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Computers in Chemistry

Computer Algebra Systems in Physical Chemistry

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It is argued that a computer algebra system should replace the FORTRAN-like languages in the undergraduate and graduate programs in chemistry. To support the argument example applications from physical chemistry are used to display the symbolic, numerical, and graphical capabilities of one such system. The code for the more complex applications is given in an appendix.

Whatever we institute, it must provide in fact the numerical tools we hoped for from FORTRAN but did not acquire.

Introduction

Many colleges and universities have a computer literacy component as part of the degree requirements for their Chemistry Major. The question that must be answered is what constitutes computer literacy. The answer has been ever-changing because of dramatic changes in the computing technology and its availability and, more recently, in the type of computer programs

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available. Certainly, word processing and graphics tools are required. Presently, both of these skills are possessed by more than ninety percent of the third-year students in my physical chemistry course. Requirements can and should build on the background of the student population. Until a few years ago most physical chemists thought that computer literacy meant some form of computational programming: BASIC, FORTRAN, and, more recently, Pascal and C. It is the thesis of this paper that the advent of the computer algebra system (CAS) requires that this view be changed.

There is and will continue to be a need for programmers versed in the "old tongues" to maintain and extend the current holdings in computational chemistry. The number of programmers required for this maintenence role is a small minority of the chemistry degree candidates and their needs should not be the focus of any general computer literacy requirement. The time required to learn a useful set of tools in any of these languages is just too great to be useful in the learning of physical chemistry. At the end of a typical introductory programming course a student cannot integrate a simple differential equation let alone the Schrödinger equation.

The spreadsheet program has a large and loyal following of users. Nearly every issue of *The Journal of Chemical Education* has an example of some problem that can be solved using a spreadsheet template. My chief argument against the spreadsheet is that the logic flow is hidden in cells that are invisible to the user unless special actions are taken. If the problem can be solved using a spreadsheet, it can be solved as well using a CAS, but the converse is not true. Learning the details of spreadsheet programming is not significantly easier than learning a CAS. Given the limited time available in students' undergraduate lives we should expend their time on the most useful computer programs.

If we are to replace the FORTRAN-like languages, we need to specify the requirements for the replacement. Whatever we institute, it must provide in fact the numerical tools we hoped for from FORTRAN but did not acquire. This requirement is amazingly easy to satisfy with any modern CAS. Probably the most pressing requirement is in the area of mathematical assistance both for our students and for ourselves; it allows for more sophisticated applications and eliminates trivial errors. When users need to integrate a differential equation, they should be able to give a command to do so. They should not have to worry about the implementation, whether the equations are stiff, or even what stiff means. Someone should worry about such things, but not third-year students. The student should know that it is necessary or important to integrate the equation and that

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it is the result of the integration that is important. The details should be hidden, but they should work.

In addition to substantial numerical and mathematical facilities, the graphics capabilities of the program need to be easy to use and impressive. The CAS must be able to import with ease tables of, for instance, the temperature dependence of the second virial coefficient and to display the result graphically. Everyone knows that tables of numbers are terribly difficult to analyze or interpret physically. It is critical that significant graphical assistance be available.

The CAS should have a reasonably shallow learning curve. The proper sequence for third-year students (or any novices) in a new language is to learn a subset and get started. As students' needs demand, they should expand their skills and then repeat this sequence. An ideal user interface would be one in which students are presented with a problem and using cut and paste operations can proceed forward to a solution, reinforcing their knowledge of the programming language but, more importantly, gaining insight into chemistry. The mathematical notation required in writing code should be as close as possible to what they have already learned in mathematics courses.

There are a number of options available in choosing a CAS. Several of these have been reviewed [1]. Some of the options are to choose an elementary program like Theorist [2], spreadsheet mimicking like MathCad [3], or full-featured like Maple [4], *Mathematica* [5], MACSYMA [6] or the like. It is an illusion to think that simple programs are useful because they can be learned quickly. If you limit a full featured system to just a few applications, the knowledge required is similarly limited and easy to learn. It is extremely important that the capabilities of the CAS be unrestricted. If the CAS will not do a job, all the time spent learning it has been wasted; one must start from scratch and learn a more powerful language.

