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ABC: a quantum reactive scattering program

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Abstract

This article describes a quantum mechanical reactive scattering program for atom–diatom chemical reactions that we have written during the past several years. The program uses a coupled-channel hyperspherical coordinate method to solve the Schrödinger equation for the motion of the three nuclei on a single Born–Oppenheimer potential energy surface. It has been tested for all possible deuterium-substituted isotopomers of the $H + H_2$, $F + H_2$, and $Cl + H_2$ reactions, and tried and tested potential energy surfaces for these reactions are included within the program as Fortran subroutines. © 2000 Elsevier Science B.V. All rights reserved.

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Keywords: Quantum reactive scattering; Hyperspherical coordinates; Chemical reaction dynamics

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PROGRAM SUMMARY

Title of program: ABC

Catalogue identifier: ADMX

Program Summary URL: http://cpc.cs.qub.cs.uk/summaries/ADMX

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland

Licensing provisions: none

Computers: SGI Origin200, Compaq DS20

Operating systems under which the program has been tested: IRIX, Digital UNIX

Programming language used: Fortran 90

Memory required to execute with typical data: 128 Mb

No. of bits in a word: 32

No. of bytes in distributed program, including test data, etc.: 246 969

Distribution format: gzipped tar file

External subprograms used: BLAS routines dgemm, dgemv, and dsyr; LAPACK routines dgetrf, dgetrs, dsytrf, dsytri, dsyev and dstev

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Keywords: Quantum reactive scattering, hyperspherical coordinates, chemical reaction dynamics

Nature of physical problem
The calculation of accurate quantum mechanical reaction probabilities and state-to-state integral and differential cross sections for atom–diatom chemical reactions.

Method of solution
The ABC program uses a coupled-channel hyperspherical coordinate method to solve the Schrödinger equation for the motion of the three nuclei (A, B, and C) on a single Born–Oppenheimer potential energy surface. The coupled-channel method used involves a simultaneous expansion of the wavefunction in the Delves hyperspherical coordinates of all three chemical arrangements ($A + BC$, $B + CA$, $C + AB$). The quantum reactive scattering boundary conditions are applied exactly, without the use of an imaginary absorbing potential, and the coupling between orbital and rotational angular momenta is also implemented correctly for each value of the total angular momentum quantum number.

Restrictions on the complexity of the problem
The present version of the program is restricted to the $H + H_2$, $F + H_2$ and $Cl + H_2$ reactions and their deuterium-substituted isotopomers. Potential energy surfaces for other reactions may be included in future releases.

Typical running time
Highly dependent on the input parameters. For the $F + HD$ test calculation given, approximately 30 minutes on a Compaq DS20 workstation.

LONG WRITE-UP

1. Introduction

A great deal of progress has been made in the quantum theory of chemical reactions since the pioneering study of the $H + H_2$ reaction by Kuppermann and Schatz in 1975 [1]. As a result of this progress, it is now possible to solve the Schrödinger equation in the same state-to-state detail for a variety of other chemical reactions including $F + H_2$ [2]. Less detailed quantum reactive scattering calculations can also be performed on a whole host of reactions, including atom-diatom reactions that proceed over deep wells in the potential energy surface such as $H + O_2$ [3] and reactions involving more than three atoms such as $OH + H_2$ [4]. The results of these calculations are often invaluable in helping us to understand the results of modern reaction dynamics experiments and to assess the role of quantum mechanical effects (such as tunneling, zero-point energy, and other interference effects) in chemical reaction dynamics. Moreover, this is likely to become even more the case in the future as the available electronic potential energy surfaces for chemical reactions continue to improve.

Although it is now possible to solve the Schrödinger equation for a number of chemical reactions, it is still not entirely straightforward. The fundamental problem is the fact that the coordinates which best describe the products of a chemical reaction are not the same as those which best describe the reactants, and this leads to technical difficulties in quantum mechanics where all regions of coordinate space have to be treated simultaneously. This problem does not arise in classical mechanics, where there is nothing to prevent one from running a classical trajectory in whatever set of coordinates one chooses and simply monitoring whether or not it reacts. Neither is there any difficulty for other molecular collision processes such as inelastic energy transfer, in which the optimum reactant and product coordinates are the same. The coordinate problem is thus a unique and complicating feature of quantum reactive scattering theory.

