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TRIATOM: programs for the calculation of ro-vibrational spectra of triatomic molecules

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The TRIATOM program suite calculates energy levels, wavefunctions, and where appropriate, dipole transition moments and spectra, for rotating and vibrating triatomic molecules. Potential energy, and where necessary, dipole surfaces must be provided. The programs use an exact (within the Born–Oppenheimer approximation) Hamiltonian, offer a choice of several body-fixed, internal coordinate systems based on two distances and an included angle and employ basis function expansions of orthogonal polynomials. The calculations are variational, and rotational excitation is treated using an efficient two-step algorithm. Constituent programs are TRIATOM which solves the vibrational problem and also performs the first step for rotationally excited systems. SELECT which optionally preselects basis functions for TRIATOM. ROTLEVD which performs the second step for rotationally excited states. DIPOLE computes either line or band transition intensities. SPECTRA uses the data generated by the other programs to give simulated absorption or emission spectra.

NEW VERSION SUMMARY

Title of program: TRIATOM

Catalogue number: ACLX

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland (see application form this issue)

Reference to original program: cat. no.: ABJW; *ref. in CPC:* 55 (1989) 149

Authors of original program: J. Tennyson and S. Miller

Does the new version supersede the original program?: yes

Licensing provisions: none

Computer: Convex C3840 running BSD unix; *Installation:* University of London Computer Centre

Other machines on which program has been tested: Cray-XMP/48, Cray-YMP/48, IBM RS6000, IBM pc-AT

Programming language used: FORTRAN 77

Memory required to execute with typical data: case dependent

Peripherals used: card reader, line printer, at least one disk file

No. of lines in distributed program, including test data, etc.: 3140

Keywords: ro-vibrational, body-fixed, finite basis representation, Gaussian quadrature, variational, vectorised

Nature of physical problem
TRIATOM calculates the bound ro-vibrational levels of a triatomic system using the generalised body-fixed coordinates developed by Sutcliffe and Tennyson [1].

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Method of solution
A basis is constructed as a product of radial (either Morse oscillator-like or spherical oscillator) functions and associated Legendre polynomials for the bending coordinate, with rotation matrices carrying the rotational motion. A secular matrix is constructed using Gaussian quadrature and diagonalised to give solutions. Input can be direct from SELECT [2]. TRIATOM provides data necessary to drive ROTLEVD [3] and DIPOLE [4].

Restrictions on the complexity of the problem
The size of matrix that can practically be diagonalised. TRIATOM dimensions arrays dynamically at execution time and in the present version the total space available is a single parameter which can be reset as required.

Typical running time
Highly case dependent. The sample data takes 17 s for $J = 0$ and 30 s for $J = 1$ (Coriolis decoupled) on the Convex C3840.

Unusual features of the program
A user supplied subroutine containing the potential energy as an analytic function (optionally a Legendre polynomial expansion) is a program requirement.

References

[1] B.T. Sutcliffe and J. Tennyson, Int. J. Quantum Chem. 29 (1991) 183.
[2] J. Tennyson, S. Miller and C.R. Le Sueur, this article, second program (SELECT).
[3] J. Tennyson, S. Miller and C.R. Le Sueur, this article, third program (ROTLEVD).
[4] J. Tennyson, S. Miller and C.R. Le Sueur, this article, fourth program (DIPOLE).

NEW VERSION SUMMARY

Title of program: SELECT

Catalogue number: ACLY

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland (see application form this issue).

Reference to original program: cat. no.: ABJX; *ref. in CPC:* 55 (1989) 149

Authors of original program: J. Tennyson and S. Miller

Does the new version supersede the original program?: yes

Licensing provisions: none

Computer: Convex C3840 running BSD unix; *Installation:* University of London Computer Centre

Other machines on which program has been tested: Cray-XMP/48, Cray-YMP/48, IBM RS6000

Programming language used: FORTRAN 77

Memory required to execute with typical data: case dependent

Peripherals used: card reader, line printer, one disk file

No. of lines in distributed program, including tests data, etc.: 2261

Keywords: basis set selection, first-order perturbation theory

Nature of physical problem
SELECT selects basis sets for TRIATOM [1].

Method of solution
A basis is selected either according to its quantum numbers and/or the value of its diagonal matrix element [2].

Restrictions on the complexity of the problem
The size of matrix that can be handled by TRIATOM.

Typical running time
Negligible compared to TRIATOM. The sample data takes 3 s on the Convex C3840.

Unusual features of the program
A user supplied subroutine containing the potential energy as an analytic function (optionally a Legendre polynomial expansion) may be needed. SELECT produces a file which drives TRIATOM.

References

[1] J. Tennyson, S. Miller and C.R. Le Sueur, this article, first program (TRIATOM).
[2] J. Tennyson, Comput. Phys. Rep. 4 (1986) 1.

NEW VERSION SUMMARY

Title of program: ROTLEVD

Catalogue number: ACLZ

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland (see application form this issue)

Reference to original program: cat. no.: ABJY; *ref. in CPC:* 55 (1989) 149

Authors of original program: J. Tennyson and S. Miller

Does the new version supersede the original program?: yes

Licensing provisions: none

Computer: Convex C3840 running BSD matrix; *Installation:* University of London Computer Centre

Other machines on which program has been tested: Cray-XMP/48, Cray-YMP/48, IBM RS6000

Programming language used: FORTRAN 77

Memory required to execute with typical data: case dependent

Peripherals used: card reader, line printer, at least two disk files

No. of lines in distributed program, including test data, etc.: 3953

Keywords: rotationally excited state, Coriolis coupling, secondary variational method, sparse matrix, vectorised

Nature of physical problem

ROTLEVD performs the second step in a two-step variational calculation for the bound ro-vibrational levels of a triatomic system [1].

Method of solution

A basis is constructed from the solutions, optionally energy ordered [2], of the Coriolis decoupled problem. The resulting sparse matrix is then diagonalised to give the solutions.

Restrictions on the complexity of the problem

The size of matrix that can practically be diagonalised. ROTLEVD dimensions arrays dynamically at execution time and in the present version the total space available is a single parameter which can be reset as required.

Typical running time

Case dependent. The sample data takes 171 s for a $J=1$ calculation on the Convex C3840.

Unusual features of the program

Most data is read directly from TRIATOM [3] or DVR1D [4]. ROTLEVD can provide data to drive DIPOLE [5].

References

[1] J. Tennyson and B.T. Sutcliffe, Mol. Phys. 58 (1986) 1067.

[2] B.T. Sutcliffe, J. Tennyson and S. Miller, Comput. Phys. Commun. 51 (1988) 73.

[3] J. Tennyson, S. Miller and C.R. Le Sueur, this article, first program (TRIATOM).

[4] J.R. Henderson and J. Tennyson, Comput. Phys. Commun. 75 (1993) 365, this issue.

[5] J. Tennyson, S. Miller and C.R. Le Sueur, this article, fourth program (DIPOLE).

NEW VERSION SUMMARY

Title of program: DIPOLE

Catalogue number: ACNA

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland (see application form this issue)

Reference to original program: cat. no.: ABJZ; *ref. in CPC:* 55 (1989) 149

Authors of original program: J. Tennyson and S. Miller

Does the new version supersede the original program?: yes

Licensing provisions: none

Computer: Convex C3840 running BSD unix; *Installation:* University of London Computer Centre

Other machines on which program has been tested: Cray-XMP/48, Cray-YMP/48, IBM RS6000

Programming language used: FORTRAN 77

Memory required to execute with typical data: case dependent

Peripherals used: card reader, line printer, at least two disk files

No. of lines in program, including test data, etc.: 3526

Keywords: transition intensities, linestrengths, vectorised

Nature of physical problem

DIPOLE calculates dipole transition intensities between previously calculated wavefunction for both rotational and ro-vibrational transitions [1] or alternatively vibrational band intensities [2].

Method of solution
Integrals over dipole surfaces are constructed using Gaussian quadrature for the primitive basis functions used in TRIATOM [3]. The wavefunctions generated by TRIATOM [3], DVR1D [4] and/or ROTLEVD [5] are then used to give transition intensities for individual pairs of states.

Restrictions on the complexity of the problem
The complexity of problem that can be solved by TRIATOM, DVR1D or ROTLEVD.

Typical running time
Case dependent. The sample data takes 20–30 s per call to DIPOLE on the Convex C3840.

Unusual features of the program
Most data is read directly from TRIATOM [3], DVR1D [4] and/or ROTLEVD [5]. DIPOLE provides data to drive SPECTRA [6].

References

[1] S. Miller, J. Tennyson and B.T. Sutcliffe, Mol. Phys. 66 (1989) 429.
[2] C.R. Le Sueur, S. Miller, J. Tennyson and B.T. Sutcliffe, Mol. Phys. 76 (1992) 1147.
[3] J. Tennyson, S. Miller and C.R. Le Sueur, this article, first program (TRIATOM).
[4] J.R. Henderson and J. Tennyson, Comput. Phys. Commun. 75 (1993) 365, this issue.
[5] J. Tennyson, S. Miller and C.R. Le Sueur, this article, third program (ROTLEVD).
[6] J. Tennyson, S. Miller and C.R. Le Sueur, this article, fifth program (SPECTRA).

NEW VERSION SUMMARY

Title of program: SPECTRA

Catalogue number: ACNB

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland (see application form this issue)

Reference to original program: cat. no.: ABLA; *ref. in CPC:* 55 (1989) 149

Authors of original program: J. Tennyson and S. Miller

Does the new version supersede the original program?: yes

Licensing provisions: none

Computer: Convex C3840 running BSD unix; *Installation:* University of London Computer Centre

Other machines on which program has been tested: Cray-XMP/48, Cray-YMP/48, IBM RS6000

Programming language used: FORTRAN 77

Memory required to execute with typical data: case dependent but small compared to DIPOLE. The sample data takes less than 1 s on the Convex C3480

Peripherals used: card reader, line printer, at least one disk file

No. of lines in distributed program, including test data, etc.: 1161

Keywords: synthetic spectra, Boltzmann distribution, partition function, vectorised, line profile, Einstein A coefficients

Nature of physical problem
SPECTRA generates synthetic, frequency ordered, emission or absorption spectra as a function of temperature. Gaussian line profiles and blended lines can be generated. Absolute intensities can be calculated if the necessary data to calculate the partition function is supplied.

Method of solution
Transitions are sorted by frequency and weighted using Boltzmann statistics.

Restrictions on the complexity of the problem
The complexity of the problem that can be solved by TRIATOM [1], DVR1D [2] or ROTLEVD [3].

