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Recent Theoretical Results on Electron-Polyatomic Molecule Collisions

C. William McCurdy
National Energy Research Supercomputer Center
Lawrence Livermore National Laboratory
Livermore, California 94550

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RECENT THEORETICAL RESULTS ON ELECTRON-POLYATOMIC MOLECULE COLLISIONS

C. W. McCurdy
Lawrence Livermore National Laboratory, Livermore, CA 94550

ABSTRACT

Until recently, the principal barrier to the accurate theoretical description of electronic collisions with polyatomic molecules was the computational problem of scattering by a nonlocal, arbitrarily asymmetric potential. Effective numerical techniques capable of solving this variety of potential scattering problem for electronic collisions have now matured, and the first applications of methods for treating many-body aspects of collisions of electrons with polyatomic molecules have begun to appear in the literature. The past two years have seen the appearance of a large collection of calculations on electron-polyatomic collisions which compare favorably with experimental determinations. In addition to the dramatic developments in methods which explicitly exploit the methods of quantum chemistry to treat the effects of electron correlation, polarization, etc., parameter-free model potential methods for electronically elastic collisions have also evolved markedly in recent years. Progress in both electronically elastic and inelastic processes is reviewed briefly.

I. INTRODUCTION

The most remarkable fact about the published literature on the accurate theoretical treatment of electron-polyatomic molecule scattering is that there is so little of it. The discipline has lagged ten or fifteen years behind theoretical developments in electron-atom scattering.[1,2] Surprisingly, this disparity in theoretical progress has occurred even for fixed-nuclei calculations and is *not* due to the inherent difficulty of treating phenomena associated with nuclear motion in molecules. The first barriers to the development of successful treatments of electron-molecule scattering were associated with the difficulties of treating collisions with arbitrarily nonspherical targets with nonlocal (exchange) potentials. Even calculations at the static-exchange level on polyatomic targets began to appear only in the late 1980s.[3,4] In this review I will maintain that the recent literature on electron-polyatomic molecule collisions gives ample evidence that the problem of scattering electrons from nonspherical, nonlocal potentials has been solved effectively by several computational approaches. More serious problems in the physics of electron-polyatomic collisions now dominate the field.

To understand recent changes in the capabilities of workers in this area, consider the following comparison. The role of configuration interaction in electron-atom scattering was already the subject of *review* talks by 1976.[5] It is accurate to say that as of 1993 the consequences in electronic collisions of the effects of configuration interaction in target states of polyatomic molecules have hardly begun to be dealt with (although considerable efforts have been made for diatomics). The reason for this disparity is that

the technology for treating the bound states of polyatomic molecules, that is, the algorithmic edifice of quantum chemistry, has proved to be difficult to couple to electron scattering calculations. Typical configuration interaction calculations on bound electronic states of polyatomics involve tens or hundreds of thousands (if not millions) of configurations of Gaussian orbitals. The awkwardness of incorporating such target descriptions in old-style scattering calculations involving single-center expansions of the continuum functions is apparent. Less obvious, but even more troublesome, is the problem of consistency in treating the N-electron target and (N+1) electron collisional correlation problems.

However, even these barriers are being surmounted, and that is the real news in this brief review.

There is another story to tell, and that concerns the evolution of model potential calculations on electronically elastic scattering from polyatomic targets. The earliest calculations (by far) on polyatomic molecules which bore comparison with experiment were of this variety, and some such methods have been improved to be parameter-free and have a well understood range of reliability.

II. THEORETICAL METHODS FOR POLYATOMIC COLLISIONS

This section presents a terse catalog of the methods which have been successfully applied in accurate calculations on polyatomic systems.

A. Variational Methods

While variational methods based on the Kato identity[6] or the Schwinger principle[7] have been historically prominent in the development of electron-atom scattering, they were slow to be applied to molecular collisions. Once the problems with resonance-like anomalies in the Kohn variational approach were overcome, that approach found immediate application in the molecular context. The key barrier to be overcome in applying the Schwinger principle was the computation of Green's function matrix elements for molecular wave functions. These two variational methods have an important feature in common, namely that they involve an explicit specification of the trial function in terms of molecular target states. The form of the trial function provides the starting point for incorporating the wave functions and techniques of quantum chemistry.

