



A CHEMICAL KINETICS NETWORK FOR LIGHTNING AND LIFE IN PLANETARY ATMOSPHERES

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ABSTRACT

There are many open questions about prebiotic chemistry in both planetary and exoplanetary environments. The increasing number of known exoplanets and other ultra-cool, substellar objects has propelled the desire to detect life and prebiotic chemistry outside the solar system. We present an ion–neutral chemical network constructed from scratch, STAND2015, that treats hydrogen, nitrogen, carbon, and oxygen chemistry accurately within a temperature range between 100 and 30,000 K. Formation pathways for glycine and other organic molecules are included. The network is complete up to H₆C₂N₂O₃. STAND2015 is successfully tested against atmospheric chemistry models for HD 209458b, Jupiter, and the present-day Earth using a simple one-dimensional photochemistry/diffusion code. Our results for the early Earth agree with those of Kasting for CO₂, H₂, CO, and O₂, but do not agree for water and atomic oxygen. We use the network to simulate an experiment where varied chemical initial conditions are irradiated by UV light. The result from our simulation is that more glycine is produced when more ammonia and methane is present. Very little glycine is produced in the absence of any molecular nitrogen and oxygen. This suggests that the production of glycine is inhibited if a gas is too strongly reducing. Possible applications and limitations of the chemical kinetics network are also discussed.

Key words: astrobiology – atmospheric effects – molecular processes – planetary systems

Supporting material: machine-readable tables

1. INTRODUCTION

The potential connection between a focused source of energy and life was first made apparent in the Miller–Urey experiment (Miller 1953), set to test a hypothesis proposed by Haldane (1928). In this experiment, a gas composed of water vapor, ammonia, methane, and molecular hydrogen was circulated past an electric discharge. After a week’s time, various biologically relevant chemicals had developed, including glycine and alanine, identified with a paper chromatogram. A follow-up study of Miller’s samples, carried out approximately 50 years later, discovered a much richer variety of prebiotic compounds than originally thought (Johnson et al. 2008). Since then, numerous related experiments have been carried out under a variety of conditions (see Miller & Urey 1959; Cleaves et al. 2008, and references therein).

The input energy source and the initial chemistry have been varied across these different experiments. An energy source may have been important for the production of prebiotic species on Earth, because the pathways to formation have considerable activation barriers, often on the order of 0.1–1 eV. Patel et al. (2015) generated prebiotic species by exposing HCN and H₂S to ultraviolet light. The experimental results from Powner et al. (2009) suggest that the aqueous synthesis of amino acids, nucleobases, and ribose is predisposed, starting from glyceraldehyde and glycoaldehyde, which they suggest would most likely form through heating and UV irradiation. Shock synthesis of amino acids due to the atmospheric entry of cometary meteors and micrometeorites or thunder is also sufficient to overcome these barriers and produce amino acids (Bar-Nun et al. 1970).

The initial chemical conditions are naturally significant to the formation of prebiotic chemistry. Of course, in an environment where hydrogen or carbon were lacking, there would be no complex hydrocarbons. Nitrogen and phosphorus are also essential to the origins of terrestrial life, although some

scientists, such as Benner et al. (2004), have speculated that life could occur under very different chemistries; presently, we lack the ability to explore this possibility. The initial chemical composition also has an effect on the production of prebiotic chemical species. For example, hydrogen can be bound in a reducing species, CH₄, in an oxidizing species, H₂SO₄, or into the neutral species of water (H₂O). Both Schlesinger & Miller (1983) and Miyakawa et al. (2002) have found that performing a Miller–Urey-like experiment in an oxidizing environment produces only trace amounts of prebiotic materials, whereas performing the experiment in a reducing environment produces a great number of prebiotic materials.

