BISTABILITY IN INTERSTELLAR GAS-PHASE CHEMISTRY
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ABSTRACT

We present an analysis of “bistability” in gas-phase chemical models of dark interstellar clouds. We identify the chemical mechanisms that allow high- and low-ionization solutions to the chemical rate equations to coexist. We derive simple analytic scaling relations for the gas densities and ionization rates for which the chemistry becomes bistable. We explain why bistability is sensitive to the H$_3^+$ dissociative recombination rate coefficient and why it is damped by gas-grain neutralization.

Subject headings: ISM: molecules — molecular processes

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1. INTRODUCTION

In this paper we reexamine and analyze the phenomenon of “bistability” that occurs in chemical models of dark interstellar clouds. Bistability was first discussed by Le Bourlot et al. (1993), who found that multiple solutions to the chemical rate equations sometimes appear in numerical computations of the gas-phase abundances of atomic and molecular species for steady state dark cloud conditions. When bistability occurs, three sets, rather than a single unique set, of chemical abundances are predicted for identical input cloud parameters such as the total gas density, the cosmic-ray (or X-ray) ionization rate, and the gas-phase supply of heavy elements. Under such circumstances, the solution that is converged to in a numerical simulation, and perhaps the actual steady state of a real physical system, depend on the initial conditions and history of the gas.

The subject of bistability begins with Pineau des Foreîts et al. (1992), who studied how the computed chemical states of dark clouds depend on the gas density and ionization rate. They found, as would be expected, that for a given ionization rate the fractional ionization of the gas decreases roughly as the square root of the gas density. However, they also found that the ionization fraction and associated chemical composition changes abruptly, or quasi-discontinuously, at a specific critical transition density. Below the critical density the clouds are in what Pineau des Foreîts et al. referred to as a “high-ionization” phase (HIP), characterized by high abundances of atomic ions. For densities greater than the critical density the clouds are in a “low-ionization” phase (LIP), with high abundances of molecular ions. Pineau des Foreîts et al. also identified a chemical instability that they, argued, is responsible for the abrupt transition that they encountered in their calculations. Bistability was subsequently discovered by Le Bourlot et al. (1993), who found that instead of a phase change at a specific critical density, the LIP and HIP “branches” can sometimes overlap for a narrow range of densities. A third (unstable) branch also appears, intermediate between the LIP and HIP solutions.

Further investigations have explored the effects of the assumed gas-phase elemental abundances, ionization rates, gas temperatures, chemical reaction rate coefficients, and gas-grain interactions on the existence and character of the multiple solutions (Le Bourlot et al. 1995a, 1995b; Shalabiea & Greenberg 1995; Lee et al. 1998; Pineau des Foreîts & Roueff 2000; Viti et al. 2001; Charnley & Markwick 2003). These studies have shown that bistability is indeed related to the transition from the HIP to LIP (or vice versa) and that it is sensitive to quantities such as the gas-phase heavy-element abundances (Le Bourlot et al. 1995a, 1995b; Viti et al. 2001) and the adopted chemical network (Lee et al. 1998), including specifically the dissociative recombination rate coefficient of H$_3^+$ (Pineau des Foreîts & Roueff 2000). In this paper we explain why the HIP and LIP can overlap, and we identify the chemical mechanisms that allow the possibility of multiple solutions.

We show that bistability can be simply understood and analyzed using just a handful of reactions. In a nutshell, when bistability occurs, atomic ions (usually S$^+$ ions) are the dominant positive charge carriers for both HIP and LIP conditions. Two modes of neutralization are then available to the gas. In the HIP, neutralization proceeds by slow radiative recombination. In the LIP, neutralization occurs by rapid dissociative recombination via the formation of intermediate molecular ions in reactions with O$_2$ molecules (e.g., S$^+$ + O$_2$ → SO$^+$ + O). Bistability occurs when a low O$_2$ abundance in the HIP can be maintained up to maximal gas densities that are greater than the minimal densities above which a large O$_2$ density is maintained in the LIP. We show by means of a simple analysis why this is possible. The explanation involves a chemical instability of a type first introduced by Pineau des Foreîts et al. (1992) but not given sufficient attention in subsequent studies.

Bistability may be of primarily theoretical interest since, as we discuss, it is a purely gas-phase chemical effect. If realistic gas-dust neutralization processes are included, the multiple solutions are damped or eliminated entirely (cf. Shalabiea & Greenberg 1995). We illustrate this by considering the effect of grain-assisted ion-electron recombination (Weingartner & Draine 2001) on the chemistry. Nevertheless, because bistability has been the subject of considerable discussion in the literature, we feel that a fresh analysis of how, why, and when it occurs is warranted.

The plan of our paper is as follows. In § 2 we present results of an illustrative numerical computation in which bistability occurs. In § 3 we discuss the key chemical instability that drives the steady state solutions to either the LIP or HIP. In § 4 we derive simple analytic formulae that show how the range of gas densities and ionization rates for which the gas becomes bistable depends on the elemental abundances and several important chemical rate coefficients. In § 5 we analyze the sensitivity of bistability to the H$_3^+$ dissociative recombination rate coefficient. In § 6 we explain
why gas-grain neutralization processes damp and eliminate bistability. We summarize in § 7.

2. COMPUTATIONS

We first illustrate the phenomenon of bistability in a detailed numerical computation. For this purpose we calculate the steady state atomic and molecular abundances for dark cloud conditions as functions of the gas density. We include only gas-phase formation and destruction processes, except for molecular hydrogen (H$_2$), which we assume is formed on grain surfaces. The chemistry is driven by cosmic-ray–impact ionization of hydrogen and helium, followed by standard sequences of ion-molecule, charge-exchange, and neutral-neutral reactions. The chemistry is also mediated by radiative and dissociative recombination, and cosmic-ray–induced photodissociation and photodissociation. The effects of externally incident far-ultraviolet (FUV) photons are excluded.