(1) The Complex Kohn Variational Method

The Kohn variational method, in a version called the "complex Kohn variational method", was first applied to electron-polyatomic molecule scattering[4] shortly after Miller and Jansen op de Haar observed[8] that a simple change in the boundary conditions (from principal-value to traveling-wave) eliminates the numerical pathology of anomalous resonances which plagued applications of the Kohn approach to electron-atom scattering. In the complex Kohn method the Kohn principle is used to determine the T matrix connecting channels Γ and Γ_0 as the stationary value of the functional

$$[T^{\Gamma\Gamma_0}] = T^{\Gamma\Gamma_0} - 2\int \Psi_\Gamma (H-E)\, \Psi_{\Gamma_0} \qquad (1)$$

The trial function is chosen to have the form

$$\Psi_{\Gamma_0} = \sum_{\Gamma} A\,[\chi_\Gamma(\vec{r}_1, \ldots, \vec{r}_N)\, F_{\Gamma\Gamma_0}(\vec{r}_{N+1})] + \sum_{\mu} d_\mu^{\Gamma_0} \Theta_\mu(\vec{r}_1, \ldots, \vec{r}_{N+1}) \qquad (2)$$

In Eq.(2) χ_Γ denotes an open-channel target state, the Θ_μ are square-integrable, antisymmetric (N+1) electron functions, and $F_{\Gamma\Gamma_0}$ is a channel continuum function whose short-range behavior is represented by an expansion in Gaussians and whose long-range behavior is explicitly specified in terms of the Riccati-Bessel functions j_l and $h_l^{(+)}$. The functions χ_Γ and Θ_μ are constructed, as are typical components of quantum-chemistry calculations on bound electron states, in terms of antisymmetric configurations of molecular spin orbitals which are in turn expanded in Gaussians centered anywhere in the molecule.

An additional twist on this approach,[4, 9] which aids in casting as much of the calculation as possible in a form which can be done by standard quantum-chemistry codes, is to use Feshbach partitioning on the trial wave function in Eq.(2) and define the Q-space (closed-channel space) as the space of the Θ_μ functions. Then H in Eq.(1) is replaced by $H_{effective}$ which includes the *ab initio* optical potential

$$H_{effective} = H_{PP} + H_{PQ}(E - H_{QQ})^{-1} H_{QP}. \qquad (3)$$

It is this form which has been applied extensively to both electronically elastic and inelastic electron-polyatomic scattering by McCurdy, Rescigno, Lengsfield, Schneider and their coworkers. Only Hamiltonian matrix elements (no Green's function matrix elements) with respect to the functions χ_Γ and Θ_μ are required so that implementing the connection to quantum chemistry codes is direct and simple.

(2) The Schwinger Multichannel (SMC) Variational Method

In the implementation of this approach to electron-polyatomic molecules collisions[5,10] the (N+1) electron wave functions of the electron-molecule scattering system are expanded in a basis and the coefficients determined by extremizing the Schwinger variational expression for the scattering amplitude

$$f(\vec{k}_m, \vec{k}_n) = -\frac{1}{2\pi} \sum_{i,j} \langle S_m(\vec{k}_m) | V | \chi_i \rangle A_{ij}^{-1} \langle \chi_j | V | S_n(\vec{k}_n) \rangle \qquad (4)$$

In Eq.(5) the χ_i are the expansion basis, $S_m(\vec{k}_m)$ is the unperturbed scattering function

$$S_m(\vec{k}_m) = \phi_{target}^{(m)}(1, 2, \ldots, N)\, exp\,(i\vec{k}_m \bullet \vec{r}) \qquad (5)$$

V is the interaction between the scattered electron and the target, and A_{ij}^{-1} are elements of the inverse of the matrix

$$A_{ij} = \langle \chi_i | A^{(+)} | \chi_i \rangle \qquad (6)$$

of the operator $A^{(+)}$. That operator is given by

$$A^{(+)} = \frac{1}{2}(PV + VP) - VG_P^{(+)}V - \frac{1}{N+1}\{\hat{H} - \frac{N+1}{2}(\hat{H}P - P\hat{H})\} \qquad (7)$$

where $\hat{H} = E - H$, and it involves the N-electron projection operator P which projects on open channels and the projected, free-particle Green's function $G_P^{(+)}$

In this procedure both the expansion basis and the target states are objects from the technology of quantum chemistry. Green's function matrix elements are required in addition to matrix elements of the Hamiltonian, but in return for expending the effort to compute them one gains considerable flexibility in the choice of the expansion basis, $\{\chi_i\}$, which can be used to exploit the efficient convergence properties of the Schwinger method. The general approach was formulated by Takatsuka and McKoy[11] and has been applied to polyatomics by McKoy and coworkers and by Huo and coworkers.

