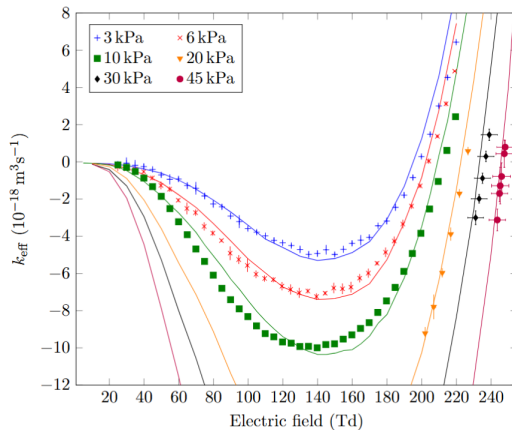


Figure: Preliminary results for HFO1234ze(E) cross section.

A Lasting Impression

- Supportive, attending talks
- Providing honest and helpful feedback
- Made me want to continue in this field

Stephen Francis Biagi (1949-2025)



*A dedicated mushroom hunter, golfer,
father, and an inspiring physicist.*

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