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International Journal of Mass Spectrometry 271 (2008) 1–7
International Journal of Mass Spectrometry
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R-matrix calculations of low-energy electron alkane collisions

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Received 31 August 2007; received in revised form 22 November 2007; accepted 3 December 2007
Available online 8 December 2007

Abstract

Ab initio electron scattering calculations are presented for methane, ethane and propane with particular emphasis on elastic cross sections. Calculations are performed with the Quantemol-N expert system which runs the UK polyatomic R-matrix code. These calculations are presented which systematically increase the size of the coupled states expansion which is used to represent polarisation effects in the scattering wave function. Agreement with experimental measurements is obtained provided sufficient coupled states are included in the expansion. Whether these coupled states expansions really converge the polarisation potential and the prospects for further calculations are discussed.

Keywords: Methane; Ethane; Propane; Elastic cross section; Quantemol-N

1. Introduction

Data on electron collisions with molecules are vital for modelling a whole range of both technological and natural phenomenon. Huo and Kim [1] stated that in new plasma reactors use of low-pressure gas and high-density plasma means frequency of electron collision with heavy particles (e.g., molecules) is increased. It is necessary therefore to account for electron collisions with feed gases. The paper also addresses the importance and availability of certain cross sections for particular organic molecules.

Electron collisions with hydrocarbon molecules are found in flames, particularly ones stimulated by spark plug ignition, and planetary atmospheres, particularly the aurora of gas giants (see [2,3] for example). Electron impact ionisation of alkane molecules, that is saturated hydrocarbons with the general formula C_nH_{2n+2}, has been considered by Kim and co-workers [4,5]. However, for many applications processes involving low-energy electrons, defined as electrons with insufficient energy to cause ionisation, are important. In this work we consider such collisions with the first three alkanes: methane ($n = 1$), ethane ($n = 2$) and propane ($n = 3$).

Low-energy electron collisions with methane have been extensively studied both experimentally [6–9,18,10–17] and theoretically [14,19–35,28]. Indeed, as is clear from the cited references, electron collisions with methane have become something of a benchmark system. Theoretically this is because the high symmetry and heavy central atom makes it an excellent system for collision methods based on single centre expansions and because of the difficulty that *ab initio*, potential-free methods have in fully reproducing polarisation effects in this system [26,28,36].

Electron collisions with the higher alkanes have attracted less attention theoretically; their lower-symmetry and lack of dominant heavy centre make them less suitable for study by methods which do not treat the target as multicentred. There are a number of experimental low-energy electron collision studies on ethane (C_2H_6) [8,12,13,37–47] but the complex Kohn study of Sun et al. [48] appears to be the only attempt to perform multicentre *ab initio* calculations including polarisation. In addition Winstead et al. [49] performed static exchange calculations on a number of systems including ethane and propane.

For propane (C_3H_8) the picture is similar with a number of experimental studies [8,12,13,38,46,50,51] but the only theoretical treatments at low energy were a recent one concentrating on vibrational excitation [52], the study of Winstead et al. [49] and McNaughten et al. [25].

A data compilation was carried out for all these systems by Shirai et al. [53] which also represents a good critical survey of

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doi:10.1016/j.ijms.2007.12.002

the experimental measurements up to 2002. Furthermore Huo and Kim [1] discuss the need for a reliable database of chemical and physical properties of the gases and surfaces involved in plasma processes, and electron collision data are part of the database. In this work we present *ab initio* studies of low-energy collisions with methane, ethane and propane. Particular emphasis is placed on elastic cross sections for which, as previous calculations have shown [54,55], the R-matrix method is capable of giving reliable results.

2. Method of calculation

The R-matrix method, in common with other multicentred *ab initio* methods for treating low-energy electron collisions [56], is based on the use of a close-coupling (CC) expansion

$$\Psi_k = A\sum_{i,j} a_{i,j,k}\Phi_i(1,\ldots,N)F_{i,j}(N+1) + \sum_i b_{i,k}\chi_i(1,\ldots,N+1), \quad (1)$$

where $\Phi_i(1,\ldots,N)$ represents the wave function of the ith state of the N-electron target, which in general is represented using a configuration interaction (CI) expansion. The continuum electron is carried orbitals $F_{i,j}$ which are antisymmetrised to the target electrons by operator A. The $N+1$-electron CI functions, $\chi_i(1,\ldots,N+1)$, allow for detailed correlation effects when the scattering electron is close to the target. These terms and the CC expansion allow for target polarisation effects [57].