We use the Boger & Sternberg (2005) network for a system consisting of 70 atomic and molecular carbon-, nitrogen-, oxygen-, sulfur-, and silicon-bearing species (see also Sternberg & Dalgarno 1995). We neglect all other heavy elements. Our oxygen-, sulfur-, and silicon-bearing species (see also Sternberg et al. 1993), N/H = 7.8 × 10$^{-7}$ (Cardelli et al. 1993), N/H = 7.5 × 10$^{-5}$ (Meyer et al. 1997), O/H = 2.84 × 10$^{-5}$ (Meyer et al. 1998), Si/H = 1.78 × 10$^{-5}$ (Cardelli et al. 1994), and S/H = 8.30 × 10$^{-6}$ (Lepp et al. 1988). We set He/H = 0.1. We assume a constant gas temperature of $T = 50$ K for the entire range of gas densities that we consider.

In our calculations we solve the equations of chemical equilibrium,

$$\sum_{j} k_{ij}(T)n_j + \sum_{j} \xi_{ij} n_j = n_i \left( \sum_{j} k_{ji} n_j + \sum_{j} \xi_{ji} \right), \quad (1)$$

for the densities $n_i$ of all species $i$ in our set. In these equations, $k_{ij}(T)$ are the temperature-dependent rate coefficients (cm$^3$ s$^{-1}$) for chemical reactions between species $j$ and $i$ that lead to the production of $i$, and $\xi_{ij}$ are the cosmic-ray destruction rates (s$^{-1}$) of species $j$ with products $i$. The parameters $\xi_{ij}$ include impact ionizations of hydrogen and helium by the cosmic-ray protons and secondary electrons, as well as photodestruction of heavy atomic and molecular species by induced UV photons. The $\xi_{ij}$ are all proportional to $\zeta \equiv 10^{-17} \zeta_{-17}$ s$^{-1}$, the cosmic-ray ionization rate of H$_2$ (Sternberg et al. 1987; Gredel et al. 1989).

The densities $n_i$ must also satisfy the supplementary equations of element and charge conservation. These are

$$\sum_{i} \alpha_{im} n_i = X_m n_{tot}, \quad (2)$$

where $\alpha_{im}$ is the number of atoms of element $m$ contained in species $i$, $X_m$ is the total abundance of element $m$ relative to the total density $n_{tot}$ of hydrogen nuclei, and

$$\sum_{i} q_in_i = 0, \quad (3)$$

where $q_i$ is the charge of species $i$. In our computations, the negative charge is carried entirely by free electrons.

H$_2$ molecules are formed primarily on dust grains and are destroyed by cosmic-ray ionization. A separate equation may then be written for the H/H$_2$ balance,

$$\zeta n_{H_2} = R n_{tot} n_{H_2}, \quad (4)$$

where $n_{H_1}$ and $n_{H_2}$ are the atomic and molecular hydrogen densities, respectively, and $R = 3 \times 10^{-18} T^{1/2}$ cm$^{-3}$ is the H$_2$ grain surface formation rate coefficient (Bihm & Lipshat 2002; Vidali et al. 2004).

For fixed gas density and gas-phase elemental abundances, the density fractions $x_i \equiv n_i/n_{tot}$ as determined by equations (1)–(4) depend on the single parameter $n_{tot}/\zeta$ (e.g., Lepp & Dalgarno 1996; Lee et al. 1998), as is readily seen by dividing each term in these equations by $n_{tot}$. We consider a range of parameters for which almost all of the hydrogen is in the form of H$_2$, so that $n_{tot} = 2n_{H_2}$. We therefore present our results as functions of the ratio $n_{H_2}/\zeta_{-17}$ (cm$^{-3}$).

We solve equations (1)–(4) numerically via Newton-Raphson (NR) iteration. In our procedure we vary the density along the HIP and LIP branches and use the solutions from the previous density step as the “initial guess” for the NR iteration in the next density step. In the bistability region we carry out repeated NR iterations with random initial guesses, so that all three branches are found.

In Figure 1 we plot the densities $n_{H_2}/\zeta_{-17}$ and density fractions $n_{H_1}/n_{H_2}$, as functions of $n_{H_2}/\zeta_{-17}$ ranging from 50 to 5 × 10$^3$ cm$^{-3}$, for several species of interest. Panels $a$ and $b$ display our results for electrons, C$^+$, S$^+$, H$_3^+$, and a sum over all molecular ions. Panels $c$ and $d$ display our results for the neutral species C, O, CO, and O$_2$. Several important features are apparent in Figure 1, some of which have been noted in previous discussions.

For our assumed elemental abundances and gas temperature, an HIP is present for densities less than $(n_{H_2}/\zeta_{-17})_{\text{max}} = 675$ cm$^{-3}$, and an LIP is present for densities greater than $(n_{H_2}/\zeta_{-17})_{\text{min}} = 370$ cm$^{-3}$. The HIP and LIP overlap, and the gas is bistable, between these minimal and maximal densities. The HIP and LIP solutions are connected by a third branch that we refer to here as the MIX solution.

In the HIP, the positive charge is carried entirely by atomic ions. S$^+$ is the dominant ion down to $n_{H_2}/\zeta_{-17} = 60$ cm$^{-3}$. At lower densities C$^+$ takes over, and for $n_{H_2}/\zeta_{-17} < 1.1$ cm$^{-3}$, H$^+$ dominates. In the LIP, the molecular ions HCO$^+$ and H$_2$O$^+$ are the primary positive charge carriers for densities greater than $n_{H_2}/\zeta_{-17} > 6 \times 10^3$ cm$^{-3}$. However, S$^+$ dominates at lower densities in the LIP. Most importantly, in our calculation S$^+$ is the primary positive charge carrier in both the HIP and LIP for the densities at which bistability occurs.

The fractional ionization increases from a minimum value $x_e = 6 \times 10^{-8}$ as the density decreases from $(n_{H_2}/\zeta_{-17})_{\text{max}}$ in the HIP. In the LIP, the fractional ionization decreases from a maximum value of $x_e = 2 \times 10^{-6}$ as the density increases from $(n_{H_2}/\zeta_{-17})_{\text{min}}$. The fractional ionization drops by a factor of $\sim 10$ in moving from the HIP to LIP in the bistability region.

