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Quantemol-N: an expert system for performing electron molecule collision calculations using the R-matrix method

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Abstract. The R-matrix method has been widely employed to *ab initio* calculations on a large variety of problems related to electron molecule scattering. The UK Molecular R-matrix Code, which are a synthesis between codes designed for quantum chemistry and electron atom scattering calculations, has proved particularly popular for these studies but is difficult for the non-specialist to use. The Quantemol-N software environment is designed for scientists with a minimal knowledge of scattering theory or quantum chemistry to use without the need of a complex and dedicated training. Their use is illustrated for low energy electron collisions with silane.

1. Introduction

Electron collisions with atoms and molecules are the major physical interaction determining the behaviour of all plasmas. Low energy electron collisions with molecules occur naturally in a number of astrophysical environments, in the upper atmosphere, in lightning bolts and within the body as a result of radiation damage [1]. From a technical perspective such collisions are important in many applications including lighting, spark plugs and lasers. Furthermore electron induced reactions in both gaseous and condensed phases initiate and drive the basic chemical processes in different regimes from industrial plasmas used for etching to damage in living tissues. For example, electron induced reactions underpin most of the multi-billion dollar modern superconductor industry since it is those reactive fragments produced by electron impact of the etching gases that react directly with the silicon substrate.

For many electron molecule problems it is difficult to make the relevant measurements in the laboratory. There is thus an increasing demand for computational procedures for obtaining reliable estimated cross section and rates for key processes. There are probably three state-of-the-art *ab initio* methods for treating low-energy electron molecule collisions including electronic excitation (see [2]). These are the Kohn variational method, the Schwinger variational method and the R-matrix method. Of these the R-matrix method [3] is the most widely used [4, 5, 6, 7, 8, 9, 10, 11].

The most advanced and the most widely used R-matrix codes are the UK molecular R-matrix codes [12]. These have been developed over a period of about 30 years from a number of

scientists based at Queen's University Belfast, Daresbury Laboratory, Royal Holloway College and, most recently, University College London. This project has been extensively supported by UK Collaborative Computational Project 2 (CCP2) on continuum states of atoms and molecules.

The UK R-matrix codes are very flexible. Besides the basic electron collision problem they have been adapted to find (diffuse) bound states [13, 14], compute differential and momentum transfer cross sections (eg [15]), treat rotational [16, 17, 18, 19] and vibrational [20, 21, 22] excitation, obtain resonance parameters, quantum defects and branching ratios [23, 24, 25, 26, 27], treat dissociative recombination both using a complete non-adiabatic method [28] and in tandem with multichannel quantum defect theory [29], study photoionisation [30, 31] and processes in intense laser fields [32, 33], and collisions with molecules physisorbed on surfaces [34, 35]. The codes have recently been extended to treat higher energies [36], larger molecules [37], electronically and more challenging problems [38, 39]. They have also been used for collisions with positrons [40, 41]. The codes are freely available, see http://www.tampa.phys.ucl.ac.uk/rmat/, but can only be used successfully by experienced scientists. The Quantemol-N software system has been developed to address this problem: it both gives an expert interface for the nonspecialist to perform *ab initio* electron-molecule scattering calculations and also provides a training tool for those wishing to learn about such calculations.

In this paper we report on the Quantemol-N package using the silane (SiH_4) molecule as a prototypical example. Electron scattering from silane is important for plasma etching [42] and has therefore been well studied in the laboratory both from an experimental [43, 44, 45, 46, 47] and a theoretical [48, 49, 50, 51, 52, 53, 54] stand-point.

2. The R-matrix Method

Use of the R-matrix method for the treatment of *ab initio* electron atom and electron molecule scattering has been comprehensively discussed elsewhere [3, 55] and will only be outlined briefly here. The basic idea of this approach is the division of configuration space into two regions by a sphere of radius a about the molecular centre-of-mass. The sphere should be big enough to enclose the charge of the N-electron target molecule. Inside the sphere it is necessary to consider electron exchange and electron-electron correlation effects and this is done by adapting quantum chemistry codes [12]; outside the sphere such effects are neglected and the scattering electron is assumed to move only in the potential given by the target. The outer region problem thus has some similarity to, but is significantly more complicated than, the same problem for an atomic target.

In the inner region, the wave function of the $(N+1)$-electron scattering system is given by

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

where $\mathcal{A}$ is the anti-symmetrisation operator, $F_{i,j}$ are continuum orbitals [55] and χ_i are two-centre L^2 functions constructed from N-electron 'target' orbitals. Φ_i represents the wave function of the i^{th} target state and itself may be represented as a configuration interaction (CI) expansion. The variational coefficients in (1) are obtained by diagonalising the inner region Hamiltonian matrix which is often the rate determining step in the calculation.

How expansion (1) is built has fairly subtle effects on the scattering model [56] which requires special programming to be implemented efficiently [38]. The standard way of performing a CI target calculation is to use a complete active space CI (CASCI) as this model keeps a balance between the target and scattering calculations [56]. In this model the valence electrons are distributed freely amongst subset of "valence" orbitals.