The atmosphere of Earth in its present state is oxidizing ($\approx 21\%$ O₂, 78% N₂). The atmosphere of the Earth during its first billion years (first 1 Gyr) would have had a very different composition, probably oxidizing or at least only weakly reducing (Kasting 1993), although Tian et al. (2005) suggest that the Earth’s atmosphere was once highly reducing. Even if the Earth never possessed a strongly reducing atmosphere, other planets and moons are known to have both reducing atmospheres and active lighting and UV photochemistry, such as Jupiter, for example. Extrasolar planets may not simply have diverse compositions, but also widely varied gas-phase C/O ratios, either intrinsically at formation, as may be the case with Wasp-12b, XO-1b, and CoRoT-2b (Madhusudhan et al. 2011; Moses et al. 2013), and possibly the interior of 55 Cancri e (Madhusudhan et al. 2012; but see also Nissen 2013); or alternatively due to oxygen depletion into the cloud particles (Bilger et al. 2013; Helling et al. 2014). The question of the C/O ratio is not a settled matter (Benneke 2015).

These diverse planetary and exoplanetary environments provide unique “laboratories” within which to explore prebiotic chemistry. There are many potential drivers for prebiotic chemistry in planets and exoplanets, from the steep thermal gradients in hot Jupiters and close-in super-Earths to the thermal production of organics and complex hydrocarbons in

Saturn's storms (Moses et al. 2015) and photochemical production of complex organics in Titan (Yung et al. 1984; Loison et al. 2015). There is some evidence that cosmic rays drive the formation of hydrogen cyanide in Neptune (Lellouch et al. 1994). Molina-Cuberos et al. (1999) have proposed pathways to formation of a rich variety of nitriles via cosmic rays in Titan's atmosphere.

As mentioned above, electric discharges may also be an important source of energy driving the production of prebiotic species, and are ubiquitous throughout the gas giants. Discharges in the form of lightning are known to occur within our solar system, on Earth, Jupiter (Little et al. 1999), Saturn (Dyudina et al. 2007), Uranus (Zarka & Pedersen 1986), and Neptune (Gurnett et al. 1990). There are some indications of lightning discharges on Venus (Taylor et al. 1979), and possibly also in Titan's nitrogen chemistry (Borucki et al. 1984), although these traces are still tentative. Lightning is hypothesized to occur on exoplanets (Aplin 2013; Helling et al. 2013) and brown dwarfs (Helling et al. 2013; Bailey et al. 2014). Simulated plasma discharges initiated within Jupiter-like gas compositions suggest that lightning on Jupiter may produce a significant amount of trace gases (Borucki et al. 1985). The comparison between experimental rates of the production of organic compounds in high-temperature plasmas to chemical equilibrium models is unsurprisingly poor (Scattergood et al. 1989), and indicates that a chemical kinetics approach will be important in explaining the results of these experiments. Chemical kinetics seems to be necessary for exploring any of these pathways to the formation of prebiotic species.

Chemical kinetics models have been applied to planetary and exoplanetary atmospheric conditions in such a diverse range that it is impractical to provide complete references, so a brief summary of the work will instead be provided. Photochemical models of the modern Earth have been applied in the context of one-dimensional (1D) models (Owens et al. 1985), up to fully coupled three-dimensional (3D) general circulation models (Roble & Ridley 1994), and even within a flexible modular framework that can be included as a module within other codes (Sander et al. 2005). The Earth's atmosphere during its first billion years has been extensively modeled (Zahnle 1986; Kasting 1993). Chemical kinetics models have also been applied to Jupiter's atmosphere, from the deep atmosphere (Fegley & Lodders 1994; Visscher et al. 2010) through the stratosphere (Zahnle et al. 1995; Moses et al. 2005). The atmosphere of the moon Titan has also been analyzed using ion-neutral chemical kinetics to better explain the abundance of rich hydrocarbons in its atmosphere and its stratospheric haze (Yung et al. 1984; Keller et al. 1998; Lavvas et al. 2008a, 2008b).

