

# A Compilation of Electron-Molecule Scattering Cross Sections

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## 1 Introduction

The intention of this project is to attempt to update the critical review and cross section data compilation of Trajmar et al. [1] to account for measurements over the past 15 years. As in the original review the emphasis will be on both differential and integral cross section measurements at low to intermediate energies (meV-1000 eV) for elastic scattering, rotational, vibrational and electronic excitation. These cross sections are of relevance in applied areas as divergent as plasma deposition and etching of semiconductors, gaseous high voltage switches and electrostatic precipitators for the processing of atmospheric pollutants. The active constituents in each of these devices are typically polyatomic molecules and as such there has been a marked increase in both experimental and theoretical studies for these complicated targets.

We will also attempt to discuss in a critical fashion the comparison between the various experimental results and between the experimental and theoretical cross sections. However it is beyond the extent of this article, and the expertise of the authors, to offer a detailed critique of the many theoretical approaches. We shall give a brief discussion of experimental techniques with particular emphasis on new developments in the measurement of absolute scattering cross sections since Trajmar et al. [1] Finally we note that whilst temporary negative ion resonances are often of great importance in low energy electron-molecule scattering the treatment of resonance dynamics is beyond the scope of this project and we will only discuss them in the context of cross section enhancement.

## 2 Scope

The extent of the review article is perhaps best illustrated by its table of contents, as given below:

<b>1.</b>	<b>Introduction</b>	<b>3.</b>	<b>Experimental Data</b>	<b>-</b>
<b>2.</b>	<b>Experimental Techniques - Recent Developments</b>		<b>Diatomic Molecules</b>	
2.1	High resolution sources	3.1	H <sub>2</sub>	
2.2	Single collision experiments	3.2	N <sub>2</sub>	
2.3	Swarm experiments	3.3	O <sub>2</sub>	
2.4	Parallel detection techniques	3.4	Halogens	
2.5	Sources of excited species	3.5	CO	
2.6	Normalisation techniques	3.6	NO	
2.7	Techniques for the generation of integral cross sections	3.7	Hydrogen Halides	
		3.8	Alkali Halides	

3.9	Cross section trends amongst diatomic molecules.	4.11	Hydrocarbons and derivatives
<b>4.</b>	<b>Experimental Data – Polyatomic Molecules</b>	4.12	Silane and derivatives
4.1	H <sub>2</sub> O	4.13	Germane and derivatives
4.2	H <sub>2</sub> S	4.14	Halocarbons and derivatives
4.3	HCN	4.15	SF <sub>6</sub>
4.4	O <sub>3</sub>	4.16	Cross section trends amongst polyatomic molecules
4.5	OCS	<b>5.</b>	<b>Epilogue</b>
4.6	CO <sub>2</sub>	<b>6.</b>	<b>Summary and Suggested Measurements</b>
4.7	N <sub>2</sub> O	<b>7.</b>	<b>References</b>
4.8	NH <sub>3</sub>	<b>8.</b>	<b>Appendix</b>
4.9	SO <sub>2</sub>	8.1	Tables of cross section data
4.10	CH <sub>4</sub>		

It is our intention that, subject to satisfying copyright requirements, all the cross section data tables will be placed on the Web for viewing and downloading.

### 3 Status of Project

At this time we have covered about 80-85% of the topic and hope that the final sections and editing can be completed in the next 6-9 months. The article will contain in excess of 260 tables of cross section data and over 200 figures, as well as a (hopefully) critical assessment of the cross sections for each gas. The reference list currently stands at 750, most of which is due to work that has been generated since the original review of Trajmar et al. [1]

### 4 Highlights

One of the nice things about a review such as this is that, in having an extensive database available at your fingertips, you can start to get a picture for any trends in the cross sections for a given molecule, or across different molecular species, and for any gaps (either experimental or theoretical) in the literature. This in turn allows one to form an opinion as to where it might be profitable to conduct new experiments or perform new calculations in the future.

We now examine just two of these areas, both of which we believe are illustrative of some very interesting physics.

### 5 Cross Section Trends Across Molecules

In the graphs in Fig. 1, we show the results of some elastic differential cross section (DCS) measurements for electron scattering from N<sub>2</sub>, CO, O<sub>2</sub>, NO, and CO<sub>2</sub>. All the illustrated data were measured at the Australian National University (ANU) with a crossed beam apparatus and employed the relative flow technique [2] to set the absolute scale.

