EquilTheTA: a web-access tool for LTE plasma thermodynamics and transport properties

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EquilTheTA is a web-access tool to calculate thermodynamic and transport properties of complex plasmas in local thermodynamic equilibrium (LTE) in a wide pressure and temperature range. Thermodynamic properties are calculated starting from the atomic and molecular internal partition functions, which are, in turn, evaluated from internal levels of the species. For atoms and atomic ions, the electronic energy levels are available in open databases and are extended by recurring to the Ritz-Rydberg approach to ensure completeness for each internal configuration. Equilibrium compositions are calculated by using a hierarchical algorithm which solves one reaction at a time [1, 2] avoiding the solution of large non-linear systems of equations. For these reasons, the method is fast and accurate and always converges. Recently, an automatic determination of the optimal reaction scheme has been implemented to speedup the convergence. Transport properties are calculated by using high order Chapman-Enskog expansion. The transport cross section database is populated by an hybrid phenomenological/multi-potential approach, ensuring accurate description of binary interactions and widening the capability of the tool. The code is accessed through a friendly interface which includes the possibility of creating a plasma mixture starting from the species and to set the thermodynamic conditions (pressure or density, temperature). As an example, Figure 1 shows molar fractions of molecules and atomic negative ions obtained in the case of a plasma of technological interest such as SiC+O_2 [3].

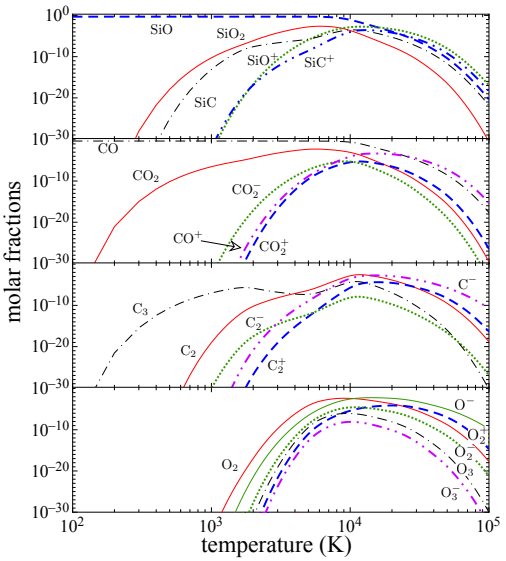

Figure 1: *Molar fractions of SiC + O_2.*

References

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