

J A E R I - M

88-228

THE ALGEBRAIC-EIKONAL APPROACH TO E-MOLECULE
COLLISION PROCESS : TWO COMPUTER CODES,
VIBA AND CROSSA, FOR CALCULATION OF
MOLECULAR SPECTRA AND SCATTERING CROSS SECTIONS

November 1988

Alberto MENGONI* and Toshizo SHIRAI

日本原子力研究所
Japan Atomic Energy Research Institute

JAERI-M レポートは、日本原子力研究所が不定期に公刊している研究報告書です。
入手の問合せは、日本原子力研究所技術情報部情報資料課（〒319-11茨城県那珂郡東海村）あて、お申しこしください。なお、このほかに財団法人原子力弘済会資料センター（〒319-11 茨城県那珂郡東海村日本原子力研究所内）で複写による実費領布をおこなっております。

JAERI-M reports are issued irregularly.

Inquiries about availability of the reports should be addressed to Information Division Department of Technical Information, Japan Atomic Energy Research Institute, Tokaimura, Naka-gun, Ibaraki-ken 319-11, Japan.

©Japan Atomic Energy Research Institute, 1988

編集兼発行 日本原子力研究所
印 刷 株高野高速印刷

The Algebraic-Eikonal Approach to e-Molecule
Collision Process: Two Computer Codes, VIBA and CROSSA, for
Calculation of Molecular Spectra and Scattering Cross Sections

Alberto MENCONI* and Toshizo SHIRAI

Department of Physics
Tokai Research Establishment
Japan Atomic Energy Research Institute
Tokai-mura, Naka-gun, Ibaraki-ken

(Received October 25, 1988)

This report contains a description of two computer codes used for the calculation of molecular spectra and scattering cross sections for e-molecule collision process on dipolar molecules in the algebraic-eikonal approach.

A brief account of the theory on which the codes are based is given in a paper on the Journal of Physics B: Atomic, Molecular and Optical Physics 21, (1988) L567.

A bibliography, more extensive than the references, is included in order to provide the interested reader with a number of papers of work on this subject.

Keywords: Electron-Molecule Collision, Molecular Spectra, Cross Section, Dipolar Molecule, Algebraic-Eikonal Approximation

* On leave from ENEA, Italy

電子-分子衝突過程への代数学的アイコナル近似の応用：
分子スペクトルと散乱断面積の計算のための計算機コード

日本原子力研究所東海研究所物理部

Alberto MENGONI*・白井 稔三

(1988年10月25日受理)

分子スペクトルの計算と電子と二重極分子の散乱断面積の代数学的アイコナル近似による計算に用いる計算機コードについて記述した。

このコードの基礎とした理論による簡単な計算は、論文として報告されている (J. Phys. B 21, (1988) L 567)。

興味をもつ読者のために、この分野に関連する論文の一覧表を付けた。

Contents

I.	VIBA	
1.	Introduction	2
2.	Structure of the code	5
3.	Input for VIBA	7
4.	Other information on VIBA	9
II.	CROSSA	
1.	Introduction	12
2.	Structure of the code	14
3.	Input for CROSSA	17
4.	Other information on CROSSA	19
	Acknowledgements	19
	References	20
	Appendix A Test Run Input and Output of VIBA	21
	Appendix B Test Run Input and Output of CROSSA	27
	Appendix C Bibliography	36

目 次

I	VIBA	1
1.	序 論	2
2.	コードの構造	5
3.	VIBAの入力	7
4.	VIBAのその他の情報	9
II	CROSSA	11
1.	序 論	12
2.	コードの構造	14
3.	CROSSAの入力	17
4.	CROSSAのその他の情報	19
	謝 辞	19
	参考文献	20
	付録 A VIBA のテストラン入出力	21
	付録 B CROSSA のテストラン入出力	27
	付録 C 文献一覧表	36

I. VIBA

1. Introduction

VIBA is a code to calculate the spectrum of diatomic molecules in the case where the Hamiltonian, which describes the rotation-vibration states of the molecule, can be expressed as :

$$H = h_0 + \varepsilon \hat{n}_\pi + \alpha \hat{n}_\pi^2 + \beta J \cdot J + \delta D \cdot D \quad (1)$$

where

$$\hat{n}_\pi = -\sqrt{3} [p^\dagger \times \tilde{p}]^{(0)}, \quad J = \sqrt{2} [p^\dagger \times \tilde{p}]^{(1)}$$

and

$$D = [p^\dagger \times \tilde{s} + s^\dagger \times \tilde{p}]^{(1)}.$$

The four boson creation (annihilation) operators $p_\mu^\dagger (\tilde{p}_\mu)$ $\mu=0,\pm 1$ and $s^\dagger (\tilde{s})$ are introduced in order to realize the algebra associated with $U(4)$. h_0 , ε , α , β and δ are the coefficients which define the spectrum uniquely.

The eigenvalues problem for the Hamiltonian (1) has a simple analytical solution $E_{\omega, J}$ or $E_{v, J}$, when the two coefficients ε and α are equal to 0:

$$E_{\omega, J} = h_0 + \delta \omega(\omega+2) + (\beta-\delta)J(J+1)$$

where ω is a quantum number labelling the states of $O(4)$.

Alternatively, defining $v \equiv (N - \omega)/2$

$$E_{v, J} = h_0 + (N^2+4N+3)\delta - 4(N+2)\delta(v+1/2) \\ + 4\delta(v+1/2)^2 + (\beta-\delta)J(J+1).$$

Here N is the total number of bosons and v is a vibrational quantum number corresponding to the various vibrational bands. Since $\omega = N$, $N-2$, $N-4$, \dots , 1 or 0 for N odd or even, v takes the values : $v = 0, 1, 2, \dots$. J is the total angular momentum of the rotation-vibration state.

This situation corresponds to the chain decomposition of the U(4) Hamiltonian:

$$U(4) \supset O(4) \supset O(3) \supset O(2)$$

$$[N] \quad \omega \quad J \quad m$$

where the quantum numbers labelling the states are written explicitly under the respective group structure.

If $\varepsilon \neq 0$ and/or $\delta \neq 0$, the Hamiltonian (1) is diagonalized in the space of fixed J with the off-diagonal terms given by:

$$\langle [N] \omega J | | \hat{n}_{\pi} | | [N] \omega J \rangle = \sqrt{(2J+1)} (3/4) N \quad \text{for } \omega = 0$$

$$= \sqrt{(2J+1)} [(N-1)/2 + J(J+1)(N+2)/2\omega(\omega+2)] \quad \text{for } \omega \neq 0$$

$$\begin{aligned} \langle [N] \omega' (= \omega+2) J | | \hat{n}_{\pi} | | [N] \omega J \rangle &= -(1/4) \sqrt{(2J+1)/\omega'} \\ &[(\omega'+J)(\omega+J+1)(\omega'-J)(\omega'-J-1)(N+2+\omega')(N+2-\omega')/(\omega'-1)(\omega'+1)]^{1/2} \end{aligned}$$

$$\begin{aligned} \langle [N] \omega' (= \omega-2) J | | \hat{n}_{\pi} | | [N] \omega J \rangle &= -1/4 \sqrt{(2J+1)/(\omega'+2)} \\ &[(N-\omega')(N+4+\omega')(\omega'+J+2)(\omega'+J+3)(\omega'-J+2)(\omega'-J+1)/(\omega'+1)(\omega'+3)]^{1/2} \end{aligned}$$

and

$$\begin{aligned} \langle [N] \omega' J | | \hat{n}_{\pi} | | [N] \omega J \rangle &= (2J+1)^{-1/2} \\ &\langle [N] \omega' J | | \hat{n}_{\pi} | | [N] \omega J \rangle. \end{aligned}$$

Moreover,

$$\begin{aligned} \langle [N] \omega' J | | \hat{n}_{\pi} \cdot \hat{n}_{\pi} | | [N] \omega J \rangle &= (2J+1)^{-1/2} \cdot \\ &\cdot \langle [N] \omega' J | | \hat{n}_{\pi} \cdot \hat{n}_{\pi} | | [N] \omega J \rangle. \end{aligned}$$

Therefore, for each J a square matrix, say $A_{i,j}$, is constructed and diagonalized numerically. The dimension of the matrix is :

$$\dim (A_{i,j}) = \text{Int}[(N-J)/2] + 1$$

where N is the total number of bosons.

VIBA also calculates the E1 electromagnetic transition rates between an initial state, labelled by $(\#_i, J_i)$ and a final state

$(\#_f, J_f)$:

$$T_{E1} \equiv (2J_i+1)^{-1} | \langle [N] \#_f J_f || \mu D || [N] \#_i J_i \rangle |^2 \quad (2)$$

where $\#_k = 1, 2, \dots$ label the 1-st, 2-nd, ... state of given J_k for $k=i$ or f .

Once the spectrum is calculated, **VIBA** makes a comparison with a terms-expansion of the rotation-vibration spectrum of type:

$$\begin{aligned} E_{v,J} = T_e + \omega_e(v+1/2) - \omega_e x_e(v+1/2)^2 \\ + B_e J(J+1) - \alpha_e(v+1/2)J(J+1). \end{aligned} \quad (3)$$

The relations between the coefficients in (1) and those in (3) are given in Mengoni and Shirai.¹⁾

VIBA has a fitting performance by which some of the coefficients in (1) can be fitted in order to better approximate the terms-expansion of eq. (3). In fact, eq. (3) contains a rotation-vibration term (the last one) which does not have a direct analogue in (1). The various coefficients that can be fitted are:

- 1) ϵ
- 2) α
- 3) ϵ and α
- 4) ϵ and α and δ
- 5) ϵ and α and δ and β
- 6) δ
- 7) β

Finally, **VIBA** writes the amplitudes of the calculated states (eigenvectors) on UNIT 10. These amplitudes are used by the code **CROSSA** for the calculation of the e-molecule scattering cross section.