Typical running time
Case dependent, but small. The sample data takes less than 1 s on the Convex C3840.

Unusual features of the program
Most data is read directly from DIPOLE [4]. Some data from TRIATOM [1], DVR1D [2] and/or ROTLEVD [3] may also be required.

References

[1] J. Tennyson, S. Miller and C.R. Le Sueur, this article, first program (TRIATOM).
[2] J.R. Henderson and J. Tennyson, Comput. Phys. Commun. 75 (1993) 365, this issue.
[3] J. Tennyson, S. Miller and C.R. Le Sueur, this article, third program (ROTLEVD).
[4] J. Tennyson, S. Miller and C.R. Le Sueur, this article, fourth program (DIPOLE).

LONG WRITE-UP

1. Introduction

The calculation of ro-vibrational energy levels and spectra for triatomic molecules at low levels of ro-vibrational excitation is now a standard technique [1]. In particular variational calculations using a finite basis representation (FBR) and with no significant approximations beyond that of assuming a potential energy surface, have been shown to give results of great significance and accuracy for spectroscopic and astrophysical observations [2]. These techniques are being used for tackling an increasing variety of problems [3].

More recently finite element techniques and in particular the discrete variable representation (DVR) have been developed which are particularly useful for studying highly excited vibrational states of triatomic systems [4]. These methods are undoubtedly powerful but can be quite difficult to use reliably [5]. For well documented reasons it is our policy to maintain both FBR and DVR codes [3].

Over a number of years Tennyson and Sutcliffe have developed an FBR based secular equation approach which initially used scattering coordinates [6–8]. This approach was implemented in programs ATOMDIAT [9] and ATOMDIAT2 [10]. Extensions to generalised body-fixed coordinates [11], basis set selection [12] and a two-step variational approach for rotationally excited states [13] were implemented in programs TRIATOM, SELECT and ROTLEV [14], respectively. A further coordinate generalisation [15], algorithmic improvements [16–18] and calculation of linestrengths [19] lead to the publication of the program suite [20] consisting of modules TRIATOM, SELECT, ROTLEVD, DIPOLE and SPECTRA. This package allowed the synthesis of stick spectra for a given triatom potential energy surface and dipole surfaces.

In this work we present a new edition of the programs TRIATOM, SELECT, ROTLEVD, DIPOLE and SPECTRA. Two major new features are available in these programs: the possibility of calculating vibrational band intensities in DIPOLE using the theory of Le Sueur et al. [21] and the implementation of Gaussian line profiles and blends in SPECTRA. SPECTRA has also been extended to give a choice between emission as well as absorption spectra, and if desired Einstein A coefficients.

Minor improvements include an extension in the use of symmetry in SELECT and extension of the use of spherical oscillator basis functions to both radial coordinates and all coordinate systems. Following experiences with the previous versions, some modifications have been made to improve the transportability of the codes.

Useful as all the above may be, a major reason for publishing an updated program suite is because of the interaction with the accompanying one-dimensional [22] and three-dimensional [23] DVR program suites. DVR methods are very much more powerful, if not essential, when studying highly excited vibrational states [4]. Our experience has shown that when DVR techniques are used for large calculations, it usually best to run smaller FBR calculations as a preparation [3]. This is especially true for the optimisation of basis set parameters and small test calculations which are both best done in the FBR. Furthermore, by exploiting the isomorphism between DVR and FBR approaches [24] program DVR1D [22] can be used to drive ROTLEVD [25,26] and DIPOLE. A similar approach is feasible for DVR3D [23] although this has not as yet been implemented.

2. Method

2.1. The ro-vibrational problem: TRIATOM

Using the generalised coordinates of Sutcliffe and Tennyson [15] defined in fig. 1, a body-fixed Hamiltonian can be written

$$\hat{H} = \hat{K}_V^{(1)} + \hat{K}_V^{(2)} + \hat{K}_{VR}^{(1)} + \hat{K}_{VR}^{(2)} + V(r_1, r_2, \theta), \tag{1}$$

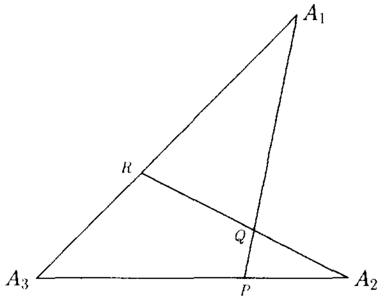

Fig. 1. Internal coordinate system of Sutcliffe and Tennyson [15]: A_i represents atom i. The coordinates are given by $r_1 = A_2 - R$, $r_2 = A_1 - P$ and $\theta = A_1\hat{Q}A_2$. The geometric parameters are defined by $g_1 = (A_3 - P)/(A_3 - A_2)$ and $g_2 = (A_3 - R)/(A_3 - A_1)$.

where V is the electronic potential. Symmetrised angular basis functions for $\hat{H}$ can be written [11]

$$|j, k, p\rangle = 2^{-1/2}(1 + \delta_{k0})^{-1/2}\left[\Theta_{jk}(\theta)\,|JMk\rangle + (-1)^p\Theta_{j-k}(\theta)\,|JM-k\rangle\right], \tag{2}$$

where $|JMK\rangle$ is a rotation matrix element [27] and Θ_{jk} an associated Legendre polynomial [28]. The total parity is given by $(-1)^{J+p}$ with $p = 0$ or 1 for e or f states, respectively. k is the projection of the total angular momentum, J, along the body-fixed z axis which can be chosen parallel to either r_1 or r_2.

Letting $\hat{H}$ act on $|j, k, p\rangle$, multiplying from the left by $\langle j', k', p'|$ and integrating over all *angular* coordinates yields an effective, diagonal in p, Hamiltonian [11]

$$\hat{K}_V^{(1)} = \delta_{j'j}\delta_{k'k}\left[\frac{\hbar^2}{2\mu_1}\frac{\partial^2}{\partial r_1^2} - \frac{\hbar^2}{2\mu_2}\frac{\partial^2}{\partial r_2^2} + \frac{1}{2}\hbar^2 j(j+1)\left(\frac{1}{\mu_1 r_1^2} + \frac{1}{\mu_2 r_2^2}\right)\right], \tag{3}$$

$$\begin{aligned}\hat{K}_V^{(2)} = &-\delta_{j'j+1}\delta_{k'k}d_{jk}\frac{\hbar^2}{2\mu_{12}}\left(\frac{\partial}{\partial r_1} - \frac{j+1}{r_1}\right)\left(\frac{\partial}{\partial r_2} - \frac{j+1}{r_2}\right)\\ &-\delta_{j'j-1}\delta_{k'k}d_{j-1,k}\frac{\hbar^2}{2\mu_{12}}\left(\frac{\partial}{\partial r_1} + \frac{j}{r_1}\right)\left(\frac{\partial}{\partial r_2} + \frac{j}{r_2}\right),\end{aligned} \tag{4}$$

$$\hat{K}_{VR}^{(1)} = \delta_{j'j}\delta_{k'k}\frac{\hbar^2}{2\mu_1 r_1^2}(J(J+1) - 2k^2) - \delta_{j'j}\delta_{k'k\pm1}\frac{\hbar^2}{2\mu_1 r_1^2}(1 + \delta_{k0} + \delta_{k'0})^{1/2}C_{Jk}^{\pm}C_{jk}^{\pm}, \tag{5}$$

$$\begin{aligned}\hat{K}_{VR}^{(2)} = &\,\delta_{j'j+1}\delta_{k'k\pm1}\frac{\hbar^2}{2\mu_{12}}(1 + \delta_{k0} + \delta_{k'0})^{1/2}C_{Jk}^{\pm}\frac{a_{j\pm k}}{r_1}\left(\frac{j+1}{r_2} - \frac{\partial}{\partial r_2}\right)\\ &+\delta_{j'j-1}\delta_{k'k\pm1}\frac{\hbar^2}{2\mu_{12}}(1 + \delta_{k0} + \delta_{k'0})^{1/2}C_{Jk}^{\pm}\frac{b_{j\pm k}}{r_1}\left(\frac{j}{r_2} + \frac{\partial}{\partial r_1}\right).\end{aligned} \tag{6}$$

The angular factors in the above equations are

$$C_{Jk}^{\pm} = [J(J+1) - k(k\pm1)]^{1/2}, \tag{7}$$

$$d_{jk} = \left[\frac{(j-k+1)(j+k+1)}{(2j+1)(2j+3)}\right]^{1/2}, \tag{8}$$

$$a_{jk} = \left[\frac{(j+k+1)(j+k+2)}{(2j+1)(2j+3)} \right]^{1/2}, \tag{9}$$

$$b_{jk} = \left[\frac{(j-k)(j-k-1)}{(4j^2-1)} \right]^{1/2}. \tag{10}$$

The reduced masses are

$$\mu_1^{-1} = g_2^2 m_1^{-1} + m_2^{-1} + (1-g_2)^2 m_3^{-1}, \tag{11}$$

$$\mu_{12}^{-1} = (1-g_1)(1-g_2) m_3^{-1} - g_2 m_1^{-1} - g_1 m_2^{-1}, \tag{12}$$

$$\mu_2^{-1} = m_1^{-1} + g_1^2 m_2^{-1} + (1-g_1)^2 m_3^{-1}, \tag{13}$$

where g_1 and g_2 define the coordinate systems used, see fig. 1.

Special case of g_1 and g_2 include scattering (Jacobi) coordinates for which

$$g_1 = \frac{m_2}{m_2 + m_3}, \qquad g_2 = 0; \tag{14}$$

bondlength–bondangle coordinates for which the g's equal either 0 or 1, and "geometric" coordinates with $g_1 = \frac{1}{2}$, $g_2 = 0$ which are useful for systems whose symmetry has been broken by isotopic substitution. Radau coordinates [29], an alternative set of orthogonal coordinates to scattering coordinates, are obtained with specific mass-dependent values of the g's:

$$g_1 = 1 - \frac{\alpha}{\alpha + \beta - \alpha\beta}, \quad g_2 = 1 - \frac{\alpha}{1 - \beta + \alpha\beta}, \quad \alpha = \left(\frac{m_3}{m_1 + m_2 + m_3} \right)^{1/2}, \quad \beta = \frac{m_2}{m_1 + m_2}. \tag{15}$$

For both the Radau and scattering (Jacobi) coordinates we have used radial coordinates defined geometrically (see fig. 1) rather than the more conventional mass weighted coordinates. Other coordinates may be used by explicitly specifying g_1 and g_2. These various options do not actually exploit the full generality of the Hamiltonian derived by Sutcliffe and Tennyson [15], but other coordinate systems can be employed with only relatively minor changes to subroutine SETCON.

