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ROTIONS: A program for the calculation of rotational excitation cross sections in electron–molecular ion collisions

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Abstract

ROTIONS is a program for the calculation of cross sections for rotational excitation of linear molecular ions by electron impact. The cross sections can be obtained from input T-matrices and from the Coulomb–Born approximation for dipole ($\Delta j = 1$) and quadrupole ($\Delta j = 2$) transitions. The Coulomb–Born results can be used to augment the low partial-wave T-matrices to an effectively infinite number of partial waves. © 1998 Elsevier Science B.V.

PACS: 34.80.Gs
Keywords: Rotational excitation cross sections; Coulomb–Born approximation; Electron impact

PROGRAM SUMMARY

Title of program: ROTIONS

Catalogue identifier: ADJA

Program Summary URL:
http://www.cpc.cs.qub.ac.uk/cpc/summaries/ADJA

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

Licensing provisions: none

Computer for which the program is designed and others on which it is operable:
Computers: Digital 8400 (known as Columbus), CRAY J90, IBM RS6000 workstations; *Installations:* Rutherford Laboratory, local

Operating systems under which the program has been tested: Unix (OSF/1, UNICOS 8, AIX 4)

Programming language used: Fortran 90

Memory required to execute with typical data: 3 Mwords

No. of bytes in distributed program, including test data, etc.: 794164

Distribution format: uuencoded compressed tar file

CPC Program Library subprograms used: COULFG [1] (catalogue number: ABNK)

Keywords: rotational excitations cross sections, Coulomb–Born approximation, electron impact

Nature of physical problem
ROTIONS calculates rotational cross sections from body-frame T-matrices and the Coulomb–Born (CB) approximation for

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electron–molecular ion collisions.

Method of solution
The body-frame T-matrices are frame transformed into the lab-frame, and the corresponding cross sections obtained. At the same energies, the CB approximation is used to obtain both total and partial rotational cross sections. The low-l partial-wave contribution to the total CB cross section is substituted by the T-matrix cross section [2].

Restrictions on the complexity of the problem
ROTIONS is restricted to the study of linear targets. The CB approximation is only applicable when the target is charged.

Typical running time
The only part of the program that takes significant time is the calculation of CB cross sections for quadrupole transitions. It can be up to 0.5 s per energy on Columbus.

Unusual features of the program
ROTIONS uses the NAG routine D01AKF [3] (not included) to perform a numerical integration.

References

[1] A.R. Barnett, Comput. Phys. Commun. 27 (1982) 147.
[2] I. Rabadán, B.K. Sarpal, J. Tennyson, J. Phys. B 31 (1998) 2077.
[3] NAG Fortran Library, The Numerical Algorithms Group Ltd. (Oxford, UK, 1996).

LONG WRITE-UP

1. Introduction

Cross sections for the rotational excitation of molecular ions by collisions with electrons have been traditionally calculated using the dipole Coulomb–Born (CB) approximation [1–3,5]. In the CB approximation, only the long-range interactions are taken into account and the dipole interaction leads to only $\Delta j = 1$ transitions.

However, our recent work [6], I hereafter, shows that the short-range interactions can be as important as the long-range ones for dipolar interactions, and the main interaction for higher multipoles. In I, we studied the cases of HeH^+, an ion with a large permanent dipole, and NO^+, an ion with a large permanent quadrupole. For HeH^+, the inclusion of short-range interactions increased the rotational excitation cross section by almost a factor of 2. It was also shown that the, previously disregarded, cross sections for quadrupole transitions are only a factor of 2 smaller than dipole ones, which can lead to significant population of the $j = 2$ rotational level [7] and, under favourable conditions, observation of $j = 2 - 1$ HeH^+ emissions in interstellar plasmas. For NO^+, quadrupole CB rotational cross sections were found to be dominated by low-l partial waves. However, low-l electron partial waves sample the internal structure of the molecular ion and, thus, are subject to short-range interactions. In I, the inclusion of short-range effects produced substantially different rotational cross sections than those given by the CB approximation.