2. Structure of the code

VIBA is a FORTRAN77 code composed of a main program, 11 subroutines and 6 functions. Except the section of the program which makes the fitting, **VIBA** is written in full double precision.

A list of the subprogram names is given in Table 1.

Table 1

MAIN

Subroutines : TRAN, PRIEN, ORDER, DIAG, XNP12, CNJJ, RCHSU, FITTA,
CALFUN, VA05A^(*), MB11A^(*).

Functions : D1, XNP1, PMSIGN, WSIXJ, WNINJ, RRAC.

(*) From Harwell Subroutine Library

We describe here in some details the most important routines of **VIBA**.

MAIN : the main program basically controls the I/O and the calls to the various sections of the code. The input for **VIBA**, mainly read by **MAIN**, is organized in NAMELIST input variables.

DIAG : is the subroutine which makes the diagonalization of the Hamiltonian. Once the coefficients of eq. (1) are read, the matrix elements A1(I,J) are computed by **DIAG**. Then a system-routine, DEIG1, is called. DEIG1 is the only external routine used by **VIBA**.

DEIG1 diagonalizes a matrix and returns its eigenvalues and eigenvectors. Of course, DEIG1 can be replaced by any equivalent routine. One must note that:

- A1(NSD,NSD) is the matrix to be diagonalized.
- REIG(NSD) and CEIG(NSD) are the real and imaginary part of the eigenvalues respectively (N.B. since Hamiltonian in eq. (1) is hermitian, it follows that the eigenvalues of A1(I,J) are real).
- VEIG(K,1), VEIG(K,2), ... are the eigenvectors of A1 with components K=1, 2,

PRIEN : besides to print the molecular spectrum (the first 25 and the last 25 states if the number of states exceed 100), PRIEN makes also the comparison of the U(4) calculated spectrum with the terms-expansion of eq. (3).

A simple statistical analysis is provided by PRIEN which gives the values of:

$$\left(\sum_i (E_i^a - E_i^b)^2 / N \right)^{1/2}$$

with a or b taking the values corresponding to the U(4), O(4) or terms-expansion energies.

TRAN : calculates the E1 electromagnetic transition rates of eq. (2). The reduced matrix elements appearing in eq. (2) are also printed together with T_{E1} .

FITTA : performs the fitting. According to the specifications given in the input, FITTA minimizes the following squares sum:

$$1/2 \sum_i [(E_i^{TS} - E_i^{U(4)}) / \sqrt{E_i^{TS}}]^2$$

where E_i^{TS} 's are the energies of the terms-expansion.

The routine used for minimization is the VA05A of the Harwell Subroutine Library. The Fortran source is inserted in **VIBA** so that no calls to external routines is required in this step of calculation.

3. Input for **VIBA**

As already mentioned, the input for **VIBA** is provided by the user through a set of NAMELIST variables. Table A.1 of appendix A provides the NAMELIST set used in the test run. The various NAMELIST input variables are described as follows:

	NAME	FUNCTION
&INP1 :	NBOST	Total number of bosons
	H0	h_0 in eq. (1)
	EPSI	ϵ in eq. (1)
	ALF	α in eq. (1)
	BET	β in eq. (1)
	DELT	δ in eq. (1)
	ERES04	Value of the energy to which the O(4) is to be scaled
	ERESU4	Value of the energy to which the U(4) is to be scaled
&LPRT :	LPLEV	=0 printing the final energy spectrum =1 printing the energy spectrum for each J

LMATD =1 printing the matrix to invert $A_1(i,j)$
 LVECT =1 printing the eigenvectors for each J
 LRESC =0 no rescaling in the spectrum
 =1 rescaling to minimum of the $O(4)$ spectrum
 =2 rescaling to the value of $ERESO4/U4$
 =3 rescaling to the value of h_0
 =4 rescaling to 0
 =5 rescaling to the minimum of the
 terms-expansion
 LSTATY =1 prints statistics
 LOUT10 =1 writes the eigenvectors on unit 10
 LJMAX0 Maximum J for out-eigenvectors on unit 10
 LPRV1 # in $J_{\#}$ to be printed
 LPRV2 Number of J to be printed for each #
 LDUNH =1 prints the comparison with terms-expansion
 =2 calculates the terms-expansion
 coefficients (see chapter I for their
 definitions) and then prints the comparison
 between the $U(4)$ spectrum and the
 terms-expansion

&INTR :
 NTRAN Number of transitions to be calculated
 DE1 Coefficient μ in the dipole operator
 JINI(K) $K=1, 2, \dots, NTRAN$ angular momentum of the
 initial state
 JFIN(K) $K=1, 2, \dots, NTRAN$ angular momentum of the
 final state
 NSIP(K) $K=1, 2, \dots, NTRAN$ # of the initial state

NSFP(K) K=1, 2, ..., NTRAN # of the final state

&IDUNH : TE T_e in eq. (3)
 OME ω_e in eq. (3)
 OMEXE $\omega_e x_e$ in eq. (3)
 BE B_e in eq. (3)
 ALFE α_e in eq. (3)

&INFT : HHH,DMAX,ACC, See long-write-up of the VA05A routine for
 MAXFUN,IPRINT definitions. Typical values
 in Table 2 for the test run

IFIT =0 no fit
 =1 ε fit
 =2 α fit
 =3 ε and α fit
 =4 ε and α and δ fit
 =5 ε and α and δ and β fit
 =6 δ fit
 =7 β fit
 NLEV1 # in $J_{\#}$ of the last level to be fitted
 NLEV2 J of the last level of each # to be fitted

4. Other information on VIBA

The print-out of **VIBA** should be self-explanatory. The test run for **VIBA** is given in appendix A together with its NAMELIST input variable set.

The only tape-unit required by **VIBA** is unit 10 on which **VIBA** writes the eigenvectors to be used by **CROSSA** for scattering cross section calculation.

The test run of **VIBA** took 2.94 sec of CPU time on the FACOM M780 computer of the JAERI Computing Center.

The storage used was 1276 Kbytes for the same run.

VIBA is composed of 1758 lines.

II. CROSSA

1. Introduction

CROSSA is a code for the calculation of the e-molecule scattering cross section. The rotation-vibration spectrum of the diatomic molecule has to be calculated by **VIBA** described in I.

The scattering cross section, for vibrationally elastic as well as for vibrationally inelastic scattering channels, is calculated in the so-called adiabatic-eikonal approximation. In this approximation, the differential cross section for channel $\#_i, J_i \rightarrow \#_f, J_f$ is given by :

$$\frac{d\sigma(\#_i, J_i \rightarrow \#_f, J_f)}{d\Omega}(q) = \frac{2}{(2J_i+1)} \sum_{m_i, m_f} |A_{i,f}(q)|^2 \quad (1)$$

where $-J_i \leq m_i \leq J_i$, $-J_f \leq m_f \leq J_f$, $q = |\mathbf{q}| = |\mathbf{k}_o - \mathbf{k}| \approx 2k_o \sin(\theta/2)$, with $k_o \approx k = \sqrt{(2\mu_e E)/\hbar}$. E is the incoming electron energy, μ_e the reduced mass of the e + Molecule system and θ the scattering angle.

The amplitude $A_{i,f}(q)$ is given by:

$$A_{i,f}(q) = i k_i^{m_f - m_i} \int db b J_{|m_f - m_i|}(qb) \cdot \\ \cdot [\delta_{i,f} - \sum_m d_{m_f, m}^{J_f}[\pi/2] d_{m_i, m}^{J_i}[\pi/2]] \cdot \\ \cdot P(b) \cdot <[N] \#_f J_f | \exp[i g(b) T_z] | [N] \#_i J_i > \quad (2)$$

where $J_x(x)$ is the Bessel function of integer order and b is the impact parameter. $d_{m', m}^{J'}[\phi]$ is the (Wigner) rotation matrix as defined by Rose.²⁾

The long-range dipole interaction is represented by the potential:

$$V_d(\mathbf{r}) = \alpha(r) \hat{\mathbf{r}} \cdot \mathbf{T} \quad (3)$$

where $\mathbf{T} = \mu \mathbf{D}$. μ is the electric dipole moment and $\alpha(r) = -e/(r^2 + R_o^2)$,

with the charge of electron e and the dipole cut-off radius R_0 .

The function $g(b)$ in eq. (2) is defined as:

$$g(b) = -\mu_e/\kappa^2 k \cdot \int \alpha(r)b/r dz \quad (4)$$

with $r = \sqrt{b^2 + z^2}$.

The function $P(b)$ in eq. (2) takes into account the polarization effects. It is calculated with an iterative procedure (see Bijker and Amado³) starting from a set of phase shifts produced by the polarization potential:

$$V_p(r) = -\alpha_0 e^2 / 2(r^2 + R_1^2)^2 \quad (5)$$

where α_0 is the static polarizability and R_1 is the polarization cut-off factor.