As a result of this complication, it has taken until comparatively recently for general computer programs for quantum reactive scattering to become available, whereas quasi-classical trajectory programs for chemical reactions and quantum mechanical programs for inelastic energy transfer have both been available now for many years. Indeed the computer program ABC that we have developed during the past several years is one of only two quantum reactive scattering programs for three-dimensional chemical reactions that have yet been released for general use. The other is a time-dependent wavepacket program called Dynasol that has been developed simultaneously by the group of Zhang [5]. Fortunately, the two programs are complementary in the way they operate and in the kind of problems they can be used to study, for reasons that we shall now outline.

The Dynasol program developed by the Zhang group avoids the coordinate problem by working exclusively with the mass-scaled Jacobi coordinates [6] of the reactant arrangement. As a result, it can be used to calculate initial state-selected reaction cross sections and thermalrate constants for a fairly wide variety of chemical reactions. However, it is less well suited to calculating detailed state-to-state quantities in which the final quantum states of the products are specified at the same time as those of the reactants. By contrast, the ABC program faces up to the coordinate problem by using a simultaneous expansion of the wavefunction in the Delves hyperspherical coordinates [6] of all three chemical arrangements ($A + BC$, $B + CA$ and $C + AB$). As a result, it is ideally suited to calculating detailed state-to-state information such as state-resolved differential reactive scattering cross sections. However, the price to be paid for this is that the use of three different hyperspherical coordinate systems leads to a significant increase in computational complexity which restricts the application of the ABC program to a considerably smaller subset of chemical reactions.

Indeed the present version of the program is restricted to just three different chemical reactions and their deuterium-substituted isotopomers: $H + H_2$, $F + H_2$ and $Cl + H_2$. These three reactions are comparatively easy to study quantum mechanically because there are no deep wells in their potential energy surfaces and because the reactant and product molecules of all three reactions contain at least one hydrogen atom. The program has been tested in a number of published calculations on the three reactions which have helped us to understand the results of recent reaction dynamics experiments [7–11]. The potential energy surfaces that were used in these calculations are included within the present version of the program as Fortran subroutines [12–14].

2. Program overview

The ABC program uses a coupled-channel hyperspherical coordinate method to solve the Schrödinger equation for the motion of the three nuclei on a single Born–Oppenheimer potential energy surface. The quantum reactive scattering boundary conditions are applied exactly, without the use of an imaginary absorbing potential [15], and the coupling between the initial and final orbital and rotational angular momenta is also implemented correctly for each value of the total angular momentum quantum number. However, the assumption that the reaction proceeds on a single adiabatic electronic potential energy surface means that the effect of spin-orbit coupling is *not* treated correctly in reactions such as $F(^2P) + H_2$. This is certainly a shortcoming of the program, and the correct inclusion of spin–orbit coupling in the $F + H_2$ and $Cl + H_2$ reactions is therefore a subject of ongoing research [16].

Table 1
Required values of J, P and p for various reactions

Reaction	J	P	p
$A + B_2$ $(j = 0)$	$0, 1, 2, \ldots$	$(-1)^J$	$+1$
$A + B_2$ $(j > 0)$	0	$+1$	$(-1)^j$
	$1, 2, 3 \ldots$	± 1	$(-1)^j$
$A + BC$ $(j = 0)$	$0, 1, 2, \ldots$	$(-1)^J$	n/a
$A + BC$ $(j > 0)$	0	$+1$	n/a
	$1, 2, 3 \ldots$	± 1	n/a

In each separate run of the ABC program, the reactive scattering Schrödinger equation is solved for specified values of the total angular momentum quantum number J and the triatomic parity eigenvalue P, and also in the case of $A + B_2$ reactions for a specified value of the diatomic parity eigenvalue p (where $p = +1$ for even and -1 for odd rotational states of the B_2 molecule). Each (J, P, p) triple therefore requires a different calculation, as indicated for some example reactions in Table 1.

The resulting output files contain parity-adapted scattering matrix elements of the form $S^{J,P}_{\alpha' v' j' k', \alpha v j k}(E)$ where α and α' are arrangement labels, v and v' are diatomic vibrational quantum numbers, j and j' are diatomic rotational quantum numbers, and k and k' are helicity (intermolecular axis angular momentum projection) quantum numbers. The primed quantities refer to the products of the reaction and the unprimed quantities to the reactants, with $\alpha = 1$ for $A + BC$, $\alpha' = 2$ for $B + CA$ and $\alpha' = 3$ for $C + AB$. The argument E of the scattering matrix is the total (collision plus internal) energy measured from the bottom of the asymptotic reactant valley.