B. The R-matrix Method for Polyatomics

While computational applications of R-matrix theory to electronic collisions with atomic[12] and diatomic[13, 14] targets date from the 1970's, only very recently, to my knowledge, has this approach been applied for the first time to a nonlinear polyatomic target in an *ab initio* calculation.[15] From a schematic view of the R-matrix method one can see the computational barriers which have to be overcome in a polyatomic application as well as how an explicit connection with the methods of quantum chemistry can be made.

The essence of the R-matrix idea in this context is to solve the (N+1)-electron problem in a region confined to a finite sphere while enforcing boundary conditions which discretize the spectrum of the (N+1)-electron Hamiltonian. Those discrete states are then used to expand the scattering wave function inside the sphere, and that expansion is matched to the asymptotic form (incorporating explicit N-electron target states) on the surface of the sphere. The point to emphasize is that the (N+1)-electron problem must be solved on a finite region—a task that no quantum chemistry code is constructed to perform.

An implementation which is suitable for polyatomic applications has been developed by Nestmann, Nesbet, Peyerimhoff and Pfingst.[15,16] They solve the key computational problems of the method for polyatomics as follows.[15]

- Cartesian Gaussians are used to form an (N+1)-electron basis.
- The electron-repulsion integrals along with nuclear attraction integrals are confined to the R-matrix sphere by using a multipole expansion to approximate an effective potential outside the sphere. Using this device to subtract off the $r > a$ contribution allows the use of standard codes for the calculation of two-electron molecular integrals.
- Correlation and polarization effects are only taken into account for selected, energetically low-lying (N+1)-electron CI roots (the R-matrix poles), which have nonvanishing amplitudes on the R-matrix sphere. Higher lying roots are approximated by a Static-Exchange calculation.

While complete details of a polyatomic application have not yet appeared in the literature, this approach shows much promise, as the preliminary results of these workers shown in Section III. amply suggest.

C. Parameter-free Model Interactions

While the more general, and potentially exact, methods described in Sections II. A. and II B. appeared a decade and a half after their atomic counterparts, model potential calculations on polyatomics are much older.[17] In very recent years considerable progress has been made on parameter-free versions of such theories by Gianturco and Jain and their coworkers. In a modern implementation[18, 19] of the method the continuum orbital, $\mu_0^\Gamma(\vec{r})$, in a given molecular symmetry (irreducible representation Γ) is the solution of

$$\{-\frac{1}{2}\nabla^2 + V_{st}^{^1A_1}(\vec{r}) + V_{ex}^{^1A_1}(\vec{r};k^2) + V_{CP}^{^1A_1}(\vec{r}) - \frac{1}{2}k^2\}\,\mu_0^\Gamma(\vec{r}) = \sum_i \lambda_i \mu_i^\Gamma(\vec{r}) \quad (8)$$

where the closed shell target is assumed to be in its $^1A_1$ ground state, and $\mu_i^\Gamma(\vec{r})$ denotes an occupied orbital. The terms in Eq.(10) are the static interaction, $V_{st}(\vec{r})$, an energy-dependent semiclassical exchange interaction, $V_{ex}(\vec{r};k^2)$, a correlation-polarization interaction $V_{CP}(\vec{r})$, and Lagrange multiplier terms on the RHS to enforce the proper nodal behavior in the continuum orbital.

Considerable exploration of the forms of the exchange and correlation-polarization interactions has lead to parameter-free versions based on the Hohenberg-Kohn theorm and perturbation theory considerations. Eq. (8) represents a tremendous simplification of the electronically elastic scattering problem and provides the groundwork, for example, for calculations of rotationally inelastic cross sections for polyatomics.[20]

D. Stabilization Calculations on Resonances

This venerable technique,[21, 22] which involves only the diagonalization of the Hamiltonian for the scattering system in a limited basis, continues to prove useful. It can be applied to largest molecules for which we can perform bound state calculations, provided the resonances are sufficiently narrow. It has been applied to a wide variety of polyatomic systems in explorations of the ways in which shape resonances change as the chemical substituents of a molecule are changed, and has been applied recently to molecules the size of tetracyanoethylene[23]—vastly larger than systems on which full scattering calculations are possible.