The $\hat{K}_{VR}$ operators given above are for the z axis embedded parallel to r_1. The appropriate operators for the other embedding are obtained by making the exchanges $r_1 \leftrightarrow r_2$ and $\mu_1 \leftrightarrow \mu_2$.

If the potential is expressed as an expansion in Legendre polynomials $P_\lambda(\theta)$, then

$$V(r_1, r_2, \theta) = \sum_\lambda V_\lambda(r_1, r_2) P_\lambda(\theta) \tag{16}$$

and the angular integration can be performed analytically

$$\langle j', k' | P_\lambda(\theta) | j, k \rangle = \delta_{k'k} (-1)^k [(2j'+1)(2j+1)]^{1/2} \begin{pmatrix} j' & \lambda & j \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} j' & \lambda & j \\ -k & 0 & k \end{pmatrix}, \tag{17}$$

where the 3-j symbols in the Gaunt coefficient are conventional [27]. This method of performing the angular integration over the potential is completely general as potentials which are not naturally expanded in Legendre polynomials can be so expressed for each (r_1, r_2) by using Gauss–Legendre quadrature. This is a computationally efficient way of forming matrix elements over the potential [30].

The motion in the radial coordinates can also be carried by basis functions. These are expressed as products of one-dimensional orthogonal sets

$$\psi_{mn}(r_1, r_2) = r_1^{-1} H_m(r_1) r_2^{-1} H_n(r_2). \tag{18}$$

In our experience the most suitable functions are a complete set based on solutions of the Morse potential [6,7]

$$|n\rangle = H_n(r) = \beta^{1/2} N_{n\alpha} \exp(-\tfrac{1}{2}y) y^{(\alpha+1)/2} L_n^{\alpha}(y), \quad y = A \exp[-\beta(r-r_e)], \tag{19}$$

where

$$A = 4D_e/\beta, \qquad \beta = \omega_e(\mu/2D_e)^{1/2}, \qquad \alpha = \text{integer}(A). \tag{20}$$

The parameters μ, r_e, ω_e and D_e can be associated with the reduced mass, equilibrium separation, fundamental frequency and dissociation energy of the relevant coordinate, respectively. In practice (r_e, ω_e, D_e) are treated as variational parameters and optimised accordingly. $N_{n\alpha} L_n^{\alpha}$ is a normalised associated Laguerre polynomial [31].

With the Morse oscillator-like functions, integrals over the differential operators in the kinetic energy operators can be computed analytically [11,12]. However, it is necessary to use Gauss–Laguerre quadrature to evaluate the integrals involving inverse powers of r and the potential.

An alternative set of radial basis functions, particularly useful for systems which have significant amplitude for $r = 0$, are spherical oscillator functions, defined by

$$|n\rangle = H_n(r) = 2^{1/2}\beta^{1/2} N_{n\alpha+1/2} \exp(-\tfrac{1}{2}y) y^{\alpha/2} L_n^{\alpha+1/2}(y), \quad y = \beta r^2 \tag{21}$$

where

$$\beta = (\mu\omega_e)^{1/2} \tag{22}$$

and (α, ω_e) are treated as variational parameters. Further details about the functions can be found elsewhere [8,9,14].

In terms of these basis functions, the approximation to the lth energy level, E_l^J, has a wavefunction

$$\Psi_l^J = \sum_k \sum_{jmn} d_{kjmn}^{Jl} |jk\rangle |m\rangle |n\rangle. \tag{23}$$

For homonuclear diatomics the wavefunction should be either symmetric or antisymmetric with respect to interchange of the like atoms. This symmetry is naturally represented in scattering coordinates where functions with j even and odd are symmetric and anti-symmetric and can be denoted $q = 0$ and $q = 1$, respectively. The wavefunction can also be symmetrised, for the case of $J = 0$, in coordinates for which $g_1 = g_2$ – these include bondlength–bondangle ($g_1 = 0$) and Radau coordinates. In this case the wavefunction can be written

$$\Psi_l^{0q} = \sum_{jmn} d_{0jmn}^{Jql} |j0\rangle 2^{-1/2}(1+\delta_{mn})^{-1/2}(|m\rangle|n\rangle + (-1)^q |n\rangle|m\rangle), \quad m \ge n+q, \quad q = 0, 1, \tag{24}$$

where $q = 0(1)$ labels the wavefunction as symmetric (antisymmetric).

2.2. Vibrational basis set selection: SELECT

A number of methods of building basis sets from the functions described above have been tested with a view to obtaining the most rapid convergence for a given problem [12]. As the vibrational basis set is a product of one-dimensional basis sets for each internal coordinate, one method is simply to take all possible product functions given by terminating each series at some maximum quantum number.

A second alternative is to use a compound quantum number NQMAX to determine which functions are selected. Allowing for selective weighting of functions in different coordinates this means that function $|jk\rangle|m\rangle|n\rangle$ is included in the basis if

$$\mathrm{NQMAX} \geq \frac{j}{d_j} + \frac{m}{d_m} + \frac{n}{d_n}. \tag{25}$$

A third alternative is to use an energy criterion in selecting the functions. In this case the diagonal matrix elements of a large set of functions are evaluated. The lowest LBASS are then selected for the final basis.

Although we have found the energy ordering criterion to be often the most efficient, all three methods have been found useful for certain systems. Furthermore, it is also possible to select a basis using a mixture of methods.

2.3. Rotational excitation: ROTLEVD

The theory outlined in section 2.1 is in principle sufficient for finding the ro-vibrational wavefunctions of arbitrary triatomics. However, as the size of the secular problem implied by this method grows rapidly with increasing angular momentum, J, alternative methods have been developed to deal with rotational excitation [18].

If k, the projection of J on the body-fixed z axis, is assumed to be a good quantum number, then the Hamiltonian of section 2.1 becomes

$$\hat{H}dJ_k = \hat{K}_V^{(1)} + \hat{K}_V^{(2)} + \delta_{k'k}\hat{K}_{VR}^{(1)} + V(r_1, r_2, \theta). \tag{26}$$

Solutions of this Hamiltonian with eigenenergy ϵ_i^{Jk} can be written

$$|i, k\rangle = \sum_{jmn} c_{jmn}^{Jki}|jk\rangle|m\rangle|n\rangle \tag{27}$$

in terms of the basis functions defined above. The functions $|i, k\rangle$ can then be used as a basis for the fully coupled problem.

The advantages of this procedure are two-fold. Firstly, the secular matrix obtained in the second step has a distinctive sparse structure which is well suited to iterative diagonalisation techniques [13,16]. Secondly, not all the functions $|i, k\rangle$ are needed to obtain converged results. A suitable basis set can be selected either by using the lowest NVIB functions for each k block, or by choosing the LBASS functions with the lowest eigenenergy, ϵ_i^{Jk}. Again, the energy selection criterion has proved the most efficient [17].

If the lth solution of the second step is written

$$\Psi_l^J = \sum_{ik} b_{ik}^{Jl}|ik\rangle, \tag{28}$$

then coefficient vectors $\boldsymbol{b}^{Jl}$ can be back transformed to yield coefficients of the wavefunction in terms of the original basis functions

$$d_{kjmn}^{Jl} = \sum_i b_{ik}^{Jl} c_{jmn}^{Jki}. \tag{29}$$

2.4. Transition intensities: DIPOLE

With the wavefunctions generated in the previous sections, dipole transition intensities for selected transitions can be calculated given appropriate dipole surfaces. For a triatomic lying in the x–z plane, the dipole surface can be expressed in a generalisation of the Legendre expansion used to express the potential [32]

$$\mu_z(r_1, r_2, \theta) = \sum_{\lambda} C_{\lambda,0}(r_1, r_2) P_{\lambda,0}(\theta), \tag{30}$$

$$\mu_x(r_1, r_2, \theta) = \sum_{\lambda} C_{\lambda,1}(r_1, r_2) P_{\lambda,1}(\theta). \tag{31}$$

Such an expansion can be obtained from any dipole surface using Gauss–Legendre quadrature, providing care is taken with the $\sin(\theta)$ factors [19].

Integrating over the dipole surface yields an expression for the transition dipole. In practice, the individual magnetic components of the wavefunctions are not computed separately. Summing over these then gives the transition line strength [16]:

$$\begin{aligned} S(f-i) = {} & \tfrac{1}{4}\left[(2J'+1)(2J''+1)\right] \\ & \times \Bigg[\sum_{\nu=-1}^{+1} \sum_{\lambda=|\nu|} \sum_{k=p''}^{J''} \sum_{j''j'} a(\nu, \nu+k, \lambda)\left[(2j'+1)(2j''+1)\right]^{1/2} \\ & \times \begin{pmatrix} J' & 1 & J'' \\ -k-\nu & \nu & k \end{pmatrix} \begin{pmatrix} j' & \lambda & j'' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} j' & \lambda & j'' \\ -k-\nu & \nu & k \end{pmatrix} \\ & \times \sum_{m''n''} \sum_{m'n'} B_{\lambda,\nu}^{m'm''n'n''} d_{k'j'm'n'}^{J'p'l'} d_{k''j''m''n''}^{J''p''l''} \left[(-1)^{J''+J'+1} + (-1)^{p''+p'}\right] \Bigg]^2, \end{aligned} \tag{32}$$

where the radial integrals, $B_{\lambda,\nu}^{m'm''n'n''}$, are again evaluated using Gauss–Laguerre quadrature and

$$a(0, n, \lambda) = 1, \quad 0 \le n \le J', \qquad a(\pm 1, 0, \lambda) = -\left[\gamma(\gamma+1)\right]^{1/2},$$

$$a(\pm 1, n, \lambda) = -\left[\tfrac{1}{2}\lambda(\lambda+1)\right]^{1/2}, \quad 0 < n \le J', \qquad a(\nu, n, \lambda) = 0, \quad n < 0, n > J', \nu = 0, \pm 1.$$

Using the linestrength, the Einstein A_{if} coefficient for spontaneous emission is given, in s^{-1}, by

$$A_{if} = \frac{1}{(2J''+1)} \frac{64\pi^4 \omega_{if}^3}{3h} S(f-i). \tag{33}$$

By taking the above formula for the ro-vibrational linestrength and separating rotational and vibrational motion, one can derive a formula for the linestrength of the whole vibrational band. In this case linestrenghts can be computed from vibrational ($J = 0$) wavefunctions using the formula [21]:

$$S_{f-i}^{\text{Vib}} = \left[\sum_{j''j'} \begin{pmatrix} j' & \lambda & j'' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} j' & \lambda & j'' \\ 0 & 0 & 0 \end{pmatrix} \sum_{m''n''} \sum_{m'n'} B_{\lambda,\nu}^{m'm''n'n''} d_{j'm'n'}^{l'} d_{j''m''n''}^{l''} \right]^2. \tag{34}$$

However, now the orientation of the axes of the dipole is crucial [21]. To get reliable answers it is necessary to use axes defined according to the Eckart embedding.