In the polyatomic version of the UK R-matrix codes [57], the target and the continuum orbitals are represented by Gaussian Type Orbitals (GTOs) and the integrals are generated

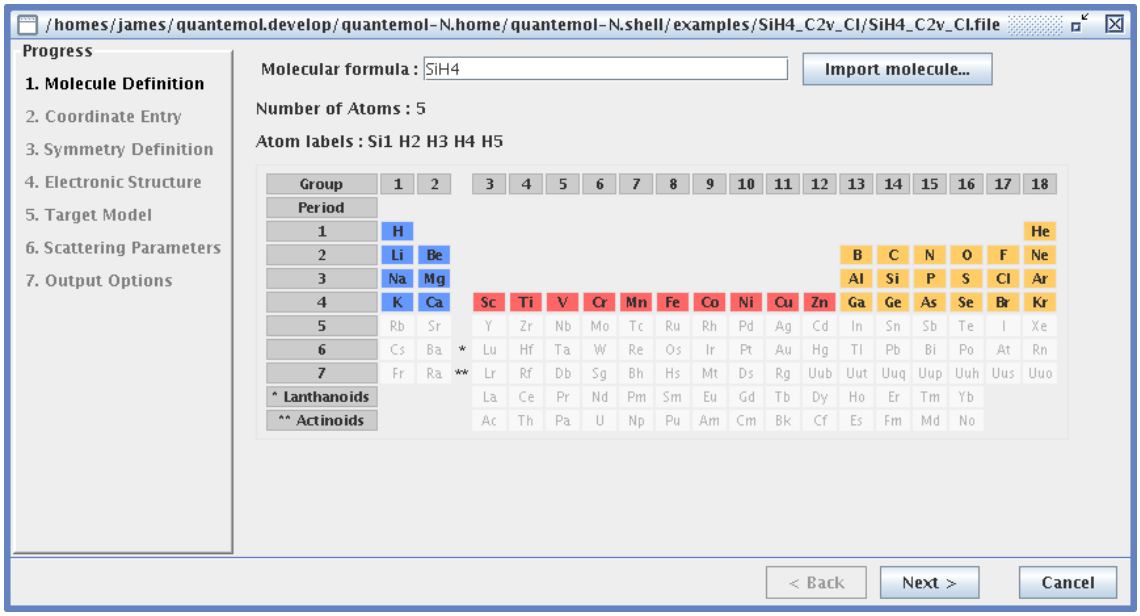

Figure 1. Panel 1: molecule definition.

using Almlöf and Taylor's Sweden Molecule package [58]. A major advantage of the R-matrix method is that this inner region problem is solved independent of the electron scattering energy; therefore repeated calculations at different scattering energies are computationally cheap.

The R-matrix itself provides the link between the inner and outer regions. In practise it is then usually propagated in the outer region potential [59] until solutions can be matched with asymptotic functions which are usually obtained from a Gailitis expansion [60].

3. The Quantemol-N approach

In the practical implementation of the R-matrix method the user has to make a large number of choices covering issues such as implementation of symmetry rules, target basis set, continuum basis set, R-matrix radius, type and number of target orbitals to retain in both the CI and as virtual orbitals, target CI representation, CI model for the scattering problem, reference configurations for each of these CI expansions, deletion threshold for the continuum orbitals, scattering grid, R-matrix propagation radius, resonance fitting and so forth. This, combined with a rather old fashioned user interface, makes the codes technically demanding to use. For this reason we have developed an expert system, Quantemol-N, which provides the user with both a friendly and intuitive graphical user interface, and a set of programs which either takes decisions on the issues listed above or provides a limited menu of choices for the user. The aim of this software is to make *ab initio* electron-molecule scattering calculations accessible to the non-specialist. As we have discovered by experience, Quantemol-N also makes it much easier and quicker for specialists to perform such calculations.

Quantemol-N is menu driven. Figures 1–7 show the series of menu screens the user completes to initiate and perform a calculation. The first panel, Fig. 1, is for specifying the chemical composition and symmetry of the molecule. Like the underlying R-matrix codes, Quantemol-N will only handle Abelian point groups which means that the highest allowable point group symmetry is D_{2h}. Other possible point group symmetries are D_2, C_{2v}, C_s, C_2 and C_i and, of course, no symmetry.

The second screen, see Fig. 2, deals the target geometry. Cartesian coordinates in Angstroms