In the remaining sections of this document examples are given of the level of assistance available from one of the best CASs, *Mathematica*. It is hoped that the examples given are sufficiently impressive that a reader will agree that a CAS should replace the FORTRAN-like languages. Additionally, it is also hoped that the coding is sufficiently transparent that the reader unfamiliar with the program will still be able to see the flow of logic. Most of the code would be transparent to a student in the author's class but the physics of the collinear collision below might take some explaining. Nevertheless, given the code,

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a student would find it easy to modify the interaction potential or initial conditions and learn something from the results.

Symbolic Capabilities

Critical Conditions for a van der Waals Gas

One of the beauties of a CAS is that (with a little practice) it can replace pencil and paper. Anything you can do with a pencil and paper can be duplicated on the computer. Major attractions of the computational approach are that there will be no sign errors, terms overlooked, etc., and that very complicated expressions are as easily handled as simple ones.

Let me solve just one nontrivial problem from physical chemistry to demonstrate that the approach is very similar to what one would do by hand. The problem is to determine the expressions for the critical pressure (P_C), molar volume (V_C), and temperature (T_C) of a van der Waals gas in terms of the van der Waals constants and the gas constant. Because the gas constant always appears multiplying the temperature, I prefer to solve for P_C, V_C, and RT_C.

Recall that at any given temperature below critical, the van der Waals equation for the pressure as a function of the volume has two extrema and a point of inflection between them. These points approach each other as the temperature increases and coincide at the critical point. The extrema satisfy the equation given by setting the slope along an isotherm to zero. The inflection point is identified as the solution to the equation given by setting to zero the second partial derivative of the pressure with respect to the molar volume along an isotherm. At the critical point these two equations are both satisfied. Our problem is to solve these simultaneous equations.

In the text to follow the input to the CAS is given in a monospaced bold font and the program output in the same, but unbolded font.

As one would expect, the first step is to write the van der Waals equation and to set to zero the expressions for the first and second derivatives of the pressure with respect to molar volume along an isotherm.

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```
P = RT/(V - b) - a/V^2
slopeEqn = D[P, V] == 0
curveEqn = D[P, {V, 2}] == 0
```

```
  a        RT
-(--) + ------
   2     -b + V
  V
2 a       RT
--- - --------- == 0
 3             2
V      (-b + V)
-6 a      2 RT
---- + --------- == 0
  4             3
 V      (-b + V)
```

The first line gives the van der Waals equation, the second equates to zero the first derivative of the pressure with respect to the molar volume at constant temperature, and the third line similarly equates to zero the second derivative.

We can mimic the pencil and paper approach by solving the `slopeEqn` for `RT` and substituting the result into the `curveEqn`.

```
Solve[slopeEqn, RT]
```

```
                     2
        2 a (b - V)
{{RT -> -----------}}
                3
               V
```

```
curveEqn /. RT -> 2 a (b - V)^2/V^3
```

```
                     2
-6 a    4 a (b - V)
---- + ----------- == 0
  4      3          3
 V      V  (-b + V)
```

In the last input line `/. RT ->` is to be read as “replace all occurrences of *RT* with” what follows. There is an alternative method of making this replacement built into *Mathematica*, but the explicit statement has the advantage of clarity.

This last equation gives us the critical molar volume, if we can solve it, and we can.

```
Solve[%, V]
```

```
{{V -> 3 b}}
```

The `%` character refers to the last output of the program. Solving this equation gives the critical molar volume as

```
Vc = 3 b ;
```

where we have suppressed the output with a terminating semicolon.

If we substitute this result for `Vc` into the `slopeEqn`, we have an equation satisfied by the critical value of `RTc`. Given this equation, we can solve it for `RTc`. We can combine these two steps as

```
Solve[ (slopeEqn /. V -> Vc), RT ]
```

```
                       2
        2 a (b - Vc)
{{RT -> -------------}}
                3
              Vc
```

We can make the identification

```
RTc = 8 a / (27 b) ;
```

Finally, the critical pressure is given by the van der Waals equation with the molar volume and temperatures replaced by their critical values.

