The Plasma Chemistry Database

W. K. Trail, C. W. Davis, and W. L. Morgan
Kinema Research & Software, Monument, Colorado
http://www. kinema. com/kinema

We are developing a comprehensive plasma chemistry database of atomic and molecular properties and collision data in Java for use on a LAN, or over the World Wide Web. The database will serve two principal functions: first, it will make this data easily accessible to scientists on the web through a graphical user interface (GUI), and second it will make the data accessible through standard SQL database calls in Java thus enabling our plasma chemistry software tools to access appropriate input data across the web or across a LAN during execution. An example of the current version of this database is on our web site.

The database, which currently contains roughly 50 species, provides atomic and molecular properties such as permanent moments, polarizabilities, electron affinities, heats of fusion, rotational constants, etc., as well as critically selected experimental or theoretical electron collision data for a wide range of processes including elastic scattering, rotational excitation, vibrational excitation, electronic excitation, attachment, dissociative attachment, ionization, and dissociation. (We will eventually add heavy particle collision data.) The collision cross sections are in two forms: raw cross sections and coefficients for analytic fits. Because reaction rates are so useful in plasma chemistry the interface provides the ability to calculate them from cross sections over a user-selected temperature range. In addition, it automatically carries out an Arrhenius fit to the resultant reaction rate and displays the coefficients.
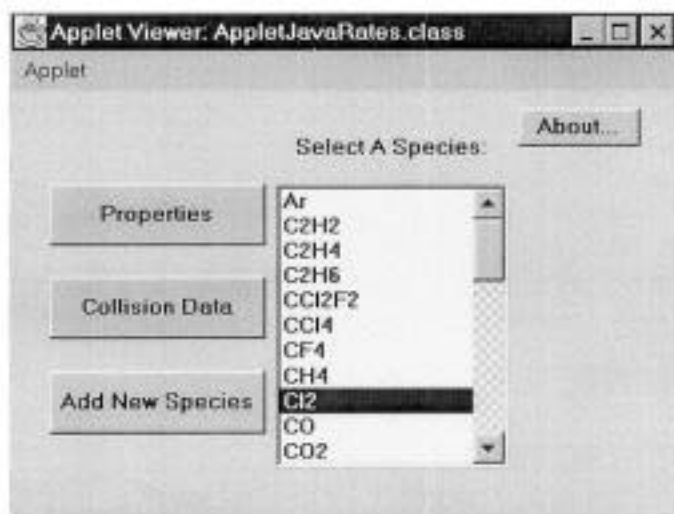

Figure 1: The main page of the graphical user interface to the database.

The first stage of this project was to build the GUI. The GUI allows the user to select an atom or molecule, and view the available raw data. All of the data are easily extracted from the interface using standard cut and paste utilities. In Fig. 1 we show the main page; the user simply selects a

species and chooses to view either 'Properties' or 'Collision Data'. In Fig. 2 we show the properties screen for Cl_2. In Fig. 3 we show the 'Collision Data' screen for momentum transfer in electron-Cl_2 scattering. The user can view the collision cross sections for other processes by clicking on the 'Next' and 'Prev.' buttons. In addition to displaying a table of cross sections for this process, this screen allows the user to calculate reaction rates from the cross sections over a selected temperature range. Also on this screen is a built in 2-D plot utility which allows the user to view a plot of the reaction rates or the cross sections. For example, in Fig. 4 we show a plot of the reaction rate for vibrational excitation of Cl_2 by electron collisions.
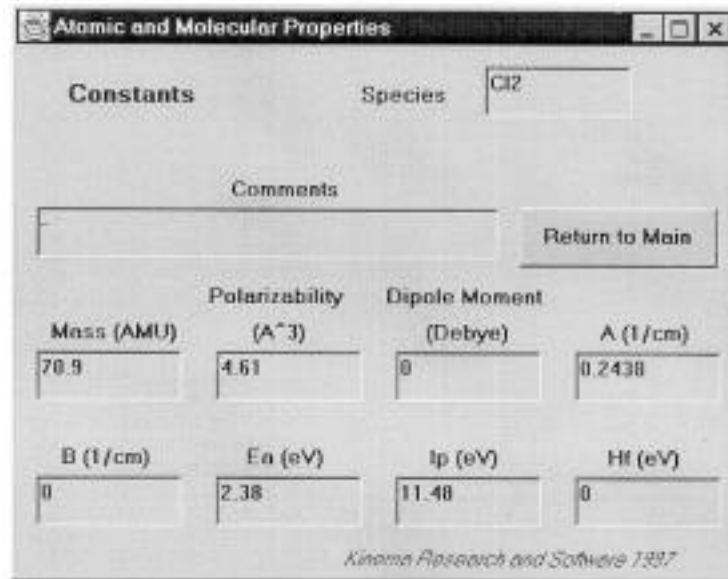

Figure 2: The 'Properties' screen for Cl_2. This page displays the mass, polarizability, dipole moment, scattering length, rotational constant, electron affinity, ionization energy, and the heat of fusion.