The free atomic carbon density and the C/CO abundance ratio is large in the HIP. The ratio C/CO $\approx 0.3$ in the bistability region and exceeds unity for $n_{H_2}/\zeta_{-17} \leq 55$ cm$^{-3}$. In the LIP the C density and the C/CO ratio are small. In our computation the C/CO ratio drops by a factor $\sim 50$ in moving from the HIP to the LIP. The drop in C/CO is associated with an increase in the O$_2$ density and the O$_2$/CO ratio. It is very significant that the C and O$_2$ densities vary in opposite directions in the transition between the HIP and LIP.
On the MIX branch the fractional ionization, and the C/CO and O2/CO ratios, are intermediate between the HIP and LIP. S+ is also the dominant positive ion on the MIX branch. However, the fractional ionization increases with gas density along the MIX.

In Table 1 we list the densities of selected atomic and molecular species for the three HIP, LIP, and MIX solutions, for \( n_{H_2} = 4.3 \times 10^5 \) cm\(^{-3} \) and \( \zeta = 1.0 \times 10^{-17} \) s\(^{-1} \). We also list the HIP/LIP density ratios for these values of \( n_{H_2} \) and \( \zeta \). Atomic ions, e.g., S\(^+\), Si\(^+\), and C\(^+\), are abundant in the HIP solution. In the LIP solution, molecular ions such as H\(^+\)\(_3\), HCO\(^+\), and H\(_2\)O\(^+\) are abundant, leading to more OH, H\(_2\)O, and O\(_2\) than in the HIP. The oxygen-bearing molecules, NO, SO, and SiO, are enhanced by the large O\(_2\) density that is maintained in the LIP. Carbon-bearing molecules, such as CN and HCN, are enhanced in the HIP because of the large atomic carbon density in this phase (see also Boger & Sternberg 2005). CS is produced by reactions of SO (enhanced in the LIP) with C (enhanced in the HIP) so that the CS density changes by only a factor of \( \sim 2 \) in moving from the LIP to the HIP.

### 3. CHEMISTRY AND INSTABILITY

Figure 1 shows that as the gas density \( n_{H_2} \) is increased along the sequence of HIP solutions, an abrupt jump to the LIP branch occurs when \( n_{H_2} \) rises above \( (n_{H_2}/\zeta)_{\text{max}} \). Similarly, as \( n_{H_2} \) is decreased along the LIP, a jump to the HIP occurs when \( n_{H_2} \) falls below \( (n_{H_2}/\zeta)_{\text{min}} \). As we now discuss, these jumps are signatures of a simple chemical instability involving electrons, S\(^+\) and H\(^+\)\(_3\) ions, C atoms, and O\(_2\) molecules. The instability can be understood by considering the gas-phase formation and destruction sequences for these species, for gas densities at which the bistable solutions occur. We first discuss the HIP and LIP, and we then consider the MIX.

We begin with H\(^+\)\(_3\). In both the HIP and LIP, this ion is formed by cosmic-ray ionization of H\(_2\) followed by proton transfer,

\[
H_2 + e \rightarrow H_2^+ + e, \quad (R1)
\]

\[
H_2^+ + H_2 \rightarrow H_3^+ + H. \quad (R2)
\]
In the HIP, the electron fraction is large, and dissociative recombination,

\[ H_3^+ + e \rightarrow H_2 + H, \]  
\[ H_3^+ + e \rightarrow H + H + H, \]

dominates the removal of the \( H_3^+ \). However, in the LIP the electron fraction is small, and the \( H_3^+ \) is removed by

\[ H_3^+ + CO \rightarrow HCO^+ + H_2. \]

For a gas temperature of 50 K, dissociative recombination dominates the destruction of \( H_3^+ \) when \( n(e)/n(CO) > 10^{-2} \).

In both the HIP and LIP, the production of \( O_2 \) is initiated by proton transfer,

\[ O + H_3^+ \rightarrow OH^+ + H_2, \]

which is followed by abstraction,

\[ OH^+ + H_2 \rightarrow H_2O^+ + H, \]  
\[ H_2O^+ + H_2 \rightarrow H_3O^+ + H, \]

dissociative recombination,

\[ H_2O^+ + e \rightarrow OH + H_2, \]  
\[ H_2O^+ + e \rightarrow H_2O + H, \]

and the neutral-neutral reaction,

\[ OH + O \rightarrow O_2 + H. \]

However, the \( O_2 \) is destroyed in different ways in the two phases. In the HIP, the density of free atomic carbon is large, and the \( O_2 \) is removed by

\[ O_2 + C \rightarrow CO + O. \]

In the LIP, the \( C \) density is small, and the \( O_2 \) is removed much less efficiently in reactions with less abundant atoms and atomic ions. An upper limit on the \( O_2 \) density in the LIP is set by cosmic-ray–induced photodissociation,

\[ O_2 + crp \rightarrow O + O. \]

Reaction (R13) is inefficient, and the \( O_2 \) density becomes large in the LIP.

In the HIP, \( C^+ \) is produced by cosmic-ray–driven helium-impact ionization of \( CO \),

\[ He + crp \rightarrow He^+ + e, \]  
\[ He^+ + CO \rightarrow C^+ + O + He. \]

This is then followed by rapid charge transfer,

\[ S + C^+ \rightarrow S^+ + C, \]

which leads to the production of \( S^+ \) and \( C \). The \( S^+ \) ions are removed by radiative recombination,

\[ S^+ + e \rightarrow S + \nu. \]

The \( C \) atoms are removed by cosmic-ray–induced photoionization,

\[ C + crp \rightarrow C^+ + e. \]

Because cosmic-ray photoionization is inefficient, a large \( C \) density is maintained in the HIP.