```
Pc = P /.{V -> Vc, RT -> RTc}
```

```
  a
-----
    2
27 b
```

The result is exactly as expected and follows from a quite intuitive symbolism.

Operator Algebra

There is a very elegant notation available in *Mathematica* to mimic the operator formalism of quantum mechanics. Consider the harmonic oscillator as an example; in the right set of units the Schrödinger equation is

$$-\frac{d^2\psi(x)}{dx^2} + x^2\psi(x) = (2n+1)\psi(x)$$

This equation can be expressed as a Hamiltonian operator operating upon the wave function to produce the wave function multiplied by some scalar number corresponding to the energy.

$$\hat{H}\psi = E\psi$$

In *Mathematica* the Hamiltonian could be coded as

```
h @ y_  := -D[y, {x, 2}] + x^2 y
```

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The $y\_$ represents a generic argument to our operator h and the second derivative operator is obvious enough on the right-hand side. We can demonstrate that $(x - 4x^3/6)\ \mathrm{Exp}[-x^2/2]$ is an eigenfunction of the Hamiltonian and determine the corresponding eigenvalue with the code

```
f[x_] := (x - 4 x^3/6 )Exp[-x^2/2]
(h @ f[x])/f[x] // Together
```

```
7
```

The first line of code merely defines our proposed eigenfunction. The second implements the idea of dividing by the eigenfunction the result of operating upon it with the Hamiltonian. The effect of `Together` is to cancel duplications in the numerator and denominator; it does with the computer what a student would do with pencil and paper.

I submit that this imitation of quantum mechanical notation is so close as to be almost intuitive. The learning curve for this part of the CAS should be shallow.

There is another problem from quantum mechanics that clearly demonstrates the utility of a CAS. This problem is not appropriate for third-year physical chemistry students but is a classic problem from a first course in quantum mechanics. It is, what we call euphemistically, character building. The problem is to demonstrate that all components of the angular momentum operator commute with the operator for the square of the angular momentum. The present solution will be limited to the y-component as sufficient to carry the point. The program identifies the square root of -1 as **I** and we will symbolize Planck's constant divided by 2π as h.

First we must define the operators for the various components of the angular momentum in Cartesian coordinates. It is then necessary to explicitly define what we mean by the square of an operator and what a commutator is.

```
ClearAll[f, h, x, y, z, lx, ly, lz, commutator]
lx      =   - I h (y D[#, z] - z D[#, y])&;
ly      =   - I h (z D[#, x] - x D[#, z])&;
lz      =   - I h (x D[#, y] - y D[#, x])&;
sqr[o _ ] =    o @ o @ # &;
```

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```
commutator[o1_, o2_] =
            (o1 @ o2 @ # - o2 @ o1 @ #)&;
```

The use of ClearAll guarantees the symbols used are not confused with those in any previous work. The combination of `#` and `&` is just an alternative way of identifying the argument of a function without using the square bracket notation. It turns out to be very useful in programming.

The commutator of the square of the angular momentum and the *y*-component is then given as

```
commutator[sqr[lx], ly] @ f[x, y, z] +
commutator[sqr[ly], ly] @ f[x, y, z] +
commutator[sqr[lz], ly] @ f[x, y, z]
```

```
                       (0,0,3)
I h (I h x (-I h y (y f       [x, y, z] -

              (0,1,1)               (0,1,2)
           2 f       [x, y, z] - z f       [x, y, z]) +

              (0,0,1)               (0,1,1)
        I h (f       [x, y, z] + y f       [x, y, z] -

              (0,2,0)
           z f       [x, y, z]) +

                (0,0,2)               (0,1,2)
        I h z (f       [x, y, z] + y f       [x, y, z] -

            (0,2,0)               (0,2,1)
           f       [x, y, z] - z f       [x, y, z])) -
```

```
                     (1,0,2)
   I h z (-I h y (y f       [x, y, z] -

          (1,1,0)               (1,1,1)
         f       [x, y, z] - z f       [x, y, z]) +

              (1,0,1)               (1,1,1)
      I h z (f       [x, y, z] + y f       [x, y, z] -

            (1,2,0)
         z f       [x, y, z]))) -

                          (0,0,3)
I h (-I h y (-I h y (-(x f       [x, y, z]) +

            (1,0,1)               (1,0,2)
         2 f       [x, y, z] + z f       [x, y, z]) +

                (0,1,1)                (1,1,0)
      I h (-(x f       [x, y, z]) + z f       [x, y, z]) +

                  (0,1,2)              (1,1,0)
      I h z (-(x f       [x, y, z]) + f       [x, y, z] +

            (1,1,1)
         z f       [x, y, z])) +

                     (0,0,2)
   I h z (-I h (-(x f       [x, y, z]) +

          (1,0,0)               (1,0,1)
         f       [x, y, z] + z f       [x, y, z]) -
```

