

JKSTARK:
Python package for the Stark-effect calculation and
symmetry classification of linear, symmetric and
asymmetric top wavefunctions in DC electric fields

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Abstract

The Controlled Molecule Imaging group (CMI) at the Center for Free Electron Laser Science (CFEL) has created the JKSTARK software to calculate, view and analyse the energy levels of adiabatic Stark energy curves of linear, symmetric-top and asymmetric top molecules.

Keywords: Asymmetric top molecule, Stark effect

1. Program summary

Program title:. JKSTARK

Licensing provisions:. Open source BSD License. See code for licensing details.

No. of lines in distributed program, including test data, etc.:. 2602

No. of bytes in distributed program, including test data, etc.:. 108606

Distribution format:. tar.gz

Programming language:. Python (version 2.6.6)

Computer:. Any Macintosh, PC, or Linux/UNIX workstations with a modern Python distribution

Email address: `jochen.kuepper@cfel.de` (Jochen Küpper)

Operating system:. Tested on Mac OS X and a variety of Linux distributions

RAM:. 2 GB for typical calculations

External routines:. numpy, scipy Python packages, utilizes BLAS and LAPACK through scipy. All available under open-source licenses.

Nature of problem:. Calculation of the Stark effect of asymmetric top molecules in arbitrarily strong DC electric fields and correct symmetry classification and labelling of the adiabatic Stark curves.

Solution method:. We set up the full M matrices of the quantum-mechanical asymmetric rotor Hamiltonian in the basis of the symmetric top wavefunctions and Wang transform the Hamiltonian. We separate the matrix according to the appropriate remaining Fourgroup symmetry, and according to J if possible, and diagonalize the individual blocks. The application of all symmetry of the system allows for the direct correlation of the asymmetric top eigenstates in the DC electric field to the field-free eigenstates, directly yielding correct adiabatic labels and correspondingly, adiabatic Stark energy curves.

Restrictions:. For practical purposes, the maximum J is limited by the available main memory. A modern PC with 8 GB of main memory allows for calculations including $J = 50$ or higher.

Running time:. 1 s–1 week on a single CPU (depending greatly on system size and RAM)

2. Introduction

Over the last year, the manipulation of complex molecules using inhomogeneous electric fields has been rejuvenated. It has been demonstrated, that it is possible to deflect, focus, and decelerate even large asymmetric top molecules [1, 2]. Moreover, it is possible to spatially separate neutral molecules according to their quantum state, their structural form, and their size using these techniques [3, 4]. Therefore, world-wide many groups in molecular physics and physical chemistry are now setting up and starting experiments on the structural-isomer and cluster-size separation using inhomogeneous electric fields for advanced studies of well-defined samples of complex molecules.

3. Description

3.1. Overview

In quantum mechanics, the energy E of a molecule is calculated from the Schrödinger equation

$$\mathcal{H}\Psi = E\Psi, \quad (1)$$

where \mathcal{H} denotes the Hamiltonian in the center-of-mass frame and Ψ is the internal wave function. Couplings between the motion of the nuclei and the motion of the electrons and nuclear spin wave functions will be neglected at any time leaving the internal wavefunction as the product of electronic, vibrational and rotational wave functions, which are denoted as Ψ_{el} , Ψ_{vib} , Ψ_{rot} , respectively:

$$\Psi = \Psi_{el}\Psi_{vib}\Psi_{rot}. \quad (2)$$

Thus, the total energy is given by the sum of electronic (E_{el}), vibrational (E_{vib}) and rotational energies (E_{rot}):

$$E = E_{el} + E_{vib} + E_{rot}. \quad (3)$$

Since this code is meant to study energy levels of very cold molecules (on the order of 1 K) and all of them are in the electronic and vibrational ground level, we shall analyze the rotational term of the Hamiltonian \mathcal{H}_{rot} .