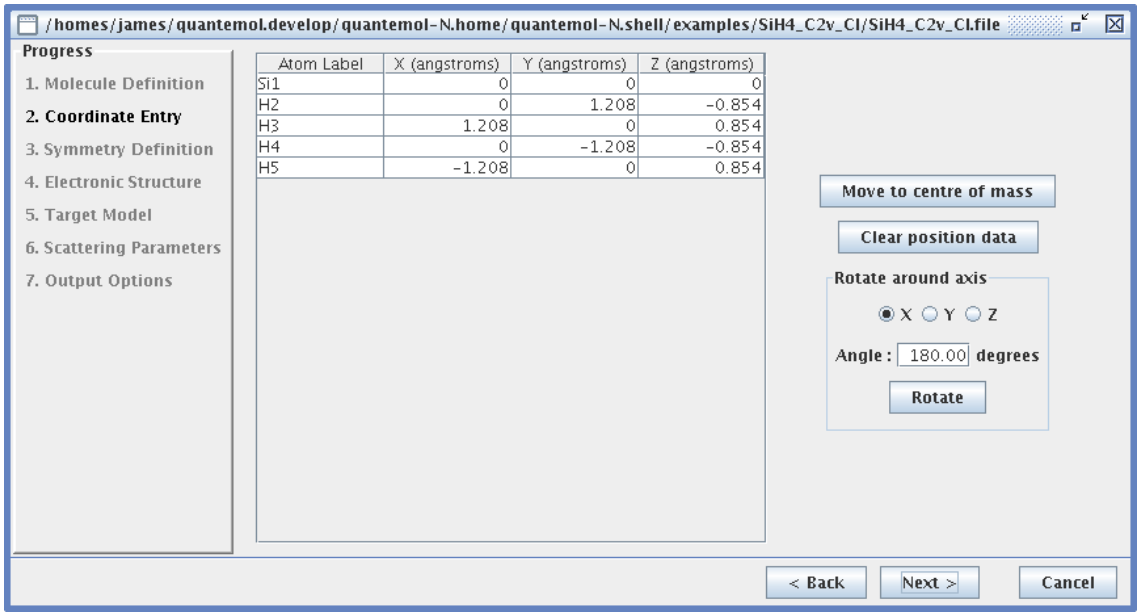

Figure 2. Panel 2: coordinate entry.

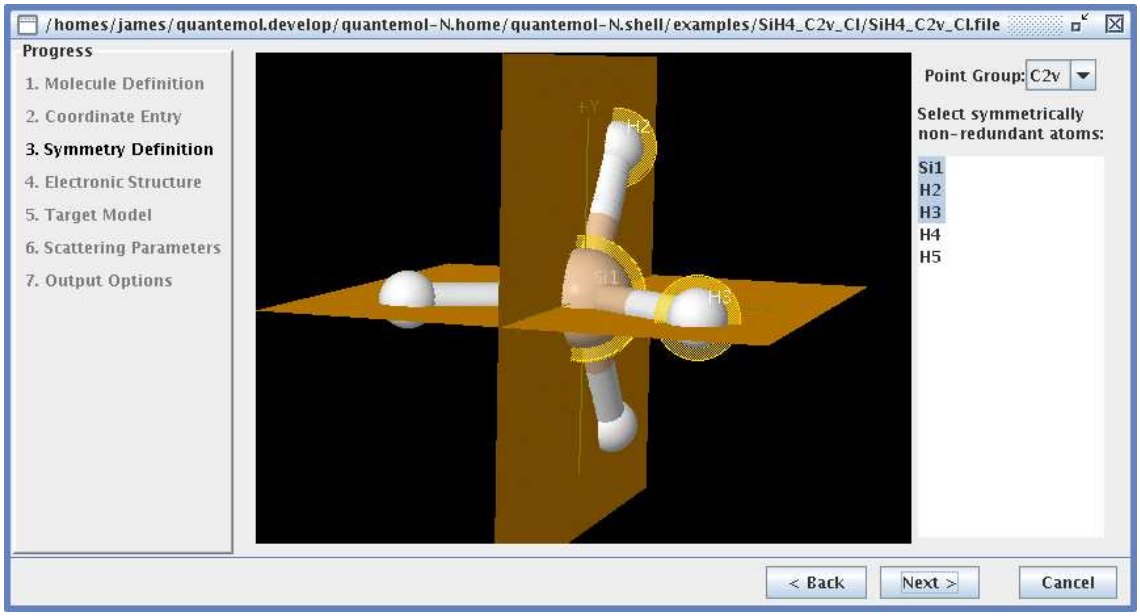

Figure 3. Panel 3: symmetry definition. The example shows silane in its equilibrium geometry with the symmetry operations for the C_{2v} point group.

are entered for symmetry unique atoms only. These geometries can be read directly from the output of various standard quantum chemistry codes including GAMESS, Gaussian 94, 98 and 03. Equilibrium geometries for most commonly occurring molecules can be found on the web [61].

Once the geometry has been specified Quantemol-N uses program jmol [62] to display the

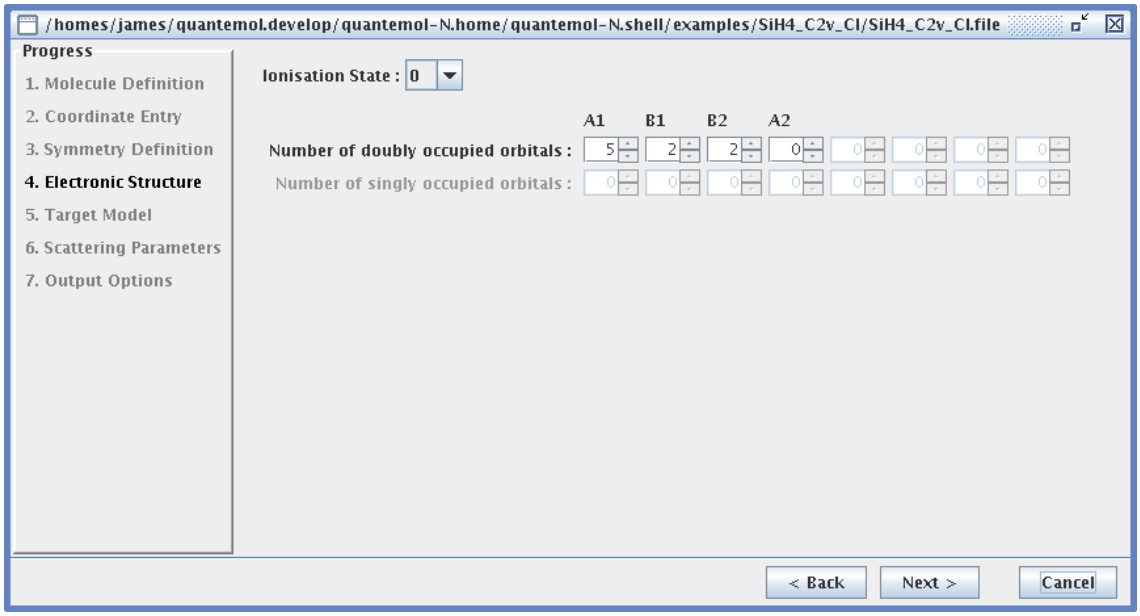

Figure 4. Panel 4: electronic structure specification. The example shows the ground state configuration of silane in C_{2v} symmetry.

molecule with the symmetry operations imposed on it, see Fig. 3. This provides an important visual check for the user that all is well.