In the R-matrix method this CC expansion is only used to represent the wave function inside a sphere centred on the target molecule's centre-of-mass. Outside this sphere, typically of radius 10–15a_0, the target wave function is assumed to have zero probability which means that the simplified problem of an electron scattering in the potential due to the target molecule can be solved.

Our specialised algorithm for solving the inner region problem [58] means that there is little extra computational cost in including large numbers of such states in the calculation see Refs. [59–61] for example. However, treating very large numbers of coupled states makes the outer region calculations slow which removes one the major advantages of the R-matrix method: the ability to consider large numbers of scattering energies at little computational cost. To mitigate this problem we tested a technique used previously [62] whereby most of the higher channels where omitted from the outer region calculation. This technique gives excellent results provided all open states and the few lowest closed ones are retained in the outer region.

The calculations presented here used the Quantemol-N software [63]. Quantemol-N provides an expert system for running the UK polyatomic R-matrix code [64,65]: it does not provide added functionality to the code but makes robust calculations considerably quicker to set up, even for experienced users. Quantemol-N automates the design of a consistent model and at the same time greatly simplifies the data input requirement thus helping to eliminate errors.

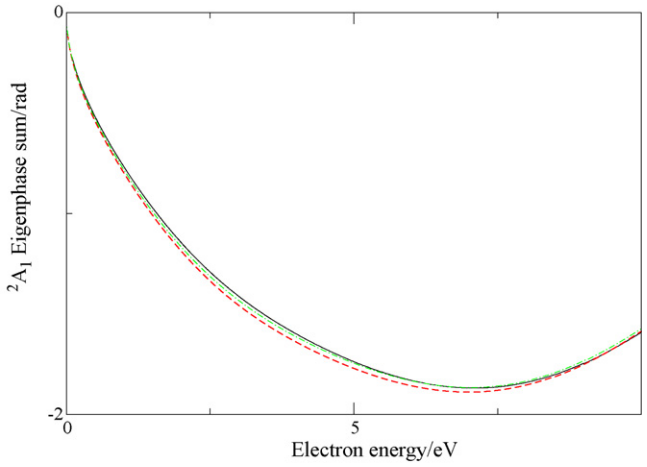

Fig. 1. $^2A_1$ eigenphase sums for propane: continuous curve full CC calculation; (dashed curve) 72 states CC in the inner region reduced to 16 in the outer region and contracted CSFs; (dot and dashed curve) 72 states in the inner region, 16 states CC in the outer region and uncontracted CSFs.

For all the calculations reported below we used continuum functions of Faure et al. [66] which includes functions up to $l = 4$ (g waves) in the partial wave expansion. Given that methane and ethane are non-polar and propane is only weakly dipolar, this basis is also adequate to represent the electron continuum as the multicentered target basis functions are used to represent higher ℓ effects in the region of the nuclear singularities. For very polar molecules, further partial waves are usually added using the Born approximation [55,67].

Convergence with respect to partial wave expansion, and other aspects of the calculation, is more thoroughly tested by comparing differential cross sections. For CH_4, we have used the programme POLYDCS to compute differential cross sections, using as input the K-matrices computed by Quantemol-N.

In this work, an R-matrix radius of 10a_0 with propagation of the R-matrix in the outer region to 100.1a_0 also proved to be adequate in all cases.

3. Results

3.1. Methane

Methane in its equilibrium geometry has tetrahedral (T_d) symmetry but standard quantum chemistry Gaussian Type Orbital (GTO) integral codes do not use point groups with degenerate representations. We therefore performed all calculations reported below using C_{2v} symmetry although some tests were also performed using even lower symmetry.

