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Los Alamos Opacity Web Page

N. H. Magee, Jr. and R. E. H. Clark
Atomic & Optical Theory Group, T-4
and
Code Integration Group, X-CI
Los Alamos National Laboratory, Los Alamos NM 87545

1 Introduction

The Los Alamos opacity data base is now available on the World Wide Web at http://t4.lanl.gov. The data base contains both the original Astrophysical Opacity Library [1] distributed worldwide in the 1980's (for historical reference) and the new improved opacities from the Light Element Detailed Configuration OPacity (LEDCOP) code [2]. Users can access the opacity data using the multigroup opacity code TOPS [3] to obtain Rosseland and Planck gray opacities, group mean opacities over selected energy ranges, the monchromatic absorption coefficients and the average ionization over a wide range of temperatures and densities. As described below, these quantities are available for all of the elements presently on the data base and TOPS will provide the same quantities for any arbitrary mixture of these elements.

2 Short History of the Opacity Data Base

The Los Alamos opacities have been distributed world wide since the 1960's, mainly for use in astrophysical modeling. At first, the opacity tables were calculated for each individual request, but this became very time consuming. All of these tables were individually calculated from scratch for each new mixture, recalculating the opacities from the individual elements over and over again. In the late 1970's, it was realized that the energy dependent absorption coefficients could be calculated once for each element and then combined with absorption coefficients of other elements to form as many mixtures as desired. There were only two restrictions for this method.

First, all molecular opacities and abundances had to be removed from the calculations since one must have all of the elemental data in the equation of state (EOS) to form molecular species. Second, the opacities had been calculated on a temperature-density ($T-\rho$) grid, but the calculation had to be switched from the ($T-\rho$) grid to a temperature-electron degeneracy ($T-\eta$) grid. The electron degeneracy parameter characterizes the electron pressure of the plasma at the ion-plasma boundary, so two elements calculated at the same η "see" the same plasma conditions and can be mixed together. Extensive comparisons were run in the late 1970's between the mixed opacities and the ab initio mixture calculations and differences were on the order of a few percent.

The Los Alamos Astrophysical Opacity Library was developed from this change in methodolgy. The first comprehensive set of elemental opacities was calculated in the late 1970's and distributed with software programs for mixing the elements together. Most of this distribution was done via magnetic tapes, with FTP being utilized in the early 1990's. Even with FTP, the data transfer was very slow since the library contained more than 300,000,000 words with more being added as new opacity calculations were being done for the library. It was then decided to place all of the detailed

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absorption coefficient data files on the Web and use the upgraded mixing program TOPS to allow users to access the full data base and download the data in as much detail as they wished.

3 Brief Code Descriptions

The Los Alamos LEDCOP opacity code uses a basis set of detailed LS terms (plus average configuration terms for complex ion stages) to calculate opacities for elements with $Z < 31$. Each ion stage is considered in detail and interactions with the plasma are treated as pertubations. Calculations are done in local thermodynamic equilibrium (LTE) and only radiative processes are included. The EOS model is based on the Saha equation [4], including degeneracy, where the bound Rydberg sequences are cut off by plasma corrections [5]. The code does not consider liquid or solid phases, but uses an explicit ion model [6] to treat all of the bound electron states of every ionization stage.

A self-consistent Hartree-Fock code [7] with relativistic corrections is used to generate both single configuration LS term energies, radial dipole matrix elements and angular factors for all ion stages and unresolved transition array (UTA) energies and variances [8] in intermediate coupling for selected ion stages. Nonhydrogenic photoionization cross sections are calculated for each configuration subshell with $l < 5$, using distorted wave continuum functions and the same Hartree-Fock structure calculations as for the bound-bound transitions in order to conserve oscillator strength across the photo-electric edges. Users should access the web page reference link for more details.

The Astrophysical Opacity Library consists of random access binary files. The TOPS code is the vehicle for accessing these data files and performing numerical integrations to obtain the Rosseland and Planck opacities. TOPS can provide opacities for an arbitrary mixture of pure elements. As mentioned previously the data is stored as a function of T and η. The TOPS code mixes elements at similar η's and then interpolates on η to obtain a material density. The user can select an arbitrary density and, for multigroup opacities, an arbitrary photon energy grid. The temperature grid is limited to subsets of the temperature grid on which the original data are tabulated; no interpolation in temperature is allowed in the TOPS code.

