

Shape resonances in electron scattering

[EIPAM 07](#)

[Electron Induced Processes At the Molecular Level](#)

[25th - 29th of May 2007, Hveragerði, Iceland](#)

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Historically [1], resonances in electron scattering on atoms and molecules have been classified into Feshbach resonances, i.e. associated with some inelastic thresholds, and resonances due to “capturing of an incoming electron into a barrier of effective, i.e. with the centrifugal force, potential”. G. Schulz [1] discovered both classes: a sharp up-and-down structure in the differential cross section at 72° degrees for electron scattering on He just below the threshold for the first electronic excitation, and 2) a maximum in the total cross sections in N_2 at about 2.1 eV. Fingerprints for resonances are, among others, sharp maxima in total cross sections, electron attachment processes occurring in a narrow energy range or maxima for vibrational excitation cross sections. In course of research, it entered into custom that almost any rise in the total and/or partial cross section, like wide maxima in total cross sections for hydrocarbons, occurring at about 8-9 eV are associated with a “resonance”. The need for re-examination of the very definition of resonances comes from the recent discovery of enhanced annihilation rates for positrons at low energies in some hydrocarbons, in the vicinity of vibrational excitation thresholds and from the electron attachment processes occurring at energies below 1 eV in many different organic molecules [2].

Ugo Fano associated theoretically resonances to *rapid* changes by $\pm 180^\circ$ in the phase shift for scattering of single partial waves. From this point of view, the maximum in the total cross section at 9 eV for electron scattering on CH_4 hardly can be classified as a resonance, and in particular as a shape resonance. One should rather speak about a maximum in the partial cross sections due to the slow passing of the phase shift by $\pi/2$, although the electron attachment processes, leading to formation of H^- and CH_2^- ions, are present in that energy region, see [3]. Note also that amplitudes of maxima in molecules CH_4 , GeH_4 , SiH_4 rise as they shift to lower collision energies, thus suggesting a dominating contribution from a single partial wave [4].

A similar rising of the total cross section maxima with lowering their energy is observed in series of linear triatomic molecules CO_2 , N_2O , OCS or for diatomic N_2 and CO . These series of targets show a big contribution to the total cross section in maxima coming from the vibrational excitation (about 1/6 of total for CO and N_2 and about 1/3 for triatomic molecules); no electron attachment is present in N_2 (this molecule, as far as we know does not form negative ions with

measurable life-times) but as much as 1% of the total cross section comes from electron attachment in triatomics [3]. If a single partial wave is attributed to the maxima in the total cross sections in N_2 and CO this would be the s -wave (not forming the centrifugal barrier!). On the other hand, differential cross sections for the lowest-level vibrational excitation show a perfect d -wave dependence in N_2 and p -wave dependence in CO, see [3].

Theoretical calculations, even in the case of N_2 , fail to predict the exact position and the amplitude of the total cross section and in the case of triatomic molecules, like N_2O they fail to predict even an approximate position of the maximum. Obviously, calculations start from molecular configurations obtained by quantum chemistry methods. At this point, it is also hard to say in the incoming electron is captured into an *overall* potential of the molecule or due to a particular *configuration of orbitals*. Therefore, the distinction between the shape resonance or a capture to a single molecular orbital is hard.

Recently, we [5] have developed an analytical method for solving the modified effective range problem. In the effective range theory the scattering is assumed to be only due to a polarization potential and the effective range is introduced to account for short range interactions. Numerous previous applications of MERT failed to work above a few tenths eV because diverging series in an approximate approach were used. For positron scattering on Ar and N_2 we showed that the analytical solutions work up to 2 eV or so [5].

In present work we applied the new MERT for electron scattering on N_2 and CO_2 . The experimental total cross sections below 1 eV have been approximated by two partial waves, and the scattering length and the effective ranges have been obtained. Extending the calculation on such a potential to higher energies, much to our surprise, we are able to reproduce the position and the amplitude of the total cross section at low energy resonances. Obviously, these are elastic cross sections obtained in our calculations.

If so, the 2.1 eV and 3.8 eV resonances in N_2 and CO_2 , respectively, could be classified as *pure* shape resonances: they occur just due to the overall form of the potential, parameterized by the molecular polarizability and four short range parameters (effective range and scattering lengths for the two, s and p waves). At this point, the rise in the partial cross sections would be just a *by-product* of the enhanced total scattering probability.

References:

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