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R-matrix calculations for polyatomic molecules: electron scattering by N_2O

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Abstract. A new computer program has been developed which allows us to use the R-matrix method to study electron scattering by polyatomic molecules. Our first application is to scattering by N_2O in its linear, equilibrium geometry for energies up to 10 eV. We confirm the earlier assignment of $^2\Pi$ symmetry to the resonance near 2 eV but we are unable to locate any resonance having $^2\Sigma$ symmetry in this energy range. We present integral and differential cross sections which are generally in excellent agreement with experiment.

1. Introduction

Nitrous oxide has been the subject of considerable scientific interest due to its role in a number of important processes. For example, it has been found to be important in the chemistry of the upper atmosphere where it may play an important role in the destruction of the ozone layer (see, for example, Wayne 1991). N_2O lasers are used in medical applications (Fox and Reid 1985) and the gas is used as an anaesthetic.

There have recently been several experimental measurements for this system. Those most relevant to the present calculations include those of Kwan *et al* (1984) and Szmytkowski *et al* (1984, 1989) who have published total cross sections and those of Azria *et al* (1975), Andrić and Hall (1984), Marinković *et al* (1986) and Johnstone and Newell (1993) who reported differential cross sections.

The 2.3 eV shape resonance was first observed by Bruche (1927) but it was not recognized as such until dissociative attachment measurements were carried out in the 1960s by Schulz (1961) and Chantry (1969). Bardsley (1969) proposed that the peak was in fact due to two resonances, the lower having $^2\Pi$ symmetry and the higher, main, peak having $^2\Sigma^+$ symmetry. The double resonance theory would appear to have been confirmed by the vibrationally inelastic measurements of Andrić and Hall (1984) who used the theory of Andrick and Read (1971) to analyse their results, though they reverse the order of the two resonances. They also identified a second resonance of Σ symmetry around 8 eV. However, the more recent measurements of Johnstone and Newell (1993) do not show any evidence for this resonance.

As far as we are aware, there have only been two previous calculations of electron scattering cross sections, by Sarpal *et al* (1996), who also used an R-matrix method and

Michelin *et al* (1996) who used a Schwinger variational method. The differences between the work of Sarpal *et al* and the present work will be discussed in detail below. Other theoretical work has concentrated on the bound states of the target molecule, but there has been one attempt to reproduce the resonant N_2O^- state. This was a multiconfiguration SCF calculation by Hopper *et al* (1976) who came to the same conclusion as Bardsley, that there were two resonant states, the lower having $^2\Sigma^+$ symmetry and the higher having $^2\Pi$ symmetry. It has been pointed out by several authors that this designation is rather odd if one compares N_2O with the iso-electronic CO_2 molecule. CO_2 has been well studied and in this case the 3 eV resonance is accepted as having $^2\Pi_u$ symmetry and the 8 eV resonance as having $^2\Sigma$ symmetry. Sarpal *et al* found no evidence for a low-lying $^2\Sigma$ resonance but did find a broad feature around 8 eV having this symmetry.

In this paper we describe our new polyatomic *R*-matrix code. The method is very similar to that used, very successfully, for diatomic targets (see, for example, Tennyson 1995). The success or failure of a particular calculation depends on the model employed, i.e. the choice of trial wavefunction. The more sophisticated of the methods currently in use, such as the *R*-matrix, the complex Kohn method, the Schwinger multichannel method or various methods based on single centre expansions (for detailed descriptions see Huo and Gianturco 1995) should, in principle, all give the same results when applied to the same model. The differences arise in computational efficiency and hence the complexity of the model to which they can be applied. The *R*-matrix model is particularly efficient since the most demanding part of any calculation, describing the system inside the *R*-matrix sphere, need only be carried out once per symmetry and geometry, since it is independent of scattering energy. The inclusion of electronically excited states poses no particular problems to us, unlike some of the other methods referred to above. In the present calculation we use two simple models, static exchange (SE), which should give identical results to those reported by Sarpal *et al* (1996) and a static-exchange-plus-polarization model (SEP) which differs in a number of important respects from their analogous model. These differences are discussed below.