4 Data Base Structure

At present, the data base contains monochromatic absorption coefficients for all of the elements from hydrogen to zinc. Older element calculations are being upgraded and the data base may be extended to higher Z elements in the future. Each element in the library is calculated on a uniform T, η and u ($u = h\nu/kT$) grid to allow the mixing of the elements to form mixtures. This provides an almost unlimited choice for users to customize opacity tables from pure elements to two element mixtures, such as the carbon-iron mix presented in this paper, to complex astrophysical mixtures containing more than 20 elements. The older 1977 element data is included so that users can baseline the changes in the opacities over the 20 year span of the calculations. The old element data can be mixed just like the newer data, and can even be mixed with the newer data since the older photon grid is a subset of the photon grid used for the newest calculations. The TOPS code automatically chooses the correct grid when the materials are mixed.

Table 1 lists the temerature, density and u ranges covered by the data base. The density range is shown rather than the electron degeneracy range since the density is a more familiar quantity. Every element in the library has approximately 1500 $T - \eta$ points, covering the ranges listed below. Therefore, each element has approximately 12,000,000 words of data. As disk space allows, the authors hope to expand the number of u grid points from the present 3,900 to 14,900.

Table 1: Ranges covered by the opacity data base.

Quantity	Range	Comments
Temperature	.5 or 1.0 eV to 100,000 eV	10 temperatures/decade.
Density	10^{-10} gm/cc to 10^{+9} gm/cc	1 to 3 densities/decade. Highest density is temperature dependent.
u	0. to 30. or 30,000.	1977 data stops at $u = 30$.

5 Sample Web Page Output

A short sample output is shown for a carbon-iron mixture at two temperatures and two densities. The default output has been chosen, so the table displays the Rosseland and Planck gray opacities and the the average number of free electrons per atom. Note that a warning message has been printed, indicating that one of the requested densities was off the table. The TOPS code will use the values from the highest calculated density for all densities above the last density point.

Table 2: Sample opacity tables for CFe mixture.

TOPS results
Opacities in cm**2/gm, T in keV, density in gm/cc
WARNING - Requested densities went off table boundaries

Temp	Den Req	Den used
1.0000E-03	1.0000E+00	7.0739E-01

Normalized composition for requested elements

No. Fraction	Mass Fraction	At. No.	Chem. Sym.	Mat Id.
5.0000E-01	1.7699E-01	6	C	l17831
5.0000E-01	8.2301E-01	26	Fe	l12142

Temperature grid used the following 2 points

1.0000E-03	1.2500E-03

Density grid used the following 2 points

1.0000E-01	1.0000E+00

Rosseland and Planck opacities and free electrons

Density	Ross opa	Planck opa	No. Free	Av Sq Free	T= 1.0000E-03
1.0000E-01	4.1416E+05	8.4327E+05	5.2602E-02	5.2604E-02	
1.0000E+00	4.5953E+05	2.5213E+06	2.3540E-02	2.3541E-02	
Density	Ross opa	Planck opa	No. Free	Av Sq Free	T= 1.2500E-03
1.0000E-01	3.3323E+05	1.2938E+06	1.0226E-01	1.0231E-01	
1.0000E+00	3.7040E+05	3.8026E+06	5.3035E-02	5.3057E-02	

6 Critical Evaluation

One of the most difficult tasks in opacity calculations has been assigning error criteria to the final results. The calculations are a complex mixture of atomic physics input data and plasma modeling.

The plasma models include the EOS occupancy determination and the broadening of the bound-bound line transition profiles. Up to 1988, there was very little organized comparison between the various theoretical codes and no experimental data. Both of these situations changed in 1988 with the meeting of the first International Opacity Code Comparison Workshop and with the publication of the first opacity transmission experiment from RAL [9] in England. Since that year, there have been three more workshops [10] with more than 15 participating groups, and more than half a dozen experiments from groups around the world.

Opacities from the various codes have changed by factors of 2 to 10 over the years since 1988, especially in $T - \rho$ regions where the $\Delta n = 0$ bound-bound line transitions are important. The authors feel that these large uncertainties are now resolved and that one can place an upper limit of 25 % on the integrated Rosseland opacities for low and moderate densities where LTE is appropriate. At higher densities, such as a few gm/cc at temperatures of 10 to 50 eV, the agreement between the independent codes can differ by more than a factor of 2 and there is almost no reliable experimental data, so it is not possible to set an uncertainty below 50 % for these regions.

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