The fourth (Fig. 4) and fifth (Fig. 5) screens deal with electronic structure issues and the model used for the target, and by implication, the scattering calculation. Here the user supplies the ground state configuration of the target and chooses between using a Self Consistent Field (SCF) and CI target calculations. The number of target states for the CI calculations is defined by the user. Only target states with the vertical excitation energies below a user-specified cutoff energy are kept. The CASCI space in the CI calculation is automatically chosen according to the first maximum energy difference between virtual molecular orbitals. Frozen molecular orbitals are defined by the first maximum energy difference between valence molecular orbitals. A further restriction on the size of the problem is introduced for electron rich or large molecules by freezing more orbitals and/or electrons in order to decrease the size of the calculations.

The target basis set is selected, usually from the library supplied by the program. This library contains 6-31G, 6-31G* and 6-311G* GTO basis for all atoms up to Cl, and for Ca and Cu. Other basis sets (DZP, TZP, cc-pVTZ etc) are defined for various atoms, particularly H. There is a user option to import other basis sets obtained from GTO basis set libraries [63]. The continuum basis GTO set [64] is automatically chosen by the program according to the charge state of the target and the selected R-matrix radius.

The final input screen, Fig. 6, deals with the outer region calculation. The number of target states per symmetry to be included in the calculation (defaulted as one for a CI target) can be altered here. The R-matrix radius, default 10 a_0, and energy grid, default 0.1 eV to 10 eV in steps of 0.02 eV, are set. The last panel before the calculations start, Fig. 7, gives a summary of the parameters and saves them for use in a future calculation.

Quantemol-N generates vertical excitation energies and graphs of eigenphase sums (Fig. 8), elastic (Fig. 9) and inelastic cross sections and rates (Fig. 11). Resonances are automatically detected and fitted to give their position and width. All this data is of course also written to simple text files to facilitate further analysis.

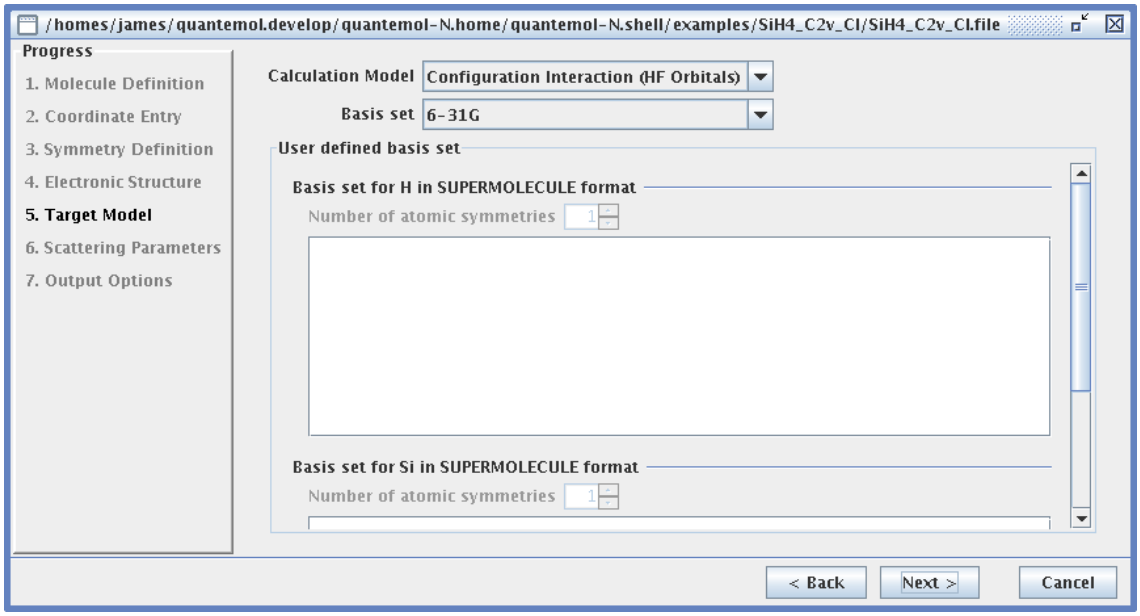

Figure 5. Panel 5: target model specification.