III. SOME RECENT COMPUTATIONAL RESULTS

Space restrictions dictate that this section can present only the briefest sampling of the kinds of results from the past two years. I therefore focus on comparisons with experimental results which suggest the level of accuracy now attainable.

The complex Kohn method has been recently applied to CH_4,[24, 25] C_2H_2,[26] SiH_4,[27] NH_3,[28] C_2H_6[29], and H_2O.[30] A principal characteristic of these calculations is their inclusion of correlation effects, either in the form of configurations contributing to target polarization included in the *ab initio* optical potential of Eq.(3) or in the form of open electronic channels. A robust and intimate interface with electronic structure codes is necessary for such calculations. Results for the electron-ethane elastic cross section from a calculation using more than 12,000 correlating configurations[29] are

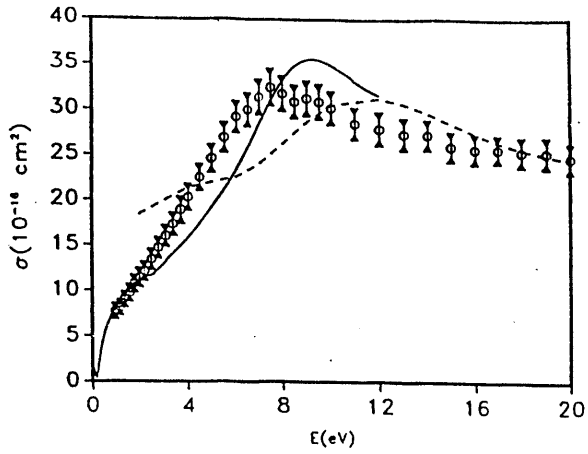

Fig. 1. Elastic cross section for ethane. Solid line, with optical potential; dashed line, static-exchange; points, experiment of Ref. 31.

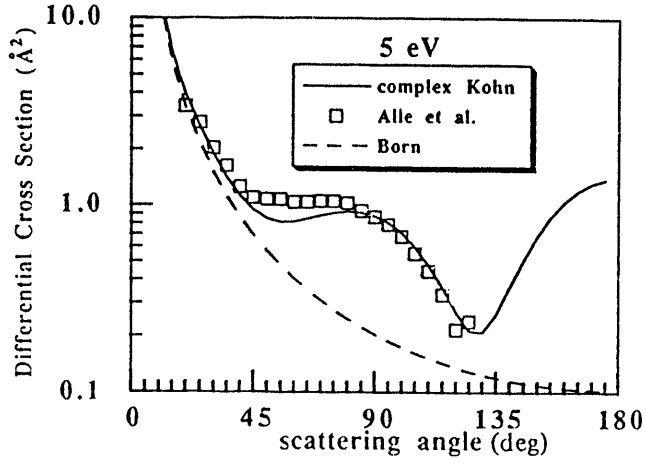

Fig. 2. Differential cross section for e^--NH_3. Solid line, with *ab initio* optical potential; dashed line Born approx.; points, experiment of Ref. 32.

compared with experiment in Fig. 1. The calculations predict a pronounced Ramsauer-Townsend minimum. Polar molecules present their own particular set of additional problems but these methods have also been applied in that case. Results for a differential cross section for electron-ammonia are compared with experiment[32] in Fig. 2. The complex Kohn method has been applied to electronic excitation of CH_2O, CH_4, and H_2O. Very recent results on the excitation of dissociative states of H_2O are shown in Fig. 3.

The Schwinger multichannel method has been applied recently to elastic scattering from CH_4, AsH_3, PH_3,[33] and isomers of C_3H_6,[34] CF_4,[35] and electronic excitation of C_2H_4,[36] CH_2O,[37] CH_4,[38] and C_5H_6.[39] Earlier