A large number of different models and basis sets were tested for methane not all of which will be reported here. Our results showed considerable sensitivity to the level of treatment used to represent polarisation effects. The simplest model is the so-called static exchange (SE) approximation in which the target wave function is frozen in its lowest configuration during the collision. Results of SE calculations, which neglect all polarisation effects, are reported here simply to allow comparison with previous calculations at this level. To allow for polarisation effects

Table 1
Vertical excitation energies, in eV, for low-lying electronic states of methane in our CAS-CI model; results of the calculations by Gil et al. [28] are given for comparison

Target state (T_d)	Present	[28]
X^1A_1	0.0	0.0
1^3F_2	12.1	12.3
1^3A_1	12.6	13.0
1^1F_2	13.7	13.5
2^3F_2	14.2	13.5
1^3E	14.7	13.2

it is necessary to allow the target to relax during the collision process.

The methane target states were represented using a complete active space (CAS) CI with the C 1s electrons frozen and the remaining eight target electrons freely distributed between, in C_{2v} notation, the $2a_1$, $3a_1$, $4a_1$, $5a_1$, $1b_1$, $2b_1$, $1b_2$, $2b_2$ orbitals. The lowest remaining virtual target orbitals for each symmetry was used to augment the continuum basis by allowing the scattering electron to occupy them. Such orbitals contribute high ℓ terms in the region of the nuclear singularities which are not well represented in the standard partial wave expansion used for the continuum basis functions. For methane two models were tested: the standard one [57] where these virtual orbitals were contracted with the continuum orbitals, i.e. included in the first sum in Eq. (1), and a second uncontracted model where no such contraction was used and the virtual orbitals were used to generated configurations in the second sum in Eq. (2). The second model increases the level of short-range polarisation included in the calculation.

The target CAS-CI gives many potential target states that can be used in the CC expansion; the lowest of these are shown in Table 1 where they are found to be in reasonable agreement with the calculations of Gil et al. [28]. As shown below our results showed considerable sensitivity to the number of these states retained in the CC expansion.

Table 2 shows our CH_4 polarisability as a function of model, computed using first-order perturbation theory as a sum over electronically excited states in the close coupling (CC) expansion:

$$\alpha = \sum_{r=1}^{N} \frac{2|\mu_{0r}|^2}{E_r - E_0} \tag{2}$$

Table 2
CH_4 polarisability, α, calculated using various models which are explained in text

Basis set	N	α/a_0^3
6-31G	32	7.59
6 31G	48	7.62
6-31G*	48	7.43
DZP	48	6.22
Experiment [68]		16.52

N is the number of target states in the close coupling expansion

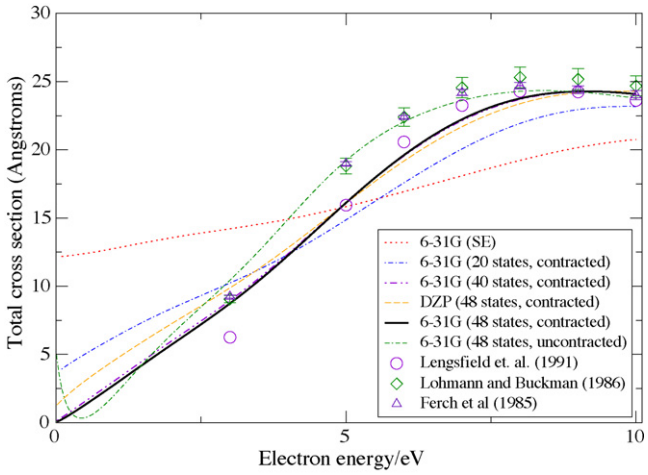

Fig. 2. Elastic cross sections for electron collisions with methane.

where μ_{0r} is the transition dipole matrix element:

$$\mu_{0r} = \langle \psi_0 | \mu | \psi_r \rangle \tag{3}$$

and r runs over the electronically excited targets states included in our CC expansion.