Within the classic approximation, any molecule can be characterized by three principal moments of inertia I_a , I_b and I_c . By convention, the principal axes a , b and c are labelled such as $I_a \leq I_b \leq I_c$. In this program we use the rotational constants instead of the moments of inertia. The rotational constants, expressed in units of MHz, are defined as

$$A = \frac{h}{8\pi^2 I_a}, \quad B = \frac{h}{8\pi^2 I_b}, \quad C = \frac{h}{8\pi^2 I_c}, \quad (4)$$

where h is Planck's constant. Throughout the code, $|J, K, M\rangle$ wavefunctions will be used for a proper description of the energy levels, where J is the total angular momentum quantum number, K characterizes the projection of the total angular momentum onto its figure axis and M is the quantum number characterizing the projection of the total angular momentum of the molecule onto a space fixed Z-axis. The quantum number of the angular momentum can take only the integral values

$$J = 0, 1, 2, 3, \dots \quad (5)$$

while K and M , which measure in units of \hbar the components of the angular momentum along its figure axis and a space-fixed Z -axis, respectively, can take the values

$$K = J, J-1, \dots, 0, \dots, -J+1, -J, \quad (6)$$

$$M = J, J-1, \dots, 0, \dots, -J+1, -J. \quad (7)$$

Nevertheless, henceforth we will only implement the $M = 0$ case.

3.2. Linear top

In a linear, polyatomic molecule the angular momentum about the principal axis a is zero whereas the two other moments of inertia along axes b and c are equal: $I_b = I_c = I$. Therefore the energy eigenvalues are

$$E_J^0 = \langle J | \mathcal{H}_0 | J \rangle = \langle J | \frac{P^2}{2I} | J \rangle = \frac{\hbar^2 J(J+1)}{8\pi^2 I}. \quad (8)$$

With the substitution of the spectral constant $B \equiv \hbar^2/8\pi^2 I$, this becomes:

$$E_J^0 = hBJ(J+1). \quad (9)$$

However, this first order term on the energy corresponds to the rigid rotor model of the molecule. The Hamiltonian for the nonrigid rotor can be written as

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_d, \quad (10)$$

where \mathcal{H} represents the centrifugal distortion energy. For the linear molecule there is only one axis of distortion and \mathcal{H}_d takes the form

$$\mathcal{H}_d = -\left(\frac{h}{\hbar^4}\right)DP^4, \quad (11)$$

where D is a constant. The first-order perturbation energy is the average of \mathcal{H}_d over the eigenfunction Ψ_J^0 of the unperturbed Hamiltonian \mathcal{H}_0 , or

$$E^{(1)} = \langle J | \mathcal{H}_d | J \rangle = -\left(\frac{h}{\hbar^4}\right)DP^4 = -hDJ^2(J+1)^2. \quad (12)$$

If we now apply an electric field \mathcal{E} to the molecule a new Hamiltonian term \mathcal{H}_{Stark} will appear. The Stark effect Hamiltonian operator can then be expressed as

$$\mathcal{H}_{Stark} = -\mathcal{E} \sum_{g=x,y,z} \mu_g \phi_{Z_g}, \quad (13)$$

where ϕ_{Z_g} are the direction cosines of the x , y , z axes with reference to the space-fixed Z -axis. Linear (and also symmetric-top) molecules have a dipole

moment component only along the symmetry axis z . For them, $\mu_z = \mu$, $\mu_x = \mu_y = 0$; the Hamiltonian then becomes simply

$$\mathcal{H}_{Stark} = -\mu \mathcal{E} \phi_{Z_z}. \quad (14)$$

Hence, now we present the Hamiltonian matrix elements corresponding to \mathcal{H}_{Stark}

$$\langle J, K, M | \mu | J, K, M \rangle = -\frac{MK}{J(J+1)} \mu \mathcal{E}, \quad (15)$$

$$\begin{aligned} \langle J+1, K, M | \mu | J, K, M \rangle &= \langle J, K, M | \mu | J+1, K, M \rangle \\ &= -\frac{\sqrt{(J+1)^2} \sqrt{(J+1)^2 - M^2}}{(J+1) \sqrt{(2J+1)(2J+3)}} \mu \mathcal{E}. \end{aligned} \quad (16)$$