2. Method

2.1. Polyatomic code

The application of the *R*-matrix method to electron–diatomic molecule scattering has been described in detail in previous papers (see, for example, Gillan *et al* 1987, Morgan 1995). Previous work was restricted to diatomic targets principally by our choice of underlying quantum chemistry code. The diatomic code used a modified verson of the IBM 'Alchemy' quantum chemistry program (McLean 1971, Noble 1982). This used Slater-type orbitals (STOs) to represent the bound electronic orbitals and numerical orbitals to describe the continuum. STOs are only really suitable for linear systems, because of the difficulty in evaluating multicentre integrals, and all modern quantum chemistry codes use Gaussian-type orbitals (GTOs), primarily to utilize the fact that all the required integrals can be evaluated in closed form. This has a major repercussion on the design of a scattering code, since it would not be easy to incorporate numerical continuum orbitals and the associated numerical quadratures. The new code therefore represents the continuum using GTOs centred at the molecular centre of mass.

To generate the necessary target molecular orbitals and transformed integrals, we have chosen the 'Molecule-Sweden' suite of codes developed by Almlof and Taylor (1984) and others. The major modification required to make a quantum chemistry code suitable for

R-matrix calculations is to restrict the range of spatial integration to a finite sphere. Rather than modify the existing integrals code, we chose to subtract from the integrals over an infinite sphere, the contribution from the outer region. This has been implemented for all the necessary integrals and the method used for evaluation of these integrals is described in the appendix.

The generation of a set of molecular orbitals for the target-plus-continuum system is non-trivial because of linear dependence problems which are a common feature of scattering calculations. The greater accuracy of integral evaluation for GTOs compared with STOs means that we have so far had to use less stringent orthogonalization techniques. The present code offers a mixture of Schmidt and symmetric (Löwden) orthogonalization procedures.

For the remaining steps, we use our previously developed codes for the construction of the Hamiltonian (Tennyson 1996) and the solution of the close-coupling equations in the outer region (Gillan *et al* 1987). These codes had to be generalized to treat the lower symmetries present in polyatomic molecules. The polyatomic code uses D_{2h} or lower symmetry.

The only other significant differences from our diatomic work was that we used a Bloch operator to make the Hamiltonian matrix Hermitian inside the R-matrix sphere. In the diatomic code we imposed fixed boundary conditions on the continuum wavefunctions and added a Buttle correction, in the outer region, to compensate for this restriction. The Buttle correction also has some effect in adding contributions from higher-energy terms omitted from the basis. However, we saw no evidence to suggest that such an addition would have a noticeable effect on the present calculations.

Before embarking on calculations with a polyatomic target, the code was tested for a number of diatomic systems including N_2, CO and H_2^+. We have also performed calculations on electron collisions with water and ozone, results of which will be published separately.

2.2. Electron–N_2O collisions

The trial wavefunctions, at a fixed geometry, have the usual form,

$$\psi_k = \sum_{ij} \phi_i(x_1 \ldots x_N) u_{ij}(x_{N+1}) a_{ijk} + \sum_i \chi_i(x_1 \ldots x_{N+1}) b_{ik} \tag{1}$$

where ϕ_i are target wavefunctions and the $u_{ij}(x)$ are continuum orbitals. The χ_i are two-centre quadratically integrable functions constructed from the target occupied and virtual molecular orbitals.

In the present calculation we only used a single SCF target wavefunction. The choice of continuum basis is a more difficult one. It is clearly computationally advantageous to represent the continuum orbitals in terms of GTOs, but there is a serious problem in choosing a basis which is sufficiently diffuse to represent wavefunctions which are oscillatory and have finite amplitudes on the R-matrix sphere, and which is sufficiently large to span the space interior to the sphere, yet does not display any linear dependence on the other orbitals used in the calculation. This problem has been addressed by Nestmann and Peyerimhoff (1990) and we use their methodology. The advantage of such an approach is that the basis is only required to provide a good approximation to an equivalent basis of orthonormal spherical Bessel functions. It is independant of the target molecule (provided that it has neutral charge) and only depends on the size of the R-matrix sphere and, to a lesser extent, on the range of scattering energies to be considered. In the present calculation we use the basis given by Sarpal *et al* (1996) which includes all angular momenta up to $l = 3$.