2.5. Synthetic spectra: SPECTRA

Integrated absorption coefficients, in cm/molecule, can be generated as a function of frequency, ω_{if}, and temperature, T, using the formula

$$I(\omega_{if}) = \frac{4.162034 \times 10^{-19} \omega_{if} g_i \left[\exp(-hc\omega''/kT) - \exp(-hc\omega'/kT)\right]}{Q(T)} S(f-i), \tag{35}$$

where $Q(T)$ is the partition function of the system, $S(f-i)$ is in D^2 and ω' and ω'' are the wavenumber of the upper and lower state in cm^{-1}, respectively. The degeneracy factor g_i for a particular level is determined by nuclear spin statistics.

The emissivity, in ergs/molecule/sr, is defined by

$$J(\omega_{if}) = \frac{(2J'+1)g_i hc\omega_{if}\exp(-hc\omega'/kT)}{4\pi Q(T)}A_{if}. \tag{36}$$

If enough energy levels of the system are known it is possible to obtain an expression for the partition function of the system

$$Q(T) = \sum_J \sum_i g_i \exp(-E_i^J/kT). \tag{37}$$

3. Program structure

Figure 2 gives the structure of the program suite showing how the various modules interconnect. The key program is TRIATOM which has to be run in all cases – it should be noted that DVR1D [22] can be used instead of TRIATOM to drive the other programs in the suite.

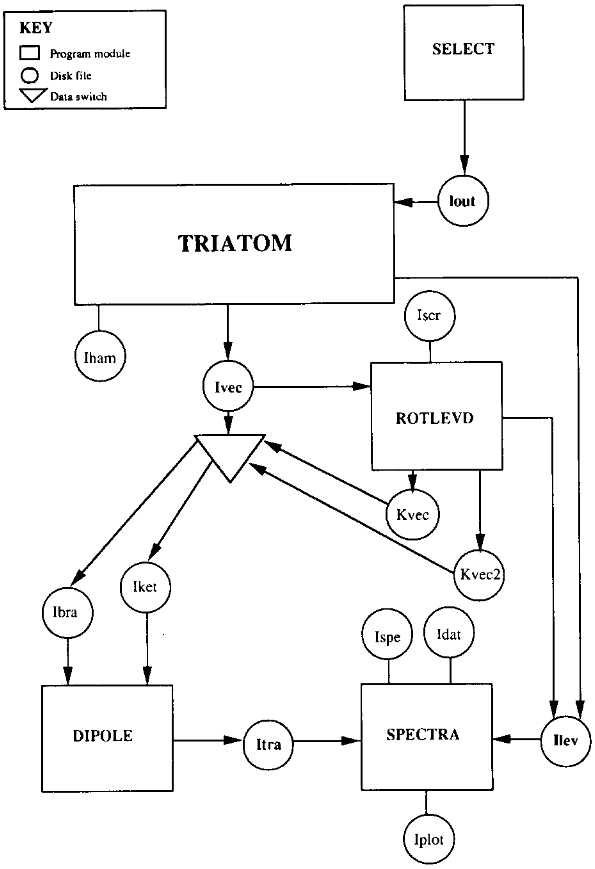

Fig. 2. Program module flow diagram. Note that SELECT and TRIATOM can be replaced by DVR1D [22].

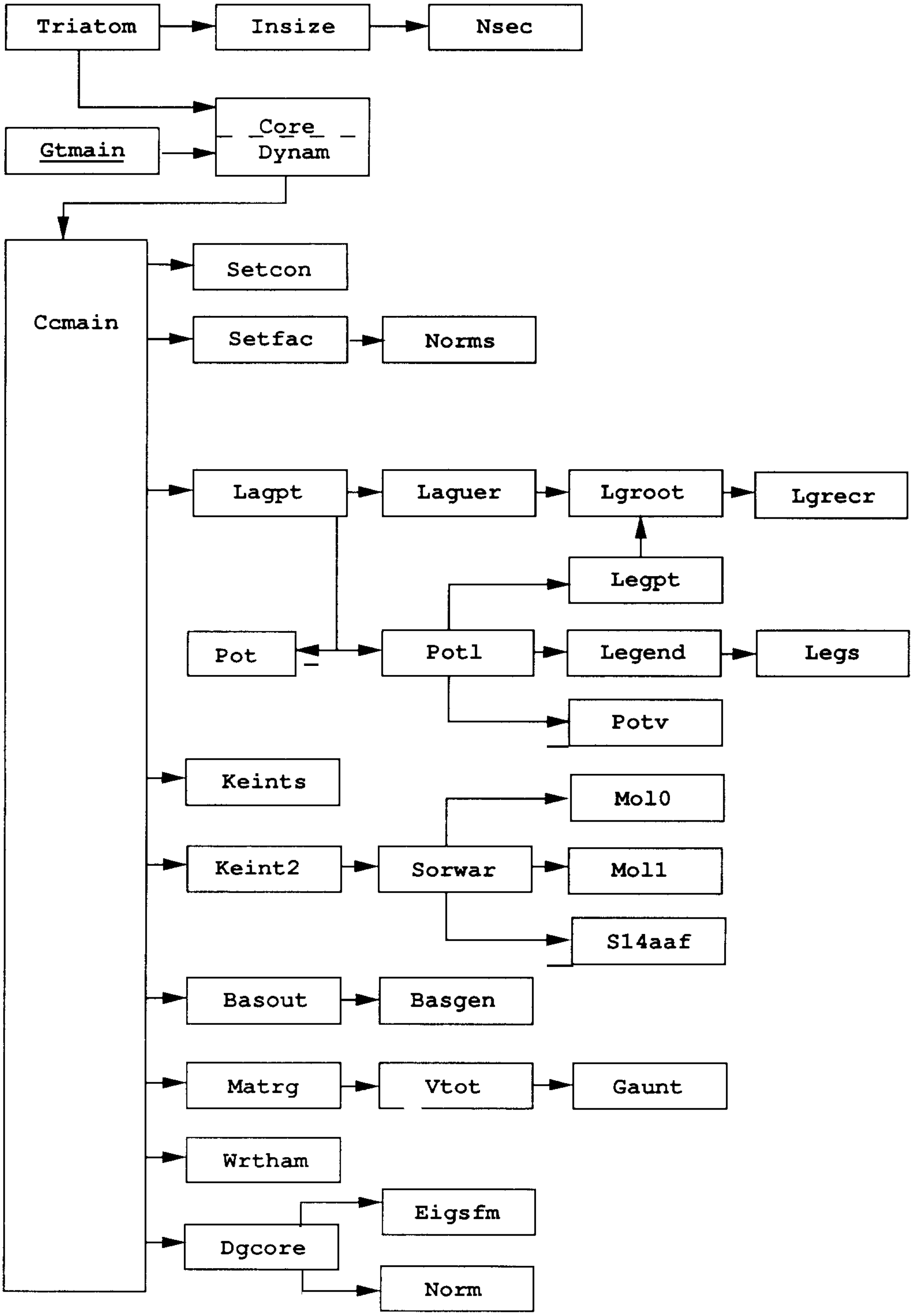

Fig. 3. Structure of program TRIATOM. Service routines TIMER, GETROW and OUTROW have been omitted.

Input for TRIATOM is either specified by the user or provided by SELECT which acts as a basis set preprocesser. If a two-step variational calculation is being performed the eigenvalues, eigenvectors and some matrix elements generated by TRIATOM are passed to ROTLEVD. The input wavefunctions for DIPOLE come from either TRIATOM or ROTLEVD. DIPOLE processes the wavefunctions in pairs and has to be run for each (J, p, symmetry) $\leftrightarrow$ (J, p, symmetry) block that is to be considered. The output from these runs is concatenated into a single file which forms the input to SPECTRA. If SPECTRA is to compute a partition function, an additional input file from TRIATOM (and ROTLEVD) containing energy levels and quantum numbers is also required.

Additional data input is needed for all modules except when TRIATOM is driven be SELECT. The amount required is kept to a minimum by passing as much information as possible from previous modules and by the use of default settings for many parameters.

All the programs follow the convention that names beginning with letters A–H and O–Y are for double precision real variables, I–N are for integers and variables whose name begins with Z are logicals. The programs should be running using real*8 length variables and should, for example, be compiled with the double precision off option on Cray machines.

All programs use dynamical assignment of array space in which one big vector is sub-divided in routine CORE. In the current versions, this array is a single fixed length array real*8 ARRAY of dimension NAVAIL (= 500000 in the versions supplied) in subroutine GTMAIN. For efficient storage management a call to a local HPALLOC, GETMAIN or MEMORY command should be implemented.

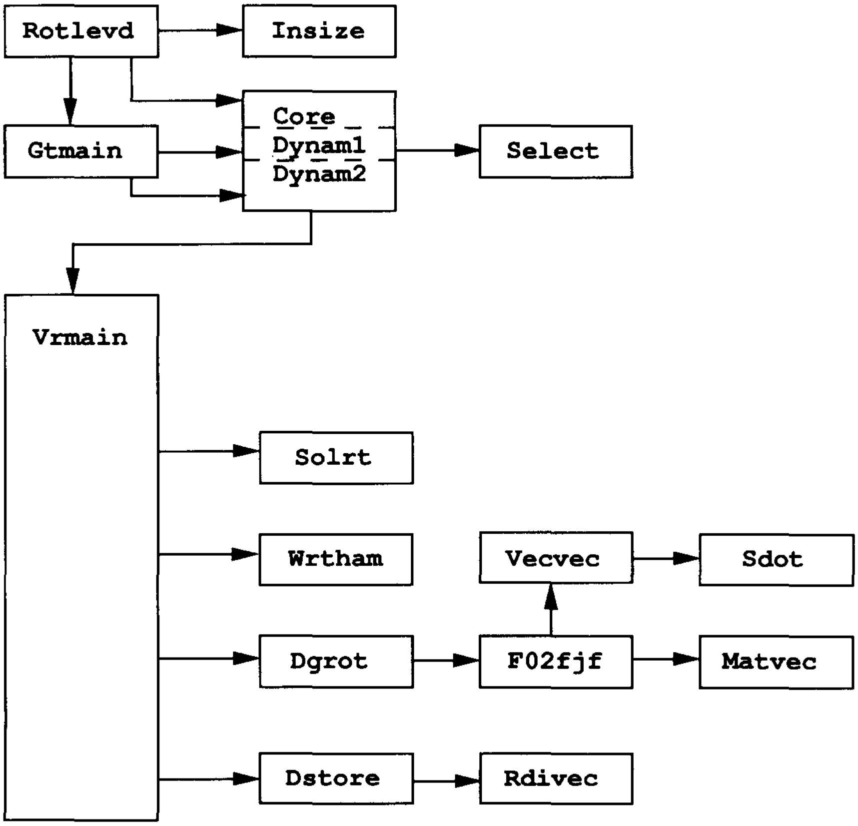

Fig. 4. Structure of program ROTLEVD. Service routines TIMER, GETROW, OUTROW and MXMB have been omitted.