Once these scattering matrix elements have been calculated for sufficiently many values of J and for sufficiently many energies, they can be used to compute any observable property of the reaction. The first stage in this process is to convert the parity-adapted S-matrix elements $S^{J,P}_{n'k',nk}(E)$ into standard helicity-representation S-matrix elements $S^{J}_{n'k',nk}(E)$ using the formulas

$$S^{J}_{n'k',nk} = S^{J}_{n'-k',n-k} = \frac{\sqrt{(1+\delta_{k'0})(1+\delta_{k0})}}{2}\left[S^{J,+1}_{n'k',nk} + S^{J,-1}_{n'k',nk}\right], \tag{1}$$

and

$$S^{J}_{n'-k',nk} = S^{J}_{n'k',n-k} = (-1)^{J}\frac{\sqrt{(1+\delta_{k'0})(1+\delta_{k0})}}{2} \times \left[S^{J,+1}_{n'k',nk} - S^{J,-1}_{n'k',nk}\right], \tag{2}$$

where n and n' are composite indices for $\alpha v j$ and $\alpha' v' j'$ and the quantum numbers k and k' are restricted such that $0 \leqslant k \leqslant \min(J, j)$ and $0 \leqslant k' \leqslant \min(J, j')$. (The quantum numbers $k = 0$ and $k' = 0$ only occur in the parity block with $P = (-1)^{J}$, but Eqs. (1) and (2) have been written with this in mind: simply set $S^{J,P}_{n'k',nk} = 0$ whenever $P = (-1)^{J+1}$ and k and/or $k' = 0$.)

The observables that can be calculated from the resulting helicity-representation S-matrix elements $S^{J}_{n'k',nk}(E)$ range from fully state-resolved differential [17]

$$\frac{d\sigma_{n'k'\leftarrow nk}}{d\Omega}(\theta, E) = \left|\frac{1}{2ik_n}\sum_{J}(2J+1)d^{J}_{k'k}(\theta)S^{J}_{n'k',nk}(E)\right|^{2}, \tag{3}$$

and integral [17]

$$\sigma_{n'k'\leftarrow nk}(E) = \frac{\pi}{k_n^2}\sum_{J}(2J+1)\left|S^{J}_{n'k',nk}(E)\right|^{2}, \tag{4}$$

reactive scattering cross sections through to considerably more averaged quantities such as initial state-selected reaction cross sections and thermal rate constants. However, as discussed in the introduction, the ABC program is ideally suited to calculating fully state-resolved quantities such as those in Eqs. (3) and (4), since other more efficient methods are available for calculating less detailed quantities in which the quantum states of the products are not resolved [18,19].

3. Methodological details

The coupled-channel hyperspherical coordinate method that is used in the ABC program is very similar to the method suggested by Schatz [20], with the following two minor modifications:

(a) The reference potentials that are used to construct the coupled-channel basis functions are taken to be the diatomic potentials of each arrangement on the surface of the hypersphere, rather than cuts through the full triatomic potential at each hyperradius ρ.

(b) The resulting multiple-arrangement basis set is canonically orthogonalized to avoid overcompleteness problems in the small-ρ exchange region [21], in the same way as atomic orbital basis sets are orthogonalized in electronic structure theory [22].

The coupled-channel hyperradial equations are solved within the ABC program using a constant reference potential log derivative method [23], with M_{tr} equally spaced sectors between $\rho = \rho_{\min}$ and $\rho_{\max}$. At each scattering energy, the scattering matrix $S^{J,P}(E)$ is then extracted from the final log derivative matrix $Y(\rho_{\max})$ by applying the reactive scattering boundary conditions in the way described by Pack and Parker [6], with one minor (but essential) modification.