The matrix elements appearing in eq. (2) are given by:

$$\begin{aligned} < [N] \#_{\pi} J_{\pi} m | \exp[i g(b) T_z] | [N] \#_i J_i m > &= \sum_{\omega} a_{\omega}^{\#_f, J_f} a_{\omega}^{\#_i, J_i} \\ \cdot < [N] \omega J_f m | \exp[i \eta(b) D_z] | [N] \omega J_i m > \end{aligned} \quad (6)$$

with:

$$\begin{aligned} < [N] \omega J_f m | \exp[i \eta(b) D_z] | [N] \omega J_i m > = \\ \sum_v < \omega/2 v \omega/2 m-v | J_f m > < \omega/2 v \omega/2 m-v | J_i m > \exp[i \eta(b)(2v-m)] \end{aligned} \quad (7)$$

and

$$\eta(b) = \mu g(b).$$

The amplitudes of the O(4) basis states are those calculated by VIBA and are indicated here by $a_{\omega}^{\#_J}$. The various components are identified by the label ω . Thus, for a given $| [N] \# J >$ state it is :

$$| [N] \# J > = \sum_{\omega} a_{\omega}^{\#_J} | [N] \omega J > \quad (8)$$

with

$w = N, N-2, N-4, \dots$

Int[(N-J)/2] + 1 values

All the preceding equations have been written for a general initial state $\#_i, J_i$. In fact it is possible to show that the differential cross section does not depend on the value of J_i . Using this result, it is possible to greatly reduce the computing time assuming $J_i = 0$. This assumption has been used in writing **CROSSA** and some of the equations written above has been consequently modified.

We point out here that the CPU time of a typical run of **CROSSA** strongly depends on the technique used for the calculation of the integral over the impact parameter b in eq. (2). In **CROSSA** this integral is calculated with the trapezoidal rule. The use of other techniques like the Gaussian method, for instance, resulted in a poor accuracy in the present numerical integration.

Typical values of the b -range and of the number of integration points are given in table B.1 of appendix B where the input NAMELIST sets of the test run are given.

2. Structure of the code

CROSSA is a FORTRAN77 code organized in a main program, 17 subroutines and 19 functions. Except the section of the program which calculates the factor $P(b)$, **CROSSA** is written in full double precision.

A list of the subprogram names is given in Table 1.

Table 1

MAIN

Subroutines : AFI, PERIMU, RAMPLJ, TRANO, WFAC, ALBE1, SPUTAB.

(*)->: AACF, SETUP, NUMINT, INTGR, MATCH, BSSL, SFRBS2, STRR,
SPRS, SKEY.

Functions : PAR, PAC, XXX, YYY, D1, CGEX, ETA, EFFE, EVODD, DWIG,
PNSIGN, XFATT, CG, RO4SU2, CO4SU2, PLEG, GP, TEIKR,
TEIKI.

(*) From the program AACF: Comp. Phys. Comm. 3 (1972) 173

The routines marked by (*)-> are part of the program AACF which calculates the phase-shifts by a spherical potential, modified here for the calculation of the factor $P(b)$ in eq. (2).

We describe below in some detail the most important routines of **CROSSA**.

MAIN : the main program in **CROSSA** controls the I/O and calculates some of the basic quantities needed for the calculation of the differential cross section. The various sets of NAMELIST variables are also read by **MAIN**.

AFI : calculates the amplitude given by eq. (2). The numerical integration over the impact parameter b is also performed by **AFI**. The Bessel functions of integer order $J_x(x)$ are requested by **AFI**. In **AFI** they are calculated using the external system-routines DBJ0, DBJ1 and DBJR for $x=0$, 1 and $x>1$. They

can be, of course, replaced by equivalent routines.

ALBE1 : makes a call to the various functions of the AACF package for the calculations of the phase shifts produced by the polarization potential. It then applies an iterative procedure which allows the calculation of a two vectors, ACCAR and ACCAI, used by SPUTAB for the calculation of the factor P(b) in eq. (2).

RAMPLI : reads the amplitude of the U(4) states from unit 10

SPUTAB : calculates the factor P(b) of eq. (2) on the basis of the results of ALBE1.

PAR : calculates the real part of the second term in the integral of eq. (2).

PAC : calculates the imaginary part of the second term in the integral of eq. (2).

CGEX : calculates the Clebsch-Gordan coefficients $\langle a b c d | A B \rangle$ including the limit of large a (> 20).

ETA : calculates $\eta(b)$ of eq. (7).

RO4SU2 : calculates the matrix element $\langle [N]\omega J_f^m | \exp[i\eta(b)D_z] | [N]\omega J_i^m \rangle$ (Real part).

CO4SU2 : calculates the matrix element $\langle [N]\omega J_f^m | \exp[i\eta(b)D_z] | [N]\omega J_i^m \rangle$ (Imaginary part).

3. Input for CROSSA

The input for **CROSSA** is provided by the following NAMELIST variables:

	NAME	FUNCTION
&INP1 :	NBOST	Total number of bosons
	DEC	Coefficient μ of the electric dipole operator T
	ROE1	R_0 cut-off of the dipole interaction potential
	ROPL	R_1 cut-off of the polarization potential
	ALFA0	Electric polarizability α_0
	NENER	Number of incoming electron energies
	ELCT	Vector containing the NENER values of the incoming electron energy
&LPRT :	LPLEV	Vector containing printing instructions : LPLEV(1) > 0 : print the values of the integrals appearing in eq. (2). LPLEV(2) > 0 : print the values of the function to be integrated LPLEV(3) > 0 : print information on the calculation of the phase shifts
	ITHQ	=1 angular range in input =2 q range in input
	ALOW	Minimum value of θ or q
	AUP	Maximum value of θ or q
	NSTEP	Number of steps in the θ or q range

&ICHAN :	NCHAN	Number of scattering channels for which the differential cross section is being calculated
	JINI	Vector containing NCHAN values of the initial state angular momentum J. N.B.: it has been noted in the introduction that $J_i=0$ is assumed by CROSSA therefore $JINI(K)=0$, $K=1, \dots, NCHAN$ <u>must</u> be supplied by the user
	NINI	Vector containing NCHAN values of the initial state quantum number $\#_i$
	JFIN	Vector containing NCHAN values of the final state angular momentum J_f
	NFIN	Vector containing NCHAN values of the final state quantum number $\#_f$
&INTGR :	BMIN	Minimum value of the impact parameter b in the numerical integration
	BMAX	Maximum value of the impact parameter b
	BMATCH	Intermediate value of the impact parameter range. The b-range is divided in two regions : $[b_{min}, b_{match}]$ and $[b_{match}, b_{max}]$
	NPOINT	Total number of integration points
	NPB1	Number of integration points in the $[b_{min}, b_{match}]$ region

4. Other information on **CROSSA**

CROSSA requires the following tape units:

unit 10 : used for reading the eigenvectors calculated by **VIBA**.

unit 13 : is a working data-set. It must be allocated and it contains data to be used by different sections of **CROSSA**.

unit 15 : contains the results of the calculation in a format similar to the computer print-out.

The print-out of **CROSSA** should be self-explanatory. We need only to specify here that:

- a) The values of q in atomic units are in fact a "rescaled" value corresponding to $4 \mu \sin(\theta/2) + q$ (\AA).
- b) On unit 15 a third value is given for the differential cross section corresponding to a "rescaled" (E / μ^4) .
 $d\sigma/d\Omega$ quantity.

The test run of **CROSSA** is given in appendix B. It took 3 min and 30 sec of CPU time on the FACOM M780 of the JAERI Computing Center.

CROSSA uses 1024 Kbytes of computer storage and is composed of 1768 lines.

Acknowledgements

We gratefully thank Dr N Shikazono and Dr S Igarasi for their encouragement in performing this work. One of us (AM) would like to express his thanks to the staff of the Nuclear Data Center for the kind hospitality offered during the stage that made this work

4. Other information on **CROSSA**

CROSSA requires the following tape units:

unit 10 : used for reading the eigenvectors calculated by **VIBA**.

unit 13 : is a working data-set. It must be allocated and it contains data to be used by different sections of **CROSSA**.

unit 15 : contains the results of the calculation in a format similar to the computer print-out.

The print-out of **CROSSA** should be self-explanatory. We need only to specify here that:

- a) The values of q in atomic units are in fact a "rescaled" value corresponding to $4 \mu \sin(\theta/2) + q$ (\AA).
- b) On unit 15 a third value is given for the differential cross section corresponding to a "rescaled" (E / μ^4) .
 $d\sigma/d\Omega$ quantity.

The test run of **CROSSA** is given in appendix B. It took 3 min and 30 sec of CPU time on the FACOM M780 of the JAERI Computing Center.

CROSSA uses 1024 Kbytes of computer storage and is composed of 1768 lines.

Acknowledgements

We gratefully thank Dr N Shikazono and Dr S Igarasi for their encouragement in performing this work. One of us (AM) would like to express his thanks to the staff of the Nuclear Data Center for the kind hospitality offered during the stage that made this work

possible. This work is partially supported by the foreign researcher inviting program of the Japan Atomic Energy Research Institute.

References

- 1) A. Mengoni and T. Shirai, J. Phys. B: Atom. Molec. Opt. Phys. **21** (1988) L567.
- 2) M.E. Rose 1957, Elementary Theory of Angular Momentum, (Wiley & Sons, New York).
- 3) R. Bijker and R.D. Amado, Phys. Rev. A **37** (1988) 1425.

possible. This work is partially supported by the foreign researcher inviting program of the Japan Atomic Energy Research Institute.

References

- 1) A. Mengoni and T. Shirai, J. Phys. B: Atom. Molec. Opt. Phys. **21** (1988) L567.
- 2) M.E. Rose 1957, Elementary Theory of Angular Momentum, (Wiley & Sons, New York).
- 3) R. Bijker and R.D. Amado, Phys. Rev. A **37** (1988) 1425.