Building the Java interface between the database and our plasma chemistry software comprises the second stage of this project. Because most of our software is written in Fortran 77 and Fortran 90, we will first develop a Java interface that essentially provides a convenient way to move data from the database to the appropriate input files. The Fortran programs will be executed from this Java interface.

For the final stage of this project we will migrate our plasma chemistry software to Java. Our programs will then be able to access the appropriate input directly from the database (over the Web) during execution. Some further advantages of a Java-only suite of programs include platform-independence, access to the massive Java class libraries, and ease of distribution (and execution) over a network.
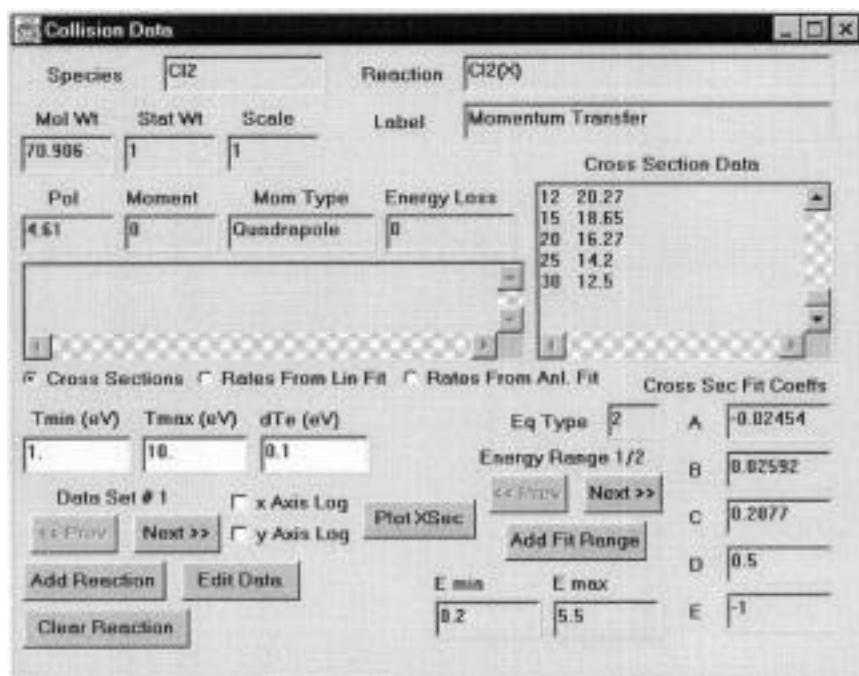
Figure 3: The 'Collision Data' screen provides information on the collision process displayed in the 'Label' field. This screen provides tools for calculating reaction rates, coefficients for fits, buttons for selecting other processes, and plotting utilities. The 'Add Reaction', 'Clear Data', and 'Edit Data' buttons in the lower left will allow users to replace, add new, or modify data in the database.
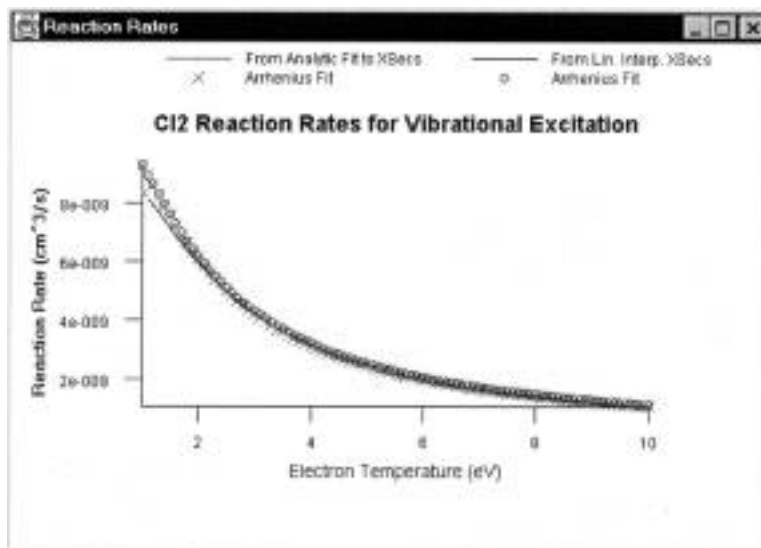

Figure 4: This is a plot of the reaction rate as calculated from the $v = 0$-1 vibrational excitation cross section. The curve labeled 'From Lin. Interp. XSecs' is the reaction rate as calculated from a linear interpolation of the raw cross section data. An Arrhenius fit to these reaction rates is represented by the circles. The curve labeled 'From Analytic Fit to XSecs' is the reaction rate as calculated from our analytic fit to the raw cross section data. An Arrhenius fit to these reaction rates is represented by the X's. (The plots are more easily viewed in color on a computer screen.)