TRIATOM can be divided into four segments which form the basis of a possible overlay structure – see fig. 3. The segments can be characterised as (1) data input and initialisation; (2) radial basis functions and matrix elements, which performs the numerical integrations using Gaussian quadrature; the points and weights are generated automatically from routines adapted [6] from Stroud and Secrest [33]; (3) angular integration and secular matrix construction, and (4) diagonalisation, which dominates the CPU requirement. A detailed consideration of each subroutine will not be given as comments are provided in the program source should more information be required.

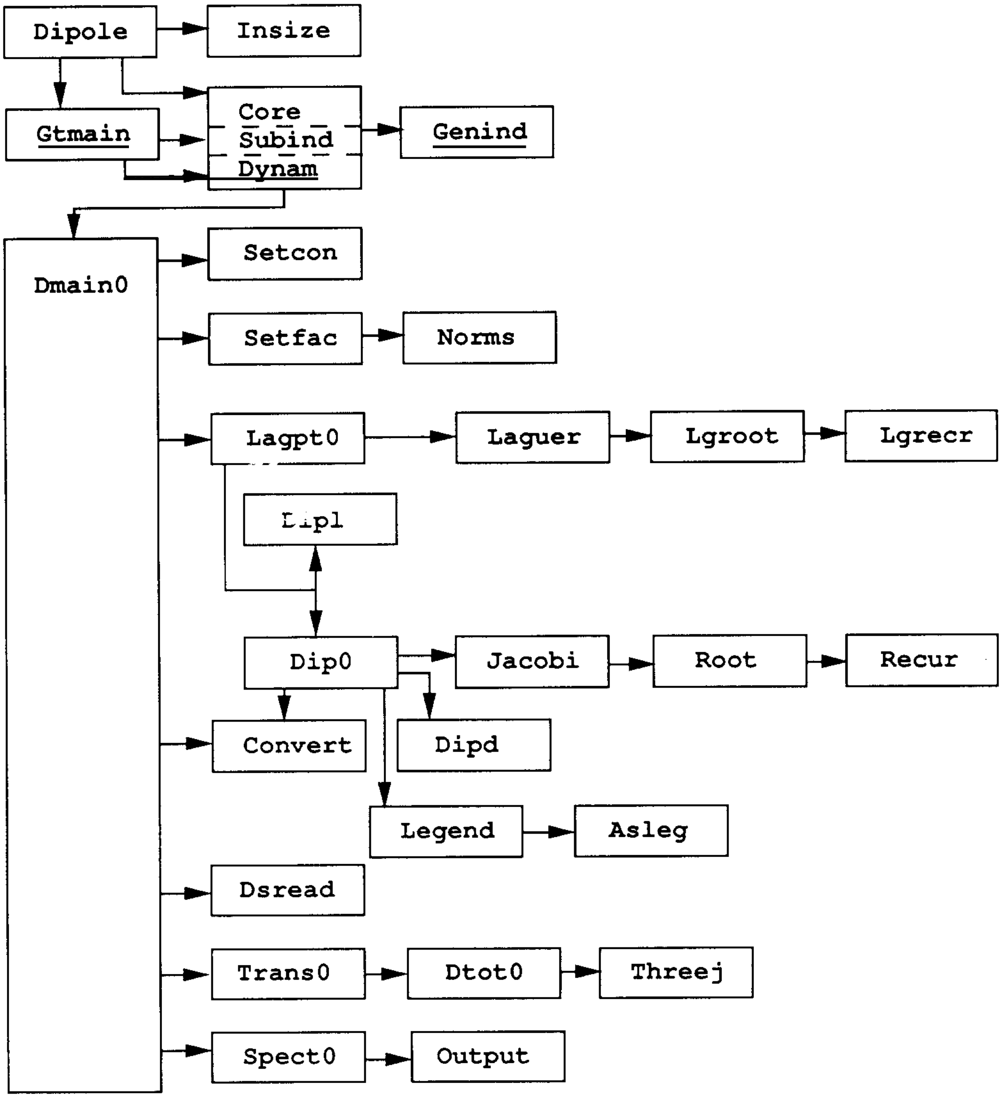

Fig. 5. Structure of program DIPOLE. Service routines TIMER, GETROW, OUTROW and MXMB have been omitted. DIPOLE actually has two parallel structures: that shown is for calculating vibrational band intensities. When calculating intensities for individual ro-vibrational transitions the high level subroutines have the same names with the zero omitted (eg DMAIN instead of DMAIN0). In this case subroutine CONVER is not used.

The CPU time and memory requirement of TRIATOM are dominated by the storage and diagonalisation of the Hamiltonian matrix. This is a real symmetric matrix and in general less than 25% of the eigenvalues and eigenvectors are required. The present implementation uses subroutine EGVQR [34] to mimic EISPACK routine EIGSFM [35]. We strongly recommend that EGVQR, which obtains *all* eigenvectors, is replaced either by the local EISPACK implementation of EIGSFM or by some real symmetric diagonaliser which yields only the NEVAL *lowest* eigenvalues and eigenvectors, and which is appropriate to the architecture of the machine being used.

Subroutine S14AAF is a NAG subroutine [36] which calculates Γ functions. The present implementation uses routine GAMMLN from "Numerical Recipes" [37] to mimic the operation of S14AAF.

SELECT is composed mainly of routine adapted from TRIATOM. Its structure is given by fig. 3, except that Segment 4 is replaced by a call to subroutine SORT which performs the basis set selection. As only the diagonal elements of HAMIL and hence the matrix element arrays are needed by SELECT, it is unlikely that an overlay will required for this step.

Figure 4 gives the structure of program ROTLEVD. A detailed consideration of the performance of the module can be found elsewhere [38]. Two subroutines deserve special comment: MXMB is a fast vector matrix multiplier – this routine uses the bulk of the CPU time [38] and thus may need optimising for the architecture of any particular machine.

The routines F02FJF to G05CAF inclusive are a NAG Library [36] subroutines suite for diagonalising sparse matrices, based on the algorithm of Nikolai [39]. The implementation given here is appropriate for IBM mainframes and it is recommended that users replace this by a local implementation where possible.

Figure 5 gives the structure of program DIPOLE. Many of the routines used in DIPOLE are the same, or very similar, to those used in TRIATOM for the evaluation of the integrals over the potential energy surface, the main difference being that the dipole moment operator is a vector. In addition, the fact that the ket and bra states considered are generated in separate TRIATOM/ROTLEVD jobs means that extra checks on compatibility are carried out in Subroutine INSIZE.

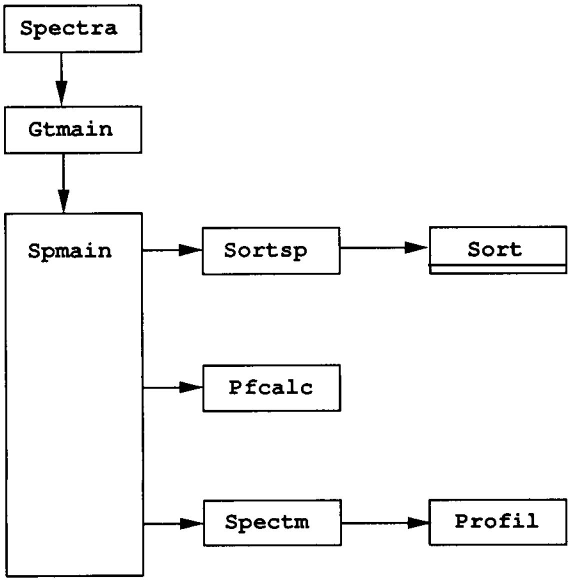

Fig. 6. Structure of program SPECTRA. Service routines TIMER, GETROW and OUTROW have been omitted.

DIPOLE also uses the fast matrix multiply routine MXMB which can be replaced at the same time as that for ROTLEVD.

When DIPOLE calculates vibrational band intensities, the calculation *must* be conducted in Eckart coordinates. DIPOLE uses routine CONVERT to find the atom coordinates in the original axis system, refered to the centre of mass. These are then used to find the rotation angle necessary to refer the dipole to the Eckart axes [21]. This requires and equilibrium geometry of the molecule to be input by the user, who is warned that the results can be sensitive to the values given.

Figure 6 gives the structures of program SPECTRA. For a large list of transitions, subroutine SORT may be beneficially replaced by specialised sorting routines; the calling sequence for NAG routines M01DEF and M01EAF [36] is given as comments in the source of SORTSP. The version of subroutine PROFIL provided gives Gaussian profiles to the lines if requested. Users may wish to adapt this subroutine to other line profiles as appropriate.

Finally, certain disk files (notably IOUT in SELECT, ILEV in TRIATOM and ROTLEVD, ITRA in DIPOLE) may be read to the end and then written to. Unfortunately whether it is necessary to BACKSPACE the file between the reads and the writes depends on the machine being used. The present implementation *does* BACKSPACE and it may be necessary to remove these statements, on certain machines such as VAXes. The occurances are all clearly labelled.

4. Program use

4.1. The potential and dipole subroutines

Both TRIATOM and SELECT require a user supplied potential energy subroutine. There are two ways of supplying the potential. If it is specified as a Legendre expansion, eq. (15), option ZLPOT = .TRUE., then the expansion must be supplied by

SUBROUTINE POT(V0,VL,R1,R2)

which returns V0 = $V_0(r_1, r_2)$ and VL(λ) = $V_\lambda(r_1, r_2)$ in Hartree for R1 = r_1 and R2 = r_2 in Bohr. If |IDIA| = 2, only even V_λ are needed. If NCOORD = 1, R1 and VL are dummies. If NCOORD = 2, R1 contains the rigid diatom bondlength, r_e, If NCOORD > 1 then V_λ has dimensions LPOT. In the present version of the codes the LiCN potential of Essers et al. [40] is provided in POT. This potential uses scattering coordinates with the CN bond frozen.