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```
                    (0,1,2)              (1,1,0)
        I h y (-(x f       [x, y, z]) + f       [x, y, z] +

              (1,1,1)
           z f       [x, y, z]) +

                    (0,2,1)                (1,2,0)
        I h z (-(x f       [x, y, z]) + z f       [x, y, z]))

     ) + I h (I h x (-I h x

             (0,2,1)             (1,0,1)
         (x f       [x, y, z] - f       [x, y, z] -

              (1,1,1)
           y f       [x, y, z]) +

                (0,1,1)               (1,1,1)
        I h y (f       [x, y, z] + x f       [x, y, z] -

              (2,0,1)
           y f       [x, y, z])) -

                     (0,2,0)             (1,0,0)
     I h z (-I h (x f       [x, y, z] - f       [x, y, z] -

              (1,1,0)
           y f       [x, y, z]) -

                (0,2,0)               (1,2,0)
        I h x (f       [x, y, z] + x f       [x, y, z] -

            (2,0,0)               (2,1,0)
           f       [x, y, z] - y f       [x, y, z]) +
```

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```
                (1,1,0)               (2,1,0)
      I h y (2 f       [x, y, z] + x f       [x, y, z] -

            (3,0,0)
         y f       [x, y, z]))) -

                          (0,2,1)
I h (-I h x (-I h x (-(x f       [x, y, z]) +

            (1,2,0)
         z f       [x, y, z]) +

             (0,0,1)               (1,0,1)
      I h (-f       [x, y, z] - x f       [x, y, z] +

            (2,0,0)
         z f       [x, y, z]) +

               (0,1,1)               (1,1,1)
      I h y (-f       [x, y, z] - x f       [x, y, z] +

            (2,1,0)
         z f       [x, y, z])) +

                     (0,1,1)
   I h y (-I h (-(x f       [x, y, z]) +

            (1,1,0)
         z f       [x, y, z]) -

               (0,1,1)               (1,1,1)
      I h x (-f       [x, y, z] - x f       [x, y, z] +

            (2,1,0)
         z f       [x, y, z]) +
```

```
                   (1,0,1)                (2,0,1)
        I h y (-2 f        [x, y, z] - x f        [x, y, z] +

              (3,0,0)
           z f       [x, y, z])))
```

The notation for the various orders of partial derivatives is fairly obvious. Do you remember this result? It is included here in all its detail only because this new medium has no penalty for space and it helps to make the point. You did this calculation by hand and so did I, but the next generations of students need not. They can suppress this result by terminating the line with a semicolon and then expand all products in the expression.

```
Expand[%]
```

```
0
```

Students must know what a partial derivative is and how to use operators, but no learning takes place in solving this problem by hand. In seconds, however, with a computer the student learns a very important point: the operator for the y-component of the angular momentum commutes with the square of the angular momentum operator.

Numerical Capabilities

Energy Eigenvalue of the Morse Oscillator

A beautiful application of a CAS is to demonstrate the origin of quantization in quantum mechanics as an immediate consequence of localizing the wavefunction near the well of a potential. If we take the Morse potential as an example and change units so the Schrödinger equation reads as

$$-\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi$$

with V given as

$$V(y) = D_e\,(1 - \exp[-\alpha(y - y_e)])^2$$

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a student can use a CAS to integrate the Schrödinger equation. A guess for the energy is made and the integration is started at $y = 0$ where the wavefunction is taken as zero and its slope unity, and the integration is carried to some large distance. The student finds quickly that only for very restricted values of the energy do solutions remain finite at large y values.