Fig. 2 presents total scattering cross sections for several of our models and compares them with previous studies. As expected our SE calculation does not give good results. However, use of the CC expansion shows a progressive and systematic improvement as states are added. Calculations with 32 or more states in the CC expansion gives results close to the measurements [9,69] and the complex Kohn calculation of Lengsfield et al. [26]. However, the apparent convergence of our results with respect to the CC expansion does not mean our calculations have completely converged the treatment of polarisation effects. As shown by Table 2, our sum over CC does not reproduce the full long-range polarisability of methane; it is known that this can only be achieved by allowing for the target continuum as well as bound states [59]. As a test of including further polarisation effects inside the R-matrix sphere we also tested a model using uncontracted virtual orbitals. This resulted in the appearance of a Ramsauer–Townsend minimum at about 0.44 eV, in good agreement with the experimental values of 0.36 eV [9] and 0.40 eV [69], see Fig. 3. Several of our CC calculations displayed narrow Feshbach resonances close to the electronic excitation thresholds. The most clear cut of these was a^2F_2 resonance at 12 eV with width 0.008 eV in our model which used a 6-31G basis set, 48 coupled states and contracted CSFs in the CC expansion.

Differential cross sections (DCS) give a more sensitive test of calculations than total cross sections since they are often measured more reliably and they are sensitive to effects which can average out in the total cross sections. We have therefore calculated DCS for incident energies 3 eV and 5 eV using the programme POLYDCS [70], with the input being our Quantemol-N fixed-nuclei C_{2v} K-matrices. These cross sections are rotationally summed for which we used the transitions J =0–0, 0–1, 0–2, 0–3, 0–4 and 0–5.

Figs. 4 and 5 compare our results with the experiments of Sohn et al. [18] and the calculations of Lengsfield et al. [26].

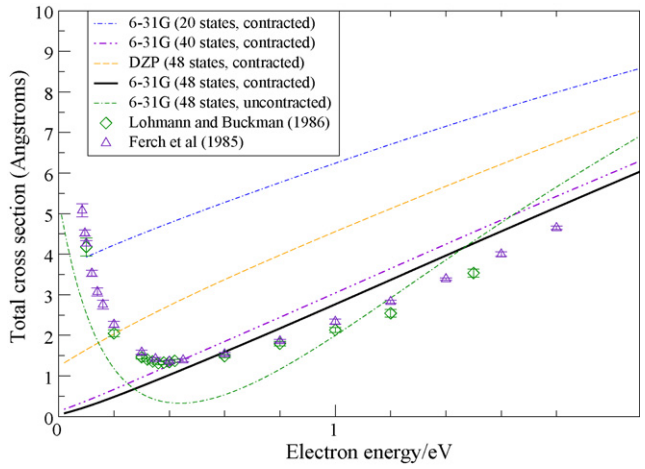

Fig. 3. Methane elastic cross sections in the region of the Ramsauer–Townsend minimum.

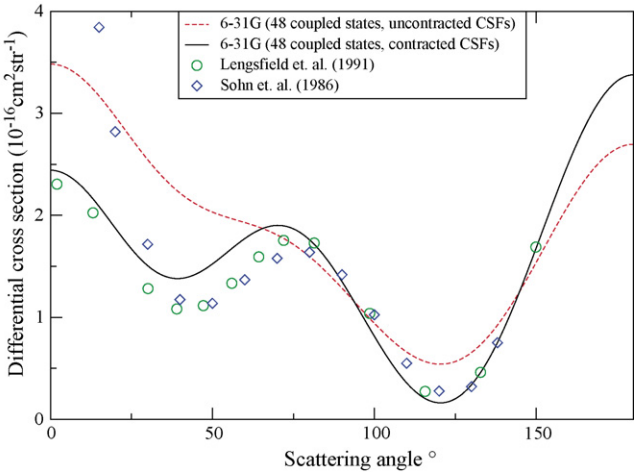

Fig. 5. Rotationally summed differential cross sections for electron collisions with methane at incident energy 5 eV.

Using contracted CSFs the present work is in good agreement with both, particularly at higher angles. The differences at small angles may well be due to a still incomplete treatment of polarisation effects although we note that it is not clear what the correct behaviour is at small angles. Clearly the agreement is not as good when uncontracted CSFs are used.