In the LIP, \( C^+ \) is also produced by helium-impact ionization (reactions [R14] and [R15]). However, because the \( O_2 \) density is large in the LIP, the \( C^+ \) ions are rapidly neutralized by the sequence

\[ C^+ + O_2 \rightarrow CO^+ + O, \]  
\[ CO^+ + e \rightarrow C + O, \]

and the \( C^+ \) density becomes small. In the LIP, charge transfer between \( C^+ \) and \( S \) (reaction [R16]) contributes negligibly to the
removal of C$^+$ or to the formation of S$^-$. The main source of S$^+$ in the LIP is cosmic-ray–induced photoionization,

$$S + crp \rightarrow S^+ + e.$$  \hfill (R21)

Crucially, O$_2$ also dominates the neutralization of S$^+$ in the LIP, via

$$S^+ + O_2 \rightarrow SO^+ + O,$$  \hfill (R22)

$$SO^+ + e \rightarrow S + O.$$  \hfill (R23)

For a gas temperature of $50$ K, neutralization of S$^+$ by O$_2$ dominates over radiative recombination when $n(O_2)/n(e) > 0.8$. Finally, the C atoms formed by reaction (R20) are also removed by reactions with O$_2$ (reaction [R12]), and the C density becomes small in the LIP.

For the gas densities of interest, most of the gas-phase sulfur is present as S and S$^+$ in both the HIP and LIP, with only a small fraction bound in molecules. S$^+$ is the primary positive charge carrier in both the HIP and LIP. However, in the HIP S$^+$ is removed by radiative recombination, but in the LIP by reactions with O$_2$. In the HIP, H$_3^+$ is removed by dissociative recombination, C is removed by cosmic-ray–induced photoionization, and O$_2$ is removed by C. In the LIP, H$_3^+$ is removed by CO, C is removed by O$_2$, and O$_2$ is limited by cosmic-ray–induced photodissociation. The abundance ratio C/O$_2$ is large in the HIP and is small in the LIP.

Now consider a gas in which S$^+$ is again the dominant charge carrier, but which differs from the HIP or LIP in that dissociative recombination contributes significantly to the removal of H$_3^+$ (as in the HIP), while, on the other hand, S$^+$ is neutralized by O$_2$ (as in the LIP). Assume also that O$_2$ is produced by the sequence (R6)–(R11) and that the O$_2$ destruction rate increases if the O$_2$ density decreases. This is possible when reaction (R12) between O$_2$ and C is the dominant destruction mechanism for both species, so that n(C) increases if n(O$_2$) decreases. For these conditions a chemical instability can occur, as we demonstrate with the following perturbation analysis.

Consider a possible solution to the steady state rate equations. With the above assumptions this requires $n(e) = n(S^+)$. Now consider a perturbative increase in the ionization fraction $x_e \equiv n(e)/n_{tot}$, carried out at fixed gas density $n_{tot}$. This will reduce H$_3^+$ by a factor that depends on the relative efficiencies of dissociative recombination versus reaction with CO in removing the H$_3^+$. The O$_2$ is removed by C (via reaction [R12]), so for a given C density the reduction in H$_3^+$ will lead to an equal reduction in O$_2$ (since O$_2$ is formed by reactions [R6]–[R11]). However, the decrease in O$_2$ will lead to an increase in C, since the C is removed by O$_2$ (again via reaction [R12]). This reduces O$_2$ further still. The S$^+$ density then increases by a factor equal to the total reduction in O$_2$ (since S$^+$ is removed by O$_2$). Finally, to close the loop, $n(e)$ must then be set equal to the new value of $n(S^+)$, since by assumption S$^+$ carries the positive charge. However, if the increase in S$^+$ is larger than the initial increase in the electron density, the cycle “runs away” in a positive feedback loop.

This H$_3^+$-O$_2$-S$^+$ cycle is illustrated schematically in Figure 2. It is clear that the cycle can also lead to a runaway decrease in the electron density, in response to a perturbative decrease in $n(e)$.

2 In this analysis we assume that most of the oxygen not locked in CO remains atomic.

For increasing electron densities, O$_2$ decreases and C increases. For decreasing electron densities, O$_2$ increases and C decreases.

The instability shuts off for sufficiently large or small fractional ionizations. For large $x_e$, radiative recombination, rather than removal by O$_2$, becomes the dominant S$^+$ neutralization process. For small $x_e$, reaction with CO replaces dissociative recombination as the H$_3^+$ removal mechanism. Either way, the H$_3^+$-O$_2$-S$^+$ instability cycle shuts off, and the gas becomes chemically stable.

In the HIP, dissociative recombination dominates the destruction of H$_3^+$, but S$^+$ is removed by radiative recombination. In the LIP, S$^+$ is removed by O$_2$, but H$_3^+$ is removed by CO. Crucially therefore, the H$_3^+$-O$_2$-S$^+$ cycle is inoperative on the HIP and LIP branches, and these solutions are chemically stable.

We now identify the maximum possible density for the HIP, ($n_{H_3} / \zeta$)$_{max}$, as the point at which O$_2$, as formed and destroyed in the HIP, becomes sufficiently abundant to begin removing the S$^+$. When this occurs, the H$_3^+$-O$_2$-S$^+$ cycle turns on (since H$_3^+$ is still being removed by electrons), and a stable HIP is no longer possible. As the density is increased above ($n_{H_3} / \zeta$)$_{max}$, the instability induces a sharp drop in $n(e)$. As the electron density drops in the runaway loop, O$_2$ increases and C decreases. The system is finally stabilized when the electron density becomes sufficiently small for reactions with CO to begin dominating the removal of H$_3^+$. The H$_3^+$-O$_2$-S$^+$ cycle then turns off, and a stable solution on the LIP is reached.