We used two scattering models, SE and SEP. In the SE model the second term in equation (1) was restricted to have the same form as the first, but with the additional electron occupying one of the virtual orbitals from the SCF basis. In contrast to our work on diatomic targets, we used all available virtual orbitals. This was not possible in the diatomic work because the diffuse nature of the highest lying virtuals, coupled with the inaccuracies inherent in numerical quadratures, gave rise to linear dependence problems. It can be argued that, ignoring questions of numerical accuracy, these very unphysical orbitals should be omitted. However, since we wished to make as close as possible a comparison with Sarpal *et al*, we used them all. In the second (SEP) model we departed from that used by Sarpal *et al*. In this model, the second term in equation (1) is constructed by allowing single electron excitations from the target wavefunction into virtual orbitals, with the scattered electron also occupying a virtual orbital. This can give rise to extremely large Hamiltonian matrices which can be expensive to diagonalize. To avoid this problem, Sarpal *et al* selected only those configurations which caused a specified lowering of the lowest SE states. We chose a different approach. Since we are able to restrict the specific configurations of the 'polarization' terms (Tennyson 1996), we chose to allow one target electron to be excited into a virtual orbital, but restrict the N electron target part of the wavefunction to have the same spin symmetry as the target wavefunction used in the first part of equation (1). A problem with all attempts to go beyond the simple SE model is to ensure that the level of approximation used to describe the $N+1$ electron anion system is consistent with that used for the N electron target. There are no triplet correlations in the SCF target and so their introduction into the $N+1$ electron wavefunction could (and would appear to) lead to an imbalance between the two parts of the trial wavefunction. Terms where the N electrons couple to give triplet spin symmetry should not have a significant effect on the polarization of the system, since there is no dipole coupling between them and the target. We feel that our model comes closer to this ideal than those where the only restriction placed on the $N+1$ electron wavefunction is that it has the correct overall symmetry. In the present calculation we froze six electrons into the the 1s orbitals of the three atoms but allowed single excitations out of all the valence shells.

In the external region we retained the dipole and quadrupole moments of the target charge distribution when solving the coupled differential equations.

3. Results and discussion

We only considered the linear geometry and used the experimental equilibrium bond lengths 2.1320 a_0 and 2.2378 a_0 for the N–N and N–O bonds respectively. Calculations were carried out in the C_{2v} point group. We restricted the range of scattering energies to below 10 eV. At higher energies, large numbers of pseudoresonances appear in our SEP model. These are due to the omission of energetically allowed channels corresponding to scattering from excited target states. However, the symmetry restriction that we have placed on the two-particle one-hole terms in the trial wavefunction has the effect of excluding all pseudoresonances except those corresponding to states having the same symmetry as the ground state ($^1\Sigma^+$).

Since we wished to make a detailed comparison with the work of Sarpal *et al*, we used the same orbital set as described in their paper. This is the [5s, 3p] contracted basis of Dunning (1971) augmented, for all three atoms, by a d function with exponent 1.8846. This gives an SCF energy of $-183.697\,98$ au, a dipole moment of -0.3431 au and a quadrupole moment of 3.628 au. Our continuum basis is that given in table 1 of Sarpal *et al*.

Our static exchange calculations gave results virtually identical to those of Sarpal *et al*. The very small differences between the two sets of results can be attributed to the fact that they omitted to subtract contributions from the two-electron integrals in the outer region. Like them, we found a low-energy resonance having $^2\Pi$ symmetry, but in neither model

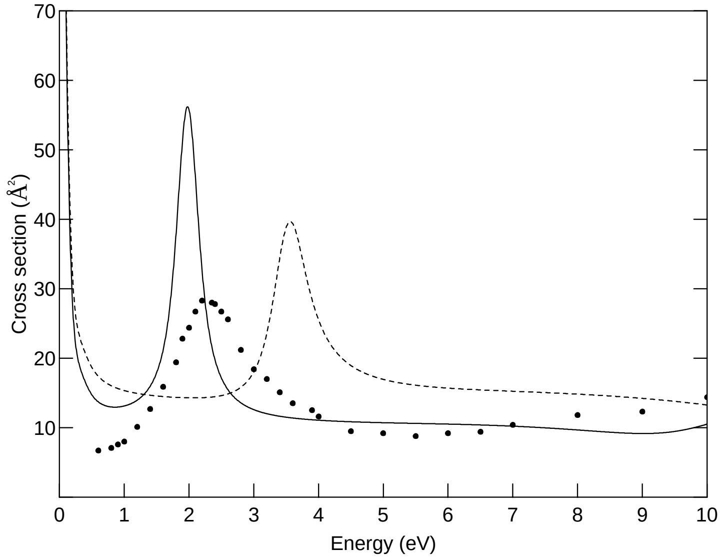


Figure 1. Integrated cross sections. Full curve, SEP model; broken curve, SE model; circles, experiment of Szmytkowski *et al*.

did we find a $^2\Sigma$ resonance below 10 eV.