Chemical kinetics models for exoplanetary atmospheres have typically been developed for hot Jupiters, especially HD 189733b and HD 209458b (Zahnle et al. 2009; Moses et al. 2011; Venot et al. 2012). Almost all of the models for hot Jupiters have been applied only in two dimensions, and so have not taken a more complete account of the atmospheric dynamics, instead relying on a parameterization of vertical mixing using the eddy diffusion coefficient, K_{zz} [$\text{cm}^2 \text{s}^{-1}$] (see Lee et al. 2015, their Section 4.2). Agúndez et al. (2014) have taken on the ambitious task of coupling a chemical kinetics model to two-dimensional (2D) dynamics for both HD 189733b and HD 209458b. Ion-neutral models have been

applied to exoplanets, taking into account photochemistry (Lavvas et al. 2014) and additionally cosmic-ray ionization (Walsh & Millar 2011; Rimmer et al. 2014). Chemical kinetics models have also been applied to the extrasolar super-Earths (Hu et al. 2012, 2013; Hu & Seager 2014), and have been used to explore possible biosignatures on rocky planets (Seager et al. 2013a, 2013b). There has also been some recent investigation into chemistry on helium-dominated exoplanets (Hu et al. 2015).

Lightning chemistry has been explored with some basic chemical kinetics models, e.g., within Earth's mesosphere (Luque & Ebert 2009 and Parra-Rojas et al. 2013) and Saturn's lower ionosphere (Dubrovina et al. 2014). Dubrovina et al. (2014) present interesting results for Saturn's lower ionosphere, predicting that TLEs within this region would produce mostly H_3^+ , what they identify as the primary positive charge carrier during the duration of the TLE and for sometime after. This would mimic the effect of cosmic-ray ionization. Parra-Rojas et al. (2013) presented similar results involving terrestrial nitrogen chemistry. The products of discharge chemistry in the upper part of both hydrogen-rich and nitrogen-rich atmospheres seem to be similar to the products of cosmic-ray chemistry in these same atmospheres.

There are many open questions about prebiotic chemistry in diverse planetary and exoplanetary environments, as well as in the lab. In this paper, we present a candidate network for exploring UV photochemistry, cosmic-ray chemistry, and lightning-driven chemistry, constructed from scratch. We will mostly explore the photochemistry and thermochemistry within this paper, leaving the exploration of lightning-driven chemistry and cosmic-ray chemistry to future work.

The largest task in developing this network has been the collation of a full set of chemical reactions that treat both reducing and oxidizing chemistries at temperatures ranging from 100 K through 30,000 K (the approximate peak temperature of lightning, see Orville 1968; Price et al. 1997) and the selection of rate constants when more than one is published. Since one interest is the investigation of the formation rate of prebiotic species in diverse environments, the network is made extensive enough to include the simplest amino acid, glycine. In this paper, we present this chemical network (STAND2015), and test in a diversity of environments. For these tests, we developed a simple 1D photochemistry/diffusion code (ARGO). ARGO was developed based on NAHOON (Wakelam et al. 2012) by including wavelength-dependent photochemistry, cosmic-ray transport, water condensation, and chemical mixing.

The STAND2015 network is presented in Section 2. We compare the predictions of our network using a simplified 1D photochemistry/diffusion code called ARGO (Section 3). The model and network are then combined and tested against other model results for HD 209458b and the early Earth, and compared to observation for Jupiter and the present-day Earth in Section 4. Finally, in Section 5 we simulate a Miller-Urey-type experiment and explore the formation of glycine under various chemical conditions. Section 6 contains a short discussion of the results and possible future applications of this model.

2. THE CHEMICAL NETWORK

The STAND2015 Atmospheric Chemical Network is an H/C/N/O network with reactions involving He, Na, Mg, Si, Cl, Ar, K, Ti, and Fe, developed from scratch. It contains all known

reactions for species of up to six hydrogen, two carbon, two nitrogen, and three oxygen atoms, for which a rate constant has been published, as well as a less complete network involving species with three or more carbon atoms, three nitrogen atoms, and/or four oxygen atoms. A chemical network is effectively a list of chemical reactions and reaction rate constants. Rate constants are used to calculate the rates of production and loss of a particular molecular or ionic species, P_i [$\text{cm}^{-3} \text{s}^{-1}$] and L_i [$\text{cm}^{-3} \text{s}^{-1}$], respectively, and i is enumerated over the list of species. Rate constants are of zeroth order (e.g., source terms, S_i [$\text{cm}^{-3} \text{s}^{-1}$]), first order (involving interactions with particles not accounted in the network, such as photons or cosmic rays, k_1 [s^{-1}]), second order (collisions between particle i and other particles within the network, k_2 [$\text{cm}^3 \text{s}^{-1}$]), or third order (collisions between particle i and other particles, as well as a third body, denoted here as k_3 [$\text{cm}^6 \text{s}^{-1}$]). The rates of production and loss for a given species, i , in terms of rate constants, are generally:

$$P_i = S_i + \sum k_1 n_j + \sum k_2 n_j n_k + \sum k_3 n_{\text{gas}} n_j n_k, \quad (1)$$

$$L_i = \sum k_1 n_i + \sum k_2 n_j n_i + \sum k_3 n_{\text{gas}} n_j n_i. \quad (2)$$