The need for this modification arises because the angular momentum basis functions that are used within the ABC program are in the helicity (k) rather than the orbital angular momentum (l) representation. If the helicity basis were complete, this would not be an issue, since the corresponding orbital angular momentum functions $|JMjl\rangle$ could be obtained from the orthogonal transformation [6]

$$|JMjl\rangle = \sum_{k=-\min(J,j)}^{\min(J,j)} |JMjk\rangle C^{Jj}_{kl}, \tag{5}$$

where

$$C^{Jj}_{kl} = \left(\frac{2l+1}{2J+1}\right)^{1/2} C(jlJ; k0k). \tag{6}$$

However, in order to make the ABC program more efficient, the helicity basis that is used within each arrangement is generally not complete for large values of the total angular momentum quantum number.

Instead, the modulus of the helicity quantum number k is restricted such that $|k| \leqslant \min(J, j, k_{\max})$, where $k_{\max}$ is an input parameter to the program. This restriction is useful in reducing the size of the angular basis set that is needed for large values of J and j, since well-converged results can often be obtained with $k_{\max}$ as small as 3 or 4 for reactions that are collinearly constrained [24,25].

The use of a truncated range of k quantum numbers implies, however, that Eq. (5) must be replaced by

$$|JMjl\rangle = \sum_{k=-\min(J,j,k_{\max})}^{\min(J,j,k_{\max})} |JMjk\rangle D_{kl}^{Jj}, \tag{7}$$

where D_{kl}^{Jj} is a component of an eigenvector of the matrix representation of the operator l^2 in the truncated helicity basis. As is well known, this matrix representation of l^2 is tri-diagonal, with diagonal elements

$$\langle JMjk|l^2|JMjk\rangle = J(J+1) + j(j+1) - 2k^2, \tag{8}$$

and off-diagonal elements

$$\langle JMjk'|l^2|JMjk\rangle = \left[J(J+1) - k'k\right]^{1/2}\left[j(j+1) - k'k\right]^{1/2}\delta_{|k'-k|,1}. \tag{9}$$

If the helicity basis were complete, the elements D_{kl}^{Jj} of the eigenvectors of this matrix would be identical to the vector-coupling coefficients C_{kl}^{Jj} in Eq. (6), and the eigenvalues would be $l(l+1)$ where $l = |J-j|, \ldots, J+j$. However, for an incomplete helicity basis of the type that is used in the ABC program, the eigenvectors of the l^2 matrix are no longer composed of standard vector coupling coefficients, and the eigenvalues have the form $l(l+1)$ where l is no longer necessarily even an integer.

In order to illustrate this, the values of l computed numerically from the eigenvalues of the l^2 matrix are shown as a function of $k_{\max}$ for the case $J = j = 3$ in Table 2. All of the calculated values lie in the range $|J - j| \leqslant l \leqslant J + j$, but equally spaced integer values of l are only obtained in the limit of a complete basis set ($k_{\max} = 3$). This result is clearly independent of whether or not one exploits the effect of parity conservation, as can be seen from the parity eigenvalues (given in parentheses) in Table 2. Thus the use of an incomplete helicity representation basis inevitably corresponds to using *non-integral* orbital angular momentum quantum numbers.

Table 2
Orbital angular momentum quantum numbers, l, and parity eigenvalues, (P), as a function of the helicity truncation parameter $k_{\max}$ for the case $J = j = 3$

$k_{\max} = 0$	$k_{\max} = 1$	$k_{\max} = 2$	$k_{\max} = 3$
			0.000 (−1)
		0.962 (−1)	1.000 (+1)
	2.000 (−1)	2.468 (+1)	2.000 (−1)
4.424 (−1)	4.217 (+1)	3.794 (−1)	3.000 (+1)
	5.844 (−1)	4.949 (+1)	4.000 (−1)
		5.994 (−1)	5.000 (+1)
			6.000 (−1)

Since the asymptotic solutions of the Schrödinger equation are most conveniently written in the orbital angular momentum representation, where the centrifugal potential $l(l+1)/2\mu R^2$ is diagonal, this complicates the application of the scattering boundary conditions. In particular, the Riccati–Bessel functions $j_l(k_n R)$ and $y_l(k_n R)$ and the modified Riccati–Bessel function $k_l(k_n R)$ that enter the scattering boundary conditions must be evaluated for non-integral values of l. This is accomplished within the ABC program using Fortran translations of Temme's excellent Algol routines for calculating Bessel functions with positive real arguments and real orders [26].

