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Increasing the accuracy of interstellar chemical models

V. Wakelam[1], **E. Herbst**[1]
and F. Selsis[2]

[1]Departments of Physics, Chemistry and Astronomy, The Ohio State University, Columbus, OH 43210, USA
email: wakelam@mps.ohio-state.edu

[2]Centre de Recherche Astronomique de Lyon, Ecole Normale Supérieure, 46 Allée d'Italie, F-69364 Lyon cedex 7, France

Abstract. Chemical models have been used for a long time to reproduce molecular abundances observed in the interstellar medium. These models usually include hundreds to thousands of reactions with rate coefficients that are "known" to have errors. The errors have some repercussions on the abundances computed by chemical models. The only rigorous way to compare the predictions of models with observed abundances is to take into account both the modeling and observational uncertainties. Although comparisons of this type have been undertaken in other fields such as planetary atmospheric photochemistry, this has never been done systematically for interstellar chemistry. One of the reasons is probably the lack of information on the rate uncertainties. Indeed, most of the rate coefficients in planetary atmospheric networks have been studied in laboratories and are given with their measured error, contrary to interstellar networks. Only the UMIST database gives even a rough estimation of the rate uncertainties.

Based on this lingering problem, we decided to include a treatment of rate uncertainties in our chemical models in order to study the consequences of this error on the computed molecular abundances. In addition, we have developed a method to identify those reactions that contribute the most to uncertainties in predicted abundances. We have applied our methods to the chemistry of both cold (dark-cloud) and warm (hot-core) regions. We have studied in particular the consequences regarding the determination of the cosmic-ray ionization rate using observed abundances and the determination of the age of hot cores using sulphur chemistry. The final goal of this study is to improve the accuracy of the chemical modeling and networks.

Keywords: ISM: abundances, ISM: clouds

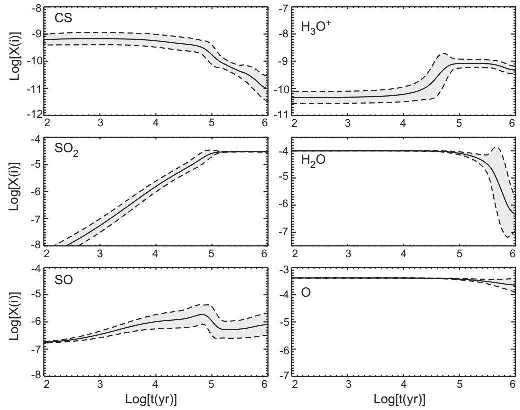

Figure 1. Evolution of fractional abundances (/H_2) of some species with 2σ errors for hot core physical conditions (T=100 K and n(H_2)=10^7 cm^{-3}).