Our integrated cross sections obtained in the SE and SEP models are compared with the experimental results of Szmytkowski *et al* (1984) in figure 1. Since N_2O is a polar molecule, the elastic integrated cross section formally diverges in the body frame. This can only be remedied by the inclusion of rotational motion in the model. Unfortunately there is no simple, yet reliable method of achieving this, except at either large or extremely small energies where the Born approximation becomes valid (Norcross and Collins 1982). We have therefore chosen to present our body frame results in which the partial wave expansion is truncated at $l = 3$. We believe that the shape of the cross section should not be affected much by this approximation, though the magnitude cannot be considered reliable. We immediately see that the SE model gives too high a position for the resonance. This is well understood to be due to the omission of polarization and correlation effects from the model. Our SEP resonance peak lies a little lower than experiment. The position was found to be 1.99 eV with a width of 0.35 eV. This contrasts with the SEP results of Sarpal *et al* who found the peak to be at 0.8 eV. We believe this excessively low value to be due to their inclusion, in the second term of equation (1), of single electron excitations from the SCF target which do not maintain the the overall symmetry of the target. To test this hypothesis, we removed this restriction from our model and obtained the even lower value of 0.6 eV. We could, of course, obtain a peak position anywhere between this value and the SE value of 3.5 eV by making an appropriate, but arbitrary, choice of which terms to omit. We also investigated the effects of reducing the size of the virtual basis. In a linear system, the B1 and B2 symmetries are degenerate and hence we need only consider one or the other. If we chose the overall B1 symmetry, our results were relatively insensitive to the number of a_1 and b_2 orbitals employed. However, the resonance position was found to be sensitive to radial correlations provided by configurations of the form $N_2O^+ + (\bar{a}1\bar{b}1)$ where $\bar{a}1$ and $\bar{b}1$ are virtual orbitals.

In figure 2 we compare our SEP results with the theory of Michelin *et al* (1996) and

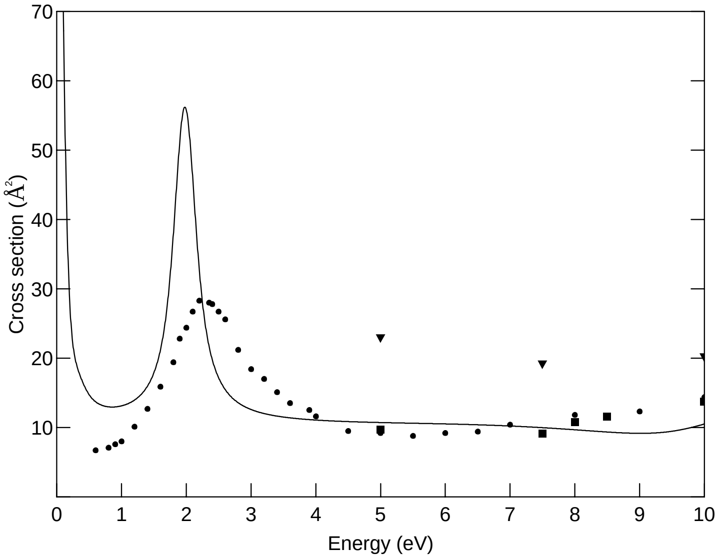


Figure 2. As in figure 1 plus squares, experiment of Johnstone and Newell; triangles, theory of Michelin *et al*.

the experiment of Johnstone and Newell (1993). Neither of these authors gave results in the resonance region below 5 eV. The upturn in our cross section as the energy approaches 10 eV is associated with a broad resonance in the $^2\Sigma$ symmetry at about 11 eV. However, it is overlaid with pseudoresonances due to the omission of excited $^1\Sigma^+$ states, the first of which has a vertical excitation energy of about 10.5 eV.