3.3. Symmetric top

A molecule in which two of the principal moments of inertia are equal is a symmetric-top rotor. In a symmetric-top molecule, one of the principal axes of inertia must lie along the molecular axis of symmetry. The principal moments of inertia which have their axes perpendicular to this axis are equal. If a , the axis of least moment of inertia ($I_a < I_b = I_c$), lies along the symmetry axis, the molecule is a prolate symmetric top. If c , the axis of the greatest moment of inertia ($I_a = I_b < I_c$), lies along the symmetry axis is an oblate symmetric top. With the a axis chosen along the symmetry axis ($I_c = I_b$) and with $P^2 = P_a^2 + P_b^2 + P_c^2$, the Hamiltonian operator may be expressed as

$$\mathcal{H}_0 = \frac{P^2}{2I_b} + \frac{1}{2} \left(\frac{1}{I_a} - \frac{1}{I_b} \right) P_a^2 \quad (17)$$

Thus, we have the eigenvalues, for instance, for the rigid prolate symmetric top

$$\begin{aligned} E_0 &= \langle J, K | \mathcal{H}_0 | J, K \rangle = \frac{1}{2I_b} \langle J, K | P^2 | J, K \rangle + \frac{1}{2} \left(\frac{1}{I_a} - \frac{1}{I_b} \right) \langle J, K | P_a^2 | J, K \rangle \\ &= \left(\frac{h^2}{8\pi^2 I_b} \right) J(J+1) + \left(\frac{h^2}{8\pi^2} \right) \left(\frac{1}{I_a} - \frac{1}{I_b} \right) K^2. \end{aligned} \quad (18)$$

With the substitution of the spectral constants, E_0 can be written

$$E_0 = h[BJ(J+1) + (A-B)K^2]. \quad (19)$$

For the oblate symmetric top, the expression of the parenthesis of the second term becomes $(C-B)$.

As in the case of the linear-top molecule, now we introduce the Hamiltonian for the nonrigid rotor \mathcal{H}_d for the symmetric-top case. The centrifugal distortion Hamiltonian has the form

$$\mathcal{H}_d = \frac{h^4}{4} \sum_{\alpha\beta\gamma\delta} \tau_{\alpha\beta\gamma\delta} P_\alpha P_\beta P_\gamma P_\delta \quad (20)$$

where $\alpha, \beta, \gamma, \delta$ represent the principal coordinate axes of the moments of inertia for the molecule (each must be summed over all three coordinate axes) and where $\tau_{\alpha\beta\gamma\delta}$ are the distortion constants. To first order, the distortion energy is

$$\begin{aligned} E_d &= \langle J, K, M | \mathcal{H}_d | J, K, M \rangle \\ &= h[D_J J^2(J+1)^2 + D_{JK} J(J+1)K^2 + D_K K^4], \end{aligned} \quad (21)$$

in which the D_J, D_{JK} and D_K are the usual first-order centrifugal stretching constants of the symmetric-top molecule. The D 's represent a combination of the τ 's. Moreover, if we now apply an electric field, just as in the case of the linear top, we will have another Hamiltonian term \mathcal{H}_{Stark} . Thus, we have the Hamiltonian matrix elements corresponding to \mathcal{H}_{Stark}

$$\langle J, K, M | \mu | J, K, M \rangle = -\frac{MK}{J(J+1)} \mu \mathcal{E}, \quad (22)$$

$$\begin{aligned} \langle J+1, K, M | \mu | J, K, M \rangle &= \langle J, K, M | \mu | J+1, K, M \rangle \\ &= -\frac{\sqrt{(J+1)^2 - K^2} \sqrt{(J+1)^2 - M^2}}{(J+1)\sqrt{(2J+1)(2J+3)}} \mu \mathcal{E}. \end{aligned} \quad (23)$$

3.4. Asymmetric top

The last, most general case we are describing in this paper is the asymmetric-top molecule. When a molecule has none of its three principal moments of inertia equal to zero and when no two are equivalent, is considered as an asymmetric top. Due to the considerably complexity of this case the rotational frequencies can no longer be expressed in convenient equations, as can be done for linear or symmetric-top molecules. But before we get further, one must first become familiar with the notation used to designate the levels. Pseudo-quantum numbers, customarily labeled by subscripts on J , are employed in the designation of the energy levels in a way that will be explain later on. First of all, we shall introduce the parameter κ that is a measure of the asymmetry of the molecule. In the conventional order, $I_a < I_b < I_c$.