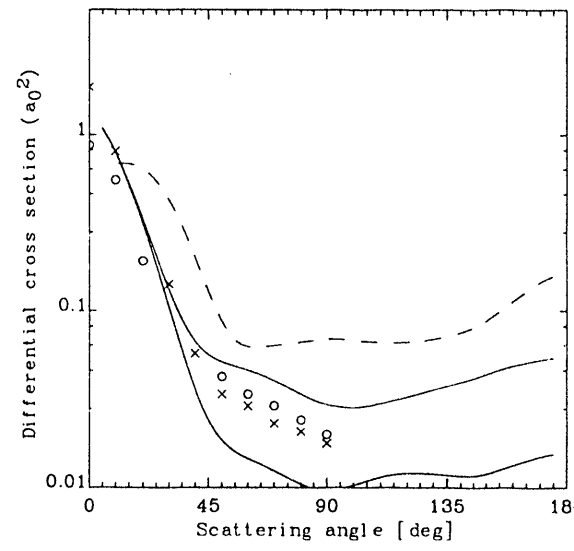

Fig. 3. Differential cross section at 20 eV for e^--H_2O. Solid lines: lower $^3B_1$, upper $^3B_1$+$^1B_1$; dashed line, $^1A_1$; circles, $^1A_1$ experiment; squares, experiment for $^3B_1$+$^1B_1$ of Ref. 33.

calculations using this method have included extensive polarization effects of closed channels, but these recent efforts have been at the static-exchange level or included some number of single configuration open channels. The static-exchange results from this method, including earlier ones, have made a compelling case for the sufficiency of this approximation for incident energies above 5 or 10 eV. Results for elastic scattering from CF_4,[35] are shown in Fig. 4 together with results by Huo.[40] A calculation of the electron-impact excitation of the $^3A_2''$ state of [1.1.1] propellane[39] (a highly symmetric form of C_5H_6) is shown in Fig. 5.

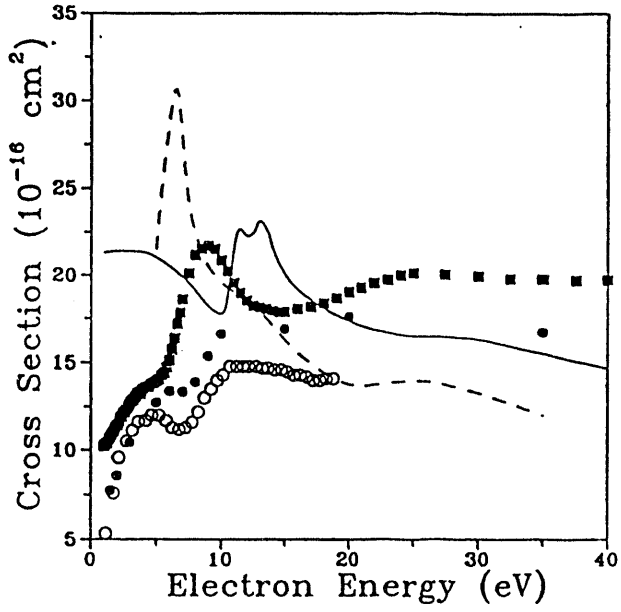

Fig. 4. Elastic cross section for CF_4. Solid line SMC of Ref 35; dashed line SMC of Ref 40; filled circles, exp., Ref. 41; open circles, exp., Ref. 42; filled squares, exp. total cross section, Ref. 43.

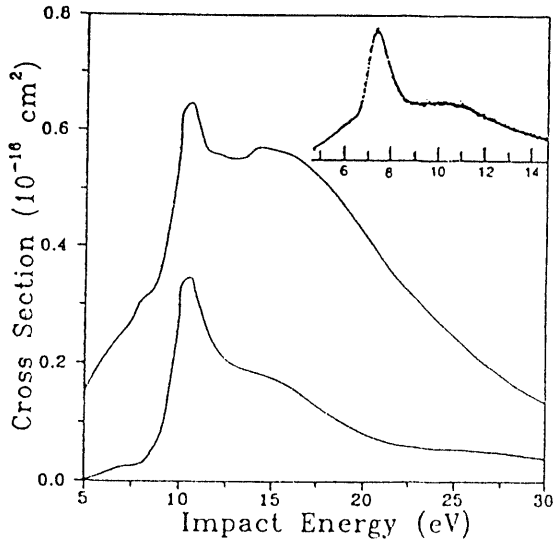

Fig. 5. SMC calculation of electron impact excitation cross section for $^3A_2''$ state of [1.1.1] propellane, upper curve and its $^2A_1'$ component, lower curve; exp. of Ref. 44.