Our differential cross sections for scattering energies of 5.0, 7.5, 8.0 and 10.0 eV are shown in figure 3. They are compared with the theoretical results of Michelin *et al* (1996) and the experiment of Johnstone and Newell (1993). The error bars on the experimental points are very small and are not shown. At 5 eV there is excellent agreement with experiment at angles above 50°. We cannot explain the discrepancy at smaller angles. Fixed nuclei differential cross sections for polar molecules diverge at 0° and so the addition of more terms to our partial wave expansion would increase, rather than decrease the small angle cross section. At 7.5 eV our agreement with experiment is not so good. The experimental results show the expected upturn as the scattering angle becomes small, but we cannot account for the structure around 65°. This structure is not apparent in the experimental results at 8 eV. Our results at this energy are in excellent agreement in the range 40–110°, but as expected have the wrong behaviour at small angles. We find a minimum around 120°, whereas the experimental minimum is near 110°. We have also used the Born closure approximation to account for the higher l values which have been omitted from our model. This approximation is only appropriate if the Born dipole approximation is valid for these higher angular momenta. We only show the results from this approximation at 10 eV (figure 3(*d*)) since it is at higher energies that the truncation of our partial wave expansion will have most effect. There is very little change except at small angles. The results of Michelin *et al* bear little resemblence to our results. They used the Born closure approximation thoughout their calculations. This could account for the structure that they observed near 20° at all energies, though we did not observe any structure in our Born closure results at any energy.

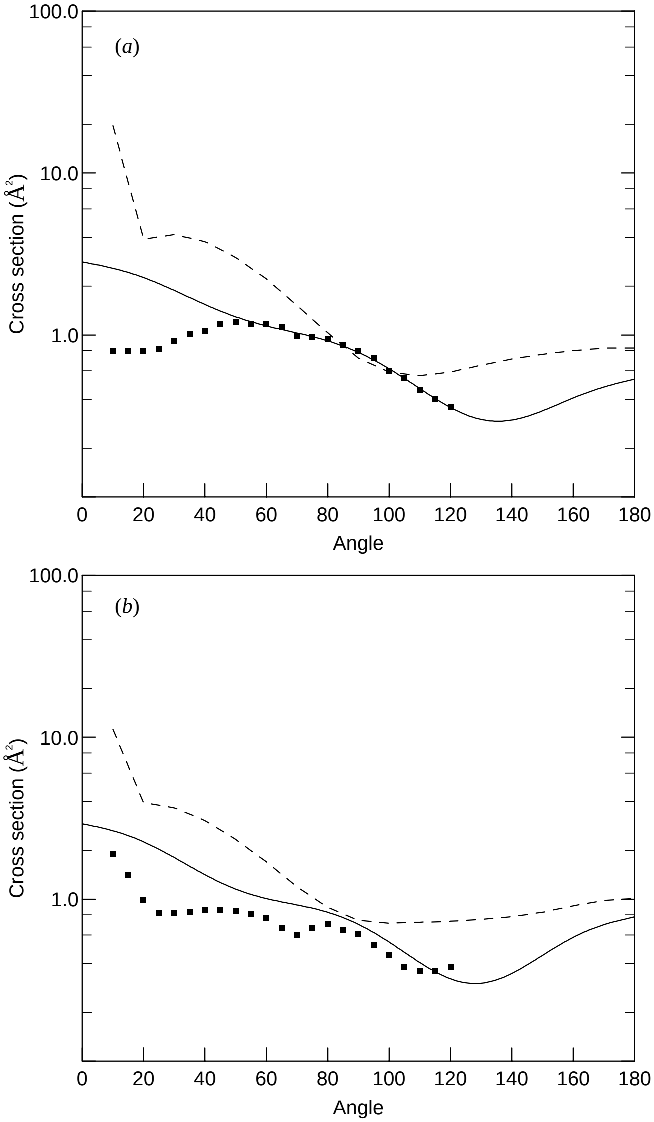
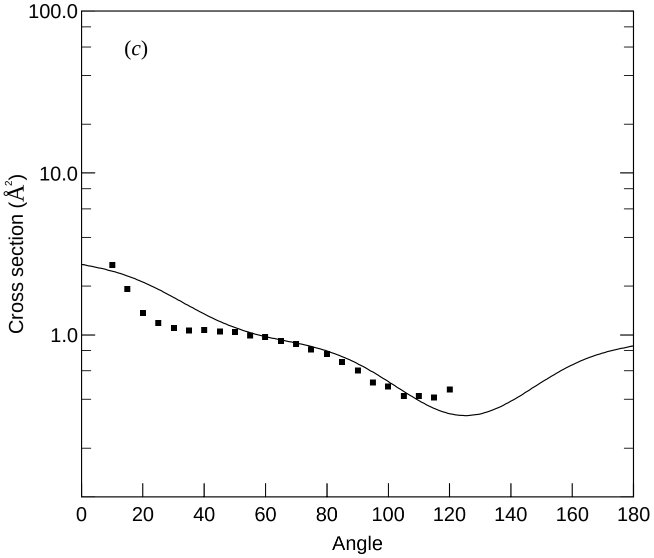