The code segment below implements these ideas and the animation which follows shows an approximately converged estimate for the energy eigenvalue. The remaining images in the animation give images a student might find with improved guesses for the energy.

```
ClearAll[alpha, depth, y, ye, n, energy, u, eqns, soln]
Needs["Graphics‘Legend‘"];
alpha  = 1.0   (* Just for convenience *)
ye     = 1.0;  (* Potential Minimum    *)
ymax   = 10;   (* Infinity             *)
depth  = 10.0; (* Well Depth           *)
energy = 2.9451454; (* The Guess       *)
u[y_] := depth (1 - Exp[-alpha (y - ye)])^2
eqns = {psi’’[y] - u[y] psi[y] == -energy psi[y],
        psi’[0] == 1,
        psi[0] == 0};
soln = NDSolve[eqns, psi, {y, 0, ymax},
         MaxSteps -> 1000];
Plot[{Evaluate[(psi[y]/.soln[[1]])] + energy,
      energy, u[y]}, {y, 0, ymax},
      PlotStyle -> {RGBColor[0, 0, 1],
                    RGBColor[1.000, 0.109, 0.147],
                    AbsoluteThickness[1]},
      PlotRange -> {0, depth},
      PlotLabel -> "Energy = "<>ToString[energy],
      PlotLegend ->{FontForm["y", {"Symbol", 12}],
                     "Energy",
                     "V(y)"},
      LegendPosition -> {0.5, -0.4}];
```

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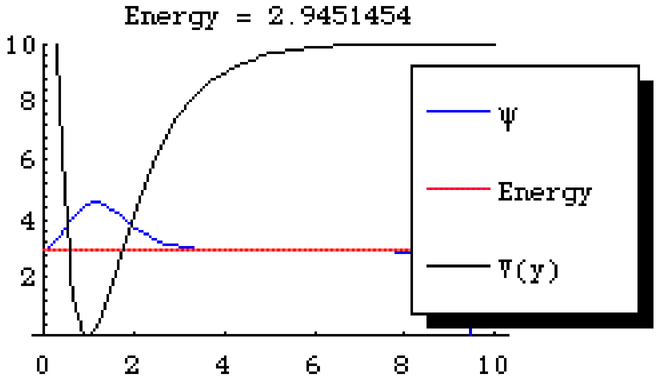

ANIMATION 1. THE APPROXIMATELY CONVERGED GROUND STATE WAVE FUNCTION FOR A MORSE OSCILLATOR SUPERIMPOSED UPON THE POTENTIAL AND OFFSET BY THE ENERGY. THE REMAINING IMAGES IN THE QUICKTIME ANIMATION DISPLAY RESULTS A USER MIGHT FIND WHILE SEARCHING FOR THE EIGENVALUE.

Most of the code above is fairly transparent and even the details are easily explained. The point that quantization results from the localization of the wavefunction by a potential well is important. I know of no easier demonstration of this point than this example. Although the point is made by the particle in a box problem, there is something artificial about that potential that seems to obscure the main point. There is nothing special about the Morse potential and a student could as well choose another form. The one requirement is that the potential be sufficiently replusive as y approaches zero to make the approximation $\psi(0) = 0$ reasonable.

Spreadsheet Impression

I offer one example of a spreadsheet-like window, but written in *Mathematica*. The example mimics a recent article [7] in *The Journal of Chemical Education*. The user adjusts the rate constants and initial concentration of A and then the “spreadsheet” does its work. It is necessary to select the cell and press the Enter key but that is a distinction with only a keystroke of difference.