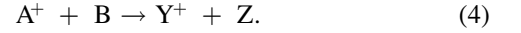
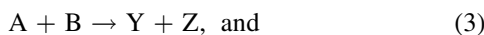
Summation is over all the relevant reactions, some involving species j and/or k , that result in the production (Equation (1)) or loss (Equation (2)) of species i . The symbol n_i [cm^{-3}] denotes the number density of species i and n_{gas} [cm^{-3}] denotes the total gas number density.

The reaction rate constants have been assembled from various databases. With only a couple hundred exceptions, the rate constants for two-body and three-body neutral reactions have been assembled from the NIST Chemical Kinetics Database (Manion et al. 2013). Virtually all of the ion–neutral reactions were taken from Ikezoe et al. (1987). Several rate constants that we have used, relevant for terrestrial atmospheric chemistry, are taken from Sander et al. (2011). The KIDA database provided the rate constants for several dissociative recombination reactions (Wakelam et al. 2012). Coefficients for the cosmic-ray ionization rate constant were taken from the OSU chemical network (Harada et al. 2010).

Rate constants were compared to the publicly available networks of Moses et al. (2011) and Venot et al. (2012), and ion–neutral rate coefficients were checked against the KIDA database (Wakelam et al. 2012)¹, as well as the OSU 09 2010 high-temperature network (Harada et al. 2010).² Some further ion–neutral reactions involving the alkali ion chemistry were appropriated from Lavvas et al. (2014). Finally, ~ 20 more reactions for suspected formation pathways for glycine have been added to the network, from Blagojevic et al. (2003) and Patel et al. (2015). The full network and references are provided in Appendix A. The following subsections contain brief discussions about the different classes of reactions, their rate coefficients and whether reverse reactions have been included.

2.1. Two-body Neutral–Neutral and Ion–Neutral Reactions

Two-body neutral–neutral and ion–neutral reactions follow the basic scheme:

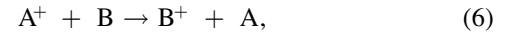


The rate constants for these reactions are approximated by the Kooij equation (Kooij 1893):

$$k_2 = \alpha \left(\frac{T}{300 \text{ K}} \right)^\beta e^{-\gamma/T}, \quad (5)$$

where T [K] is the gas temperature³, k_2 [$\text{cm}^3 \text{s}^{-1}$] is the rate constant, and α [$\text{cm}^3 \text{s}^{-1}$], β , and γ are constants characterizing the reaction. All of these reactions are reversed in our network and we use the rate coefficients for the best characterized direction for each reaction, which is typically the exothermic direction. For neutral–neutral reactions, even when exothermic, there is often a sizable barrier to reaction, allowing certain elements to be locked into non-equilibrium configurations at low temperatures effectively for eternity, because the barrier to the lower energy state is too large to be overcome in the current environment.

Ion–neutral reactions do not typically have barriers in the exothermic direction, and in many cases the rate constants are altogether temperature-independent, closely approximating the Langevin approximation. A notable exception are charge-exchange reactions,



which, due to the differences in energy between ionic and neutral ground states, often contains barriers on the order of a few $\times 100$ K.

The rate constants for the forward reactions are given in Appendix A with the label “2n,” reactions 577–1352. These reactions are reversed following the scheme described in Appendix B. The ion–neutral reactions are also reversed, and are listed in Appendix A with “2i,” reactions 1353–2569.