Figure 3. Differential cross sections for various scattering energies, (*a*) 5.0 eV, (*b*) 7.5 eV, (*c*) 8.0 eV, and (*d*) 10.0 eV. Full curve, present SEP results; squares, experiment of Johnstone and Newell; broken curve, theory of Michelin *et al*. At 10 eV the full curve represents SEP+Born closure, the chain curve represents SEP only.

4. Conclusion

These results, for low-energy scattering from N_2O, are the first from the new UK polyatomic R-matrix code. This code differs in several important respects from our earlier diatomic code and from the code developed in Bonn (Pfingst *et al* 1995), although the R-matrix method underlying all three codes is the same.

As expected, our SE results are virtually identical to those of Sarpal *et al* (1996). Our SEP model is quite different from theirs and we obtain a position for the $^2\Pi$ resonance which



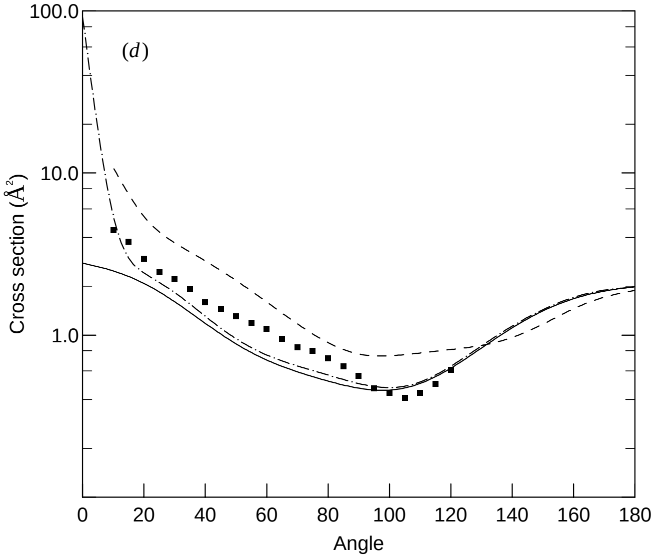


Figure 3. (Continued)

is closer to that observed experimentally. We do not find any resonance of $^2\Sigma$ symmetry below 10 eV. As pointed out by Sarpal *et al*, the interpretation of the early experimental data was based on a simple model of a resonance which ignored the possibility of strong mixing between partial waves. Several of these experiments (for example Azria *et al* 1975, Andrić and Hall 1984) measured vibrational excitation, including bending modes. When the molecule is bent the two degenerate $^2\Pi$ states will split into non-degenerate A′ and A″ states, which could account for the conclusion that there are two resonances in the region of 2 eV.

Our differential cross sections are generally in excellent agreement with the recent measurements of Johnstone and Newell (1993), though discrepancies exist at both small and large angles. Our results are not in agreement with the calculations of Michelin *et al* whose cross sections are generally much larger than ours and have a completely different shape.

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Appendix. Evaluation of tail integrals

We need to evaluate the contribution to all of the spatial integrals from the region outside of the R-matrix sphere. Here we describe the evaluation of the two-electron integrals, since these are the most complicated. The one-electron integrals can be evaluated in a similar manner.

The basic two-electron integral has the form,

$$\left\langle u_i(\boldsymbol{r}_1)u_j(\boldsymbol{r}_2)\frac{1}{|\boldsymbol{r}_1-\boldsymbol{r}_2|}u_k(\boldsymbol{r}_1)u_l(\boldsymbol{r}_2)\right\rangle \tag{A1}$$

where the $u(\boldsymbol{r})$ are atom-centred orbitals which, in our case, are Cartesian Gaussians of the form

$$(x-x_n)^i(y-y_n)^j(z-z_n)^k\mathrm{e}^{-\alpha(r-r_n)^2} \tag{A2}$$

where nucleus n is located at the point (x_n, y_n, z_n). The numerical subscripts label the electrons.