3.2. Ethane

Experimental studies of electron scattering by ethane have focused upon the Ramsauer–Townsend minimum region (particularly interesting given that the molecule has a quadrupole moment), and a distinctive shape resonance was found at 7.5 eV [38]. McCorkle et al. [47] confirmed the existence of the minimum at 0.14 eV by the measurement of its momentum transfer cross section σ_m. Although scarce there have been a few theoretical studies devoted to electron scattering by ethane. A particular one is the *ab initio* study of Sun et al. [48]. They applied the complex Kohn variational method at the static exchange (SE) and static exchange plus polarisation (SEP) level. Their enquiry made use of polarised SCF trial wave functions, which was necessary to obtain reliable cross sections in the region of the Ramsauer–Townsend minimum. Although their integral, differential and momentum transfer cross sections agreed well with experimental data, the shape resonance shifted to higher energy.

The study by Winstead et al. [49] also studied ethane by application of the Schwinger multichannel method at the static exchange level. They computed differential elastic, integral elastic and momentum transfer cross sections, The data obtained were in good agreement with available experimental ones, although there was some disagreement between their theoretical momentum transfer cross section and the corresponding experimental one. They stated that it could only be partially explained by shift in the position of the resonance. They also noted that in the case of ethane there was insensitivity with respect to variation of basis sets. Specifically use of a large basis set made little difference to their results.

Ethane has D_{3d} point group symmetry. In our work the calculations on ethane used a 6-31G* GTO basis for the target and worked within the C_{2h} symmetry group, the first system to be

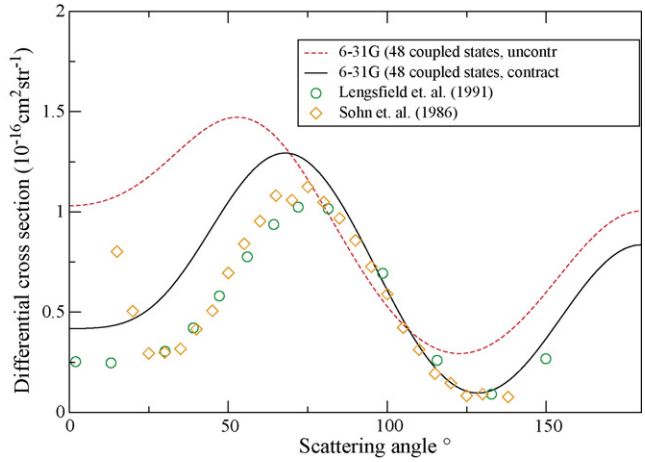

Fig. 4. Rotationally summed differential cross sections for electron collisions with methane at incident energy 3 eV.

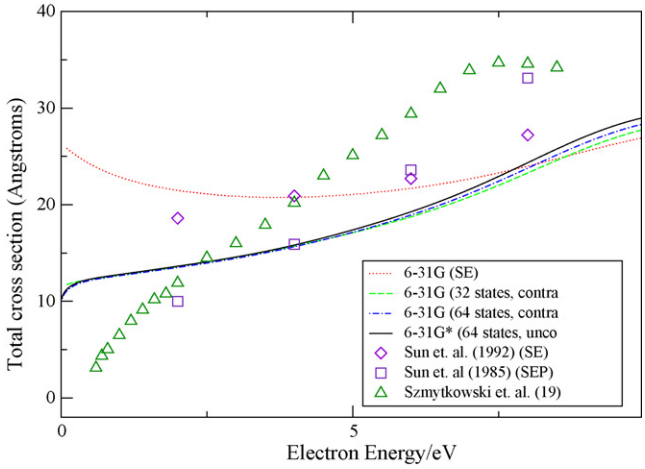

Fig. 6. Elastic cross sections for electron collisions with ethane, experimental data is from Szmytkowski and Krzyzstofowicz.