Appendix A Test Run Input and Output of VIBA

Table A.1 Test Run Input for VIBA.

```

&INP1 NBOST = 55,
HO =42841.12 , EPSI=-40.0,ALF = 0.0, BET ==-2.597 ,DELT ==-13.190
&END
&LPRT LMATD=0, LPLEV=0, LPRV1=5, LPRV2=5,
LVECT=0, LRESC=5, LOUT10=0, LJMAX0=8, LDUNH=1, LSTATY=1, &END
&INTR NTRAN= 5, DE1=1.108,
JINI( 1) = 0, JFINC( 1) = 0, NSIP( 1)=1, NSFP( 1)=1,
JINI( 2) = 1, JFINC( 2) = 0, NSIP( 2)=1, NSFP( 2)=1,
JINI( 3) = 0, JFINC( 3) = 0, NSIP( 3)=2, NSFP( 3)=1,
JINI( 4) = 1, JFINC( 4) = 0, NSIP( 4)=2, NSFP( 4)=1,
JINI( 5) = 2, JFINC( 5) = 1, NSIP( 5)=2, NSFP( 5)=1,
&END
&IDUNH TE=0.0, OME=2990.89, OMEXE=52.472, BE=10.593, ALFE=0.3069, &END
&INFT IFIT=1, NLEV1= 3, NLEV2= 8,
HHH=0.50, DMAX=100.0, ACC=0.010, MAXFUN=1000, IPRINT= 0, &END

```

Test Run Output

** RESULTS O(4) BASIS **

TOTAL NUMBER OF BOSONS : 55
 HO : 0.42841D+05
 EPSI : -0.40000D+02
 ALF : 0.0
 BET : -0.25970D+01
 DELT : -0.13190D+02
 TOTAL NUMBER OF STATES : 812

#	V	J	E(04)	J	E(U4)
1	0	0	0.14823D+04	0	0.14823D+04
2	0	1	0.15035D+04	1	0.15028D+04
3	0	2	0.15459D+04	2	0.15437D+04
4	0	3	0.16094D+04	3	0.16051D+04
5	0	4	0.16942D+04	4	0.16870D+04
6	0	5	0.18001D+04	5	0.17894D+04
7	0	6	0.19272D+04	6	0.19122D+04
8	0	7	0.20755D+04	7	0.20555D+04
9	0	8	0.22450D+04	8	0.22192D+04
10	0	9	0.24357D+04	9	0.24034D+04
11	0	10	0.26476D+04	10	0.26081D+04
12	0	11	0.28806D+04	11	0.28333D+04
13	0	12	0.31348D+04	12	0.30789D+04
14	0	13	0.34103D+04	13	0.33450D+04
15	0	14	0.37069D+04	14	0.36315D+04
16	0	15	0.40246D+04	15	0.39385D+04
17	0	16	0.43636D+04	16	0.42660D+04
18	1	0	0.43841D+04	0	0.43838D+04
19	1	1	0.44053D+04	1	0.44042D+04
20	1	2	0.44477D+04	2	0.44451D+04
21	1	3	0.45112D+04	3	0.45063D+04
22	1	4	0.45960D+04	4	0.45880D+04
23	1	5	0.47019D+04	17	0.46140D+04
24	0	17	0.47238D+04	5	0.46901D+04
25	1	6	0.48290D+04	6	0.48126D+04
787	20	15	0.42012D+05	4	0.41467D+05
788	24	1	0.42023D+05	5	0.41471D+05
789	24	2	0.42066D+05	7	0.41509D+05
790	22	10	0.42112D+05	9	0.41525D+05
791	23	7	0.42120D+05	6	0.41531D+05
792	24	3	0.42129D+05	8	0.41607D+05
793	21	13	0.42189D+05	1	0.41730D+05
794	24	4	0.42214D+05	3	0.41736D+05
795	23	8	0.42290D+05	5	0.41748D+05
796	24	5	0.42320D+05	7	0.41780D+05
797	22	11	0.42345D+05	0	0.41845D+05
798	25	0	0.42371D+05	2	0.41859D+05
799	25	1	0.42393D+05	4	0.41894D+05
800	25	2	0.42435D+05	6	0.41948D+05
801	24	6	0.42447D+05	1	0.42079D+05
802	23	9	0.42481D+05	3	0.42103D+05
803	25	3	0.42498D+05	5	0.42149D+05
804	25	4	0.42583D+05	0	0.42313D+05
805	24	7	0.42595D+05	2	0.42330D+05
806	26	0	0.42635D+05	4	0.42371D+05
807	26	1	0.42656D+05	1	0.42585D+05
808	25	5	0.42689D+05	3	0.42617D+05
809	26	2	0.42699D+05	0	0.42864D+05

810	26	3	0.427620+05	2	0.428850+05
811	27	0	0.427930+05	1	0.431750+05
812	27	1	0.428150+05	0	0.434880+05

AVERAGE DEVIATION (O(4)--U(4)) : 0.499969220+03

*** COMPARISON WITH TERMS EXPANSION ***

COEFFICIENTS (CM**-1) :

```

TE      : 0.0
OME     : 0.29909D+04
OMEXE   : 0.52472D+02
BE      : 0.10593D+02
ALFE    : 0.30690D+00

```

#	V	J	E(04)	E(TERMS)	#	J	E(U4)
1	0	0	0.14823D+04	0.14823D+04	1	0	0.14823D+04
2	0	1	0.15035D+04	0.15032D+04	1	1	0.15028D+04
3	0	2	0.15459D+04	0.15450D+04	1	2	0.15437D+04
4	0	3	0.16094D+04	0.16076D+04	1	3	0.16051D+04
5	0	4	0.16942D+04	0.16911D+04	1	4	0.16870D+04
6	0	5	0.18001D+04	0.17955D+04	1	5	0.17894D+04
18	1	0	0.43841D+04	0.43683D+04	2	0	0.43838D+04
19	1	1	0.44053D+04	0.43885D+04	2	1	0.44042D+04
20	1	2	0.44477D+04	0.44291D+04	2	2	0.44451D+04
21	1	3	0.45112D+04	0.44899D+04	2	3	0.45063D+04
22	1	4	0.45960D+04	0.45709D+04	2	4	0.45880D+04
23	1	5	0.47019D+04	0.46723D+04	2	5	0.46901D+04
40	2	0	0.71804D+04	0.71493D+04	3	0	0.71798D+04
41	2	1	0.72016D+04	0.71689D+04	3	1	0.72001D+04
42	2	2	0.72440D+04	0.72082D+04	3	2	0.72408D+04
44	2	3	0.73075D+04	0.72672D+04	3	3	0.73019D+04
46	2	4	0.73923D+04	0.73458D+04	3	4	0.73833D+04
47	2	5	0.74982D+04	0.74440D+04	3	5	0.74851D+04
68	3	0	0.98712D+04	0.98253D+04	4	0	0.98702D+04
69	3	1	0.98924D+04	0.98444D+04	4	1	0.98905D+04
70	3	2	0.99347D+04	0.98824D+04	4	2	0.99310D+04
71	3	3	0.99983D+04	0.99396D+04	4	3	0.99919D+04
73	3	4	0.10083D+05	0.10016D+05	4	4	0.10073D+05
75	3	5	0.10189D+05	0.10111D+05	4	5	0.10175D+05
99	4	0	0.12456D+05	0.12396D+05	5	0	0.12455D+05
100	4	1	0.12478D+05	0.12415D+05	5	1	0.12475D+05
101	4	2	0.12520D+05	0.12452D+05	5	2	0.12516D+05
103	4	3	0.12584D+05	0.12507D+05	5	3	0.12576D+05
104	4	4	0.12668D+05	0.12581D+05	5	4	0.12657D+05
107	4	5	0.12774D+05	0.12673D+05	5	5	0.12758D+05
133	5	0	0.14936D+05	0.14863D+05	6	0	0.14934D+05
134	5	1	0.14957D+05	0.14880D+05	6	1	0.14954D+05
136	5	2	0.15000D+05	0.14916D+05	6	2	0.14995D+05
137	5	3	0.15063D+05	0.14969D+05	6	3	0.15055D+05
138	5	4	0.15148D+05	0.15041D+05	6	4	0.15136D+05
141	5	5	0.15254D+05	0.15130D+05	6	5	0.15236D+05

AVERAGE DEVIATION < O(4)--TERMS > : 0.1467583D+04
< U(4)--TERMS > : 0.1022631D+04

AVERAGE DEVIATION (O(4)--TERMS) : 0.5872206D+02 *
(U(4)--TERMS) : 0.5245550D+02 *

STARTING THE FITTING PROCEDURE :
 INITIAL VALUES : EPSI= -40.00000 ALF= 0.0 BET= -2.59700 DELT= -13.1900
 IFIT = 1 EPSI SEARCH
 NLEV1 : 3 NLEV2 : 8 NSTOT : 36

*** END OF THE FITTING PROCEDURE ***
 FINAL VALUES : EPSI= -78.98755 ALF= 0.0 BET= -2.59700 DELT= -13.1900

** RESULTS O(4) BASIS **

TOTAL NUMBER OF BOSONS : 55
 HO : 0.42841D+05
 EPSI : -0.78988D+02
 ALF : 0.0
 BET : -0.25970D+01
 DELT : -0.13190D+02
 TOTAL NUMBER OF STATES : 812