The first *ab initio* calculation on a polyatomic target using the R-matrix method has been performed this year. That calculation is on elastic scattering from CH_4 and includes the effects of polarization using CI for the lower R-matrix roots as discussed above. CH_4 has become an important test case because several other calculations have treated the Ramsauer-Townsend minimum region which is critically sensitive to correlation effects, and because good experiments are available. Preliminary results from the R-matrix calculation[15] are shown in Fig. 6.

Parameter-free model potential calculations have been performed on a large array of polyatomic systems, with some recent examples including H_2S,[20] NH_3,[20] H_2O,[48] SiH_4,[49,52]

H_2S,[50] GeH_4,[51,52] CF_4.[52] Additional light is shed on the capabilities of the method in

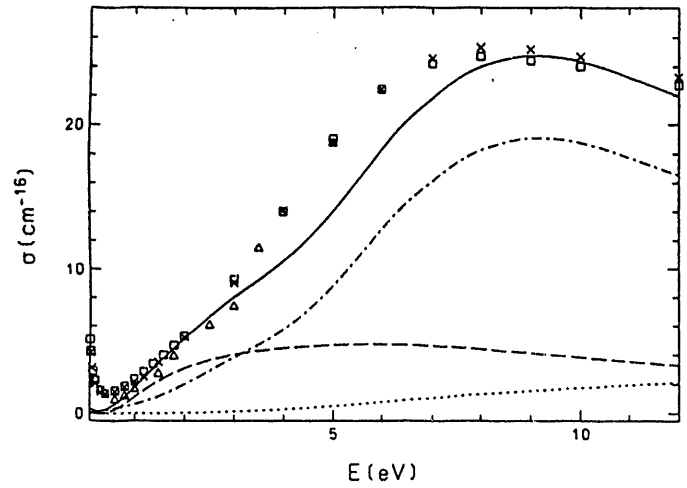

Fig. 6. R-matrix results for elastic scattering cross section for CH_4. Solid, integral cross section; Partial cross sections: $^2A_1$ (dashed), $^2T_2$ (dash-dot) and ^2E (dotted). Experiments: squares, Ref. 45, crosses, Ref. 46, triangles, Ref. 47.

positron scattering from CH_4, SiH_4,[53] and H_2O.[54] The differential cross section for GeH_4 shown in Fig. 7 indicates the level of accuracy attained in many cases for energies greater that about 10 eV. Another recent development in this approach is the incorporation of a complex optical potential to model inelastic effects. Fig. 8 shows the results of such a calculation.[56]

Finally, Fig. 9 shows a stabilization calculation on tetracyanoethylene at the Hartree-Fock level of the sort used routinely now to identify shape resonance features in electron-transmission spectra of large organic molecules.

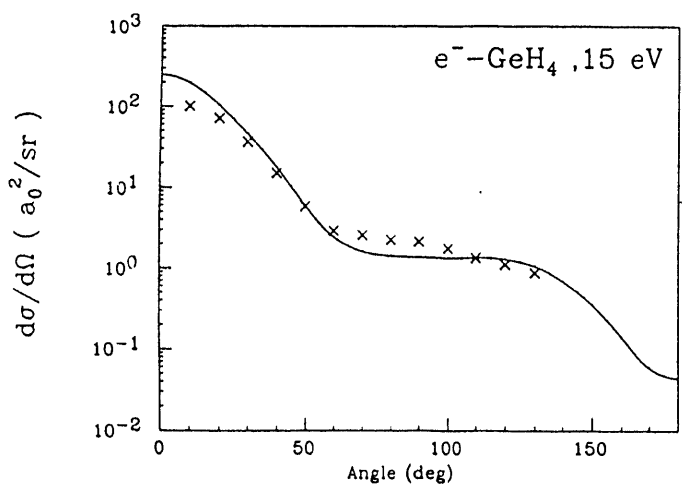

Fig 7. Differential cross section at 15 eV for GeH_4 from a parameter-free model potential calculation. Crosses are experimental points from Ref. 55.