Similarly, we identify the minimum possible density for the LIP, ($n_{H_3} / \zeta$)$_{min}$, as the point at which the fractional ionization, as determined for the LIP, becomes sufficiently large for dissociative recombination to begin dominating the removal of H$_3^+$. When this occurs, the H$_3^+$-O$_2$-S$^+$ cycle turns on (since S$^+$ is still removed by O$_2$), and a stable LIP is no longer possible. As the density is decreased below ($n_{H_3} / \zeta$)$_{min}$, the instability induces a sharp rise in $n(e)$. As the electron density increases, O$_2$ decreases and C increases. The electron density rises until it becomes sufficiently large (and the O$_2$ density sufficiently small) for radiative recombination to dominate the neutralization of S$^+$. The instability then shuts off, and a stable solution on the HIP is reached.

The MIX branch can now also be understood. It represents the locus of equilibrium solutions, with varying $n_{H_3}$, for which the H$_3^+$-O$_2$-S$^+$ cycle is operative, but for which any change in
electron density is precisely matched by a corresponding change in the S$^+$ density. For these solutions, dissociative recombination and reactions with CO both contribute to the removal of H$_2^+$, and S$^+$ is removed by O$_2$. Furthermore, reaction (R12) is the dominant destruction mechanism, for both O$_2$ and C. As the electron fraction increases along the MIX, the O$_2$ formation rate decreases, but by a factor that is smaller than the increase in electron density. The density of C atoms (which remove the O$_2$) increases such that the total increase in O$_2$, and the resulting increase in S$^+$, exactly matches the increase in electron density.

Figure 3 summarizes the key characteristics of the HIP, LIP, and MIX branches, as described above. The triangles indicate the three “legs” of the H$_2^+$-O$_2$-S$^+$ instability cycle in each of the three phases. [See the electronic edition of the Journal for a color version of this figure.]

4. ANALYSIS

4.1. HIP and $n_{max}$

For stable HIP conditions the electron density must be sufficiently large for dissociative recombination to dominate the removal of H$_2^+$, and the O$_2$ density must be sufficiently small for radiative recombination to dominate the removal of S$^+$. We now show analytically that consistent solutions that satisfy these HIP conditions are possible, provided the density is less than a critical maximum gas density.

We first derive an expression for the O$_2$ density in the low-density limit of the HIP. We show that in this limit the O$_2$ density is small and radiative recombination dominates the removal of S$^+$. We then show that our low-density expression for O$_2$ remains consistent only up to a maximal gas density. We identify this as the maximum possible density for HIP solutions. We then verify that dissociative recombination dominates the removal of H$_2^+$, a necessary condition for the HIP, for all densities below this critical density.

In the HIP, O$_2$ is produced by the sequence (R6)–(R11) and is removed by reaction (R12) with atomic carbon. This gives

$$n(O_2) = \frac{n(H_2^+)/n(O)k_{d,OH}}{n(C)k_{12}},$$

where $k_6 = 8.0 \times 10^{-10}$ cm$^3$ s$^{-1}$ are the rate coefficients (at 50 K) of reactions (R6) and (R12), respectively, and $d_{OH} = 0.74$ is the fraction of atomic carbon is produced by helium-impact ionization of CO followed by immediate charge transfer neutralization (reactions [R15] and [R16]) and is removed by cosmic-ray–induced photodissociation (reaction [R18]). Because reaction (R15) dominates the removal of He$^+$, the rate of C formation equals the cosmic-ray ionization rate of helium. Therefore,

$$n(C) / n_{He} = \frac{X_{He}}{\rho_{18}} = 10^{-4},$$

independent of $n_{He}/C$. In this expression $\rho_{18} = 1.02 \times 10^3$ is the efficiency of reaction (R18), and $X_{He} = 0.1$ is the helium abundance. It is clear that a large C density is indeed expected in the HIP, since $n(C)/n_{He} = 10^{-4}$ is comparable to the typical total gas-phase carbon abundance (e.g., $X_C = 1.32 \times 10^{-4}$ in our...
The large C density keeps the O2 abundance small in the HIP.
The O2 density is proportional to H3+_, which in turn, depends on the electron density. For electrons we set n(e) = n(S+). The S+ is produced the same way as atomic carbon, i.e., by helium-impact ionization of CO followed by charge transfer (reactions [R15] and [R16]). We assume that the S+ is removed by radiative recombination. This gives

\[ x_e = n(e)/n_{H2} = \left( \frac{X_{He} \zeta}{k_{17} n_{H2}} \right)^{1/2} = 2.9 \times 10^{-4} \left( \frac{\zeta_{-17}}{n_{H2}} \right)^{1/2}, \]  

(7)

where the radiative recombination rate coefficient \( k_{17} = 1.2 \times 10^{-11} \text{ cm}^3 \text{s}^{-1} \). In this limit the fractional ionization varies as \( \langle n_{H2}/\zeta \rangle^{-1/2} \). For \( n_{H2}/\zeta_{-17} = 100 \text{ cm}^{-3} \), equation (7) gives \( x_e = 2.9 \times 10^{-5} \) in good agreement with 2.3 \times 10^{-5}, which is computed numerically (see Fig. 1).

H3+ is produced by cosmic-ray ionization and is removed by dissociative recombination, so that

\[ n(H3^+) / n_{H2} = \frac{\zeta}{k_{3,4 n(e)}} = \left( \frac{k_{17} \zeta}{X_{He} n_{H2}} \right)^{1/2} = 2.0 \times 10^{-7} \left( \frac{\zeta_{-17}}{n_{H2}} \right)^{1/2}, \]  

(8)

where \( k_{3,4} = 1.7 \times 10^{-7} \text{ cm}^3 \text{s}^{-1} \) is the total rate coefficient for dissociative recombination. The H3+ abundance also varies as \( \langle n_{H2}/\zeta \rangle^{-1/2} \). For \( n_{H2}/\zeta_{-17} = 100 \text{ cm}^{-3} \), equation (8) gives \( n(H3^+)/n_{H2} = 2.0 \times 10^{-8} \), as also computed numerically.