Short-range interactions in electron–molecular ion collisions can be introduced using close-coupling (CC) methods. In the case of electron-neutral molecule collisions, CC methods have been implemented to study rotational, vibrational and electronic transitions [8]. However, implementations in the case of electron–molecular ion scattering only cover, so far, vibrational and electronic excitation [9]. With ROTIONS, we extend the range of applications to the study of rotational transitions.

ROTIONS uses, as its starting point, the body-frame (BF) T-matrices produced by reliable CC methods to obtain, through a frame-transformation to the laboratory frame, rotational cross sections. As the number of partial waves used to represent the projectile electron in CC methods is necessarily limited, the cross sections thus obtained lack the contribution of high partial waves. In ROTIONS, the contribution of these high-partial waves to the rotational cross section is evaluated using the CB approximation. This approximation has been implemented only for transitions with $\Delta j \leq 2$. Transitions with $\Delta j > 2$ can be significant [4,6], but the high-l CB contribution to the rotational cross sections is negligible for these transitions, and they can be safely evaluated using BF T-matrices alone. On the other hand, ROTIONS can be used to calculate CB rotational excitation cross sections with $\Delta j \leq 2$ alone.

In I, we calculated rotational cross sections from T-matrices obtained for three different treatments of nuclear motion: (i) the fixed-nuclei approximation, in which the T-matrices are obtained at the target equilibrium geometry; (ii) the adiabatic approximation, with the T-matrices obtained by vibrational averaging fixed-nuclei T-matrices calculated at different geometries; and (iii) the non-adiabatic approximation, in which the T-matrices are obtained from wavefunctions that include nuclear motion terms. Results from fixed-nuclei and adiabatic T-matrices were found in I to be very similar, while those from non-adiabatic T-matrices contained Feshbach resonances associated with nuclear excited states of the molecular Rydberg states. These resonances appear as oscillations around a background cross section similar to the fixed-nuclei and adiabatic ones. Their effect tends to be washed out when averaging in energy around the resonance, so this detailed treatment is probably unnecessary to obtain reliable rotational excitation rates.

Rotational excitation cross sections calculated from BF T-matrices and the CB approximation do not have the correct behaviour at threshold due to the assumed degeneracy of rotational states. Threshold effects are important at low energy collisions, especially for light systems such as HeH^+ [6], and a kinematic correction [10,11] is implemented in ROTIONS (see Section 2.4).

ROTIONS has been implemented within the UK molecular R-matrix package [9,12]. This means that the T-matrices are read according to the output format of the R-matrix package. However, as long as the T-matrix files are produced in this format (detailed in Section 5), ROTIONS is 'CC-method' independent.

When several spin states of the total system have to be considered in the rotational excitation of a target state from BF T-matrices, each spin-state requires a separate calculation with ROTIONS. Similarly, if the system is homonuclear, molecular symmetries g and u need to be treated separately. To obtain the total rotational cross section including contributions from different spin states and symmetries g/u, when applicable, the user has to sum the separate results allowing for spin-statistical weights; the present spin weighting is appropriate for a $^1\Sigma^+$ target state. On the other hand, rotational cross sections in the CB approximations are independent of the total spin-state and, in the case of homonuclear molecules, the rotational transitions $j = 0 \rightarrow 2$ include both even and odd l-waves (i.e., g and u symmetries).

The next section contains the outline of the theory implemented in ROTIONS, Section 3 presents the structure of the code and the task of each subroutine, Section 4 describes the input data required and Section 5 the format of the T-matrix file. Section 6 describes the test data, test run and output.

2. Theory

The method ROTIONS implements is described in detail in I, which made extensive use of earlier work on this problem [2,11,13–15]. Here, we summarise the method.