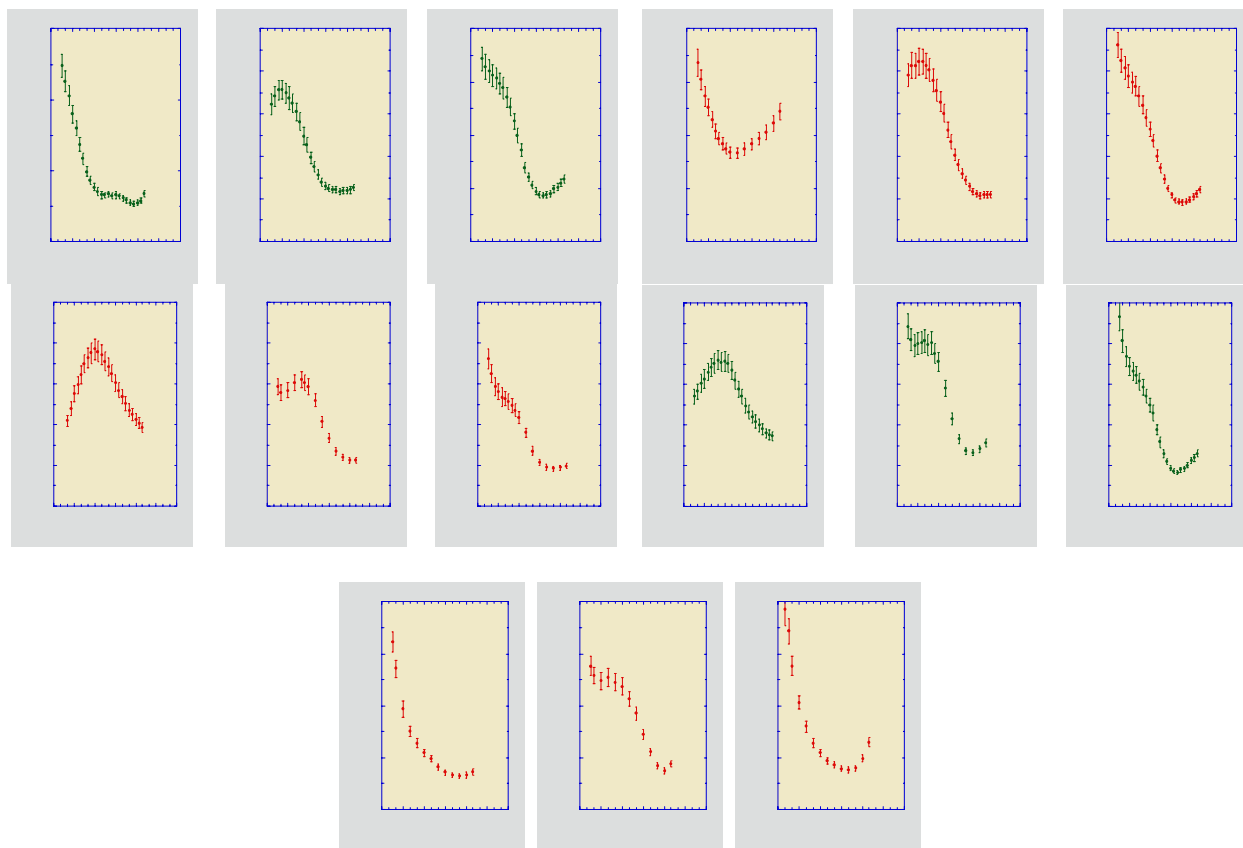


Figure 1: Elastic differential cross section (DCS) measurements for electron scattering from  $N_2$ ,  $CO$ ,  $O_2$ ,  $NO$  and  $CO_2$ . See text for explanation.

For each of these molecules we observe an interesting behavior in the elastic DCS at forward angles. This occurs at energies above the shape resonance in each molecule but below about 10 eV. This behavior appears to be associated with those systems that possess a strong, low energy shape resonance. Where the resonances are at relatively low energy and are “sharp”, e.g.  $O_2$  and  $NO$ , the DCS at low energy ( $\sim 1$  eV) dips strongly at forward scattering angles. It then passes through a transition from weak forward scattering to a forward-peaked DCS in the energy region 4-7 eV. In the other systems ( $N_2$ ,  $CO$ ,  $CO_2$ ), which all have a broad shape resonance that peaks between 2-4 eV, the DCS in the resonance region are strongly forward peaked but then decrease in magnitude at forward angles as the energy increases just above the resonance.