Thus, when $I_b \rightarrow I_c$, the prolate symmetric top is approached; and when $I_b \rightarrow I_a$, the oblate symmetric top is approached. Then we define κ as

$$\kappa = \frac{2B - A - C}{A - C}, \quad (24)$$

with A, B, C the rotational constants with respect to the a, b, c axes. The limiting values for κ , -1 and +1, correspond to the prolate and oblate symmetric tops, respectively. The most asymmetric top has $\kappa = 0$. An asymmetric rotor has $(2J + 1)$ distinct rotational sublevels for each value of J , whereas the symmetric rotor has only $(J + 1)$. With an increase in asymmetry, the "K splitting" increases until there is no longer any close correspondence between the two levels and the degenerate K levels of the symmetric top. Nevertheless, by connecting the K levels for a given J of the limiting prolate symmetric top with those of the limiting oblate symmetric top in the ordered sequence one may obtain a qualitative indication of the levels of the asymmetric rotor. Hence, from now on we will be using the following notation $J_{K_a K_c}$ in order to label the energy levels. The first subscript, K_a represents the K value of the limiting prolate top while the second one, K_c , represents the K value of the limiting oblate top. Note that the highest sublevels of the prolate symmetric top have the highest K values, whereas the highest sublevels for the oblate symmetric top have the lowest K values. Analogously to the linear and symmetric top cases, we shall now present the eigenvalues of the Hamiltonian corresponding with the rigid rotor approximation.

$$\langle J, K, M | \mathcal{H}_0 | J, K, M \rangle = \frac{(B + C)}{2} (J(J + 1) - K^2) + AK^2, \quad (25)$$

$$\begin{aligned} \langle J, K + 2, M | \mathcal{H}_0 | J, K, M \rangle &= \langle J, K, M | \mathcal{H}_0 | J, K + 2, M \rangle \\ &= \frac{(B - C)}{4} \sqrt{J(J + 1) - K(K + 1)} \sqrt{J(J + 1) - (K + 1)(K + 2)}. \end{aligned} \quad (26)$$

And now, the distortable rotor terms according to Watson's A reduction

$$\langle J, K, M | \mathcal{H}_d | J, K, M \rangle = \Delta_J (J(J + 1))^2 - \Delta_{JK} J(J + 1) K^2 - \Delta_K K^4, \quad (27)$$

$$\begin{aligned} \langle J, K + 2, M | \mathcal{H}_d | J, K, M \rangle &= \langle J, K, M | \mathcal{H}_d | J, K + 2, M \rangle \\ &= (-\delta_J J(J + 1) - \frac{\delta_K}{2} ((K + 2)^2 + K^2)) \\ &\times \sqrt{(J(J + 1) - K(K + 1))(J(J + 1) - (K + 1)(K + 2))}, \end{aligned} \quad (28)$$

where $\Delta_J, \Delta_{JK}, \Delta_K, \delta_J$ and δ_K are the quartic distortion coefficients. If we apply an electric field \mathcal{E} to the molecule a Hamiltonian term \mathcal{H}_{Stark} will appear. The Stark effect Hamiltonian operator can then be expressed as

$$\mathcal{H}_{Stark} = -\mathcal{E}\boldsymbol{\mu}, \quad (29)$$

where μ can be projected on the three principal axes of the molecule in order to split the Hamiltonian term \mathcal{H}_{Stark} in three different parts corresponding to the components of $\boldsymbol{\mu} : \mu_a, \mu_b$ and μ_c . Then, according to the component along the principal axis a of the molecule we have

$$\langle J, K, M | \mu_a | J, K, M \rangle = -\frac{\mu_a \mathcal{E} M K}{J(J+1)}, \quad (30)$$

$$\begin{aligned} \langle J+1, K, M | \mu_a | J, K, M \rangle &= \langle J, K, M | \mu_a | J+1, K, M \rangle \\ &- \mu_a \mathcal{E} \frac{\sqrt{(J+1)^2 - K^2} \sqrt{(J+1)^2 - M^2}}{(J+1) \sqrt{(2J+1)(2J+3)}}. \end{aligned} \quad (31)$$