2.1. T-matrix rotational cross sections

ROTIONS starts with energy dependent BF T-matrices. These are frame-transformed to the laboratory-frame (LAB),

$$T^J_{j'l',jl} \simeq \sum_{\Lambda=-l}^{l} A^{J\Lambda}_{j'l'} \, T^{\Lambda}_{l',l} \, A^{J\Lambda}_{jl} , \tag{1}$$

using the rotational frame transformation matrix A [11]. The cross sections are, then, obtained using the equation

$$\sigma^{\mathrm{TM}}(j \rightarrow j') = \frac{\pi}{k_i^2(2j+1)} \sum_{J=0}^{\infty} \sum_{l=|J-j|}^{J+j} \sum_{l'=|J-j'|}^{J+j'} (2J+1)|T^J_{j'l',jl}|^2 , \tag{2}$$

where k_i is the projectile kinetic momentum, $T^J_{j'l',jl}$ are the LAB T-matrices obtained from the BF T-matrices $T^\Lambda_{j'l',jl}$, l labels the projectile angular momentum, j the target rotational state and J is the total angular momentum of the target plus projectile system. The sum over J is, in practice, limited by the number of partial waves included in the T-matrices, LMAX$\geq l, l'$.

2.2. Coulomb–Born rotational cross sections

CB cross sections are (optionally) evaluated at the energies where the BF T-matrices are given or at a user-specified energy grid if no T-matrices are given. If $\Delta j = 1$, the dipole CB cross section is obtained; if $\Delta j = 2$, the corresponding quadrupole CB cross section. No implementation has been made for transitions with $\Delta j > 2$.

The total dipole CB cross section is obtained by the closure formula

$$\sigma_1^{\rm CB}(j \to j') = \frac{3Q_1^2}{4\pi}\frac{2j'+1}{k_i^2}\begin{pmatrix} j & j' & 1 \\ 0 & 0 & 0 \end{pmatrix} f_{E1}(\eta_i, \xi)\,, \tag{3}$$

where Q_1 is the permanent dipole moment of the target, $\eta = -1/k$, $\xi = \eta_f - \eta_i$ and f_{E1} is a dipole Coulomb excitation function expressed in terms of hypergeometric functions.

The partial dipole CB ($\sigma_1^{\rm PCB}$), total quadrupole CB ($\sigma_2^{\rm CB}$) and partial quadrupole CB ($\sigma_2^{\rm PCB}$) cross sections are obtained using the equation

$$\sigma_\lambda^{\rm CB,PCB}(j \to j') = 16\pi\frac{k_f}{k_i}Q_\lambda^2\frac{2j'+1}{2\lambda+1}\begin{pmatrix} j & j' & \lambda \\ 0 & 0 & 0 \end{pmatrix}\sum_{l_il_f}(2l_i+1)(2l_f+1)\begin{pmatrix} l_i & l_f & \lambda \\ 0 & 0 & 0 \end{pmatrix}^2 \left|M_{l_i,l_f}^{-\lambda-1}\right|^2, \tag{4}$$

where $\lambda = 1$ for the dipole and $\lambda = 2$ for quadruple transitions, and M_{l_i,l_f} are radial matrix elements defined as

$$M_{l_i,l_f}^{-\lambda-1} = \frac{1}{k_ik_f}\int_0^\infty F_{l_f}(k_fr)r^{-\lambda-1}F_{l_i}(k_ir)\,{\rm d}r\,. \tag{5}$$

Here, $F_l(kr)$ is the regular radial Coulomb function of angular momentum l.

The sum in Eq. (4) is performed up to $l_i = l_f =$ LMAX, in the case of the partial CB cross sections, and up to $l_i = l_f =$ LMAXQ for the total quadrupole CB cross section; LMAXQ has to be high enough to obtain convergence (LMAXQ=40 is a safe value).

The integrals in Eq. (5) are evaluated numerically only for M_{02}^{-3} and M_{20}^{-3}. The remaining elements are obtained using recurrence relations. In the dipole case, all radial matrix elements are obtained with recurrence relations from the first two monopoles, which have an analytical solution in terms of a hypergeometric function, see I.