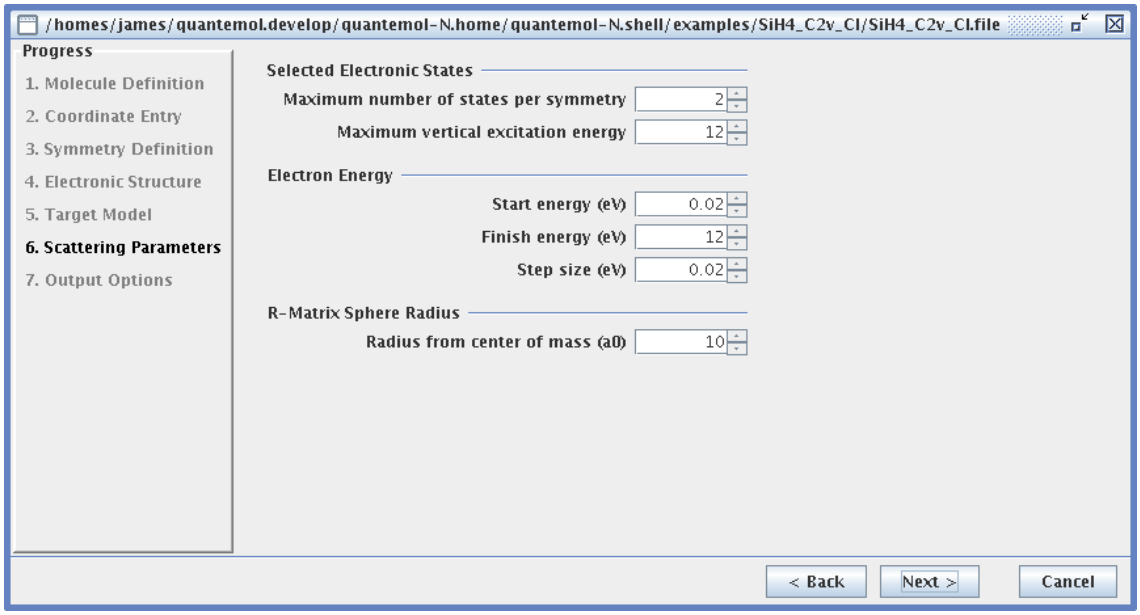

Figure 6. Panel 6: specification of the scattering parameters.

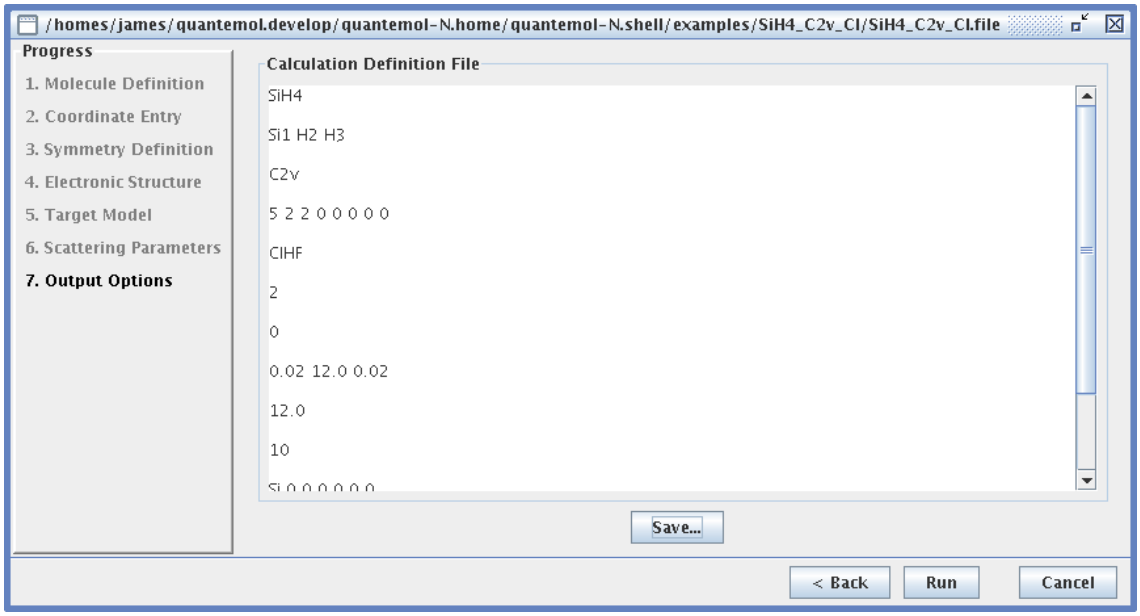

Figure 7. Panel 7: calculation definition file, a summary of the parameters input in the previous windows.

4. Sample calculation

Test calculations for many molecules have been performed using the Quantemol-N code eg [65, 66]. Such tests are stored and therefore the programme comes with an extensive, and increasing, set of sample calculations. Here we present results for low-energy electron collisions with silane.

Calculations were performed for silane in its tetrahedral equilibrium geometry which corresponds to an Si-H distance of 2.80 a_0. A variety of test calculations were performed including the use of target basis sets 6–31G, 6–31G* and 6–311G* and C_2 instead of C_{2v} symmetry. These all gave essentially the same results. Calculations were repeated for two of the Quantemol-N default models: static exchange (SE) and close-coupling (CC). In both cases the results presented are for a 6–31G target basis and two target states per symmetry; other parameters correspond to the default settings.

The SE model uses an SCF ground state wavefunction as the only state in the close-coupling expansion and does not allow for target polarisation. The SE model misses much of the essential physics, especially at low energies, but besides computational simplicity it is also has the advantage that it does not suffer from artificial resonances at higher energies which are a feature of CC methods. Furthermore the SE model is well defined and is therefore useful for comparing between codes. Our SE calculations used an R-matrix radius $a = 10$ a_0, and retained one virtual orbital of each symmetry in the scattering basis, where available, to allow for short-range effects omitted by the continuum orbitals. We used the continuum orbitals of Faure et al [64], which include up to g ($\ell = 4$) symmetry functions. In the outer region the R-matrix was propagated to 100.1 a_0.