Inserting equations (6), (7), and (8) into equation (5) gives

\[ n(O2) / n_{H2} = \frac{2X_{O2} X_{He}^{1/2} k_{6}}{k_{12} X_{He}^{1/2} k_{3,4} d_{OH} p_{18}} \left( \frac{\zeta_{-17}}{n_{H2}} \right)^{1/2} = 1.1 \times 10^{-5} \left( \frac{\zeta_{-17}}{n_{H2}} \right)^{1/2}, \]  

(9)

where \( X_{O2} \equiv X_0 - X_C = 1.5 \times 10^{-4} \) and where we have assumed that most of the oxygen not bound in CO remains atomic. The O2 abundance varies as \( \langle n_{H2}/\zeta \rangle^{1/2} \). For \( n_{H2}/\zeta_{-17} = 100 \text{ cm}^{-3} \), equation (9) gives \( n(O2)/n_{H2} = 1.1 \times 10^{-6} \), close to 3.0 \times 10^{-7}, which is computed numerically.

The O2 density, as given by equation (9), is sufficiently small for removal of S+ by O2 to be negligible compared to radiative recombination. This can be seen by considering the ratio of the S+ removal rates, equation (9) is valid so long as cosmic-ray photons dominate the removal of the C atoms. When this occurs the C density becomes small, and the O2 density must become large (see eq. [5]). We identify this as the point where O2 becomes sufficiently abundant to begin removing the S+. However, because H3+ continues to be removed by dissociative recombination, the H3+ - O2-S+ instability cycle turns on at this point, and a stable HIP is no longer possible.

Thus, the HIP can be maintained so long as the O2 density given by equation (9) is small enough for cosmic-ray photo-ionization to dominate the removal of the C atoms. This condition,

\[ \frac{k_{22} n(O2)}{k_{17} n(e)} = \frac{2X_{O2} X_{He}^{1/2} k_{6}}{k_{12} X_{He}^{1/2} k_{3,4} d_{OH} p_{18}} \left( \frac{n_{He}}{\zeta_{-17}} \right)^{1/2} < 1, \]  

(11)

provides a maximal density for HIP solutions. For our standard elemental abundances and rate coefficients,

\[ \left( \frac{n_{He}}{\zeta_{-17}} \right)_{\text{max}} = 7.63 \times 10^2 \text{ cm}^{-3}. \]  

(12)

This is slightly larger than our numerically computed density of 675 cm^{-3} at which the transition to the LIP occurs (see Fig. 1).

For consistency we must verify that dissociative recombination dominates the removal of H3+ for densities as high as \( \langle n_{H2}/\zeta \rangle_{\text{max}} \). Dissociative recombination dominates when the ratio

\[ \frac{k_{3,4 n(e)}}{k_{3,4 n(CO)}} = \left( \frac{X_{He}}{k_{17}} \right)^{1/2} \frac{X_{He}}{k_{3,4}} \frac{1}{X_C} \left( \frac{\zeta}{n_{H2}} \right)^{1/2} \gg 1, \]  

(13)

where \( k_{3,4} = 1.7 \times 10^{-6} \text{ cm}^3 \text{s}^{-1} \) is the rate coefficient of reaction (R5). For \( \langle n_{H2}/\zeta \rangle_{\text{max}} = 7.63 \times 10^2 \text{ cm}^{-3} \) this ratio equals 8.0, so consistency is obtained.

4.2. LIP and \( n_{\text{min}} \)

In the LIP, the electron density must be sufficiently small for CO to dominate the removal of H3+, and the O2 density must be sufficiently large for O2 to dominate the removal of S+. We now show that these conditions can be satisfied, provided the gas density is greater than a critical minimum density.

To show this, we first derive an expression for the electron density assuming that S+ is removed by abundant O2, with an upper limit for the O2 density set by cosmic-ray--induced photo-dissociation. We show that CO then dominates the removal of H3+ for densities greater than a minimum critical density. We then verify that the assumption that O2 dominates the removal of S+ is consistent for densities greater than this critical density.

For the electron density in the LIP we again assume that \( n(e) = n(S^+) \). In the LIP, S+ is produced by cosmic-ray--induced photoionization, and we assume that it is removed by O2. This gives

\[ n(e)/n_{H2} = \frac{2X_{sp} p_{21}}{k_{22} n(O2)}, \]  

(14)

where \( p_{21} = 2.0 \times 10^3 \) is the efficiency of reaction (R21). H3+ is removed by CO, so that

\[ n(H3^+)/n_{H2} = \left( \frac{\zeta}{k n(CO)} \right) = \left( \frac{1}{k} \right) \frac{\zeta}{n_{H2}} = 2.2 \times 10^{-5} \zeta_{-17}/n_{H2}. \]  

(15)

where we have assumed that in the LIP all of the carbon is locked in CO. For \( n_{He}/\zeta_{-17} = 10^2 \), equation (14) gives \( n_{He}/n_{H2} = 2.2 \times 10^{-8} \), in good agreement with the numerically computed 1.0 \times 10^{-8}. 
For $O_2$ we again assume the production sequence (R6)–(R11). If the $O_2$ is removed by only cosmic-ray—induced photodissociation,

$$\frac{n(O_2)}{n_{H_2}} = \frac{n(H_3^+)n(O)k_{dOH}}{\zeta p_{13}n_{H_2}} = \frac{k_8}{k_5} \frac{1}{p_{13}} \frac{d_{OH}}{X_O} \frac{X_O}{X_C} = 2.3 \times 10^{-4},$$

(16)

where $p_{13} = 1.7 \times 10^3$ is the efficiency of reaction (R13). This is actually an upper limit for the $O_2$ abundance because additional chemical reactions contribute to the removal of the $O_2$ in the LIP. In this approximation the $O_2$ density is independent of $n_{H_2}/\zeta$, consistent with our numerical computations (see Fig. 1). Because the upper limit is close to the total available oxygen not locked in CO, we set $n(O_2)/n_{H_2} = 2f_{o_2}/X'_O$, where the $O_2$ fraction $f_{o_2}$ is 1. In our numerical computation $f_{o_2} \approx 0.2$ (see Fig. 1).