2.3. Final rotational cross section

The final cross section, which includes the low-l partial wave information from the T-matrices, and the high-l cross section from the CB calculations, is obtained simply by

$$\sigma(j \to j') = \sigma^{\rm TM}(j \to j') + \sigma_\lambda^{\rm CB}(j \to j') - \sigma_\lambda^{\rm PCB}(j \to j')\,. \tag{6}$$

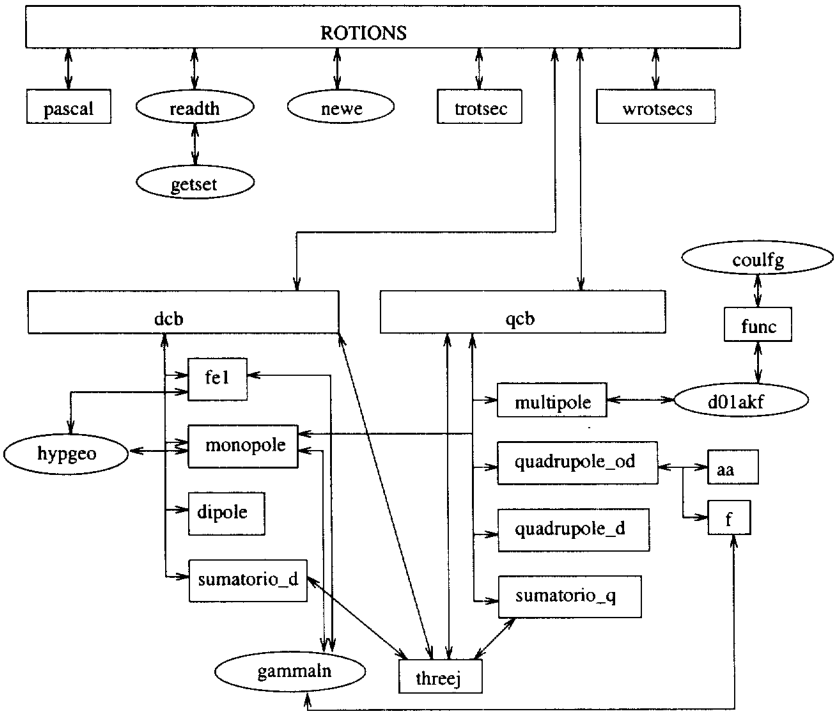

Fig. 1. Flow diagram of the program ROTIONS. Routines in ovals have been taken from existing libraries.

2.4. Threshold correction

The theory implemented in ROTIONS assumes that the rotational states of the target are degenerate, which leads to rotational excitation cross sections that do not go to zero at threshold. This is (optionally) corrected by multiplying the rotational cross sections by a kinematic ratio [10,11]

$$\sigma^{\mathrm{tc}}(j \to j') = \frac{k_f}{k_i}\,\sigma(j \to j'), \tag{7}$$

where k_i and k_f are the initial and final projectile momentum, respectively. We note that this correction can lead to cross sections that do not obey detailed balance [7] and de-excitation cross sections should be evaluated, in this case, from the excitation ones, using the detailed balance relation.

3. Description of the program

Fig. 1 shows the linkage of the subroutines in ROTIONS. What follows is a description of each subroutine. Further comments are given within the code.

ROTIONS is the central driving routine. It reads the input parameters and drives the calculation accordingly.

PASCAL initializes a 100×100 matrix with binomial coefficients to use in the calculation of 3j-symbols.

READTH, GETSET, NEWE are routines taken from the UK molecular R-matrix package [12] to read the T-matrix files, and set the collision energy range.

TROTSEC calculates the T-matrix rotational excitation cross sections (σ^{TM}) from BF T-matrices by performing the frame transformation of Eq. (2).

DCB calculates the dipole CB rotational cross sections, $\sigma_1^{\mathrm{CB,PCB}}$.

FE1 evaluates the total CB rotational cross sections of Eq. (3).

MONOPOLE obtains the monopole radial matrix elements: Eq. (5) for $\lambda = 0$.

DIPOLE uses monopole radial matrix elements to calculate dipole ones ($\lambda = 1$).