If a general potential function, ZLPOT = .FALSE., is to be used then

SUBROUTINE POTV(V,R1,R2,XCOS)

must be supplied. POTV returns the potential V in Hartree for an arbitrary point given by R1 = r_1, R2 = r_2 (both in Bohr) and XCOS = cos θ. The H_2S potential of Senekowitch et al. [41] is provided. This routine is in subroutine POTS with POTV giving a flexible conversion of coordinates systems.

DIPOLE requires a subroutine defining the dipole surfaces. If ZLPOT = .TRUE. and the surfaces are supplied as a Legendre expansion, eqs. (20) and (21), then

SUBROUTINE DIPL(D0,DL,R1,R2,NU)

must be supplied, where for R1 = r_1, R2 = r_2 (in Bohr) and NU = $\nu = 0$ or 1, the routine returns D0 = $C_{0,\nu}(r_1, r_2)$ and DL = $C_{\lambda,\nu}(r_1, r_2)$ in atomic units. If $\nu = 1$, D0 is not required. If |IDIA| = 2, only terms with λ even are required. In the present version of the codes the LiCN dipole surfaces of Brocks et al. [32] is provided in DIPL. These surfaces use scattering coordinates with the CN bond frozen.

It should be noted that the option of expressing the dipoles as a Legendre expansion is not available when calculating vibrational band intensities. In this case it is necessary to explicitly sum the Legendre series and implement the dipoles surfaces in DIPD (see below).

If a general dipole function, ZLPOT = .FALSE., is to be used then

```
SUBROUTINE DIPD(DIPC,R1,R2,XCOS,NU)
```

must be supplied. DIPD returns the NU-th component of the dipole in atomic units (1 a.u. = 2.5417662 Debye) at point R1 = r_1, R2 = r_2 (both in Bohr) and XCOS = $\cos\theta$ where NU = 0 corresponds to μ_z and NU = 1 μ_x.

TRIATOM and SELECT include COMMON /MASS/ XMASS(3),G1,G2 where XMASS contains the atomic masses in atomic units (as opposed to amu), G1 = g_1 and G2 = g_2. This is to enable users to write flexible potential subroutines which allow for changes in coordinates or isotopic substitution. See, for example, the version of POTV supplied. DIPOLE includes COMMON /MASS/ XMASS(3),G1,G2,ZEMBED which also allows the dipole surface to take account of the embedding used.

4.2. Input for TRIATOM

TRIATOM requires 8 lines of card input for *all* runs, extra cards are required if the basis set is selected. Cards giving data not required or for which the defaults [given below in parenthesis] are sufficient should be left blank. This input can optionally all be generated by SELECT.

Card 1: NAMELIST /PRT/

ZPHAM[F]	= T requests printing of the Hamiltonian matrix.
ZPRAD[F]	= T, request printing of the radial matrix elements.
ZPMIN[F]	= T, request only minimal printing.
ZPVEC[F]	= T, request printing of the eigenvectors.
ZDIAG[T]	= T, request diagonalisation of Hamiltonian matrix.
ZROT[F]	= T, TRIATOM to perform first step in a two-step variational calculation.
ZLADD[F]	= T, maximum j in angular basis (LMAX) incremented with (J, k); = F, maximum j fixed (only used if ZROT = T).
ZEMBED[T]	= T, z axis embedded along r_2; = F, z axis embedded along r_1.
ZMORS1[T]	= T, use Morse oscillator-like functions for r_1 coordinate; = F, use spherical oscillator functions.
ZMORS2[T]	= T, use Morse oscillator-like functions for r_2 coordinate; = F, use spherical oscillator functions.
ZLPOT[F]	= T, potential supplied in POT; = F, potential supplied in POTV.
ZVEC[F]	= T, data for ROTLEVD to be written to stream IVEC.
IVEC[4]	output stream for ROTLEVD data (unformatted).
ZPFUN[F]	= T, eigenvalues concatenated on stream ILEV. Warning, the first eigenvalues on this file must be for $J = 0$, $q = 0$.
ILEV[14]	output stream for eigenvalue data (formatted).
IHAM[10]	stream for Hamiltonian matrix (scratch, unformatted).

Card 2: NCOORD (I5)
NCOORD[3] the number of vibrational coordinates of the problem:
= 1 for a diatomic (is useful for basis set optimisation),
= 2 for an atom rigid diatom system (not valid for |ISYM| = 2),
= 3 for a full triatomic.

Card 3: NPNT2,NMAX2,JROT,NEVAL,LMAX,LPOT,IDIA,KMIN,NPNT1,NMAX1,ISYM,NBASS, NRAD(14I5)
NPNT2[2*NMAX2 + 1] order of Gaussian quadrature in the r_2 coordinate.
NMAX2 order of the largest radial basis function $H_n(r_2)$, giving an r_2 basis of NMAX2 + 1 functions.
JROT[0] |JROT| is the total angular momentum quantum number of the system.
> 0, the off-diagonal Coriolis terms are included.
< 0, they are neglected and k (KMIN) is treated as a good quantum number.
= 0 or NCOORD = 1, there are no Coriolis terms.
NEVAL[10] number of eigenvalues and eigenvectors required.

If NCOORD = 1 the rest of the card is ignored

LMAX order of the highest associated Legendre polynomials in the basis.
If IDIA = 2, the parity of the angular basis is given by the parity of LMAX.
LPOT[2*LMAX2 + 1] highest value of λ in the Legendre expansion of the potential.
If ZLPOT = T,LPOT must be consistent with subroutine POT.
If ZLPOT = F,LPOT + 1 + MOD(LPOT,2) point Gauss-Legendre integration is used for the θ coordinate.
IDIA = − 1 for generalised coordinates,
= 0 for Radau or other orthogonal coordinates,
= 1 for scattering coordinates with a hetronuclear diatomic,
= 2 for scattering coordinates with a homonuclear diatomic,
= −2 for midpoint coordinates with a symmetric potential (e.g. where the symmetry has been broken by isotopic substitution).
KMIN = k for JROT < 0,
= $(1 - p)$ for JROT > 0 (including ZROT = T).
Note: if KMIN = 2 in ROTLEVD, KMIN must be 1 in TRIATOM.
NPNT1[2*NMAX1 + 1] order of Gaussian quadrature in the r_1 coordinate.
NMAX1 order of the largest radial basis function $H_m(r_1)$, giving an r_1 basis of NMAX1 + 1 functions.
ISYM[0] ≠ 0 for bondlength-bondangle coordinates ($g_1 = g_2 = 0$) or other symmetric cases ($g_1 = g_2$):
= 1 for hetronuclear case,
= 2 for symmetric AB_2 case,
= −2 for anti-symmetric AB_2 case.
|ISYM| = 2 cannot be used with JROT > 0 or ZROT = T.
NBASS[0] number of basis functions in the secular problem:
= 0 determined internally,
> 0 basis preselected and to be read in (see card 9).

NRAD[0]	largest number of radial functions in any block: if NBASS = 0, set internally as (NMAX1 + 1)*(NMAX2 + 1), If NBASS > 0, must be specified.

Card 4: TITLE (9A8)
A 72 character title.

Card 5: (XMASS(I),I = 1,3) (3F20.0)
XMASS(I) contains the mass of atom I in atomic mass units.
If NCOORD = 1, XMASS(3) is set to zero, the diatom comprising atoms 1 and 2.

Card 6: G1,G2 (2F20.0)
Parameters g_1 and g_2 determine the coordinate system used if IDIA = -1 or IDIA = 0 and ISYM = 1.
Otherwise this card is ignored and:
if IDIA > 0, G1 = $m_2/(m_2+m_3)$, G2 = 0,
if IDIA = -2, G1 = $\frac{1}{2}$, G2 = 0,
if IDIA = 0 and ISYM = ± 2, G1 = $1+s-(s^2+2s)^{1/2}$, where $s = m_3/m_2$.
If ISYM = ± 2 then G2 = G1.

Card 7: RE1,DISS1,WE1 (3F20.0)
If NCOORD = 1, this card is read but ignored.
If NCOORD = 2, RE1 is the fixed diatomic bondlength, DISS1 and WE1 ignored.
If NCOORD = 3, then:
If ZMORS1 = T, RE1 = r_e, DISS1 = D_e and WE1 = ω_e are Morse parameters for the r_1 coordinate.
If ZMORS1 = F, RE1 is ignored; DISS1 = α and WE1 = ω_e are spherical oscillator parameters for the r_1 coordinate.

Card 8: RE2,DISS2,WE2 (3F20.0)
If |ISYM| = 2, this card is read but ignored.
If ZMORS2 = T, RE2 = r_e, DISS2 = D_e and WE2 = ω_e are Morse parameters for the r_2 coordinate.
If ZMORS2 = F, RE2 is ignored; DISS2 = α and WE2 = ω_e are spherical oscillator parameters for the r_2 coordinate.

Card 9 onwards: (IK(I),IL(I),IM(I),IN(I),I = 1,NBASS) (36I2)
If NBASS = 0, not read.
If NBASS > 0, basis set labels as generated by SELECT: IK(I) = k, IL(I) = j, IM(I) = $m+1$ and IN(I) = $n+1$ for the Ith basis function.

4.3. Input for SELECT

Card 1: LBASS,NQMAX,NQJ,NQM,NQN,IFLAG,IOUT (7I5)

LBASS[0]	select the LBASS lowest basis functions ordered by their diagonal elements.
NQMAX[0]	$= N_{\max}$, maximum total quantum number for a basis function.
NQJ[1]	$= d_j$, weight of $P_{jk}(\theta)$ in determining $N_{\max}$.
NQM[1]	$= d_m$, weight of $H_m(r_1)$ in determining $N_{\max}$.
NQN[1]	$= d_n$, weight of $H_n(r_2)$ in determining $N_{\max}$.
IFLAG[0]	$\neq 0$: select basis for different (J, k) or symmetry from the full calculation.
IOUT[7]	output stream for TRIATOM data file (formatted).

Cards 2–9: These are the same as cards 1–8 of the TRIATOM input, except:
If IFLAG > 0, then TRIATOM card 3 is repeated: first to characterise the basis for the selection run, second to characterise the TRIATOM run.
If NQMAX > 0, then NMAX1 and NMAX2 default to NQM * NQMAX and NQN * NQMAX, respectively.

4.4. Card input for ROTLEVD

Most of the data for ROTLEVD, which must have been prepared previously by TRIATOM, is read from stream IVEC. Three lines of data are read from cards.