Now for the b axis

$$\begin{aligned} \langle J, K+1, M | \mu_b | J, K, M \rangle &= \langle J, K, M | \mu_b | J, K+1, M \rangle \\ &= -M \mu_b \mathcal{E} \frac{\sqrt{(J-K)(J+K+1)}}{2J(J+1)}, \end{aligned} \quad (32)$$

$$\begin{aligned} \langle J+1, K+1, M | \mu_b | J, K, M \rangle &= \langle J, K, M | \mu_b | J+1, K+1, M \rangle \\ &= \mu_b \mathcal{E} \frac{\sqrt{(J+K+1)(J+K+2)} \sqrt{((J+1)^2 - M^2)}}{2(J+1) \sqrt{(2J+1)(2J+3)}}, \end{aligned} \quad (33)$$

$$\begin{aligned} \langle J+1, K-1, M | \mu_b | J, K, M \rangle &= \langle J, K, M | \mu_b | J+1, K-1, M \rangle \\ &= -\mu_b \mathcal{E} \frac{\sqrt{(J-K+1)(J-K+2)} \sqrt{((J+1)^2 - M^2)}}{2(J+1) \sqrt{(2J+1)(2J+3)}}. \end{aligned} \quad (34)$$

And finally, the \mathcal{H}_{Stark} matrix elements involving μ_c

$$\begin{aligned} \langle J, K+1, M | \mu_c | J, K, M \rangle &= \langle J, K, M | \mu_c | J, K+1, M \rangle \\ &= iM \mu_c \mathcal{E} \frac{\sqrt{(J-K)(J+K+1)}}{2J(J+1)}, \end{aligned} \quad (35)$$

$$\begin{aligned}
\langle J+1, K+1, M | \mu_c | J, K, M \rangle &= \langle J, K, M | \mu_c | J+1, K+1, M \rangle \\
&= -i\mu_c \mathcal{E} \frac{\sqrt{(J+K+1)(J+K+2)}\sqrt{((J+1)^2 - M^2)}}{2(J+1)\sqrt{(2J+1)(2J+3)}}, \tag{36}
\end{aligned}$$

$$\begin{aligned}
\langle J+1, K-1, M | \mu_c | J, K, M \rangle &= \langle J, K, M | \mu_c | J+1, K-1, M \rangle \\
&= -i\mu_c \mathcal{E} \frac{\sqrt{(J-K+1)(J-K+2)}\sqrt{((J+1)^2 - M^2)}}{2(J+1)\sqrt{(2J+1)(2J+3)}}. \tag{37}
\end{aligned}$$

Although the energy levels can be found by diagonalizing the Hamiltonian matrix, a further simplification can be obtained by consideration of the symmetry properties of the Hamiltonian. The symmetry properties may be deduced from its ellipsoid of inertia, which is symmetric not only to an identity operation E but also to a rotation of 180° , C_2 , about any of its principal axes of inertia. This set of symmetry operations form a group known as the Four-group designated by $V(a, b, c)$. These symmetry operations cause the angular momentum to transform in the following manner:

$$E : P_a \rightarrow P_a, P_b \rightarrow P_b, P_c \rightarrow P_c, \tag{38}$$

$$C_2^a : P_a \rightarrow P_a, P_b \rightarrow -P_b, P_c \rightarrow -P_c, \tag{39}$$

$$C_2^b : P_a \rightarrow -P_a, P_b \rightarrow P_b, P_c \rightarrow -P_c, \tag{40}$$

$$C_2^c : P_a \rightarrow -P_a, P_b \rightarrow -P_b, P_c \rightarrow P_c. \tag{41}$$