Table 3
Calculated vertical excitation energies, T_e, in eV for the low-lying states of ethane in our CAS-CI model

Target state (D_{3d})	T_e	[71]
X^1A_{1g}	0.0	0.0
1^3E_g	12.2	9.01
1^3A_{1g}	12.8	9.05
1^1E_g	12.9	9.16
1^3E_u	13.3	9.85

Compare to the calculations of Buenker and Peyerimhoff [71].

Table 4
Calculated vertical excitation energies, T_e, in eV for the low-lying states of propane in our CAS-CI model

Target state (C_{2v})	T_e	[72]
X^1A_1	0.0	0.0
1^3B_1	12.2	9.49
1^3B_2	12.3	9.00
1^3A_1	12.3	8.91
1^1B_1	12.8	9.69

Data from Richartz et al. [72] is provided for the purposes of comparison.

treated with this point group by the UK polyatomic R-matrix code. Again the carbon 1s electrons were frozen and a CAS-CI representation $(2a_g\ 3a_g\ 4a_g\ 5a_g\ 2a_u\ 3a_u\ 4a_u\ 1b_g\ 1b_u)^{14}$ was used. Excitation energies for this model are given in Table 3 where they are compared to the *ab initio* results of Buenker and Peyerimhoff [71]. The significant difference is because our target model does not account for the Rydberg-like nature of the excited states.

In the scattering calculation one virtual orbital was allocated to each symmetry where target orbitals were available to do so. A 64 state CC with uncontracted CSFs calculation was used. The averaged target polarisability α for this model was found to be $5.89a_0^3$, significantly smaller than $28.52a_0^3$ obtained experimentally [68].

Results for elastic scattering from ethane are given in Fig. 6. Given the lack of agreement between experiment and the present work, more target states are needed to improve matters. The expected Ramsauer–Townsend minimum is absent from the cross-section and this is perhaps not surprising given that the target polarisability is a sixth of the experimental value.

We did not detect the shape resonance predicted by Sueoka and Mori [38] even in calculations using an expanded number of virtual orbitals. Instead the CC model we employed yields several narrow Feshbach resonances between 12 and 13 eV.

3.3. Propane

The experimental study of McCorkle et al. of [47] included propane, whose momentum transfer cross section also yielded a Ramsauer–Townsend minimum at 0.14 eV. Boesten et al. [50] also reported a broad shape resonance with a peak of 7.5 eV which they found from analysis of vibrationally inelastic differential cross sections.

Winstead et al. [49] used the multi-channel Schwinger method at the static exchange level, using distributed memory parallel computers. Their results had the correct overall magnitudes and was able to reproduce the broad shape resonance, although in static exchange approximation the position was higher than the observed value of 7.5 eV.

Propane has C_{2v} symmetry. Our target model used a 6-31G* GTO basis and a valence CAS-CI defined by $(3a_1\ 4a_1\ 5a_1\ 6a_1\ 7a_1, 1b_1\ 2b_1\ 2b_2\ 3b_2\ 4b_2\ 5b_2\ 1a_2)^{20}$. This model gives a dipole moment of 0.065 D (compare with the experimental value of 0.084 D [68]). Vertical excitation energies for the lowest states are given in Table 4. Alongside our results we give the results of Richartz et al. [72]. Like ethane, propane also has low lying Rydberg orbitals, again this is not modelled in the present study.

Our target model, which used 72 target states, yielded an (averaged) polarisability of $3.72a_0^3$ compared with $39.96a_0^3$ [68] obtained experimentally.

Up to 72 target states were included in the coupled states expansion. In the outer region however, a reduced states calculation was performed using only 16 of those (electronically) excited states. With regard to virtual orbitals one was allocated to each symmetry where target orbitals were available to do so. Fig. 5 gives total cross sections, which are in disagreement with experiment. This is expected to be due to poor modelling of target polarisation and more closed channel wave functions would still be needed.