The electron fraction, $x_e$, is then

$$\frac{n(e)}{n_{H_2}} = \frac{X_S}{X_O} \frac{1}{k_{22}f_{o_2}/n_{H_2}} = 7.4 \times 10^{-5} \frac{1}{f_{o_2}} \frac{1}{n_{H_2}} \frac{1}{\zeta}. $$

(17)

In this limit $x_e$ varies as $(n_{H_2}/\zeta)^{-1}$. For $f_{o_2} = 0.2$, equation (17) gives $x_e = 3.7 \times 10^{-7}$, in good agreement with $4.1 \times 10^{-7}$ in Figure 1.

The electron density as given by equation (17) is independent of $n_{H_2}$, whereas the CO density decreases with $n_{H_2}$. Reactions with CO can therefore dominate the removal of $H_3^+$ only down to a minimal density set by the condition

$$k_{57}(CO) \frac{n(O)}{k_{47}n(e)} = \frac{2X_O}{X_S} \frac{k_{22}}{k_{47}p_{21}} \frac{1}{f_{o_2}} \frac{m_{H_2}}{\zeta} > 1.$$  

(18)

This relation provides a minimal critical density

$$\left(\frac{n_{H_2}}{\zeta} \right)_{\text{min}} = \frac{28}{f_{o_2}} \text{ cm}^{-3}$$

(19)

for which LIP solutions are possible. For $f_{o_2} = 0.2$, this is slightly smaller than the numerically computed value of $370 \text{ cm}^{-3}$ at which the transition from the LIP to HIP occurs (see Fig. 1). When the gas density falls below the critical density, electrons remove $H_3^+$, but $O_2$ continue to remove $S^+$. The $H_3^+-O_2-S^+$ instability cycle therefore turns on, and the gas is driven from the LIP to the HIP.

For consistency we must now verify that reactions with $O_2$ dominate the removal of $S^+$ everywhere in the LIP. This requires that

$$k_{22}(O_2) \frac{n(O_2)}{k_{17}n(e)} = \frac{2X_O^2}{X_S} \frac{k_{22}^2}{k_{17}p_{21}} \frac{m_{H_2}}{\zeta} = 5.1f_{O_2} \frac{m_{H_2}}{\zeta} \gg 1$$

(20)

for all LIP densities, down to the minimal density. Inserting $(n_{\zeta-17})_{\text{min}}$ as given by equation (19) gives $k_{22}(O_2)/k_{17}n(e) = 142/f_{o_2}$. We conclude that consistent LIP solutions are obtained even for $f_{o_2}$ as small as $\sim 0.01$ (for which the $O_2$ density in the LIP is still much larger than in the HIP).

5. SCALING

The key result of the above analysis is that for our standard parameters $(n_{\zeta-17})_{\text{max}}$, as given by equation (12), is greater than $(n_{\zeta-17})_{\text{min}}$, as given by equation (19). The gas is therefore bistable between the maximal HIP density and the minimum LIP density. The MIX branch must therefore “switch back” from the maximal HIP density to the minimal LIP density.

For $O_2$ we again assume the production sequence (R6)–(R11). If the $O_2$ is removed by only cosmic-ray—induced photodissociation,
density. An HIP can therefore be maintained to higher densities before O₂ becomes significant in removing S⁺. An increased H₃⁺ recombination efficiency also implies that electrons become competitive with CO in removing H₃⁺ at larger densities in the LIP. Quantitatively, equation (11) shows that (n_{H₂}/C⁻)_{max}, the density above which O₂ begins removing S⁺, is proportional to k₃.₄/n₁. However, (n_{H₂}/C⁻)_{min}, the density below which electrons begin removing the H₃⁺, varies only linearly with k₃.₄. Therefore, as k₃.₄ is increased, (n_{H₂}/C⁻)_{max} falls below (n_{H₂}/C⁻)_{min} and bistability disappears. As k₃.₄ is increased, (n_{H₂}/C⁻)_{max} grows more rapidly and eventually exceeds (n_{H₂}/C⁻)_{min}, and the gas becomes bistable for an increasing range of densities. For example, if k₃.₄ is increased by a factor of 5 relative to our standard value, Figure 4 shows that (n_{H₂}/C⁻)_{max} increases by about a factor of 25, and (n_{H₂}/C⁻)_{min} increases by about a factor of 5. This is consistent with expressions (11) and (18).

A similar scaling analysis may be carried out for the other parameters that control (n_{H₂}/C⁻)_{min} and (n_{H₂}/C⁻)_{max}. For example, if the oxygen abundance is reduced, our analysis shows that the regime of bistability should move to higher values of (n_{H₂}/C⁻) as found numerically by Viti et al. (2001; see their Figs. 5 and 7). For a lower oxygen abundance (n_{H₂}/C⁻)_{max} is increased because the HIP can be maintained to a higher density before O₂ becomes abundant enough to remove the atomic ions. The reduced O₂ density leads to a higher electron density in the LIP, so (n_{H₂}/C⁻)_{min} is increased as well.

Our numerical and analytic results show how the onset of the H₃⁺-O₂-S⁺ instability cycle depends on the O₂ and electron densities as determined by the elemental abundances and by the H₃⁺ dissociative recombination rate coefficient. However, Figure 4 reveals an additional interesting feature. For k₃.₄ equal to 0.2 times our standard value, the gas again becomes marginally bistable at (n_{H₂}/C⁻) ≈ 9 cm⁻³. At such low densities the dominant atomic ion in the HIP is C⁺ rather than S⁺ (see Fig. 1). The instability, and the transition from HIP to LIP, is therefore modified by the addition of an identical H₃⁺-O₂-C⁺ cycle, with reactions (R19) and (R20) operating to neutralize the C⁺. The behavior in this numerical example is a bit more complicated because S⁺ is still the dominant ion in the LIP at the transition density. We note that at such low densities realistic clouds would likely become “diffuse” and optically thin to external FUV radiation, with a resulting reduction in O₂ and further modifications to the chemistry. We do not consider such effects here.