#	V	J	E(04)	J	E(U4)
1	0	0	0.14823D+04	0	0.14823D+04
2	0	1	0.15035D+04	1	0.15021D+04
3	0	2	0.15459D+04	2	0.15417D+04
4	0	3	0.16094D+04	3	0.16011D+04
5	0	4	0.16942D+04	4	0.16802D+04
6	0	5	0.18001D+04	5	0.17792D+04
7	0	6	0.19272D+04	6	0.18979D+04
8	0	7	0.20755D+04	7	0.20364D+04
9	0	8	0.22450D+04	8	0.21947D+04
10	0	9	0.24357D+04	9	0.23728D+04
11	0	10	0.26476D+04	10	0.25707D+04
12	0	11	0.28806D+04	11	0.27883D+04
13	0	12	0.31348D+04	12	0.30258D+04
14	0	13	0.34103D+04	13	0.32830D+04
15	0	14	0.37069D+04	14	0.35600D+04
16	0	15	0.40246D+04	15	0.38568D+04
17	0	16	0.43636D+04	16	0.41734D+04
18	1	0	0.43841D+04	0	0.43830D+04
19	1	1	0.44053D+04	1	0.44027D+04
20	1	2	0.44477D+04	2	0.44420D+04
21	1	3	0.45112D+04	3	0.45011D+04
22	1	4	0.45960D+04	17	0.45097D+04
23	1	5	0.47019D+04	4	0.45798D+04
24	0	17	0.47238D+04	5	0.46783D+04
25	1	6	0.48290D+04	6	0.47964D+04
787	20	15	0.42012D+05	9	0.41103D+05
788	24	1	0.42023D+05	0	0.41200D+05
789	24	2	0.42066D+05	2	0.41214D+05
790	22	10	0.42112D+05	4	0.41248D+05
791	23	7	0.42120D+05	6	0.41302D+05
792	24	3	0.42129D+05	8	0.41378D+05
793	21	13	0.42189D+05	1	0.41532D+05
794	24	4	0.42214D+05	3	0.41558D+05
795	23	8	0.42290D+05	5	0.41606D+05
796	24	5	0.42320D+05	7	0.41677D+05
797	22	11	0.42345D+05	0	0.41877D+05
798	25	0	0.42371D+05	2	0.41894D+05
799	25	1	0.42393D+05	4	0.41935D+05
800	25	2	0.42435D+05	6	0.41999D+05
801	24	6	0.42447D+05	1	0.42258D+05
802	23	9	0.42481D+05	3	0.42288D+05

803	25	3	0.42498D+05	5	0.42344D+05
804	25	4	0.42583D+05	0	0.42647D+05
805	24	7	0.42595D+05	2	0.42666D+05
806	26	0	0.42635D+05	4	0.42711D+05
807	26	1	0.42656D+05	1	0.43068D+05
808	25	5	0.42689D+05	3	0.43101D+05
809	26	2	0.42699D+05	0	0.43493D+05
810	26	3	0.42762D+05	2	0.43513D+05
811	27	0	0.42793D+05	1	0.43948D+05
812	27	1	0.42815D+05	0	0.44405D+05

AVERAGE DEVIATION (O(4)--U(4)) : 0.9704236D+03

*** COMPARISON WITH TERMS EXPANSION ***

COEFFICIENTS (CM**-1) :

TE : 0.0
 OME : 0.29909D+04
 OMEXE : 0.52472D+02
 BE : 0.10593D+02
 ALFE : 0.30690D+00

#	V	J	E(O4)	E(TERMS)	#	J	E(U4)
1	0	0	0.14823D+04	0.14823D+04	1	0	0.14823D+04
2	0	1	0.15035D+04	0.15032D+04	1	1	0.15021D+04
3	0	2	0.15459D+04	0.15450D+04	1	2	0.15417D+04
4	0	3	0.16094D+04	0.16076D+04	1	3	0.16011D+04
5	0	4	0.16942D+04	0.16911D+04	1	4	0.16802D+04
6	0	5	0.18001D+04	0.17955D+04	1	5	0.17792D+04
18	1	0	0.43841D+04	0.43683D+04	2	0	0.43830D+04
19	1	1	0.44053D+04	0.43885D+04	2	1	0.44027D+04
20	1	2	0.44477D+04	0.44291D+04	2	2	0.44420D+04
21	1	3	0.45112D+04	0.44899D+04	2	3	0.45011D+04
22	1	4	0.45960D+04	0.45709D+04	2	4	0.45798D+04
23	1	5	0.47019D+04	0.46723D+04	2	5	0.46783D+04
40	2	0	0.71804D+04	0.71493D+04	3	0	0.71780D+04
41	2	1	0.72016D+04	0.71689D+04	3	1	0.71975D+04
42	2	2	0.72440D+04	0.72082D+04	3	2	0.72367D+04
44	2	3	0.73075D+04	0.72672D+04	3	3	0.72954D+04
46	2	4	0.73923D+04	0.73458D+04	3	4	0.73737D+04
47	2	5	0.74982D+04	0.74440D+04	3	5	0.74716D+04
68	3	0	0.98712D+04	0.98253D+04	4	0	0.98673D+04
69	3	1	0.98924D+04	0.98444D+04	4	1	0.98867D+04
70	3	2	0.99347D+04	0.98824D+04	4	2	0.99256D+04
71	3	3	0.99983D+04	0.99396D+04	4	3	0.99840D+04
73	3	4	0.10083D+05	0.10016D+05	4	4	0.10062D+05
75	3	5	0.10189D+05	0.10111D+05	4	5	0.10159D+05
99	4	0	0.12456D+05	0.12396D+05	5	0	0.12451D+05
100	4	1	0.12478D+05	0.12415D+05	5	1	0.12470D+05
101	4	2	0.12520D+05	0.12452D+05	5	2	0.12509D+05
103	4	3	0.12584D+05	0.12507D+05	5	3	0.12567D+05
104	4	4	0.12668D+05	0.12581D+05	5	4	0.12644D+05
107	4	5	0.12774D+05	0.12673D+05	5	5	0.12741D+05
133	5	0	0.14936D+05	0.14863D+05	6	0	0.14929D+05
134	5	1	0.14957D+05	0.14880D+05	6	1	0.14948D+05
136	5	2	0.15000D+05	0.14916D+05	6	2	0.14986D+05
137	5	3	0.15063D+05	0.14969D+05	6	3	0.15044D+05
138	5	4	0.15148D+05	0.15041D+05	6	4	0.15120D+05
141	5	5	0.15254D+05	0.15130D+05	6	5	0.15216D+05

AVERAGE DEVIATION (O(4)--TERMS) : 0.1467583D+04
 (U(4)--TERMS) : 0.6761316D+03

AVERAGE DEVIATION (O(4)--TERMS) : 0.5872206D+02 *
 (U(4)--TERMS) : 0.4485390D+02 *

FINAL STATE J # ENERGY	INITIAL STATE J # ENERGY	E1-PROBABILITY	
0 1 0.14823D+04	0 1 0.14823D+04	0.12277D+01	0.11080D+01
FINAL STATE J # ENERGY		E1-PROBABILITY	
0 1 0.14823D+04	1 1 0.15021D+04	0.12826D+04	-0.62031D+02
FINAL STATE J # ENERGY		E1-PROBABILITY	
0 1 0.14823D+04	0 1 0.14823D+04	0.12277D+01	0.11080D+01
0 1 0.14823D+04	0 2 0.43830D+04	0.26657D-31	-0.16327D-15
FINAL STATE J # ENERGY		E1-PROBABILITY	
0 1 0.14823D+04	1 1 0.15021D+04	0.12826D+04	-0.62031D+02
0 1 0.14823D+04	1 2 0.44027D+04	0.52235D-02	0.12518D+00
FINAL STATE J # ENERGY		E1-PROBABILITY	
1 1 0.15021D+04	2 1 0.15417D+04	0.15377D+04	0.87683D+02
1 1 0.15021D+04	2 2 0.44420D+04	0.60397D-02	0.17378D+00

Appendix B Test Run Input and Output of CROSSA

Table B.1 Test Run Input for CROSSA.

```
&INP1 NBOST = 55, ROE1=0.50, DEC=1.108, ALFA0=2.59, ROPL=0.680,
NENER= 5, ELCT(1)=1.0,ELCT(2)=2.0,ELCT(3)= 3.0,
ELCT(4)=4.0,ELCT(5)=5.0, &END
&LPRT LPLEV(1)=0, LPLEV(2)=0, LPLEV(3)=0,
ITHQ=1, ALOW=10.0, AUP=180.00, NSTEP=17, &END
&ICHAN NCHAN= 3,
JINI(1) = 0, NINI(1)=1, JFIN(1) = 0, NFIN(1)=1,
JINI(2) = 0, NINI(2)=1, JFIN(2) = 1, NFIN(2)=1,
JINI(3) = 0, NINI(3)=1, JFIN(3) = 2, NFIN(3)=1,
&END
&INTGR BMIN=0.01, BMATCH=5.01, BMAX=1005.01,
NPOINT=1251, NPB1=251, &END
```

Test Run Output

*** C R O S S A - 0(4) BASIS STATES ***

CONSTANTS :

ELECTRIC DIPOLE MOMENT DEC = 0.110800D+01 (D)
 ELECTRON ENERGY = 1.000 (EV)
 WAVE NUMBER = 0.51232D+00 (A**-1)
 RO (DIPOLE) = 0.50000D+00 (A)
 RO (POLARIZATION) = 0.68000D+00 (A)
 POLARIZABILITY (ALFA0) = 0.25900D+01 (A**3)
 NUMBER OF BOSONS = 55
 $\langle (1)1^- || D(1) || (1)0^+ \rangle$ = 0.55984D+02
 EPSIO = 0.30397D-01
 BMIN = 0.01
 BMATCH = 5.01
 BMAX = 1005.01
 INTEGRATION POINTS IN BMIN->BMATCH : 251
 TOTAL # OF INTEGRATION POINTS : 1251