One may locate the position of a Ramsauer–Townsend minimum by checking that the s-wave or, in the case of propane A_1, phase shift passes through zero. This occurs when the polarisation (attractive) part of the scattering potential cancels the exchange (repulsive) part of the same potential and is a purely s-wave, low-energy phenomenon. Fig. 1 shows the $^2A_1$ phase shift for propane. As the eigenphase does not pass through zero the observed [47] minimum is absent from our calculated cross sections, see Fig. 7. The fact that the polarisability given by the CC model used in the present work is less than a tenth of the experimental value may explain this absence.

Like Winstead et al. [49] we do not detect any clear evidence for the shape resonance reported by Boesten et al. [50]; we per-

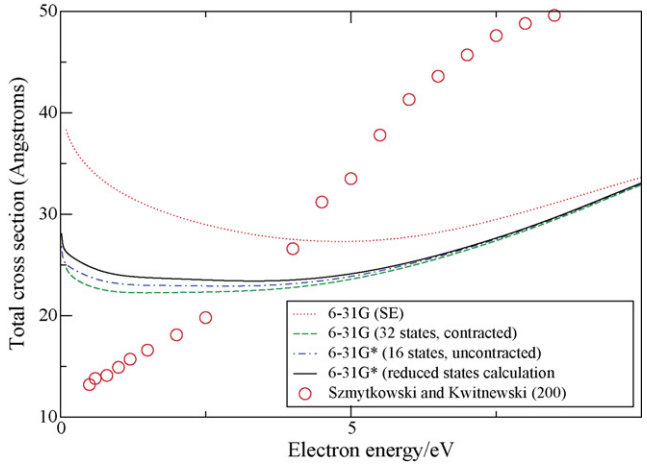

Fig. 7. Elastic cross sections for electron collisions with propane, experimental data is from Szmytkowski and Kwitnewski [73].

formed specific calculations to confirm this. Conversely our CC calculations yielded Feshbach resonances of various symmetries with positions between 12 eV and 13 eV and widths between 0.004 eV and 0.01 eV. Given that the electronic eigenstates are too high and not Rydberg-like these values should be regarded as upper bounds of the true values.

4. Conclusion

This paper has addressed the problem of electron scattering by the first three alkanes (methane, ethane and propane) using the new software Quantemol-N, a software that provides a user interface to the expert UK R-matrix suite of codes.

For methane it has been shown that increasing the number of coupled states in the close-coupling expansion converges the total cross section to values in good agreement with the previous studies. However, although there is convergence with respect to the CC expansion, this does necessarily mean that one has attained a complete converged treatment of target polarisation or the long-range polarisability. An uncontracted CSFs model, which increases polarisation effects, was used to achieve such an improved treatment. The model gives the Ramsauer–Townsend at 0.44 eV, in good agreement with experiment values of 0.36 eV [9] and 0.40 eV [69].

Rotationally summed differential cross sections for incident energies 3 eV and 5 eV for methane are computed in good agreement with previous experimental and theoretical data, particularly for angles greater than 75° when contracted CSFs are employed. With uncontracted CSFs however, the agreement is not as good, despite the integral cross sections being in excellent agreement across the incident electron energy spectrum considered.

The cases of ethane and propane have proved much more difficult. In these cases a large number of coupled states were included in the close coupling expansion (64 and 72, respectively). It is clear that such a number of closed channel target states is still insufficient to attain a converged treatment of the long range polarisability and by inference of polarisation effects in general. One consequence of this is the absence of a Ramsauer–Townsend minimum in our elastic cross sections for both molecules.

For all three systems we find narrow, Feshbach resonances at energies close to the excited target states we include in our close-coupling expansion. The location of Feshbach resonances is very sensitive to the precise excitation energy of the parent target state employed in the calculation. The energies predicted for these resonances should therefore be considered as upper limits to the true positions as our excited state energies are systematically too high due to the neglect of the Rydberg character of the electronically excited target states in our models. Molecular R-matrix calculations including Rydberg states have been performed before [74] and such a study on the alkanes could well be the subject of future work.

In general this work confirms, as stated in the introduction, that *ab initio* electron scattering from the longer chain alkanes is much more difficult to model than it is from methane.

Acknowledgements

HNV thanks A.G. Harvey and B.C. Silva for very useful discussion.

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