Card 1: NAMELIST/PRT/

TOLER[0.0d0]	tolerance for convergence of the eigenvalues, zero gives machine accuracy. 1.0D-4 is usually sufficient for most applications.
ZPVEC[F]	= T, request printing of the eigenvectors.
THRESH[0.1d0]	threshold for printing eigenvector coefficients, zero requests the full vector (only used if ZPVEC = T).
ZPHAM[F]	= T, requests printing of the Hamiltonian matrix.
ZPRAD[F]	= T, requests printing of the radial matrix elements.
ZPTRA[F]	= T, requests printing of the transformed vectors.
IVEC[4]	stream for input data from TRIATOM (unformatted).
ZVEC[F]	= T, eigenvalue and eigenvector data to be written to disk file. (= T forced if ZTRAN = T).
JVEC[3]	stream for first set of eigenvalue/vector output (unformatted).
JVEC2[2]	stream for second set of eigenvalue/vector output (unformatted), KMIN = 2 only.
ZTRAN[F]	= T, eigenvector transformed back to original basis.
KVEC[8]	stream for first set of transformed eigenvector output (unformatted).
KVEC2[9]	stream for second set of transformed eigenvector output (unformatted), KMIN = 2 only.
ISCR[1]	stream for scratch file storing array OFFDG (unformatted).
IRES[0]	restart flag: = 1, full restart, = 2, restart second diagonalisation only (for KMIN = 2 only), = −1, perform vector transformation only (stream JVEC must be supplied).
ZPFUN[F]	= T, eigenvalues concatenated on stream ILEV. The first eigenvalues on this file must (with $J = 0$, j even) be already present.
ILEV[14]	stream for eigenvalue data (formatted).

Card 2: NVIB,NEVAL,KMIN,IBASS,NEVAL2 (5I5)

NVIB	number of vibrational levels from TRIATOM for each k to be read, and perhaps selected from, in the second variational step.
NEVAL[10]	the number of eigenvalues required for the first set.
KMIN[0]	= 0, f or $p = 1$ parity calculation. = 1, e or $p = 0$ parity calculation. = 2, do both e and f parity calculation.
IBASS[0]	= 0 or > NVIB * (JROT + KMIN), use all the vibrational levels. Otherwise, select IBASS levels with the lowest energy.
NEVAL2[NEVAL]	the number of eigenvalues required for the second set.

Card 3: TITLE (9A8)
A 72 character title.

4.5. Card input for DIPOLE

DIPOLE processes batches of transitions between states defined by the the bra and ket input files. These files are produced either by TRIATOM – stream IVEC – or ROTLEVD – stream JVEC of JVEC2. They contain most of the data necessary to characterise the run. This data must be consistent which means that runs creating the bra and ket files must have identical input for cards 5–9 in TRIATOM, otherwise an error condition will result. To generate transitions with $\Delta J = 0$, the same input files should be used for the bra and ket. In this case the diagonal transition dipoles are simply the vibrational averaged dipole of the relevant state.

DIPOLE takes most of its input from the output streams IVEC (from TRIATOM) or JVEC and JVEC2 (from ROTLEVD). It has the option to produce output files for SPECTRA to calculate simulated spectra at a given temperature. The user must supply the following three lines of input on card:

Card 1: NAMELIST/PRT/

ZLPOT[F]	= T, the dipole surfaces supplied DIPL (not allowed if $J' = J'' = 0$); = F, the dipole surfaces supplied in DIPD.
ZPRINT[F]	= T, supplies extra print out for debugging purposes.
ZTRA[F]	= T, writes data for SPECTRA to stream IOUT.
ZSTART[F]	= T, initiates the output file for the data for SPECTRA. = F, writes data to the end of existing file on stream ITRA.
IKET[11]	input stream from TRIATOM/ROTLEVD for the Ket (unformatted).
IBRA[12]	input stream for the Bra (unformatted).
ITRA[13]	output stream to SPECTRA (if ZTRA = T) (unformatted).

Card 2: TITLE (9A8)
A 72 character title.

Card 3: LPOT,NPNT1,NPNT2,NV1,NV2 (5I5)

LPOT	highest value of λ in the Legendre expansion of the dipole. If ZLPOT = T, LPOT must be consistent with Subroutine DIPL. If ZLPOT = F, LPOT + 1 + MOD(LPOT,2) point Gauss–Legendre integration is used for the θ coordinate.
NPNT1[2*NMAX1 + 1]	order of Gaussian quadrature in the r_1 coordinate.
NPNT2[2*NMAX2 + 1]	order of Gaussian quadrature in the r_2 coordinate.
NV1[all]	number of ket eigenfunctions considered.
NV2[all]	number of bra eigenfunctions considered.

Card 4: ER1,ER2,ECOS (3F20.0)
Only read if $J'' = J' = 0$, when
ER1 = equilibrium value of r_1 in a_0, in specified coordinate system.
ER2 = equilibrium value of r_2 in a_0, in specified coordinate system.
ECOS = equilibrium value of $\cos\theta$, in specified coordinate system.

Input and output on streams IKET, IBRA and IOUT are in atomic units. The data printed at the end of DIPOLE is given in wavenumbers, Debye for the transition dipoles and s^{-1} for the Einstein A coefficients.

4.6. Card input for SPECTRA

SPECTRA takes most of its input from stream ITRA generated by DIPOLE. Data for generating partition functions may optionally be provided TRIATOM/ROTLEVD stream ILEV. The user must supply at least 6 (5 if ZSPE = .FALSE. or ZSORT = .FALSE.) cards in input, cards 5 and 6 can be repeated to generate spectra from the same transitions for different conditions.

Card 1: NAMELIST/PRT/

ZOUT[F]	= .TRUE., print sorted transition frequencies and line strengths. ZOUT is set automatically to .TRUE. if ZSPE is .FALSE.
ZSORT[T]	= .TRUE., sort transition data and write it to stream ISPE. = .FALSE., sorted transition data is to be read from stream ISPE.
ZSPE[T]	= .FALSE., if the program is to stop after sorting only.
ZPFUN[T]	= .TRUE., calculate the partition function from data on stream ILEV; = .FALSE., the partition function is not calculated but set to 1.0
ITRA[13]	input stream transitions file from DIPOLE (unformatted).
ILEV[14]	formatted input stream with energy levels for the partition function. The first eigenenergy on ILEV must be the Ground State for $J = 0$, ($q = 0$). This is the zero energy of the problem.
ISPE[15]	stream for the sorted transitions (unformatted).

Card 2: TITLE (9A8)
A 72 character title.

Card 3: NAMELIST/SOR/
If ZSORT = .FALSE. this card should *not* be supplied.

EMIN[$-$1.0d27]	minimum value of energy of lower state, E'', in cm^{-1} for which data printed.
EMAX[$+$1.0d27]	maximum value of energy of lower state, E'', in cm^{-1} for which data printed.
JMAX[all]	maximum value of J'', the angular momentum of the lower state, for which data printed.
SMIN[0.0]	lowest relative linestrength to be printed out.

Card 4: GE, GO (2D10.0)

GE[1.0ed0]	nuclear-spin times symmetry-degeneracy factors for homonuclear diatomic-containing molecules for the j even states.
GO[1.0d0]	nuclear-spin times symmetry-degeneracy factors for homonuclear diatomic-containing molecules for the j odd states.

Card 5: TEMP,XMIN,WMIN,WMAX,DWL (5D10.0)

TEMP	temperature in K.
XMIN	lowest relative intensity printed.
WMIN[0.0]	minimum transition frequency required in cm^{-1}.
WMAX[all]	maximum transition frequency required in cm^{-1}.
DWL[0.0]	profile half width, in cm^{-1} or μm depending on ZFREQ, used if ZPROF = T.

Card 6: NAMELIST/SPE/

EMIN1[−1.0d27] minimum value of energy of lower state, E'', in cm^{-1} for which data printed.
EMAX1[+1.0d27] maximum value of energy of lower state, E'', in cm^{-1} for which data printed.
EMIN2[−1.0d27] minimum value of energy of upper state, E', in cm^{-1} for which data printed.
EMAX2[+1.0d27] maximum value of energy of upper state, E', in cm^{-1} for which data printed.

JMAX[all]	maximum value of J'', the lower state angular momentum, for which data printed.
ZEMIT[F]	= F, calculates integrated absorption coefficient. = T, calculates emissivities.
ZPROF[F]	= T, gives spectrum at 3000 points with Gaussian line profiles; only used with ZPLOT = T, when results are on stream IPLOT. = F generates stick spectrum.
IDAT[19]	Scratch file used to construct profiles (formatted), used if ZPROF = T and ZPLOT = T.
ZPLOT[F]	= T, writes computed spectrum to stream IPLOT.
IPLOT[20]	output stream for formatted file containing spectral data.
ZFREQ[T]	= T, stream IPLOT contains wavenumber (cm^{-1}) as first column. = F, stream IPLOT contains wavelength (μm) as first column.
ZEINST[F]	= T, stream IPLOT contains spin weighted Einstein A coefficient as second column. In this case ZEMIT = T. is forced. = F, stream IPLOT contains intensity as second column.

Cards 5 and 6 are repeated for each set of spectral conditions required.

4.6. Test output

Runs of SELECT, TRIATOM, ROTLEVD, DIPOLE and SPECTRA for the H_2S molecule have been prepared using the potential (in POTV and POTS) and dipole (in DIPD and DIPS) surfaces of Senekowitch et al. [41]. These runs mimic benchmark calculations on H_2S transisitions performed by Carter et al. [42], although the size of the calculations have been reduced in the test data.