CALCULATION FOR CHANNEL : 1

JI= 0(1) ---> JF= 0(1)

ANGLE	Q (A**-1)	Q (A.U.)	X-SECTION (CM**2)	X-SECTION (A.U.)
10.0	0.0893	0.1520	0.22605D-14	0.80777D+02
20.0	0.1779	0.3028	0.16989D-14	0.60711D+02
30.0	0.2652	0.4513	0.12119D-14	0.43307D+02
40.0	0.3504	0.5963	0.79468D-15	0.28398D+02
50.0	0.4330	0.7368	0.46159D-15	0.16495D+02
60.0	0.5123	0.8718	0.22334D-15	0.79808D+01
70.0	0.5877	1.0000	0.80210D-16	0.28663D+01
80.0	0.6586	1.1207	0.21562D-16	0.77051D+00
90.0	0.7245	1.2328	0.29070D-16	0.10388D+01
100.0	0.7849	1.3356	0.80901D-16	0.28909D+01
110.0	0.8393	1.4282	0.15548D-15	0.55559D+01
120.0	0.8874	1.5099	0.23462D-15	0.83841D+01
130.0	0.9286	1.5802	0.30564D-15	0.10922D+02
140.0	0.9628	1.6384	0.36190D-15	0.12932D+02
150.0	0.9897	1.6841	0.40190D-15	0.14362D+02
160.0	1.0091	1.7170	0.42732D-15	0.15270D+02
170.0	1.0207	1.7369	0.44099D-15	0.15758D+02
180.0	1.0246	1.7435	0.44525D-15	0.15911D+02

CALCULATION FOR CHANNEL : 2

JI= 0(1) ---> JF= 1(1)

ANGLE	Q (A**-1)	Q (A.U.)	X-SECTION (CM**2)	X-SECTION (A.U.)
10.0	0.0893	0.1520	0.54233D-14	0.19380D+03
20.0	0.1779	0.3028	0.14960D-14	0.53458D+02
30.0	0.2652	0.4513	0.60130D-15	0.21487D+02
40.0	0.3504	0.5963	0.28793D-15	0.10289D+02
50.0	0.4330	0.7368	0.18638D-15	0.66601D+01
60.0	0.5123	0.8718	0.13278D-15	0.47449D+01
70.0	0.5877	1.0000	0.97291D-16	0.34767D+01
80.0	0.6586	1.1207	0.77394D-16	0.27656D+01
90.0	0.7245	1.2328	0.60555D-16	0.21639D+01
100.0	0.7849	1.3356	0.50291D-16	0.17971D+01

110.0	0.8393	1.4282	0.36757D-16	0.13135D+01
120.0	0.8874	1.5099	0.30987D-16	0.11073D+01
130.0	0.9286	1.5802	0.29100D-16	0.10399D+01
140.0	0.9628	1.6384	0.23979D-16	0.85689D+00
150.0	0.9897	1.6841	0.23480D-16	0.83904D+00
160.0	1.0091	1.7170	0.24030D-16	0.85872D+00
170.0	1.0207	1.7369	0.22782D-16	0.81411D+00
180.0	1.0246	1.7435	0.23561D-16	0.84193D+00

CALCULATION FOR CHANNEL : 3

JI= 0(1) ---> JF= 2(1)

ANGLE	Q (A**-1)	Q (A.U.)	X-SECTION (CM**2)	X-SECTION (A.U.)
10.0	0.0893	0.1520	0.19629D-16	0.70144D+00
20.0	0.1779	0.3028	0.12071D-16	0.43136D+00
30.0	0.2652	0.4513	0.87566D-17	0.31291D+00
40.0	0.3504	0.5963	0.69295D-17	0.24762D+00
50.0	0.4330	0.7368	0.58317D-17	0.20839D+00
60.0	0.5123	0.8718	0.51500D-17	0.18403D+00
70.0	0.5877	1.0000	0.47212D-17	0.16871D+00
80.0	0.6586	1.1207	0.44459D-17	0.15887D+00
90.0	0.7245	1.2328	0.42590D-17	0.15219D+00
100.0	0.7849	1.3356	0.41187D-17	0.14718D+00
110.0	0.8393	1.4282	0.40006D-17	0.14296D+00
120.0	0.8874	1.5099	0.38931D-17	0.13912D+00
130.0	0.9286	1.5802	0.37933D-17	0.13555D+00
140.0	0.9628	1.6384	0.37036D-17	0.13235D+00
150.0	0.9897	1.6841	0.36280D-17	0.12964D+00
160.0	1.0091	1.7170	0.35706D-17	0.12759D+00
170.0	1.0207	1.7369	0.35349D-17	0.12632D+00
180.0	1.0246	1.7435	0.35228D-17	0.12588D+00

*** C R O S S A - 0(4) BASIS STATES ***

CONSTANTS :

ELECTRIC DIPOLE MOMENT DEC	=	0.11080D+01 (D)
ELECTRON ENERGY	=	2.000 (EV)
WAVE NUMBER	=	0.72452D+00 (A**-1)
RO (DIPOLE)	=	0.500000D+00 (A)
RO (POLARIZATION)	=	0.680000D+00 (A)
POLARIZABILITY (ALFAO)	=	0.259000D+01 (A**3)
NUMBER OF BOSONS	=	55
< (1)>1- D(1) (1)>0+ >	=	0.55984D+02
EPSIO	=	0.21494D-01
BMIN	=	0.01
BMATCH	=	5.01
BMAX	=	1005.01
INTEGRATION POINTS IN BMIN->BMATCH :		251
TOTAL # OF INTEGRATION POINTS	:	1251

CALCULATION FOR CHANNEL : 1

JI= 0(1) ---> JF= 0(1)

ANGLE	Q (A**-1)	Q (A.U.)	X-SECTION (CM**2)	X-SECTION (A.U.)
10.0	0.1263	0.1520	0.23779D-14	0.84975D+02
20.0	0.2516	0.3028	0.18377D-14	0.65669D+02
30.0	0.3750	0.4513	0.14064D-14	0.50259D+02

40.0	0.4956	0.5963	0.10328D-14	0.36908D+02
50.0	0.6124	0.7368	0.70161D-15	0.25072D+02
60.0	0.7245	0.8718	0.41803D-15	0.14938D+02
70.0	0.8311	1.0000	0.20046D-15	0.71634D+01
80.0	0.9314	1.1207	0.71799D-16	0.25657D+01
90.0	1.0246	1.2328	0.46692D-16	0.16685D+01
100.0	1.1100	1.3356	0.11991D-15	0.42849D+01
110.0	1.1870	1.4282	0.26419D-15	0.94409D+01
120.0	1.2549	1.5099	0.43997D-15	0.15722D+02
130.0	1.3133	1.5802	0.61008D-15	0.21801D+02
140.0	1.3617	1.6384	0.75033D-15	0.26813D+02
150.0	1.3997	1.6841	0.85177D-15	0.30437D+02
160.0	1.4270	1.7170	0.91642D-15	0.32748D+02
170.0	1.4435	1.7369	0.95107D-15	0.33986D+02
180.0	1.4490	1.7435	0.96182D-15	0.34370D+02

CALCULATION FOR CHANNEL : 2

JI= 0(1) ---> JF= 1(1)

ANGLE	Q (A**-1)	Q (A.U.)	X-SECTION (CM**2)	X-SECTION (A.U.)
10.0	0.1263	0.1520	0.25340D-14	0.90552D+02
20.0	0.2516	0.3028	0.58105D-15	0.20764D+02
30.0	0.3750	0.4513	0.21650D-15	0.77366D+01
40.0	0.4956	0.5963	0.10156D-15	0.36290D+01
50.0	0.6124	0.7368	0.58005D-16	0.20728D+01
60.0	0.7245	0.8718	0.39977D-16	0.14286D+01
70.0	0.8311	1.0000	0.30145D-16	0.10772D+01
80.0	0.9314	1.1207	0.23828D-16	0.85147D+00
90.0	1.0246	1.2328	0.18127D-16	0.64774D+00
100.0	1.1100	1.3356	0.12428D-16	0.44409D+00
110.0	1.1870	1.4282	0.73862D-17	0.26394D+00
120.0	1.2549	1.5099	0.37367D-17	0.13353D+00
130.0	1.3133	1.5802	0.15891D-17	0.56784D-01
140.0	1.3617	1.6384	0.14160D-17	0.50600D-01
150.0	1.3997	1.6841	0.20346D-17	0.72707D-01
160.0	1.4270	1.7170	0.29931D-17	0.10696D+00
170.0	1.4435	1.7369	0.41022D-17	0.14659D+00
180.0	1.4490	1.7435	0.46979D-17	0.16788D+00

CALCULATION FOR CHANNEL : 3

JI= 0(1) ---> JF= 2(1)