The CC model differs from the SE model in that it is based upon a Complete Active Space (CAS) CI target wave functions in which the Si 1s electrons are frozen and all configuration generated by distributing the remaining 16 electrons among the 12 lowest orbitals are used in the CI expansion. In compact notation, and remembering that the calculation is being performed in C_{2v} symmetry, this CAS-CI can be written:

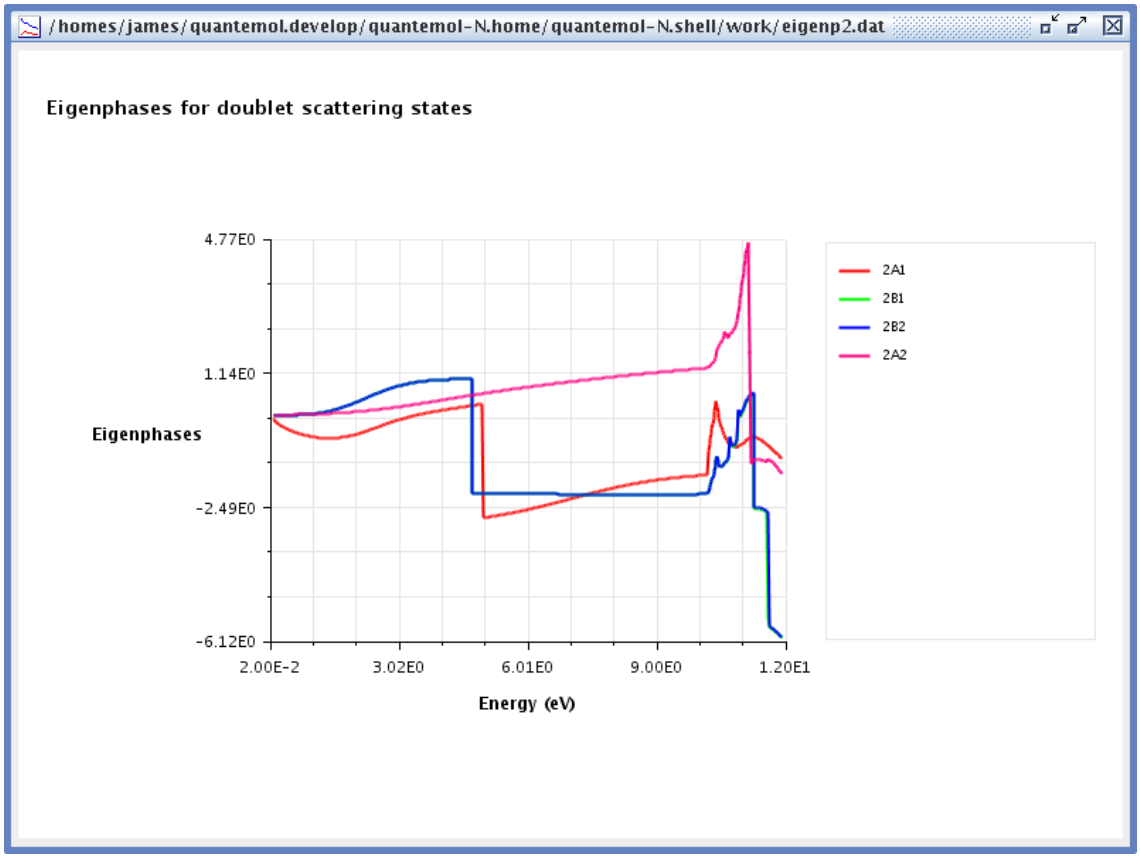

Figure 8. Quantemol-N graphical output: Eigenphases for a 16-state close-coupling calculation for silane performed in C_{2v} symmetry.

$1a_1^2$ $(2a_1\ 3a_1\ 4a_1\ 5a_1\ 6a_1\ 1b_1\ 2b_1\ 3b_1\ 1b_2\ 2b_2\ 3b_2)^{16}$
The lowest two states for each symmetry were retained in the CC expansion: this gives 16 states in all when both singlet and triplet symmetries are accounted for. In our model the 15 excited states lie between 10.26 and 11.66 eV above the $^1A_1$ ground state.

Figure 12 compares the present results with those obtained previously. Our SE calculations are in complete agreement with those of Winstead and McKoy [51] who performed Schwinger variational calculations on silane using the same model. Our CC calculations agree well with the Kohn variational calculations of Sun et al [53] except at low energies. Sun et al used an optical potential rather than CC expansion to model target polarisation effects. It can be seen that our CC are calculations are in excellent agreement with the experiments of Sueoko et al [47] over the entire energy range considered.

Another property of low-energy electron-silane scattering is the presence of a Ramsauer-Townsend minimum in the total cross section. This minimum is absent in SE calculations, which neglect effects due to polarisation of the target charge cloud, as it is the result of a subtle cancellation between the multipole potential and polarisability. Table 1 compares calculated values with the experimental value of Ohmari et al [43]; again our CC value is in very good agreement with the value inferred experimentally suggesting that this model provides a good *ab initio* treatment of polarisation effects, at least at low scattering energies.