SUMATORIO_D performs the sum of Eq. (4).

QCB evaluates the quadrupole CB cross sections, $\sigma_2^{\mathrm{CB,PCB}}$.

MULTIPOLE obtains two quadrupole radial matrix elements by numerical integration of Eq. (5). It can also be used to obtain any multipole of the same equation.

QUADRUPOLE_OD computes the off-diagonal quadrupole radial matrix elements. It uses functions **AA** and **F** that specify the recurrence relations between monopole radial matrix elements and quadrupole ones.

QUADRUPOLE_D computes the diagonal quadrupole radial matrix elements.

SUMATORIO_Q obtains the partial and total CB rotational cross sections by performing the sum (4) up to l_i, l_f = LMAX and l_i, l_f = LMAXQ, respectively (LMAXQ≥LMAX).

FUNC is a function that contains the integrand of Eq. (5).

HYPGEO is a routine to evaluate complex hypergeometric functions taken from Numerical Recipes [16].

D01AKF is a NAG routine [17], not provided, which evaluates the integral of Eq. (5). It integrates the function supplied in function FUNC over the range *AQ* to *BQ* and returns the result in *XM*. D01AKF uses an 1-D quadrature, adaptative, finite interval, method suitable for oscillating functions.

COULFG is a CPC library routine (catalogue number ABNK) [18], not supplied. It evaluates the regular radial Coulomb function for a given energy and at a given distance.

GAMMLN evaluates $\ln \Gamma(z)$, where z a complex number. It is a modified version of a Numerical Recipes [16] routine.

THREEJ Obtains the 3j-symbols required.

WROTSECS is the routine to print out the rotational cross sections obtained. It makes the units conversions required and sorts the different cross sections into columns, suitable for display with a graphics package.

4. Input data

A single namelist /RXSECIN/ is required. The default values are given in brackets. This is read from the standard input.

NAME	Character*80 variable to contain a title for the output.
ANR_OP	[1] = 1, threshold corrected cross sections, see Eq. (7), are computed; = 0, no threshold correction.
BE	Rotational constant of the ion. Units: cm^{-1}.
CB_OP	[0] = 0, only T-matrices are used to obtain rotational cross sections. = 1, T-matrix and CB rotational cross sections are obtained. = 2, only the CB rotational cross sections are obtained. CB_OP = 1, 2 will only work if the target is charged and if Δj = 1 or 2.
EMIN	[0.0] Minimum scattering energy (in units as specified by ieunit).
EMAX	[1×10^8] Maximum scattering energy (in units as specified by ieunit).
GRID	[1] Energy grid mode to use when CB_OP=2: 1 = linear, 2 = logarithmic.

ITFORM	['F'] T-matrix data format: 'F' = Formatted, 'U' = Unformatted.
IEUNIT	[1] Units of the input and output scattering energies. 1 = eV, 2 = Hartree, 3 = Ryd.
ION	[1] Charge of the target.
IPRNT	[6*0] Debug print switches: IPRNT(1) = 1 print all input data. IPRNT(4) = 1,2,3 are increasing debug levels for the rotational cross section calculations.
IWRITE	[6] Logical unit for standard output.
IXSN	[1] Units of the cross sections on output. 1 = a_0^2, 2 = Å^2, 3 = πa_0^2.
IXSOUT	[8] Logical unit to output the cross sections.
J	[0] Initial rotational quantum number of the target.
JP	[1] Final rotational quantum number of the target.
MJJ	[6] Maximum total angular momentum to be considered in the rotational cross sections calculations from BF T-matrices.
LUTMV	[NSYM*12] Vector of dimension NSYM containing the logical unit numbers for the T-matrix data sets.
MAXI	[1] Label of highest initial state for which cross sections are required.
MAXF	[0] Label of highest final state for which cross sections are required.
NTSET	[1] Set number of T-matrix input.
NSYM	[0] Number of molecular symmetries to be considered.
NUMENER	[0] Number of energies to be read from the T-matrix files. If = 0, all energies will be read. If CB_OP = 2, this is the number of energies to set up an energy grid.
Q1	[0.0] Permanent dipole moment of the target (in Debye).
LMAX	[5] Maximum value of l (partial waves) to be used in the partial CB rotational cross sections.
LMAXQ	[40] Number of partial waves to use for the total CB quadrupole rotational cross sections.
Q2	[0.0] Permanent quadrupole of the target in atomic units.
AQ	[0.1] Lower limit for the numerical integral of the quadruple radial matrix elements M_02 and M_20.
BQ	[2×10^4] Upper limit for the numerical integral of the quadrupole radial matrix elements M_02 and M_20.