Reversible First Order Reactions
k_1▮>
A <▮▮▮▮▮> B
<▮k_2
Keq = k_1/k_2

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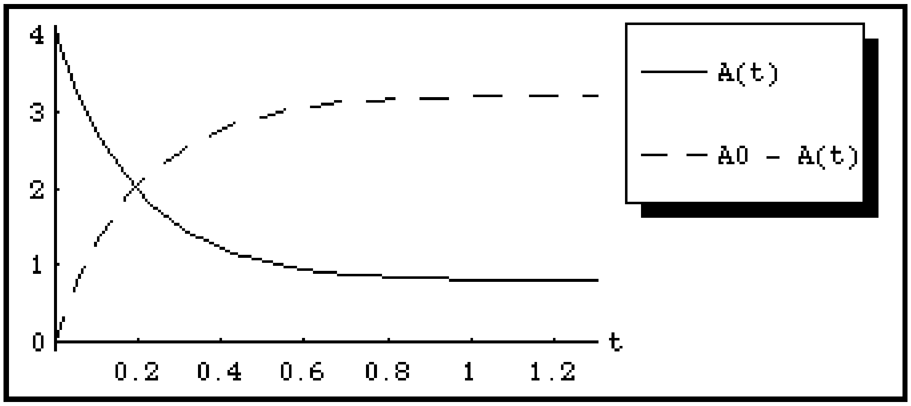
```
Needs["Graphics'Legend'"]
k1 = 4;   k2 = 1;   eqConstant := k1/k2 (* Keq *) ;



   a0 = 4;   (*  b0 = 0  *)   aEq := k2 a0/(k1 + k2);



a[t_] := aEq  +  (a0 - aEq) Exp[-(k1 + k2) t]
             tRange = {t, 0, 1.3};

Print[Subscripted[K[eq]]," =  ",eqConstant,"       ",
      Subscripted[A[Eq]]," =  ",aEq]
Plot[{a[t], a0 - a[t]}, {t, 0, 1.3},
      AxesLabel -> {"t",""},
      PlotRange -> {{0, 1.3}, All},
      PlotStyle -> {GrayLevel[0],
                    Dashing[{0.05, 0.05}]},
      PlotLegend -> {"A(t)", "A0 - A(t)"},
      LegendPosition -> {1, 0}
     ];
```

```
                          4
K   =  4        A   =   -
 eq              Eq     5
```



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Graphical Capabilities

The graphical tools available in a modern CAS are truely impressive and probably well-known to the reader. Most issues of *The Journal of Chemical Education* [8] contain two- and three-dimensional renderings taken directly from some CAS. Instead of reviewing what is available in a static publication, I would like to take advantage of this new medium and show how animation can cast light upon two areas of physical chemistry. At the same time readers will be able to judge whether the programming requirements necessary to solve the problems exceed their significance. The program coding required is probably just beyond the skill level of our third-year students. However, they would have no trouble following the logic of the programs. The programs themselves appear in the appendix that accompanies this paper.

PseudoRotations in the Bending Modes of CO_2

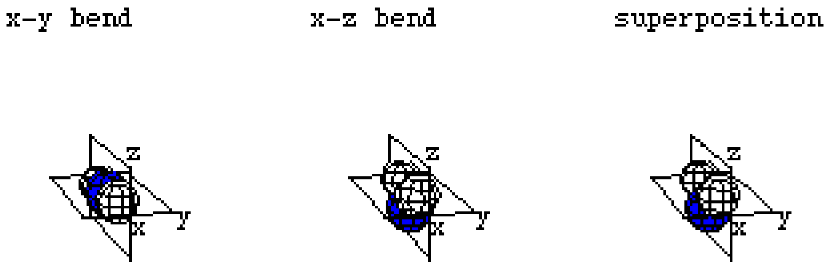
In the third-year course in physical chemistry I limit discussion of the coupling of rotation and vibration to linear diatomic molecules. The infrared absorption spectrum splits nicely into a p and an r branch. The absence of the q branch is explained on the basis of conservation of angular momentum and knowledge that the photon is a spin 1 particle. Many texts include the spectra of polyatomic as well as diatomic linear molecules. In all bending modes of the polyatomic molecules the q branch is clearly visible. That a linear combination of two degenerate orthogonal bending modes out of phase by $\pi/2$ can lead to a pseudorotation is nicely demonstrated with the animation included here.

Colinear Collision of an H *atom and a* Cl_2 *Molecule*

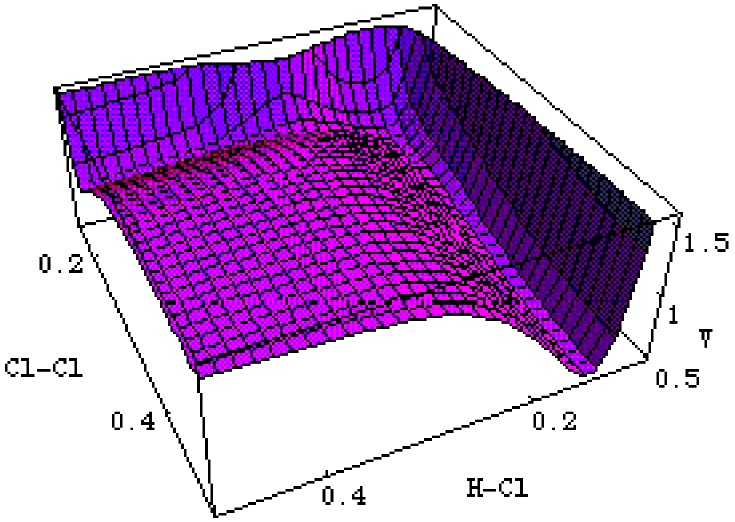
When we introduce theories of kinetics in physical chemistry, we always talk about collisions and possibly sketch a few trajectories superimposed upon a potential diagram, but that is about it. The likely or even possible collision trajectories for even simple potentials are unfamiliar to us and necessarily to our students. The reason for this void is the difficulty in generating the coordinates of a trajectory and the lack of an easy means of displaying the results.