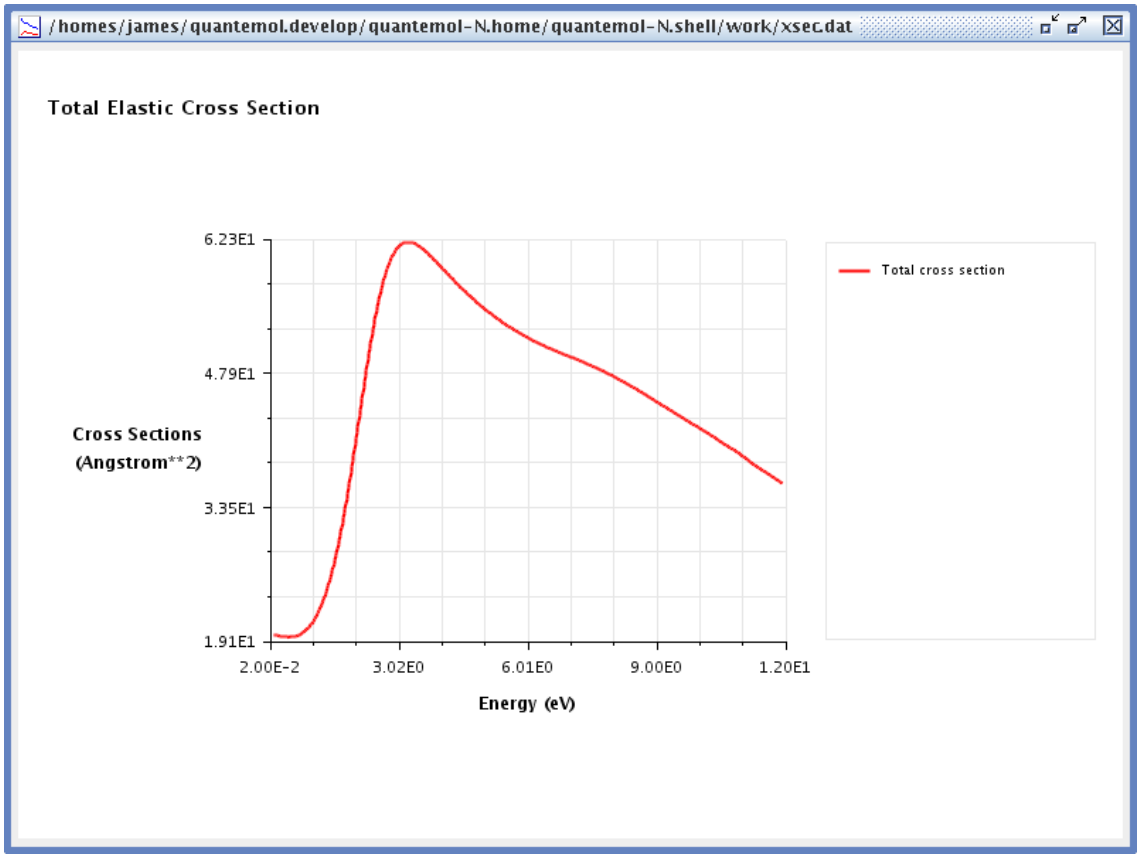

Figure 9. Quantemol-N graphical output: Elastic cross sections for a 16-state close-coupling calculation for silane performed in C_{2v} symmetry.

Table 1. Position of the Ramsauer-Townsend minimum in various calculations and the experiment of Ohmari et al [43].

Model	Position/eV
Sun et al (1992) [53]	0.30
Jain and Thompson (1987) [48]	0.50
Ohmari et al (1986) [43]	0.35
This work, 6-31G (CC)	0.40

5. Conclusions

The R-matrix method has proved to be highly successful for treating a variety of collision problems in atomic and molecular physics [3]. In particular the UK molecular R-matrix codes have become widely used for the treatment of low (and now intermediate [36]) energy electron-molecule scattering. We have developed an expert system, Quantemol-N, for running these codes. Quantemol-N is designed so that *ab initio* electron-molecule scattering calculations can be performed by the non-specialist. As we demonstrate with the results for electron-silane collisions presented here and by results published elsewhere [65, 66], the code is capable of giving excellent results with little more input than a knowledge of the equilibrium geometry of the target molecule. Further information on Quantemol-N can be found at www.quantemol.com.