2.2. Three-body Neutral Reactions, Dissociation Reactions, and Radiative Association Reactions

Reactions that involve a third body occur primarily in the two forms:



where M represents any third body. Decomposition reactions are well studied at high temperatures, being important for various combustion processes. Just as in Section 2.1, we choose the reactions best characterized, which in this case often involve endothermic reactions. The rate coefficients for the majority of these reactions follow the Lindemann form (Lindemann et al. 1922). In this form, we first determine the rate constants in the low-pressure (k_0 [$\text{cm}^6 \text{s}^{-1}$]) and high-pressure (k_∞ [$\text{cm}^3 \text{s}^{-1}$]) limits:

$$k_0 = \alpha_0 \left(\frac{T}{300 \text{ K}} \right)^{\beta_0} e^{-\gamma_0/T}, \quad (9)$$

$$k_\infty = \alpha_\infty \left(\frac{T}{300 \text{ K}} \right)^{\beta_\infty} e^{-\gamma_\infty/T}. \quad (10)$$

¹ <http://kida.obs.u-bordeaux1.fr/>

² <http://faculty.virginia.edu/ericherb/research.html>

³ Surface chemistry is not considered in this paper, and the temperature of all chemical species including electrons is set equal to the gas-phase temperature.

These are combined with the number density of the neutral third species, $[M]$ [cm^{-3}] to determine the reduced pressure, $p_r = k_0[M]/k_\infty$, and this can then be utilized to set the pressure-dependent effective “two-body” rate:

$$k_2 = \frac{k_\infty p_r}{1 + p_r}. \quad (11)$$

Sometimes this expression is multiplied by a dimensionless function $F(p, T)$ to more accurately approximate the transition between the low-pressure and high-pressure limits, and this provides the Troe form (Troe 1983). The coefficients for the Troe form are not explicitly given.

We favor using the rate constants for three-body combination reactions, and reversing these reactions to determine the rate of thermal decomposition. In many cases, however, the rate constants are unavailable. When we have only the rate coefficients for the decomposition reactions, we add an additional 500 K barrier to both the decomposition and three-body combination rate constants. This barrier is added in order to limit runaway three-body reactions that can result from reversing decomposition reactions at low temperatures.

Additionally, we incorporate a small number of radiative association reactions, of the form:



where γ is the radiated photon that carries the excess energy from the association. We appropriate the Kooij form for this reaction, as with two-body neutral–neutral reactions, in order to determine the rate constant k_{ra} [$\text{cm}^3 \text{s}^{-1}$]. We then apply this rate constant, along with the rate constant for the corresponding three-body reaction, to the adduct form of the overall rate constant (Hébrard et al. 2013, their Equation (B.2)):

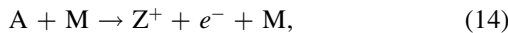
$$k = \frac{(k_0[M]F + k_r)k_\infty}{k_0[M] + k_\infty}, \quad (13)$$

where the function F is from the Troe form of the transition from high to low pressure.

The rate constants for the forward reactions are given in Appendix A with the labels “2d” for the neutral species and “3i” for ion–neutral species. These reactions are reversed in the manner described by Appendix B. Reactions 1–420 are reactions of this type, for which each odd number reaction gives the low-pressure rate constant k_0 [$\text{cm}^6 \text{s}^{-1}$] and each even number reaction gives the high-pressure rate constant k_∞ [$\text{cm}^3 \text{s}^{-1}$]. Reactions labeled “ra” are radiative association reactions, numbered 2974–2980.

2.3. Thermal Ionization and Recombination Reactions

A special set of three-body reactions are thermal ionization and three-body recombination reactions, which proceed by the pair of equations (analogous to Equations (7) and (8)):



For which we again use published rates wherever possible for the ionization reactions, (Equation (14)), but in many cases

here use the simple approximation:

$$k_0 = \left(\frac{8\pi e^8}{m_e k_B T} \right)^{1/2} e^{-I/k_B T}, \quad (16)$$

where $e = 4.9032 \times 10^{-10}$ esu is the elementary charge, $k_B = 1.38065 \times 10^{-16}$ erg K^{-1} is the Boltzmann constant, $m_e = 9.1084 \times 10^{-28}$ g is the mass of the electron, and I is the ionization energy (here in units of erg) which we determine from the change in the Gibbs free energy for the reaction. k_∞ is then estimated from k_0 .