Sun et al. [3] noted, in their calculations of  $N_2$  elastic DCS, that above the resonance, where the  $\Pi_g$  symmetry is no longer dominant, it is essential to include higher order partial waves and additional symmetries to reproduce the observed behavior. In the case of diatomic systems it is interesting to note that each of the above molecules possess similar dipole polarisabilities and so it is tempting to speculate that it is this which may be responsible for the angular behavior of the DCS. However, as it also appears that this effect is present in a class of polyatomic molecule systems the problem is deserving of some careful theoretical attention.

## 6 Polyatomic Molecule Scattering Theory

Most polyatomic molecule scattering calculations have concentrated on DCS and integral cross sections (ICS) for the elastic scattering process, although some calculations for excitation of the vibrational modes of molecules are available in the literature. In this latter case both DCS and ICS are also typically reported. An extensive series of calculations have been performed for elastic scattering from methane which, because of its near-spherical symmetry, has become something of a prototypical system for low energy electron-polyatomic molecule scattering calculations. A summary of the available experimental and theoretical data for this molecule can be found in the recent publication of Bundschu et al. [4]

In Fig. 2, we show the level of agreement that has been obtained amongst experimental groups and between theory and experiment for  $\text{CH}_4$ . While we only show DCS at 1 eV and 3 eV, the level of accord in these figures is indicative of that found up to about 5.5 eV. Note the very good agreement between the two most recent experimental measurements [4] [5], both of which independently applied the relative flow technique, and between these measurements and the calculation of Gianturco and Sanna [4].

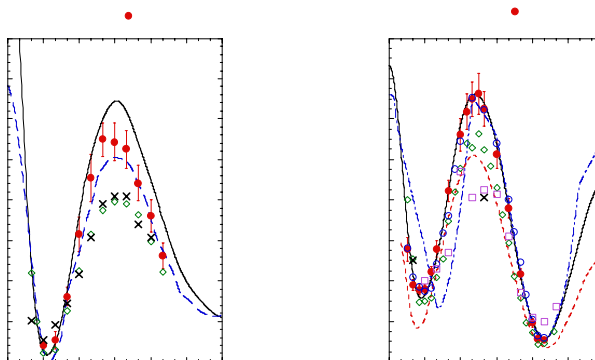


Figure 2: Comparison of theory and experiment for  $\text{CH}_4$  at 1 eV and 3 eV. See text for explanation.

Unfortunately, this level of agreement between theory and experiment for low energy elastic polyatomic molecule scattering is quite unique. In general, for energies less than 10 eV, one usually finds quite poor agreement between the calculations and measurements, as we now specifically illustrate for  $e^- + \text{CO}_2$  scattering.

In the next figure, we show the situation in  $\text{CO}_2$  at energies of 1 and 5 eV. Whilst it is clear that the level of agreement between the various experiments is only fair, the major point that we wish to make here is the serious discrepancies between experiment and theory. Neither the model of Takekawa and Itikawa or that of Gianturco and Stoecklin adequately reproduces the shape or magnitude of these low energy DCS, even when additional symmetries were employed in the latter case.

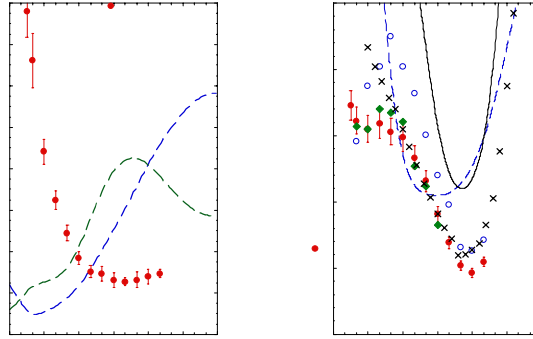


Figure 3: Comparison of theory and experiment for CO<sub>2</sub> at 1 eV and 5 eV. See text for explanation.

## References

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