5. *T*-matrix file format

The files containing the *T*-matrices can be formatted or unformatted. For the formatted option, the header of the files is read with the following code (or equivalent):

```
 READ(LUTMT,FMT='(5I5)') KEY,NSET,NREC
 READ(LUTMT,FMT='(A80)') TITLE
 READ(LUTMT,FMT='(5I5,F15.8)') MGVN,STOT,GUTOT,NCHAN,NAPPR,MAXNE,NVIB,
&                              NDIS,NTARG,MAXCHI,MAXCHF,R
 DO I=1,MAXCHF
    READ(LUTMT,*) ICHL(I),LCHL(I),MCHL(I),ECHL(I)
 END DO
 DO IE=1,MAXNE
    READ(LUTMT,*) I,NEREP(I),(EINC(J,I),J=1,2)
 END DO
```

while the *T*-matrices are read with

```
DO IE=1,NE
   READ(LUTMT,FMT='(3I5,F10.6)') MVI,MVJ,MVD,EN(IE)
   READ(LUTMT,FMT='(4E20.13)') ((TR(I,J,IE),I=1,MVI),J=1,MVJ+MVD)
   READ(LUTMT,FMT='(4E20.13)') ((TI(I,J,IE),I=1,MVI),J=1,MVJ+MVD)
END DO
```

For the unformatted option, the code used is the same but without specifying the formatting labels.

The meaning of the variables is as follows:

KEY	12.
NSET	*T*-matrix data set number within the file.

NREC	Number of records in the file. If the file is formatted, then
	`NREC=1+NETOT*(2*((MAXCHI*MAXCHF+3)/4)+1)+1+MAXCHF+MAXNE;`
	if the file is unformatted,
	`NREC=1+3*NETOT+1+MAXCHF+MAXNE.`

TITLE	A character*80 title.
MGVN	Molecular symmetry of the electron plus target system. $0 = \Sigma$, $1 = \Pi$, $2 = \Delta$, etc.
STOT	Spin multiplicity of the total system.
GUTOT	g/u symmetry of the total system. 1 = g, −1 = u, 0 = not applicable.
NCHAN	Number of channels.
NAPPR	Theory approximation: 1 = fixed-nuclei *T*-matrix, 2 = adiabatic *T*-matrix, 3 = non-adiabatic *T*-matrix.
MAXNE	Number of energy subranges.
NVIB	Number of vibrational levels.
NDIS	Number of dissociative channels.
NTARG	Number of target electronic states.
MAXCHI	Maximum number of initial channels.
MAXCHF	Maximum number of final channels.
R	Internuclear distance (a_0).
ICHL(I)	Number of the electronic state of the Ith channel.
LCHL(I)	l-value of the Ith channel.
MCHL(I)	m-value of the Ith channel.
ECHL(I)	Threshold energy of the Ith channel.
NEREP(IE)	Number of energies in the IEth energy subrange.

EINC(1,IE)	Initial value of the energy in the IEth subrange.
EINC(2,IE)	Increment in the energy value in the IEth subrange.
MVI	Number of initial channels.
MVJ	Number of final channels.
MVD	Number of dissociative channels.
EN	Vector with the energies where the T-matrix has been calculated (in Ryd).
TR	Real part of the T-matrix.
TI	Imaginary part of the T-matrix.