Three-body recombination and ionization reactions have been well studied, and in many cases have well characterized rate constants. Here we treat the three-body recombinations as the reverse reactions for the collisional ionization reactions, but the studied rate coefficients for these reactions generally have a temperature dependence of $T^{-4.5}$, at least for $T > 1$ K (Hahn 1997). This creates a problem for reversibility. Using these rates will not allow us to reproduce chemical equilibrium for plasmas and this is largely because we are not properly treating the time-dependent plasma conditions in which these rates are often measured. Many of these rate constants may accurately describe the time to achieve an equilibrium electron density in a regime where a strong ionizing source has recently been removed from the environment.

With this in mind, we instead set the recombination rate constants such that, when dissociative recombination reactions are disabled, the Saha equation is upheld.

These reactions and rate coefficients are also given in Appendix A. The ionization reactions are labeled “ti” and numbered 421–576. As with Section 2.2, the odd reactions are k_0 [$\text{cm}^6 \text{s}^{-1}$] and the even numbers are k_∞ [$\text{cm}^3 \text{s}^{-1}$].

Finally, we include a series of dissociative recombination reactions, which take the form:



These have rate constants parameterized in the form of Equation (5). The reverse reactions can in principle be calculated, and their rate constants could be calculated straightforwardly using the same principles used for the three-body reactions. This would effectively be analogous to the rates of three-body recombination for any third body, and we do not find that reversing these reactions changes the results much. When we compare with chemical equilibrium, however, we disable these reactions. The dissociative recombination reactions are taken only from the OSU 09 2010 high-temperature network (Harada et al. 2010), and shown in Appendix A, numbered 2777–2973, and labeled “dr.”

2.4. Photochemistry and Cosmic-ray Chemistry

Photochemistry is considered for the species H, H^- , He, C, $\text{C}^{(1\text{D})}$, $\text{C}^{(1\text{S})}$, N, O, $\text{O}^{(1\text{D})}$, $\text{O}^{(1\text{S})}$, H^- , C_2 , CH, CN, CO, H_2 , N_2 , NO, O_2 , OH, CO_2 , H_2O , HO_2 , HCN, NH_2 , NO_2 , O_3 , C_2H_2 , H_2CO , H_2O_2 , NH_3 , NO_3 , CH_4 , HCOOH, HNO_3 , N_2O_3 , C_2H_4 , C_2H_6 , CH_3CHO , C_4H_2 , C_4H_4 , Na, K, and HCl. The photoionization and photodissociation cross sections are taken almost entirely from PHIDRATES⁴ (Huebner & Carpenter 1979; Huebner et al. 1992; Huebner & Mukherjee 2015), with the exception of C_4H_2 , C_4H_4 , and N_2O_3 , the cross sections of

⁴ phidrates.space.swri.edu

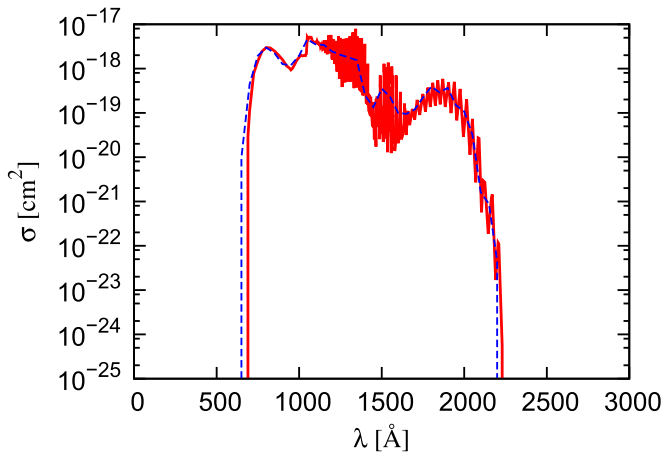


Figure 1. Photodissociation cross sections of $\text{NH}_3 \rightarrow {}^1\text{NH} + \text{H}_2$, σ [cm^2], as a function of wavelength, λ (\AA), from PHIDRATES (original data from McNesby et al. 1962; Schurath et al. 1969, red line). The data is compared to our binned fit (blue line).

which are taken from the MPI-Mainz UV/VIS Spectral Atlas⁵ (Keller-Rudek et al. 2013).

