



Astronomy and Astrophysics

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Editorial

The nature of bistability in large gas-phase chemical networks of dense interstellar clouds at 10 K is examined. The dependence of bistability on the parameter ζ/nH , the cosmic ray ionization rate divided by the total hydrogen density, for a wide range of elemental depletions is investigated in detail. We confirm that bistability can exist at steady-state for a range of ζ/nH , but we also confirm that the range of bistability is very dependent on elemental depletions, and also dependent on which network is utilized. In particular, bistability is a more salient feature in the new neutral-neutral model than it is in the new standard model. With the former model, we find that for some gas-phase elemental abundances, the bistability range is non-existent while for others the bistability range includes gas densities as high as $1\ 105\ \text{cm}^{-3}$ assuming a standard value for ζ . When all of our new neutral-neutral model results are plotted on one diagram with the fractional electron abundance as ordinate and the parameter ζ/nH as abscissa, it is found that bistability is confined to a vertical band which is narrower at small ζ/nH (high densities). Above and below the band lie the so-called “high metal” and “low metal” single-phase results. The intermediate electron abundances at which bistability occurs are best obtained by relatively high abundances of the element sulfur because this element, unlike real metals, is a “soft” ionizer; i.e., its abundance is not totally in ionized forms. We present newly obtained steady-state results for a variety of molecules in both the HIP (high ionization phase) and LIP (low ionization phase) solutions for a bistable model at a rather high density near $3\ 104\ \text{cm}^{-3}$ with a standard cosmic ray ionization rate. Both the steady-state results as well as a variety of early-time results are compared with observations in TMC-1 and L134N.

The phenomenon of bistability in gas phase chemical models of interstellar clouds is by now well known (Pineau des Forets et al. 1992, Le Bourlot et al. 1993, 1995a,b, Shalabiea & Greenberg 1995). The term bistability refers to the existence of two stable steady-state chemical solutions – labelled the high ionization phase (HIP) and the low ionization phase (LIP) – over a certain range of gas densities and cosmic ray ionization rates. The two solutions, obtained both by solution of algebraic equations and by following the time dependence of differential equations until no further changes occur, arise from different initial conditions. In addition to a high degree of ionization, the HIP solution is characterized by a high C/CO abundance ratio, while the LIP solution is characterized by a much lower C/CO abundance ratio. Other chemical differences have also been explored (Gerin et al. 1997). When selected results, such as the C/CO abundance ratio, are plotted against density or cosmic ray ionization rate, the nature of bistability emerges (Flower & Pineau des Forets 1996).

Starting, for example, from high density with initial abundances either rich in molecules or rich in atoms (with the exception of H₂), and proceeding to lower densities at a fixed ionization rate, one encounters only one solution with relatively low ionization at steady-state until at a certain critical point, a sharp phase transition occurs to the HIP solution for the initial abundances rich in atoms. If initial abundances rich in molecules are used, no sharp transition occurs at this density, and a second solution – the LIP solution – is obtained. At a lower density critical point, the LIP solution reached from molecular initial conditions undergoes a phase transition of its own and merges with the HIP solution. At still lower densities, there exists only one solution, with relatively high ionization.

If initial abundances rich in molecules are used, no sharp transition occurs at this density, and a second solution - the LIP solution - is obtained. At a lower density critical point, the LIP solution reached from molecular initial conditions undergoes a phase transition of its own and merges with the HIP solution. At still lower densities, there exists only one solution, with relatively high ionization. HIP and LIP phases show differing abundances of deuterated species. The relevance of bistability to the actual interstellar medium, however, rests on questions such as whether or not it is an artifact of incomplete models and over how wide a region of parameter space it occurs. Bistability has by now been investigated in both small- and moderately-sized model networks, although it has not been studied in any detail with the largest chemical networks, which might be expected to be the most stable. The dependence of the range of bistability on elemental depletions has also been looked at to some degree (Le Bourlot et al. 1995a). In addition, the effect of grain chemistry on the nature of bistability has been investigated and debated (Shalabiea & Greenberg 1995, Le Bourlot et al. 1995b). There is thus still an element of controversy concerning bistability, and a more thorough investigation of the phenomenon is indicated. In this paper, we report such a thorough investigation with a very large gas-phase chemical network – the so-called “new neutralneutral” model of Bettens et al.

In this global study, we have used a variety of elemental abundances, which can be regarded as variations of three primary sets of abundances. Two of these sets are the well-known “low metal” and “high metal” abundances (e.g. Leung et al. 1984; Graedel et al. 1982) in which the elements C, N, and O are depleted according to Morton (1975). The “high metal” and “low metal” results differ in abundances for the elements S, Si, Na, Mg, and Fe, with the former containing a modest depletion of 2 for sulfur and stronger depletions of 50, 10, 60, 110, respectively for the other elements while the “low metal” values contain additional depletions of 100 for each. Although the “high metal” abundances give a reasonable description of diffuse cloud gas-phase measurements, the “low metal” results typically yield substantially better agreement with observation in cold dense interstellar clouds (Graedel et al. 1982), without, it would appear, violating any obvious elemental constraints based on gas-phase observations. In addition to these two sets of primary abundances, we have also started with a set of abundances we refer to as the “dense core” abundances. These are derived by Flower et al. (1995) from the solar values of Anders & Grevesse (1989) via an analysis based on a review article by van Dishoeck et al. (1993). A final point of discussion concerns the effect of including dust chemistry on the phenomenon of bistability.