The symmetry group of the Hamiltonian is extremely important in quantum mechanics because a knowledge of it allows the classification of quantum states and simplification thereby of the energy matrix. Each asymmetric rotor wave function may be classified according to its behaviour under $V(a, b, c)$. A wave function that is, for instance, symmetric for a twofold rotation about axis a and antisymmetric for a two fold rotation about the other two axes may be classified as belonging to species B_a of the group. A function that is invariant with respect to all symmetry operations of the group obviously belongs to species A . Each wave function could then be classified according to one of the symmetry species A, B_a, B_b and B_c of V , and hence the matrix elements of the Hamiltonian $\langle \Psi_i | \mathcal{H} | \Psi_j \rangle$ would be nonzero only between states of the same symmetry. As a consequence, the secular determinant for any value of J will factor into four independent subdeterminants, one for considerably simplifies the diagonalization problem and has the further advantage that pairs of degenerate or nearly degenerate K levels are separated into different submatrices.

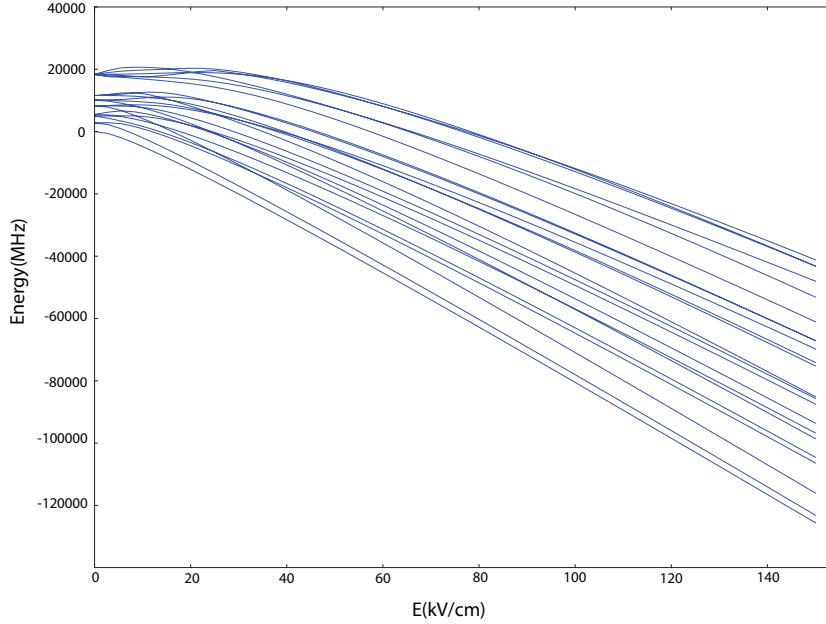


Figure 1: Energy curves for indole molecule from $J=0$ up to $J=2$

3.5. Results

We have successfully calculated Stark curves for several different molecules, such as indole, water, 2,6-difluoro-iodobenzene, 4-aminobenzonitrile, benzonitrile, iodobenzene, etc. One of the calculations for indole molecules is shown in Figure 1 where the energy of the molecule is presented as a function of the applied electric field \mathcal{E} . Here we can clearly see that the lowest energy levels of this molecule are high-field-seeking.

We have also calculated the energy curves for OCS using three different algorithms. These enable us to calculate the Stark curves of a molecule by considering it as an asymmetric-top, symmetric-top or as a linear molecule, whenever is possible. In the case of OCS, we have calculated the energy levels up to $J = 32$ through three different algorithms with the following computation times:

- Asymmetric-top code: 12min 21.28s
- Symmetric-top code: 5min 11.7s (2.4 times faster)
- Linear code: 9.46s (78.36 times faster)

Furthermore, the maximum difference founded in the energy values using the three different algorithms is approximately 0.02%. In Figure 2 we can