6. Test data

The present test run corresponds to the calculation of the rotational excitation cross section of HeH^+ ($j = 0 \rightarrow 1$) by electron impact. We use the T-matrices for electron–HeH^+ collisions at the HeH^+ equilibrium geometry calculated by Sarpal et al. [19]. Four molecular symmetries are considered: $^2\Sigma^+$, $^2\Pi$, $^2\Delta$ and $^2\Phi$, which should be available in files fort.50, fort.51, fort.52 and fort.53, respectively. These T-matrices were obtained using three target states and electron partial waves up to $l = 5$.

The standard input for the present test run is given below. ROTIONS will read this input and produce a standard output plus the file fort.8 containing the rotational excitation cross sections. The standard output contains information about the T-matrices that are input and, depending of the options specified, total rotational excitation cross sections from T-matrices and/or from the CB approximation. The columns of data in the file fort.8 correspond to the several cross sections in Eq. (6). The results are threshold corrected according to Eq. (7).

Acknowledgements

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References

[1] R.F. Boĭkova, V.D. Ob"edkov, Sov. Phys. JETP 27 (1968) 772.
[2] S.-I. Chu, A. Dalgarno, Phys. Rev. A 10 (1974) 788.
[3] D.R. Flower, Astron. Astrophys. 73 (1979) 237.
[4] A.J. Lim, I. Rabadán, J. Tennyson, Mon. Not. R. Astr. Soc. (1998), to be submitted.
[5] D.A. Neufeld, A. Dalgarno, Phys. Rev. A 40 (1989) 633.
[6] I. Rabadán, B.K. Sarpal, J. Tennyson, J. Phys. B 31 (1998) 2077.
[7] I. Rabadán, B.K. Sarpal, J. Tennyson, Mon. Not. R. Astr. Soc. (1998), in press.
[8] W.M. Huo, F.A. Gianturco, eds., Computational Methods for Electron Molecule Collisions (Plenum Press, New York, 1995).
[9] C.J. Gillan, J. Tennyson, P.G. Burke, in: Computational Methods for Electron Molecule Collisions (Plenum Press, New York, 1995) p. 239.
[10] N. Chandra, A. Temkin, Phys. Rev. A 13 (1976) 188.
[11] M.A. Morrison, W. Sun, in: Computational Methods for Electron Molecule Collisions (Plenum Press, New York, 1995) p. 131.
[12] L.A. Morgan, J. Tennyson, C.J. Gillan, Comput. Phys. Commun. 114 (1998) 120, this issue.
[13] K. Alder, A. Bohr, T. Huss, B. Mottelson, A. Winther, Rev. Mod. Phys. 28 (1956) 432.
[14] H. van Regemorter, Mon. Not. R. Astr. Soc. 121 (1960) 213.
[15] S.-I. Chu. Phys. Rev. A 12 (1975) 396.
[16] W.H. Press, B.P. Flannery, S.A. Teukilsky, W.T. Vetterling, Numerical Recipes in Fortran (Cambridge Univ. Press, Cambridge, 1995).
[17] NAG Fortran Library, The Numerical Algorithms Group Ltd. (Oxford, UK, 1996).
[18] A.R. Barnett, Comput. Phys. Commun. 27 (1982) 147.
[19] B.K. Sarpal, J. Tennyson, L.A. Morgan, J. Phys. B 24 (1991) 1851.

TEST RUN INPUT

```
&rxsecin
 name=' HeH+ equilibrio rotational XS ',
 numener=10, nsym=4,
 lutmtv=50,51,52,53, itform='F',
 ieunit=1, ixsn=2,
 anr_op=1, cb_op=1,
 lmax=5, q1=1.66, q2=1.397864,
 j=0, jp=1, mjj=6,
 be=33.47278,
 aq=1.d-3,bq=2.d3,
 maxi=3, maxf=6,
&END
```