This program segment is a first attempt at filling this void, although it exceeds the coding capabilities of most third-year students. Nevertheless, the code could be run and modified easily by a student to good advantage.

The collision geometry is that of a hydrogen atom entering from the left toward a colinearly oscillating chlorine molecule entering from the right. The separation distance between



ANIMATION 2. THE LEFT-HAND IMAGE IS THAT OF A CO_2 BEND LIMITED TO THE *x-y* PLANE. THE MIDDLE FIGURE HAS THE CORRESPONDING *x-z* MODE CLEARLY OUT OF PHASE WITH THE *x-y* BEND. THE RIGHT-HAND IMAGE IS THE RESULT OF BOTH BENDING MODES BEING EXCITED SIMULTANEOUSLY AND THE ROTATION IS CLEARLY VISIBLE IN THE ANIMATION.

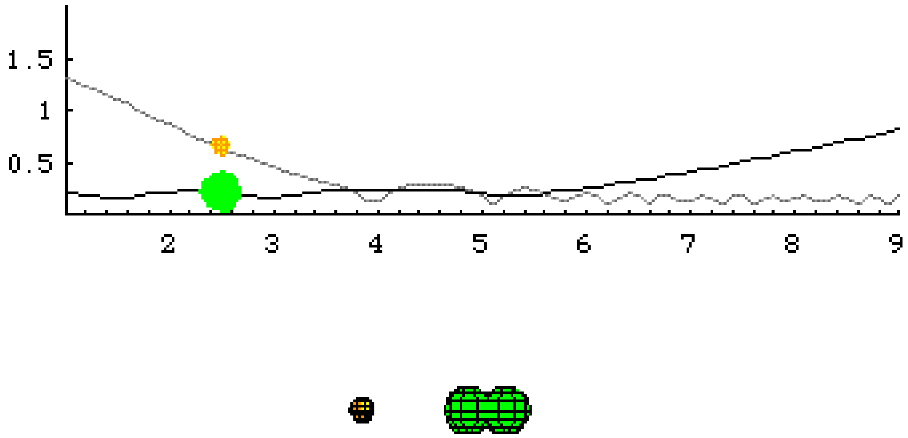


ANIMATION 3. AN IDEALIZED INTERACTION POTENTIAL BETWEEN AN H ATOM AND A CL_2 MOLECULE. THE H ATOM ENTERS THE VALLEY IN THE UPPER LEFT PASSING OVER THE BARRIER TO THE VALLEY ON THE RIGHT. THE CL ATOM THEN EXITS DOWN THE RIGHT-HAND VALLEY LEAVING A VIBRATING HCL MOLECULE.

---

the hydrogen atom and the left-most chlorine atom is one coordinate and the chlorine–chlorine atom separation distance is the other. The interaction potential for this collision system is a modification of the Morse potential for an HCl molecule and Cl_2 molecule. The functional form of the potential is given inside the code in the appendix. The resulting shape of the potential is displayed here with an animation.

Although the interaction potential itself is highly artificial, the reader sees from Animation 3 the general shape is that expected for a reaction with an activation energy.



ANIMATION 4. UPPER FIGURE: THE H-CL (HALFTONE) AND CL-CL (BLACK) DISTANCES AS FUNCTIONS OF TIME. LOWER FIGURE: AT THE TIME INDICATED BY THE GREEN AND GOLD DOTS IN THE UPPER FIGURE, THE ATOMS ARE REPRESENTED AS SPHERES SEPARATED BY THE CORRESPONDING DISTANCES.