4. Example calculation

A suitable test run of the ABC program is provided by the F + HD reaction at low collision energies in the reaction threshold region. This particular reaction exhibits a pronounced quantum mechanical resonance in the HF + D product channel which cannot be reproduced by quasi-classical trajectory calculations. Our test run is only for zero total angular momentum ($J = 0$), and cannot therefore be compared directly with any scattering experiment. However, the resonance that is seen in the test calculation survives angular momentum averaging to appear as a distinct feature in the F + HD → HF + D integral cross section, and this feature *has* been observed experimentally [11].

Table 3
Input parameters for the test calculation on the $F + HD(v = 0, j = 0)$ reaction

Parameter	Explanation
`mass = 19,1,2`	Masses of the three atoms in atomic mass units.
`jtot = 0`	Total angular momentum quantum number J.
`ipar = 1`	Triatomic parity eigenvalue P.
`jpar = 0`	Diatomic parity eigenvalue p.
`emax = 1.7`	Maximum internal energy in any channel (in eV).
`jmax = 15`	Maximum rotational quantum number of any channel.
`kmax = 4`	Helicity truncation parameter k_{max}.
`rmax = 12.0`	Maximum hyperradius ρ_{max} (in bohr).
`mtr = 150`	Number of log derivative propagation sectors.
`enrg = 0.233`	Initial scattering energy (in eV).
`dnrg = 0.001`	Scattering energy increment (in eV).
`nnrg = 48`	Total number of scattering energies.
`nout = 0`	Maximum value of v for which output is required.
`jout = 0`	Maximum value of j for which output is required.

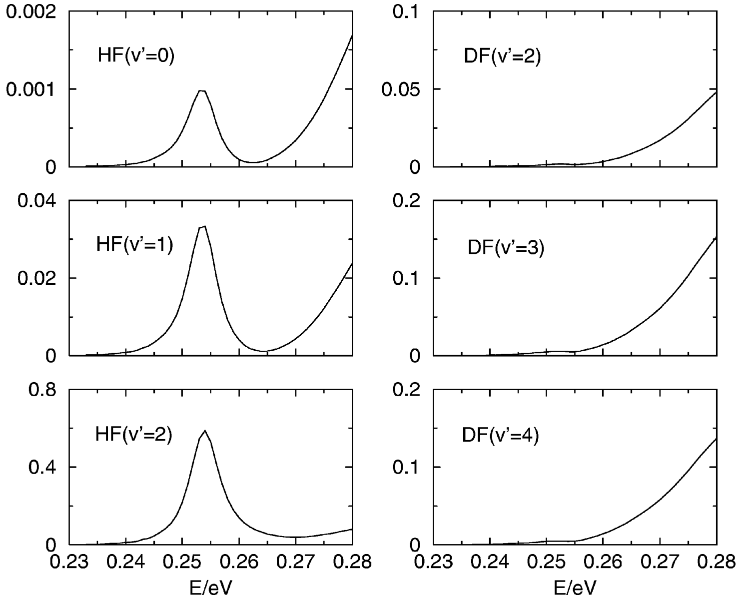

Fig. 1. Reaction probabilities for the $F + HD(v = j = 0) \rightarrow HF(v') + D$ and $DF(v') + H$ reactions on the SW potential energy surface.

The namelist input data that defines the test calculation is shown in Table 3. The atomic masses in the first line of this table only need to be input as integers, since the program adds more significant figures automatically. The appropriate potential energy surface (presently either the LSTH potential for $H + H_2$ [12],

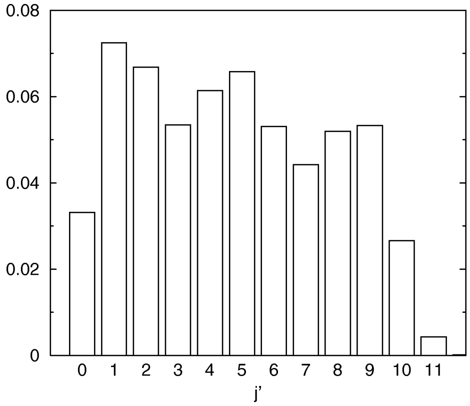

Fig. 2. Reaction probabilities for the $F + HD(v = j = 0) \rightarrow HF(v' = 2, j') + D$ reaction at $E = 0.254$ eV.