The integration in the above formula is over all values of $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$, but we only require the contribution outside the R-matrix sphere. If none of the orbitals $u(\boldsymbol{r})$ in the integral represent a continuum orbital, then, since we have assumed that the target charge cloud is completely enclosed by the R-matrix sphere, there is no contribution. Also, we require only integrals where only one electron in the trial wavefunction occupies a continuum orbital. From these considerations it can be seen that the only integrals for which there will be a contribution from the outer region will be those, 'direct'-type, integrals where either $u_i(\boldsymbol{r}_1)$ *and* $u_k(\boldsymbol{r}_1)$ are continuum orbitals or else $u_j(\boldsymbol{r}_2)$ *and* $u_l(\boldsymbol{r}_2)$ are continuum orbitals. It is clear from the symmetry of the integrals that we need only consider one of these cases. We choose the latter and simplify our notation by writing equation (A1) as

$$\left\langle u_i(\boldsymbol{r}_1)f_s(\boldsymbol{r}_2)\frac{1}{|\boldsymbol{r}_1-\boldsymbol{r}_2|}u_k(\boldsymbol{r}_1)f_t(\boldsymbol{r}_2)\right\rangle \tag{A3}$$

where u now denotes a target orbital and f denotes a continuum orbital.

We make the usual multipolar expansion of the operator in terms of real spherical harmonics $S_{lm}^q(\hat{\boldsymbol{r}})$

$$\frac{1}{|\boldsymbol{r}_1-\boldsymbol{r}_2|}=\sum_{lmq}\frac{r_<^l}{r_>^{l+1}}S_{lm}^q(\hat{\boldsymbol{r}}_1)S_{lm}^q(\hat{\boldsymbol{r}}_2)=\sum_{lmq}\frac{1}{r_>^{2l+1}}r_1^lS_{lm}^q(\hat{\boldsymbol{r}}_1)\ r_2^lS_{lm}^q(\hat{\boldsymbol{r}}_2). \tag{A4}$$

Using equations (A3) and (A4) we can write our required tail integral as

$$\sum_{lmq}\iint \frac{1}{r_>^{2l+1}} u_i(\boldsymbol{r}_1) r_1^l S_{lm}^q(\hat{\boldsymbol{r}}_1) u_k(\boldsymbol{r}_1) f_s(\boldsymbol{r}_2) r_2^l S_{lm}^q(\hat{\boldsymbol{r}}_2) f_t(\boldsymbol{r}_2)\,\mathrm{d}\boldsymbol{r}_1\,\mathrm{d}\boldsymbol{r}_2 \tag{A5}$$

where the integration over $\boldsymbol{r}_2$ is over the outer region only. The integration over the atom-centred coordinate $\boldsymbol{r}_1$ is over all space, but since we are assuming that the $u(\boldsymbol{r}_1)$ are zero outside the R-matrix sphere, we can regard this as being only over the inner region. We can now identify $r_>$ with r_2, the radial coordinate of the continuum electron and equation (A5) separates into

$$\sum_{lmq}\int u_i(\boldsymbol{r}_1) r_1^l S_{lm}^q(\hat{\boldsymbol{r}}_1) u_k(\boldsymbol{r}_1)\,\mathrm{d}\boldsymbol{r}_1 \int \frac{1}{r_2^{2l+1}} f_s(\boldsymbol{r}_2) r_2^l S_{lm}^q(\hat{\boldsymbol{r}}_2) f_t(\boldsymbol{r}_2)\,\mathrm{d}\boldsymbol{r}_2. \tag{A6}$$

The term $r^l S_{lm}^q(\hat{\boldsymbol{r}})$ can be written as a polynomial of degree l in x, y and z and so the integral over $\boldsymbol{r}_1$ can be evaluated, in closed form, by standard techniques. The integral over $\boldsymbol{r}_2$ is slightly more complicated since the range of the radial coordinate is from the R-matrix radius to infinity. This can also be evaluated in closed form and is most easily achieved by using polar coordinates rather than Cartesians.

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