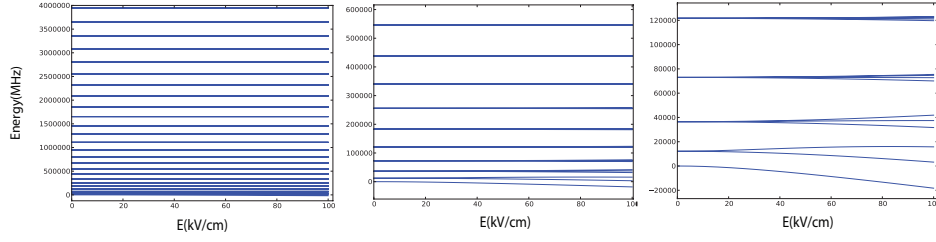


Figure 2: Energy curves for OCS molecule from $J = 0$ up to $J = 26$, $J = 10$ and $J = 5$

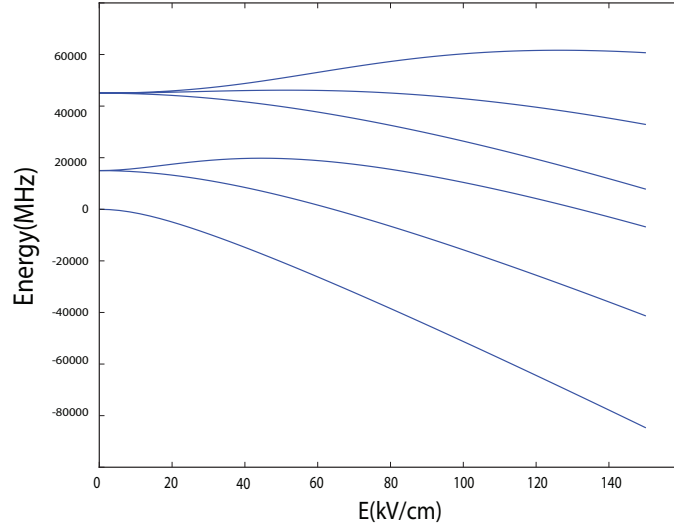


Figure 3: Energy curves for iodomethane molecule from $J = 0$ up to $J = 2$

see a three-figure representation of the energy levels for an OCS molecule after a calculation for levels from $J = 0$ up to $J = 26$, $J = 10$ and $J = 5$, respectively.

We have also simulated the Stark curves for iodomethane, which is a symmetric-top molecule, with both the symmetric and asymmetric-top algorithms. The results for the calculated times for the energy levels from $J = 0$ up to $J = 27$ were:

- Asymmetric-top code: *6min 25.86s*
- Symmetric-top code: *2min 9.29s* (3 times faster)

A representation of the three first Stark curves for iodomethane is shown in Figure 3.

4. Installation instructions

Installation is as simple as running the generic Python install command `python setup.py install`. This requires write access to the packages directory tree of the Python distribution. Alternatively, on Unix-like systems the provided shell-script `user-install.sh` can be used to install the program into `somewhere` in the user `$HOME` directory. This method requires the user to define the shell variable `PYTHONHOME` to include this directory in the package search path.

5. Alternative software

Several programs exist for the simulation of rotationally resolved spectra of asymmetric top molecules in dc electric fields [5, 6, 7]. Inherently these programs work by calculating the energies of all states possibly involved in the relevant transitions, i.e., they do perform similar calculations to jkstark. Only PGopher provides direct access to the Stark curves of individual or a few states, but its graphical/text based access is not well suited for the storage of many precisely calculated Stark curves for further use in trajectory simulation codes. For example, even for relatively small molecules like benzonitrile or indole thousands of Stark curves need to be calculated and stored, with hundreds of energies per curve for specific dc field strengths.

6. Outlook

The current program has been successfully used in the calculation of Stark energy maps of various asymmetric top molecules, including, for example, benzonitrile, 3-aminophenol, indole, and indole-water clusters. However, for molecules containing large nuclear quadrupole constants the corresponding quadrupole coupling terms need to be implemented. This real challenge here is to still automatically symmetrize the Hamiltonian and the resulting states. Moreover, especially many of the small molecules employed in electric-field manipulation experiments are open-shell, i.e., they possess electric angular momentum. The respective Hamiltonians should also be implemented in JK-STARK. We will implement extensions as they are relevant for the simulation of our manipulation experiments, but we are happy to support third parties to extend our code to their needs, under the provision that is is provided to all users after a reasonable amount of time.

Acknowledgments

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