the SW potential for $F + H_2$ [13], or the BW potential for $Cl + H_2$ [14]) is also chosen automatically on the basis of these atomic masses. The parameter `jpar` is not actually used for the $F + HD$ reaction, since it only has any significance for $A + B_2$ reactions (see Table 1); this parameter has nevertheless been included for completeness because it forms part of the input to the ABC program. The parameter `kmax` is also not used when $J = 0$, for reasons that should be clear from Section 3. The particular value $k_{\mathrm{max}} = 4$ is given in the table because this has been found to be adequate for calculating converged integral and differential cross sections for the $F + HD(v = 0, j = 0)$ reaction at collision energies slightly higher than those considered here [8].

Since this test calculation involves a lot of scattering energies (`nnrg = 48`), and the exothermicity of the $F + HD$ reaction leads to a lot of open channels in the $HF + D$ and $DF + H$ product arrangements, the resulting output file is rather long. Rather than list the output file, we have therefore summarized some of the results it contains in Figs. 1 and 2. The most interesting thing that can be seen from these results is the fact that there is a pronounced quantum mechanical resonance in the reaction at an energy close to 0.254 eV. Fig. 1 shows that the resonance decays exclusively to give the $HF + D$ product and displays a state-specific preference for the production of $HF(v' = 2)$. The product rotational (j') distribution of the resonance decay can also be extracted from the output of the calculation, and this turns out to be remarkably broad as shown in Fig. 2. A more detailed discussion of these and other aspects of the resonance has recently been given by Skodje et al. [11].

Although it is only for total angular momentum $J = 0$, this test calculation is not entirely trivial because of the large number of coupled channels and scattering energies involved. The computer times taken to complete the calculation on two contemporary computer workstations are given for reference in Table 4. For comparison, an analogous calculation on the same reaction (but using a different quantum reactive scattering method [27]) took approximately 16 hours on a Cray 2 supercomputer back in 1991 [28]. Interestingly, this earlier calculation also found a virtually identical resonance in the $F + HD \rightarrow HF + D$ reaction, even though the best available (T5A [29]) potential energy surface at that time had little in common with the SW potential energy surface in use today. The first ever theoretical observation of this resonance was in a collinear model calculation

Table 4
$F + HD$ test case run times on two contemporary computer workstations

Computer:	SGI Origin200	Compaq DS20
Processor:	R10000	Alpha 21264
Clock frequency:	225 MHz	500 MHz
Operating system:	IRIX 6.5 IP27	Digital UNIX V4.0F
Fortran compiler:	MIPSpro f90	DIGITAL f90
Compiler options:	-ansi -Ofast	-std -fast -fpe1 -assume byterecl
Blas/Lapack:	-lscs	-ldxml
Run time:	1h3m6s	32m10s

performed by Schatz and co-workers in 1975 [30], whereas the first conclusive experimental observation of the resonance was in a state-of-the-art molecular beam experiment reported by Liu and co-workers earlier this year [11].

5. Final remarks

In addition to the $F + HD$ test calculation described above, two other example calculations are included in the ABC program distribution: the $Cl + HD$ reaction for total angular momentum $J = 5$ and the $H + D_2$ reaction for $J = 10$. The purpose of these additional calculations is to test the two remaining potential energy surfaces that are contained within the program and to illustrate the helicity truncation procedure outlined in Section 3 (with $k_{\max} = 3$ for $Cl + HD$ and $k_{\max} = 5$ for $H + D_2$). If all three example calculations run successfully it is almost certain that the program has been correctly installed.

The input data for the $Cl + HD$ and $H + D_2$ calculations has the same form as the $F + HD$ input data in Table 3. It is clear from this input data that each value of J (`jtot`), P (`ipar`) and p (`jpar`) requires a separate calculation, as we have already discussed in some detail in Section 2. If integral and differential cross sections are required they can be computed by inserting the resulting scattering matrices into the formulas that are given in that section. Fortran programs for calculating integral and differential cross sections in this way from the output of the ABC program have been written by the first two authors and are available from them on request.

Finally, it should be stressed that there are still many ways in which the ABC program could be improved. In particular, there is no obvious reason why future versions of the program should not contain either potential energy surfaces for additional reactions or a more rigorous treatment of spin-orbit coupling in reactions such as $F(^2P) + H_2$ [16].

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