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TEST RUN OUTPUT

```
     Program SELECT (Version of 22 Aug 1992)


     BASIS SET SELECTION PROGRAM:
     8 LINES OF INPUT DATA TRANSFERED TO STREAM  7

     SELECTION CRITERIA:
     LOWEST  400 BASIS FUNCTIONS CHOSEN

     FULL TRIATOMIC VIBRATIONAL PROBLEM WITH

       13    POINT NUMERICAL INTEGRATION FOR
        7    TH ORDER R1 RADIAL BASIS FUNCTIONS
       13    POINT NUMERICAL INTEGRATION FOR
        7    TH ORDER R2 RADIAL BASIS FUNCTIONS
       24    TH ORDER ANGULAR BASIS FUNCTIONS
       50    TERMS IN THE POTENTIAL EXPANSION
     1600    CANDIDATE BASIS FUNCTIONS

     TITLE: H2S: J=0 USING BONDLENGTH-BONDANGLE COORDINATES

     LOWEST  400 FUNCTIONS SELECTED FROM    0.5129179734D-01 HARTREE TO    0.1332150779D+00 HARTREE

      BASIS SET LIMITS RESET:
     LMAX  WAS   24 RESET TO   24
     NMAX1 WAS    7 RESET TO    6
     NMAX2 WAS    7 RESET TO    6
     NBASS WAS 1600 RESET TO  400

     Program TRIATOM (Version of 15 Sept 1992)

LOWEST    5 EIGENVALUES IN WAVENUMBERS

 0.329745977066D+04      0.448790101862D+04      0.566949168078D+04      0.591788868010D+04      0.592844065195D+04


     TITLE: H2S: J=1 USING BONDLENGTH-BONDANGLE COORDINATES

     ***  VIBRATIONAL PART OF ROT-VIB CALCULATION  ***
                    J =  1  K =  0
     ***  OPTION TO NEGLECT CORIOLIS INTERACTIONS  ***


LOWEST  200 EIGENVALUES IN WAVENUMBERS

 0.331642039760D+04      0.450676709526D+04      0.568826419149D+04      0.593656330853D+04      0.594712981259D+04

     ***  VIBRATIONAL PART OF ROT-VIB CALCULATION  ***
                    J =  1  K =  1
     ***  OPTION TO NEGLECT CORIOLIS INTERACTIONS  ***


LOWEST  200 EIGENVALUES IN WAVENUMBERS

 0.331679080564D+04      0.450779580425D+04      0.568999028509D+04      0.593694187015D+04      0.594748070067D+04

     PROGRAM ROTLEVD (VERSION OF 12 Sept 1992):


     ROTATIONAL PART OF ROT-VIB CALCULATION  WITH:
      200   LOWEST VIBRATIONAL EIGENVECTORS SUPPLIED FROM
      400   DIMENSION VIBRATION SECULAR PROBLEM
      200   LOWEST VIBRATIONAL EIGENVECTORS ACTUALLY USED
       10   LOWEST ROTATIONAL EIGENVECTORS REQUIRED FOR
      350   DIMENSION ROTATION SECULAR PROBLEM
            WITH BASIS SELECTED BY ENERGY ORDERING

     TITLE:  H2S J=1, BLBA CO-ORDINATES


     J =  1 ROTATIONAL STATE,     350 BASIS FUNCTIONS
            E PARITY, SYMMETRIC |JK> + |J-K> FUNCTIONS IN BASIS

LOWEST  10 EIGENVALUES IN WAVENUMBERS

 0.331115075845D+04      0.331253701910D+04      0.450172612360D+04      0.450328577958D+04      0.568346790639D+04

 0.568521027599D+04      0.593138602715D+04      0.593273954513D+04      0.594200205322D+04      0.594325594700D+04

     J =  1 ROTATIONAL STATE,     173 BASIS FUNCTIONS
            F PARITY, ANTI-SYMMETRIC |JK> - |J-K> FUNCTIONS IN BASIS

LOWEST   5 EIGENVALUES IN WAVENUMBERS

 0.331679080564D+04      0.450779580425D+04      0.568999028509D+04      0.593694187015D+04      0.594748070067D+04

Program DIPOLE (Version of 11 Sept 1992):

H2S 0E TO 0E TRANSITIONS; GENERAL G1,G2; BLBA COORDS.
```

```
    GIVEN EQUILIBRIUM POSITIONS CORRESPOND TO
    THE FOLLOWING CARTESIAN POSITIONS

                             X                  Z
    ATOM 1             -0.07477790         2.45177613
    ATOM 2              2.44701955        -0.16998003
    ATOM 3             -0.07477790        -0.07192687

IE1 IE2   KET ENERGY   BRA ENERGY    FREQUENCY  Z TRANSITION    X TRANSITION       DIPOLE       S(F-I)       A-COEFFICIENT

  1   1     3297.460     3297.460        0.000   0.681268E+00   0.708272E+00   0.982739E+00   0.965776E+00    0.000000E+00
  1   2     3297.460     4487.901     1190.441   0.102073E-01   0.106119E-01   0.147242E-01   0.216802E-03    0.114707E+00
  1   3     3297.460     5669.492     2372.032  -0.255053E-02  -0.265163E-02   0.367918E-02   0.135364E-04    0.566586E-01
  1   4     3297.460     5917.889     2620.429   0.500317E-02   0.520153E-02   0.721718E-02   0.520876E-04    0.293937E+00
  1   5     3297.460     5928.441     2630.981   0.455234E-02  -0.437872E-02   0.631641E-02   0.398970E-04    0.227874E+00

    Program DIPOLE (Version of 11 Sept 1992):

    H2S 0E TO 1E TRANSITIONS; GENERAL G1,G2; BLBA COORDS.

IE1 IE2   KET ENERGY   BRA ENERGY    FREQUENCY  Z TRANSITION    X TRANSITION       DIPOLE       S(F-I)       A-COEFFICIENT

  1   1     3297.460     3311.151       13.691   0.487134E+00  -0.486871E+00   0.263149E-03   0.692476E-07    0.185776E-10
  1   2     3297.460     3312.537       15.077  -0.471017E+00  -0.511689E+00   0.982706E+00   0.965711E+00    0.346014E-03
  1   3     3297.460     4501.726     1204.266   0.419270E-02  -0.418815E-02   0.455269E-05   0.207270E-10    0.378430E-08
  1   4     3297.460     4503.286     1205.826   0.540274E-01  -0.699653E-01   0.159379E-01   0.254018E-03    0.465584E-01
  1   5     3297.460     5683.468     2386.008   0.365641E-02  -0.365503E-02   0.138275E-05   0.191199E-11    0.271508E-08
  1   6     3297.460     5685.210     2387.751   0.989454E-03   0.277054E-02   0.375999E-02   0.141375E-04    0.201197E-01
  1   7     3297.460     5931.386     2633.926  -0.411693E-02   0.410370E-02   0.132211E-04   0.174797E-09    0.333908E-06
  1   8     3297.460     5932.740     2635.280   0.328378E-02   0.450673E-02   0.779052E-02   0.606921E-04    0.116116E+00
  1   9     3297.460     5942.002     2644.542  -0.297983E-02  -0.339611E-02   0.637594E-02   0.406525E-04    0.785995E-01
  1  10     3297.460     5943.256     2645.796  -0.454762E-02   0.456205E-02   0.144275E-04   0.208152E-09    0.403024E-06

    H2S 1E TO 1F TRANSITIONS; GENERAL G1,G2; BLBA COORDS.

IE1 IE2   KET ENERGY   BRA ENERGY    FREQUENCY  Z TRANSITION    X TRANSITION       DIPOLE       S(F-I)       A-COEFFICIENT

  1   1     3311.151     3316.791        5.640  -0.576754E+00  -0.626842E+00   0.120360E+01   0.144864E+01    0.271700E-04
  1   2     3311.151     4507.796     1196.645   0.661830E-01  -0.856606E-01   0.194776E-01   0.379378E-03    0.679592E-01
  1   3     3311.151     5689.990     2378.840  -0.124482E-02  -0.342071E-02   0.466553E-02   0.217671E-04    0.306322E-01
  1   4     3311.151     5936.942     2625.791   0.379722E-02   0.525634E-02   0.905357E-02   0.819671E-04    0.155132E+00
  1   5     3311.151     5947.481     2636.330   0.557479E-02  -0.557690E-02   0.210417E-05   0.442754E-11    0.848091E-08

     Program SPECTRA (Version of 10 Sept 1992)

     H2S SPECTRUM FOR J=0 AND 1 LEVELS.

     TEMPERATURE SET TO:     10.00K

    PARTITION FUNCTION Q =      0.194711E+01
    ESTIMATED ERROR IN Q =      0.716357E+01 %

    MAXIMUM ABSORPTION COEFFICIENT =    0.275671E-17
         UNITS ARE CM./MOLECULE.

    INTEGRATED BAND ABSORPTION =   0.306872E-17

       100 TRANSITIONS WITHIN SPECTRAL RANGE
        18 TRANSITIONS INCLUDED
        82 TRANSITIONS NEGLECTED

    IPAR   J2  P2  I2   J1  P1  I1      E2         E1        FREQ        S(F-I)      ABS I(W)     REL I(W)       A(IF)

      1     1   1   1    1   0   1     19.331     13.691      5.640    0.145E+01    0.135E-18    0.491E-01    0.272E-04
      1     1   0   2    0   0   1     15.077      0.000     15.077    0.966E+00    0.276E-17    0.100E+01    0.346E-03
      1     0   0   2    1   0   2   1190.441     15.077   1175.364    0.183E-03    0.526E-20    0.191E-02    0.934E-01
      1     1   0   3    1   1   1   1204.266     19.331   1184.935    0.276E-03    0.433E-20    0.157E-02    0.480E-01
      1     1   1   2    1   0   1   1210.336     13.691   1196.645    0.379E-03    0.135E-19    0.491E-02    0.680E-01
      1     1   0   4    0   0   1   1205.826      0.000   1205.826    0.254E-03    0.655E-19    0.238E-01    0.466E-01
      1     0   0   3    1   0   2   2372.032     15.077   2356.955    0.123E-04    0.706E-21    0.256E-03    0.503E-01
      1     1   0   5    1   1   1   2386.008     19.331   2366.677    0.178E-04    0.557E-21    0.202E-03    0.246E-01
      1     1   1   3    1   0   1   2392.531     13.691   2378.840    0.218E-04    0.154E-20    0.560E-03    0.306E-01
      1     1   0   6    0   0   1   2387.751      0.000   2387.751    0.141E-04    0.722E-20    0.262E-02    0.201E-01
      1     0   0   4    1   0   2   2620.429     15.077   2605.352    0.456E-04    0.290E-20    0.105E-02    0.253E+00
      1     1   0   7    1   1   1   2633.926     19.331   2614.595    0.735E-04    0.255E-20    0.923E-03    0.137E+00
      1     0   0   5    1   0   1   2630.981     13.691   2617.290    0.361E-04    0.282E-20    0.102E-02    0.203E+00
      1     1   1   4    1   0   1   2639.482     13.691   2625.791    0.820E-04    0.642E-20    0.233E-02    0.155E+00
      1     1   0  10    1   1   1   2645.796     19.331   2626.465    0.544E-04    0.189E-20    0.686E-03    0.103E+00
      1     1   1   5    1   0   2   2650.021     15.077   2634.944    0.659E-04    0.424E-20    0.154E-02    0.126E+00
      1     1   0   8    0   0   1   2635.280      0.000   2635.280    0.607E-04    0.342E-19    0.124E-01    0.116E+00
      1     1   0   9    0   0   1   2644.542      0.000   2644.542    0.407E-04    0.230E-19    0.834E-02    0.786E-01
```