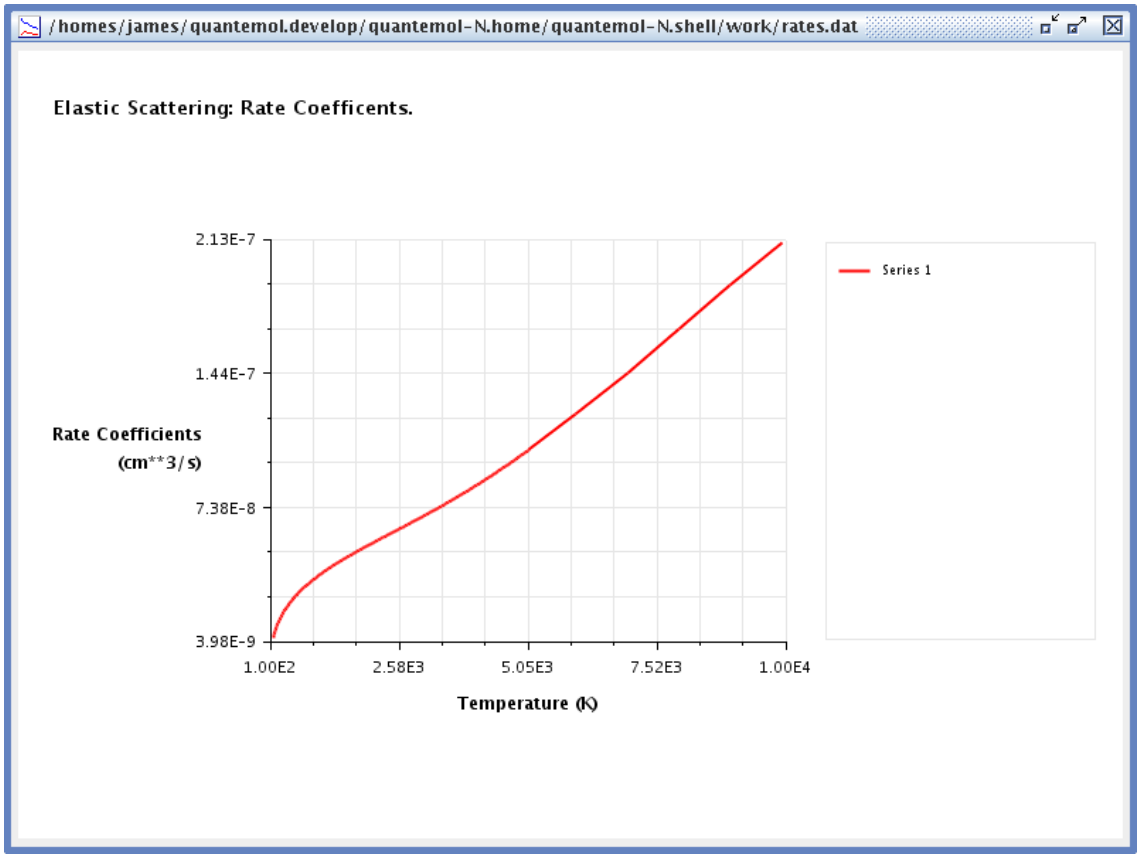

Figure 10. Quantemol-N graphical output: Rates for electron-silane elastic scattering.

Figure 11. Rates

Acknowledgements

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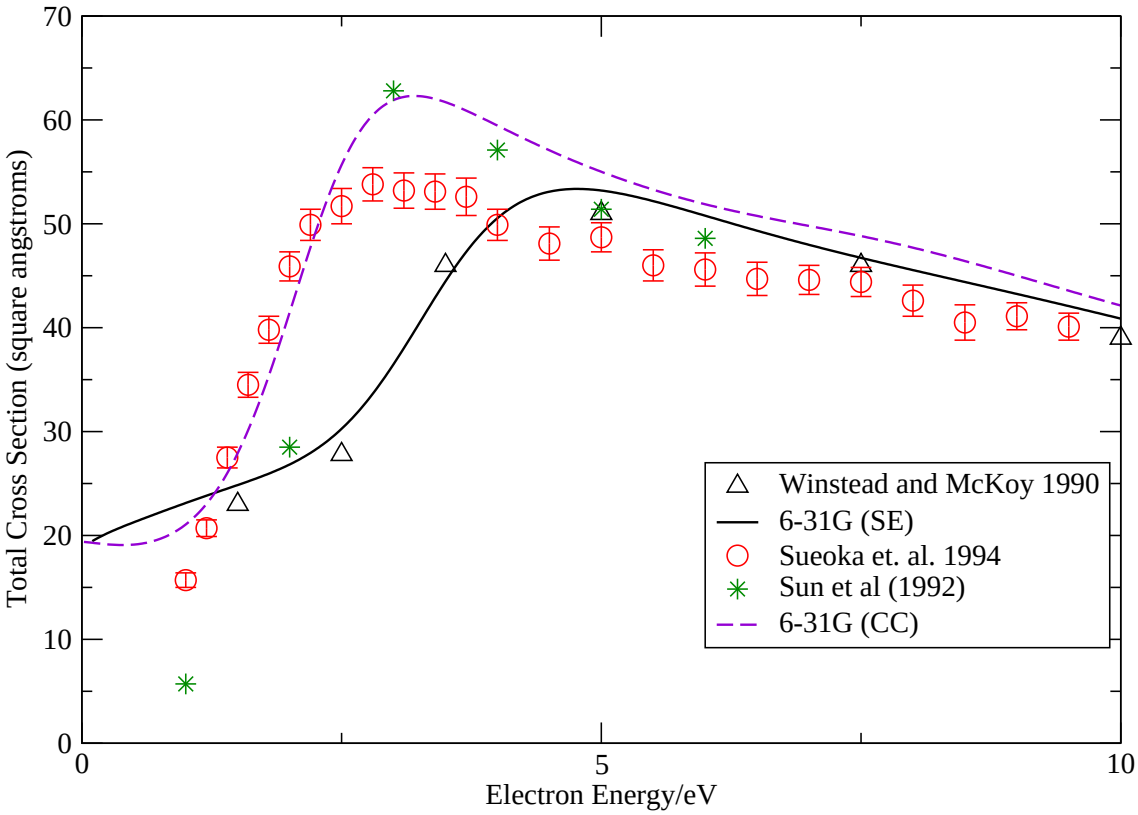

Figure 12. Total cross section for electron-silane collisions. Curves are for the SE and CC models of this work, see text for details. Points are the measurements of Soueko et al [47], the SE calculations of Winstead and McKoy [51] and the polarised target calculation of Sun et al [53].

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