Given the interaction potential, it is necessary to set up the equations of motion and integrate them for some set of initial conditions. This task is accomplished with the code segment titled **H Cl2 Collision Segment #1** in the appendix. It is this segment that a student could modify by changing the initial conditions (i.e., the total energy, the vibrational energy, the initial position of the hydrogen atom, or the shape of the interaction potential). The program assumes the Cl2 molecule is at the minimum extreme of its vibration and this should be left unchanged so there is a clear way to separate the initial kinetic and vibrational energies.

After running segment #1 the separation distances H–Cl and Cl–Cl are in hand. There remains only to display them appropriately. Animation 4 shows the separation distances plotted as functions of time with a gold dot on the H–Cl curve and a green dot on the Cl–Cl curve at a time when the separation distances are those shown on the image of the spheres below it.

Animation 4, especially if it is stepped through slowly, should aid a novice in interpreting literature figures of the separation distances as functions of time.

The code generating Animation 4 is identified as segment #3 in the appendix.

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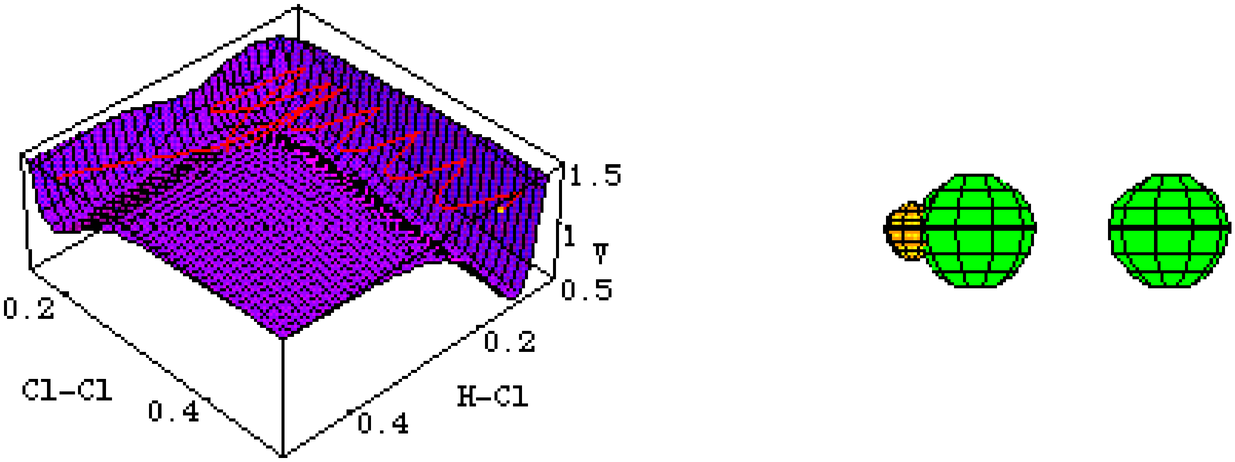

ANIMATION 5. LEFT FIGURE: THE COLLISION TRAJECTORY (RED LINE) SUPERIMPOSED UPON THE POTENTIAL ENERGY PLOT. THE THIRD DIMENSION OF THE TRAJECTORY IS THE TOTAL ENERGY OF THE COLLISION. RIGHT FIGURE: AT THE TIME THE TRAJECTORY IS LOCATED AT THE GOLD DOT IN THE LEFT FIGURE, THE H (GOLD) ATOM AND CL (GREEN) ATOMS ARE SHOWN AS SPHERES WHOSE CENTERS ARE SEPARATED BY THE CORRESPONDING DISTANCES.

As a second display of a collision, Animation 5 shows the trajectory plotted with the three-dimensional potential. It appears as a gold dot moving along the trajectory leaving a red trail. The third dimension of the trajectory is the total energy of the collision system. To see the structure of a collision it is necessary to restrict the time period displayed.

For the given set of initial conditions the trajectory follows the path seen in Animation 5. For other locations of the H atom at time zero (r0HCl in code segment 1) other types of reactive encounters appear as well as non reactive collisions.

It is the author's opinion that the ability to create images such as those of Animation 5 is sufficient in itself to justify learning and using a CAS.

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