6. GAS-GRAIN RECOMBINATION

We have shown that bistability arises in purely gas-phase models, consistent with previous findings. When the HIP and LIP solutions “overlap,” neutralization of atomic ions (S⁺ in our models) proceeds by either slow radiative recombination in the HIP or via the formation of intermediate molecular ions (S⁺ + O₂ → SO⁺ + O) followed by rapid dissociative recombination in the LIP. The two solutions are separated by a chemical instability, which we have identified in our models as the H₃⁺-O₂-S⁺ cycle.

Our analysis suggests that bistability will be damped, or eliminated entirely, if additional neutralization processes are included that interrupt the H₃⁺-O₂-S⁺ cycle. We demonstrate this by considering how the single process of “grain-assisted recombination” of atomic ions affects the chemistry. In this process, atomic ions recombine via electron transfer from grains to the ions during collisions with the grains (Draine & Sutin 1987; Weingartner & Draine 2001). The grain-assisted recombination rate may be expressed as k₉μ_plot, where μ_plot is the total density of hydrogen nuclei. For any ion, k₉ is an effective rate coefficient that depends on the dust-to-gas ratio, grain size distribution, grain charge, and gas temperature. This process dominates radiative recombination when 2k₉ > k₉x_s, where k₉ is the radiative recombination rate coefficient. For k₉ ≈ 10⁻¹¹ cm³ s⁻¹ (appropriate for S⁺) and a fractional ionization x_s ≈ 10⁻³, it occurs for densities near (n_{H₂}/C⁻)_{max} in our computation (see Fig. 1), grain-assisted recombination dominates radiative recombination for k₉ ≈ 5 × 10⁻¹¹ cm³ s⁻¹. This is well below the maximum values of k₉ ≈ 10⁻¹⁴ cm³ s⁻¹ found by Weingartner & Draine, so this process is potentially relevant in determining the ionization balance.

Furthermore, grain-assisted recombination will interfere with the H₃⁺-O₂-S⁺ cycle and render it ineffective when k₉ > f₀₂x_s/k₂₂, where, as previously defined, f₀₂x_s is the fraction of oxygen bound in O₂ and k₂₂ = 1.5 × 10⁻¹¹ cm³ s⁻¹ is the rate coefficient of reaction (R22). For k₉ ≈ 0.2 and x_s = 1.5 × 10⁻³, the H₃⁺-O₂-S⁺ instability cycle is quenched when k₉ ≈ 5 × 10⁻¹⁰ cm³ s⁻¹. Bistability and the sharp transition from HIP to LIP should then disappear.

We illustrate this in Figure 5, where we plot x_s versus n_{H₂}/C⁻, for k₉ ranging from zero (as in Figs. 1 and 4) to 1.0 × 10⁻¹⁴ cm³ s⁻¹, for all atomic ions. All other parameters are as in the calculation in § 2. As k₉ is increased, the diminished electron density leads to more H₃⁺ and O₂ in the HIP, so that (n_{H₂}/C⁻)_{max} is reduced. Similarly, the onset of dissociative recombination in the LIP occurs at lower densities, and (n_{H₂}/C⁻)_{min} is reduced. Thus, at first the bistability region shifts to lower densities as k₉ is increased. However, as estimated above, when k₉ exceeds ~3 × 10⁻¹⁶ cm³ s⁻¹, bistability is eliminated entirely, because the H₃⁺-O₂-S⁺ (and H₃⁺-O₂-C⁺) cycles are fully quenched, and neutralization occurs entirely by grain recombination.

These results strongly suggest that for realistic clouds, in which gas-grain neutralization is a likely important process, bistability will not occur. The precise value of k₉ in dark clouds may be variable, as the grain population can be modified by coagulation (Draine 1985; Flower et al. 2005) and other processes. However, even with the removal of all grains with sizes below ~15 Å, the rate coefficient k₉ ≈ 10⁻¹² cm³ s⁻¹ (e.g., McKee 1989), which is sufficiently large to suppress bistability. We thus confirm and explain the results of Shalabiea & Greenberg (1995), who found that bistability is eliminated when gas-grain
processes, including grain-assisted recombination, are incorporated in the numerical computations.

7. SUMMARY

The nonlinearity of equations (1)–(4) is a mathematical prerequisite for bistability and the appearance of multiple solutions (Le Bourlot et al. 1993, 1995a, 1995b; Lee et al. 1998; Pineau des Forêts & Roueff 2000; Charnley & Markwick 2003). However, the purpose of our paper has been to identify and analyze the chemical mechanisms underlying the bistability phenomenon. We have shown that a simple chemical instability, involving atomic ions (typically S⁺), O₂ molecules, and H₃⁺ ions, allows multiple solutions to appear near the transition points from low-density high-ionization (HIP) to high-density low-ionization (LIP) conditions in the gas-phase chemistry. The instability drives the O₂ density to either small (HIP) or large (LIP) values. Bistability occurs when a low O₂ abundance in the HIP can be maintained up to maximal densities that are greater than the minimal densities above which a large O₂ density is maintained in the LIP.

Two modes of neutralization are then simultaneously available to the gas. The slow (HIP) mode is radiative recombination (usually S⁺ + e → S + ν).

The fast (LIP) mode is formation of molecular ions followed by dissociative recombination (usually S⁺ + O₂ → SO⁺ + O, SO⁺ + e → S + O).

We have derived simple analytic scaling relations for the range of gas densities and ionization rates for which bistability occurs. Our formulae show how the bistable range depends on the assumed gas-phase abundances and several reaction rate coefficients, including the dissociative recombination rate coefficient of H₊. Bistability is eliminated when the two modes of gas-phase neutralization are superseded by gas-grain processes such as grain-assisted recombination of the atomic ions. This likely happens for the range of electron and O₂ densities in which bistability typically occurs in purely gas-phase models. We conclude that the bistability phenomenon probably does not occur in realistic dusty interstellar clouds, although it remains of theoretical interest.

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