TEST RUN OUTPUT

The (edited) standard output of ROTIONS for the test run is

```
Program ROTIONS  (last modified 20-Mar-1998 )

HeH+ equilibrio rotational XS

The charge of the target is  1

The cross sections will include the ANR correction.

Coulomb-Born cross sections will be obtained.

--------------------------------------------------T-matrix  1

T-matrices will be read from set  1 on unit 50
 (HEH 2-PHI  T-MATRIX                                                          )

Symmetry data  MGVN = 0   STOT = 2   GUTOT = 0

Fixed nuclei data for R = 1.455

Number of target states       =   3
Number of scattering channels =  18
Channel data corresponding to stored T-matrix elements
 Element  Target   L    M    Energy
   1         1     0    0   0.00000
   2         1     1    0   0.00000
   3         1     2    0   0.00000
   4         1     3    0   0.00000
   5         1     4    0   0.00000
   6         1     5    0   0.00000
   7         2     0    0   1.59352
   8         2     1    0   1.59352
   9         2     2    0   1.59352
  10         2     3    0   1.59352
  11         2     4    0   1.59352
  12         2     5    0   1.59352
  13         3     0    0   1.93844
  14         3     1    0   1.93844
  15         3     2    0   1.93844
  16         3     3    0   1.93844
  17         3     4    0   1.93844
  18         3     5    0   1.93844

Input Energy grid (Ryd)
Number of points       400
Initial values     0.00200
Increments         0.00200

The number of partial waves is  6 (l= 0 to  5)

Cross-sections can be computed for   400 energies in the T-matrix file
from 0.27211E-01 to  10.884      eV

Only the first   10 T-matrices will be used
```

```
 ---> T-matrix  1; starting pointers with next=       1

 T-matrices in symmetry  1 have been read for    10 energies

....
lines deleted
....

 **** Rotational excitation cross sections from T-matrices

        energy (eV)  X Section(A^2)   Col. strength
    1      0.02721     282.628        0.643
    2      0.05442     158.606        0.721
    3      0.08163     110.816        0.756
    4      0.10885      85.787        0.780
    5      0.13606      70.390        0.800
    6      0.16327      59.950        0.818
    7      0.19048      52.392        0.834
    8      0.21769      46.658        0.849
    9      0.24490      42.151        0.862
   10      0.27211      38.511        0.876

 **** Coulomb-Born rotational cross sections.

            ei (eV)        ef (eV)        TCB (A^2)
    1       0.027211       0.018911       816.409
    2       0.054423       0.046123       487.382
    3       0.081634       0.073334       357.758
    4       0.108846       0.100545       288.423
    5       0.136057       0.127757       244.846
    6       0.163268       0.154968       214.655
    7       0.190480       0.182180       192.336
    8       0.217691       0.209391       175.056
    9       0.244903       0.236602       161.211
   10       0.272114       0.263814       149.819


 *** Task has been successfully completed ***
```

The file fort.8, with the rotational excitation cross sections for $\mathrm{HeH}^+(j = 0 \rightarrow 1)$, reads

```
#  HeH+ equilibrio rotational XS
#
# key=  3  R-matrix & TCB & ACB XS
# Number of energies=   10
#
# Rotational transition: j= 0--> 1
#
# Energy in  eV ; Cross sections in ANGS**2
#
# Threshold energy   0.83001958E-02  eV
#
# Number of partial waves in PCB (lmax) = 5
#
#    Energy         TM+TCB-PCB       TM CS           TCB CS          PCB CS
  0.27211400E-01   1018.5171       282.62834       816.40898       80.520252
```

```
0.54422800E-01  596.13701       158.60627       487.38157       49.850828
0.81634200E-01  430.69199       110.81645       357.75774       37.882199
0.10884560      342.66886       85.786554       288.42278       31.540476
0.13605700      287.65414       70.389888       244.84618       27.581928
0.16326840      249.75565       59.949535       214.65547       24.849351
0.19047980      221.89748       52.391744       192.33595       22.830218
0.21769120      200.45071       46.657863       175.05625       21.263401
0.24490260      183.36010       42.151415       161.21076       20.002074
0.27211400      169.37262       38.510827       149.81919       18.957388
```