ANGLE	Q (A**-1)	Q (A.U.)	X-SECTION (CM**2)	X-SECTION (A.U.)
10.0	0.1263	0.1520	0.71380D-17	0.25507D+00
20.0	0.2516	0.3028	0.41099D-17	0.14686D+00
30.0	0.3750	0.4513	0.28871D-17	0.10317D+00
40.0	0.4956	0.5963	0.22789D-17	0.81436D-01
50.0	0.6124	0.7368	0.19722D-17	0.70475D-01
60.0	0.7245	0.8718	0.18433D-17	0.65868D-01
70.0	0.8311	1.0000	0.18264D-17	0.65266D-01
80.0	0.9314	1.1207	0.18762D-17	0.67046D-01
90.0	1.0246	1.2328	0.19565D-17	0.69915D-01
100.0	1.1100	1.3356	0.20389D-17	0.72859D-01
110.0	1.1870	1.4282	0.21039D-17	0.75183D-01
120.0	1.2549	1.5099	0.21427D-17	0.76569D-01
130.0	1.3133	1.5802	0.21553D-17	0.77019D-01
140.0	1.3617	1.6384	0.21481D-17	0.76760D-01
150.0	1.3997	1.6841	0.21301D-17	0.76118D-01

160.0	1.4270	1.7170	0.21103D-17	0.75411D-01
170.0	1.4435	1.7369	0.20956D-17	0.74884D-01
180.0	1.4490	1.7435	0.20902D-17	0.74691D-01

*** C R O S S A - 0(4) BASIS STATES ***

CONSTANTS :

ELECTRIC DIPOLE MOMENT DEC = 0.11080D+01 (D)
ELECTRON ENERGY = 3.000 (EV)
WAVE NUMBER = 0.88736D+00 (A**-1)
RO (DIPOLE) = 0.50000D+00 (A)
RO (POLARIZATION) = 0.68000D+00 (A)
POLARIZABILITY (ALFA0) = 0.25900D+01 (A**3)
NUMBER OF BOSONS = 55
< (1)1- || D(1) || (1)0+ > = 0.55984D+02
EPSIO = 0.17550D-01
BMIN = 0.01
BMATCH = 5.01
BMAX = 1005.01
INTEGRATION POINTS IN BMIN->BMATCH : 251
TOTAL # OF INTEGRATION POINTS : 1251

CALCULATION FOR CHANNEL : 1

JI= 0< 1) ---> JF= 0< 1)

ANGLE	Q (A**-1)	Q (A.U.)	X-SECTION (CM**2)	X-SECTION (A.U.)
10.0	0.1547	0.1520	0.27815D-14	0.99394D+02
20.0	0.3082	0.3028	0.21111D-14	0.75440D+02
30.0	0.4593	0.4513	0.15426D-14	0.55123D+02
40.0	0.6070	0.5963	0.10583D-14	0.37818D+02
50.0	0.7500	0.7368	0.67285D-15	0.24044D+02
60.0	0.8874	0.8718	0.39140D-15	0.13986D+02
70.0	1.0179	1.0000	0.20416D-15	0.72954D+01
80.0	1.1408	1.1207	0.99950D-16	0.35717D+01
90.0	1.2549	1.2328	0.74028D-16	0.26454D+01
100.0	1.3595	1.3356	0.12204D-15	0.43612D+01
110.0	1.4538	1.4282	0.23044D-15	0.82348D+01
120.0	1.5369	1.5099	0.37445D-15	0.13381D+02
130.0	1.6084	1.5802	0.52509D-15	0.18764D+02
140.0	1.6677	1.6384	0.65869D-15	0.23538D+02
150.0	1.7142	1.6841	0.76221D-15	0.27237D+02
160.0	1.7478	1.7170	0.83249D-15	0.29749D+02
170.0	1.7680	1.7369	0.87214D-15	0.31166D+02
180.0	1.7747	1.7435	0.88483D-15	0.31619D+02

CALCULATION FOR CHANNEL : 2

JI= 0< 1) ---> JF= 1< 1)

ANGLE	Q (A**-1)	Q (A.U.)	X-SECTION (CM**2)	X-SECTION (A.U.)
10.0	0.1547	0.1520	0.20556D-14	0.73455D+02
20.0	0.3082	0.3028	0.34737D-15	0.12413D+02
30.0	0.4593	0.4513	0.12037D-15	0.43013D+01
40.0	0.6070	0.5963	0.40007D-16	0.14296D+01
50.0	0.7500	0.7368	0.21178D-16	0.75680D+00
60.0	0.8874	0.8718	0.15654D-16	0.55940D+00
70.0	1.0179	1.0000	0.14378D-16	0.51380D+00
80.0	1.1408	1.1207	0.13837D-16	0.49446D+00

90.0	1.2549	1.2328	0.12351D-16	0.44136D+00
100.0	1.3595	1.3356	0.98507D-17	0.35201D+00
110.0	1.4538	1.4282	0.63175D-17	0.22575D+00
120.0	1.5369	1.5099	0.33518D-17	0.11978D+00
130.0	1.6084	1.5802	0.13395D-17	0.47866D-01
140.0	1.6677	1.6384	0.34833D-18	0.12447D-01
150.0	1.7142	1.6841	0.56931D-18	0.20344D-01
160.0	1.7478	1.7170	0.13094D-17	0.46791D-01
170.0	1.7680	1.7369	0.19666D-17	0.70275D-01
180.0	1.7747	1.7435	0.21952D-17	0.78444D-01

CALCULATION FOR CHANNEL : 3

JI= 0(1) ---> JF= 2(1)

ANGLE	Q (A**-1)	Q (A.U.)	X-SECTION (CM**2)	X-SECTION (A.U.)
10.0	0.1547	0.1520	0.31989D-17	0.11431D+00
20.0	0.3082	0.3028	0.16715D-17	0.59730D-01
30.0	0.4593	0.4513	0.11064D-17	0.39536D-01
40.0	0.6070	0.5963	0.84761D-18	0.30289D-01
50.0	0.7500	0.7368	0.73675D-18	0.26328D-01
60.0	0.8874	0.8718	0.71626D-18	0.25595D-01
70.0	1.0179	1.0000	0.75629D-18	0.27026D-01
80.0	1.1408	1.1207	0.83508D-18	0.29841D-01
90.0	1.2549	1.2328	0.93271D-18	0.33330D-01
100.0	1.3595	1.3356	0.10307D-17	0.36831D-01
110.0	1.4538	1.4282	0.11138D-17	0.39801D-01
120.0	1.5369	1.5099	0.11732D-17	0.41924D-01
130.0	1.6084	1.5802	0.12074D-17	0.43147D-01
140.0	1.6677	1.6384	0.12206D-17	0.43618D-01
150.0	1.7142	1.6841	0.12202D-17	0.43603D-01
160.0	1.7478	1.7170	0.12137D-17	0.43372D-01
170.0	1.7680	1.7369	0.12073D-17	0.43141D-01
180.0	1.7747	1.7435	0.12047D-17	0.43049D-01

*** C R O S S A - 0(4) BASIS STATES ***

CONSTANTS :

ELECTRIC DIPOLE MOMENT DEC	=	0.11080D+01 (D)
ELECTRON ENERGY	=	4.000 (EV)
WAVE NUMBER	=	0.10246D+01 (A**-1)
RO (DIPOLE)	=	0.50000D+00 (A)
RO (POLARIZATION)	=	0.68000D+00 (A)
POLARIZABILITY (ALFA0)	=	0.25900D+01 (A**3)
NUMBER OF BOSONS	=	55
< (1)1- II D(1) II (1)0+ >	=	0.55984D+02
EPSIO	=	0.15198D-01
BMIN	=	0.01
BMATCH	=	5.01
BMAX	=	1005.01
INTEGRATION POINTS IN BMIN->BMATCH	:	251
TOTAL # OF INTEGRATION POINTS	:	1251

CALCULATION FOR CHANNEL : 1

JI= 0(1) ---> JF= 0(1)

ANGLE	Q (A**-1)	Q (A.U.)	X-SECTION (CM**2)	X-SECTION (A.U.)
10.0	0.1786	0.1520	0.25060D-14	0.89550D+02

20.0	0.3559	0.3028	0.19030D-14	0.68004D+02
30.0	0.5304	0.4513	0.14134D-14	0.50506D+02
40.0	0.7009	0.5963	0.10024D-14	0.35822D+02
50.0	0.8661	0.7368	0.67239D-15	0.24028D+02
60.0	1.0246	0.8718	0.42200D-15	0.15080D+02
70.0	1.1754	1.0000	0.24263D-15	0.86703D+01
80.0	1.3172	1.1207	0.13050D-15	0.46634D+01
90.0	1.4490	1.2328	0.88884D-16	0.31762D+01
100.0	1.5698	1.3356	0.11745D-15	0.41972D+01
110.0	1.6787	1.4282	0.20313D-15	0.72588D+01
120.0	1.7747	1.5099	0.32138D-15	0.11484D+02
130.0	1.8573	1.5802	0.44517D-15	0.15908D+02
140.0	1.9257	1.6384	0.55388D-15	0.19793D+02
150.0	1.9794	1.6841	0.63704D-15	0.22764D+02
160.0	2.0181	1.7170	0.69282D-15	0.24758D+02
170.0	2.0415	1.7369	0.72399D-15	0.25871D+02
180.0	2.0493	1.7435	0.73391D-15	0.26226D+02

CALCULATION FOR CHANNEL : 2

JI= 0(1) ---> JF= 1(1)