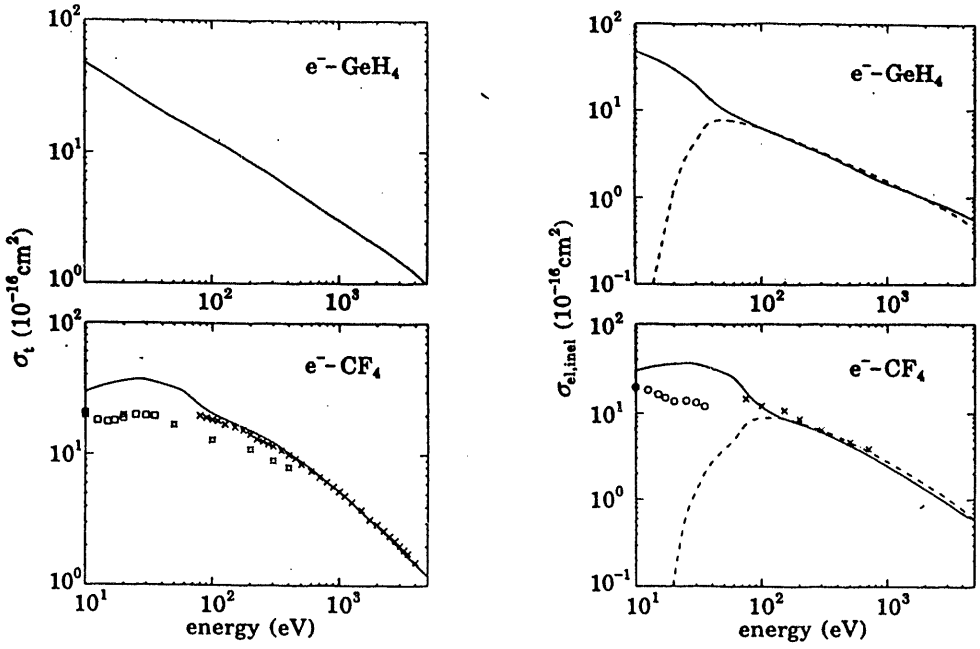

Fig. 8. Left column, Total (elastic plus inelastic) cross sections for CF_4 and GeH_4 compared with experiments summarized in Ref. 56. Right column, elastic (solid) and inelastic (dashed) cross sections from the same calculation compared with results of Huo (Ref. 40) (circles) and experiment of Ref. 57.

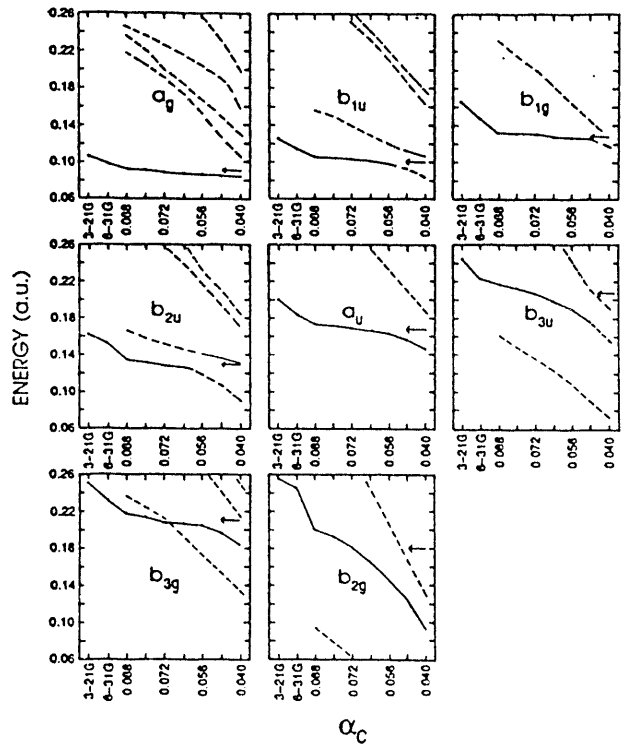

Fig. 9. Stabilization calculation of unfilled orbital energies of tetracyanoethylene as functions of scale factor α.

CONCLUSION AND ACKNOWLEDGEMENTS

Only a minimum impression of the range of new work on electron-polyatomic scattering is given by the few examples included in this review. Sadly, space does not permit inclusion of the entire range of work on vibrational excitation and dissociative attachment of polyatomics which appeared over the last two years.

I would like to thank the authors who made their work available prior to publication for inclusion in this review as well as those who helped by sending re/preprints. I apologize for the many omissions of outstanding work in this area. This work was performed under the auspices of the U. S. Department of Energy by the Lawrence Livermore National Laboratory under contract No. W-7405-ENG-48.

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