ANGLE	Q (A**-1)	Q (A.U.)	X-SECTION (CM**2)	X-SECTION (A.U.)
10.0	0.1786	0.1520	0.15430D-14	0.55139D+02
20.0	0.3559	0.3028	0.25054D-15	0.89529D+01
30.0	0.5304	0.4513	0.74476D-16	0.26614D+01
40.0	0.7009	0.5963	0.21443D-16	0.76626D+00
50.0	0.8661	0.7368	0.10703D-16	0.38246D+00
60.0	1.0246	0.8718	0.95591D-17	0.34159D+00
70.0	1.1754	1.0000	0.12798D-16	0.45734D+00
80.0	1.3172	1.1207	0.14056D-16	0.50229D+00
90.0	1.4490	1.2328	0.14201D-16	0.50747D+00
100.0	1.5698	1.3356	0.12484D-16	0.44611D+00
110.0	1.6787	1.4282	0.80992D-17	0.28942D+00
120.0	1.7747	1.5099	0.49775D-17	0.17787D+00
130.0	1.8573	1.5802	0.28740D-17	0.10270D+00
140.0	1.9257	1.6384	0.17700D-17	0.63252D-01
150.0	1.9794	1.6841	0.15563D-17	0.55614D-01
160.0	2.0181	1.7170	0.19098D-17	0.68246D-01
170.0	2.0415	1.7369	0.22898D-17	0.81826D-01
180.0	2.0493	1.7435	0.24373D-17	0.87097D-01

CALCULATION FOR CHANNEL : 3

JI= 0(1) ---> JF= 2(1)

ANGLE	Q (A**-1)	Q (A.U.)	X-SECTION (CM**2)	X-SECTION (A.U.)
10.0	0.1786	0.1520	0.16974D-17	0.60657D-01
20.0	0.3559	0.3028	0.80851D-18	0.28892D-01
30.0	0.5304	0.4513	0.50172D-18	0.17929D-01
40.0	0.7009	0.5963	0.36255D-18	0.12956D-01
50.0	0.8661	0.7368	0.30088D-18	0.10752D-01
60.0	1.0246	0.8718	0.29003D-18	0.10364D-01
70.0	1.1754	1.0000	0.31926D-18	0.11409D-01
80.0	1.3172	1.1207	0.37927D-18	0.13553D-01
90.0	1.4490	1.2328	0.45691D-18	0.16327D-01
100.0	1.5698	1.3356	0.53636D-18	0.19167D-01
110.0	1.6787	1.4282	0.60390D-18	0.21580D-01
120.0	1.7747	1.5099	0.65186D-18	0.23294D-01
130.0	1.8573	1.5802	0.67956D-18	0.24284D-01

140.0	1.9257	1.6384	0.69099D-18	0.24692D-01
150.0	1.9794	1.6841	0.69212D-18	0.24733D-01
160.0	2.0181	1.7170	0.68861D-18	0.24607D-01
170.0	2.0415	1.7369	0.68480D-18	0.24471D-01
180.0	2.0493	1.7435	0.68324D-18	0.24415D-01

*** C R O S S A - O(4) BASIS STATES ***

CONSTANTS :

ELECTRIC DIPOLE MOMENT DEC = 0.11080D+01 (D)
ELECTRON ENERGY = 5.000 (EV)
WAVE NUMBER = 0.11456D+01 (A**-1)
R0 (DIPOLE) = 0.50000D+00 (A)
R0 (POLARIZATION) = 0.68000D+00 (A)
POLARIZABILITY (ALFA0) = 0.25900D+01 (A**3)
NUMBER OF BOSONS = 55
< (1)1- || D(1) || (1)0+ > = 0.55984D+02
EPSIO = 0.13594D-01
BMIN = 0.01
BMATCH = 5.01
BMAX = 1005.01
INTEGRATION POINTS IN BMIN->BMATCH : 251
TOTAL # OF INTEGRATION POINTS : 1251

CALCULATION FOR CHANNEL : 1

JI= 0(1) ---> JF= 0(1)

ANGLE	Q (A**-1)	Q (A.U.)	X-SECTION (CM**2)	X-SECTION (A.U.)
10.0	0.1997	0.1520	0.23259D-14	0.83116D+02
20.0	0.3979	0.3028	0.17422D-14	0.62258D+02
30.0	0.5930	0.4513	0.12897D-14	0.46086D+02
40.0	0.7836	0.5963	0.92172D-15	0.32937D+02
50.0	0.9683	0.7368	0.63011D-15	0.22517D+02
60.0	1.1456	0.8718	0.40955D-15	0.14635D+02
70.0	1.3141	1.0000	0.25079D-15	0.89618D+01
80.0	1.4727	1.1207	0.14822D-15	0.52968D+01
90.0	1.6201	1.2328	0.10247D-15	0.36618D+01
100.0	1.7551	1.3356	0.11296D-15	0.40365D+01
110.0	1.8768	1.4282	0.17016D-15	0.60805D+01
120.0	1.9842	1.5099	0.25552D-15	0.91309D+01
130.0	2.0765	1.5802	0.34797D-15	0.12435D+02
140.0	2.1530	1.6384	0.43088D-15	0.15397D+02
150.0	2.2131	1.6841	0.49529D-15	0.17699D+02
160.0	2.2563	1.7170	0.53901D-15	0.19261D+02
170.0	2.2824	1.7369	0.56367D-15	0.20142D+02
180.0	2.2911	1.7435	0.57155D-15	0.20424D+02

CALCULATION FOR CHANNEL : 2

JI= 0(1) ---> JF= 1(1)

ANGLE	Q (A**-1)	Q (A.U.)	X-SECTION (CM**2)	X-SECTION (A.U.)
10.0	0.1997	0.1520	0.10381D-14	0.37097D+02
20.0	0.3979	0.3028	0.21729D-15	0.77649D+01
30.0	0.5930	0.4513	0.53298D-16	0.19046D+01
40.0	0.7836	0.5963	0.14676D-16	0.52445D+00
50.0	0.9683	0.7368	0.65134D-17	0.23275D+00
60.0	1.1456	0.8718	0.85241D-17	0.30460D+00

70.0	1.3141	1.0000	0.12818D-16	0.45805D+00
80.0	1.4727	1.1207	0.14177D-16	0.50661D+00
90.0	1.6201	1.2328	0.14697D-16	0.52518D+00
100.0	1.7551	1.3356	0.11332D-16	0.40494D+00
110.0	1.8768	1.4282	0.87524D-17	0.31276D+00
120.0	1.9842	1.5099	0.59148D-17	0.21136D+00
130.0	2.0765	1.5802	0.43228D-17	0.15447D+00
140.0	2.1530	1.6384	0.32582D-17	0.11643D+00
150.0	2.2131	1.6841	0.29023D-17	0.10371D+00
160.0	2.2563	1.7170	0.27904D-17	0.99714D-01
170.0	2.2824	1.7369	0.28377D-17	0.10141D+00
180.0	2.2911	1.7435	0.28271D-17	0.10102D+00

CALCULATION FOR CHANNEL : 3

JI= 0(1) ---> JF= 2(1)

ANGLE	Q (A**-1)	Q (A.U.)	X-SECTION (CM**2)	X-SECTION (A.U.)
10.0	0.1997	0.1520	0.10225D-17	0.36538D-01
20.0	0.3979	0.3028	0.45722D-18	0.16338D-01
30.0	0.5930	0.4513	0.27507D-18	0.98294D-02
40.0	0.7836	0.5963	0.18997D-18	0.67887D-02
50.0	0.9683	0.7368	0.14651D-18	0.52354D-02
60.0	1.1456	0.8718	0.13320D-18	0.47600D-02
70.0	1.3141	1.0000	0.14867D-18	0.53125D-02
80.0	1.4727	1.1207	0.18872D-18	0.67440D-02
90.0	1.6201	1.2328	0.24294D-18	0.86812D-02
100.0	1.7551	1.3356	0.29830D-18	0.10659D-01
110.0	1.8768	1.4282	0.34486D-18	0.12323D-01
120.0	1.9842	1.5099	0.37823D-18	0.13516D-01
130.0	2.0765	1.5802	0.39874D-18	0.14249D-01
140.0	2.1530	1.6384	0.40920D-18	0.14623D-01
150.0	2.2131	1.6841	0.41304D-18	0.14760D-01
160.0	2.2563	1.7170	0.41342D-18	0.14773D-01
170.0	2.2824	1.7369	0.41269D-18	0.14747D-01
180.0	2.2911	1.7435	0.41229D-18	0.14733D-01

Appendix C Bibliography

We give here, in addition to the references of in our paper (1988) and II, a brief list of works on subjects related to the algebraic-eikonal approach to e-Molecule collision process:

- 1) O.S. van Roosmalen and A.E.L. Dieperink, "Properties of a Generalized Pseudo-spin System: Application of the Time Dependent Mean Field Method to an SU(4) Invariant Hamiltonian," Ann. Phys. **139** (1982) 198.
- 2) Y. Alhassid and J. Wu J, " An algebraic Approach to the Morse Potential Scattering, Chem. Phys. Lett. **109** (1984), 81.
- 3) J.N. Ginocchio, T. Otsuka, R.D. Amado and D.A. Sparrow, "Medium energy probes and the interacting boson model of nuclei," Phys. Rev. C **33** (1986) 247.
- 4) Y. Alhassid, J. Engel and F. Iachello, " Algebraic Approach to Dissociation from Bound States," Phys. Rev. Lett. **57** (1986) 9.
- 5) A. Frank, F. Iachello and R. Lemus, "Algebraic Method for Molecular Electronic Spectra," Chem. Phys. Lett. **131** (1986) 380.
- 6) Y. Alhassid, E.A. Hinds and D. Meschede, "Dynamical Symmetries of the Perturbed Hydrogen Atom: The van der Waals Interaction," Phys. Rev. Lett. **59** (1987) 1545.