We divide the cross sections between 200 bins each ≈ 50 \AA wide. A comparison between our binned cross sections and the raw cross sections from PHIDRATES is plotted for an example reaction (Figure 1). The cross sections, both in the database and here are of the form $\sigma(\lambda)$ with σ in units cm^2 and wavelength in units of \AA . The resolution for the UV cross sections is fairly low, and cannot encapsulate the fine structure of the UV emission lines or the UV cross sections. This is especially important when treating ionospheres of gas giants, since, e.g., the fine structure in the H_2 bands leave small spectral windows through which photons can penetrate and effectively ionize deeper in the atmosphere. Such a low-resolution spectrum will effectively close these windows and underestimate the ion production in the ionosphere (Kim & Fox 1994; Kim et al. 2014). High resolution is also an important for capturing where the UV flux and cross sections both peak; a low-resolution cross section can, in this case, underestimate the destruction rate of the species with this resonant photochemical cross section. As can be seen below, these issues do not significantly affect the comparisons of this model for HD 209458b, Jupiter, or Earth. For photoionization deep in the atmosphere, where high resolution is essential, the network itself need not be modified. The transport of UV photons line by line would need to be calculated.

The tabulated chemical cross sections are combined with $F(\lambda, z)$ [photons $\text{cm}^{-2} \text{s}^{-1} \text{\AA}^{-1}$], the radiant flux density onto a unit sphere (hereafter called the actinic flux) located at atmospheric height, z [cm], to determine the photochemical rate constants,

$$k_{\text{ph},i}(z) = \tau_f \int_{1 \text{\AA}}^{10^4 \text{\AA}} \sigma_i F(\lambda, z) d\lambda, \quad (18)$$

where i is indexed over the molecules listed above, for which photochemistry is considered. τ_f is a dimensionless parameter representing the fraction of time (over a period much longer than the longest characteristic timescale for the atmosphere) the particular atmospheric region is irradiated; for tidally locked

planets, $\tau_f = 1$ (dayside) or 0 (nightside), the diurnal average for a rotating planet is $\tau_f = 1/2$. The photoionization and photodissociation reactions are listed in Appendix A, reactions numbered 2570–2693, and labeled “pi” for photoionization reactions and “pd” for photodissociation reactions.

Cosmic-ray ionization and dissociation is parameterized by ζ (Rimmer & Helling 2013), to treat both direct ionization by galactic cosmic rays and ionization by secondary particles produced in air showers. The cosmic-ray ionization rate depends on the chemical species in question, since different species will have different chemical cross sections for the photons produced by cosmic rays, and this is accounted for by multiplying $\zeta(z)$ by a constant $\kappa_{\text{CR},i}$ such that:

$$k_{\text{CR},i}(z) = \kappa_{\text{CR},i} \zeta(z). \quad (19)$$

We treat low-energy cosmic rays ($E < 1$ GeV) for these objects as though they have been significantly shielded by the astrospheres of the host stars, and therefore set the fitting parameters for the incident cosmic-ray flux to $\alpha = 0.1$ and $\gamma = -1.3$ in the equation for the flux of cosmic-ray particles:

$$j(E) = \begin{cases} j(E_1) \left(\frac{p(E)}{p(E_1)} \right)^\gamma, & \text{if } E > E_2 \\ j(E_1) \left(\frac{p(E_2)}{p(E_1)} \right)^\gamma \left(\frac{p(E)}{p(E_2)} \right)^\alpha, & \text{if } E_{\text{cut}} < E < E_2 \\ 0, & \text{if } E < E_{\text{cut}} \end{cases} \quad (20)$$

where $p(E) = \frac{1}{c} \sqrt{E^2 + 2EE_0}$, $E_0 = 9.38 \times 10^8$ eV, $E_1 = 10^9$ eV, and $E_2 = 2 \times 10^8$ eV, and the flux at E_1 is set to $j(E_1) = 0.22 \text{ cm}^{-2} \text{ s}^{-1} \text{ sr}^{-1} (\text{GeV/nucleon})^{-1}$. All of these parameters except α are observationally well constrained (Indriolo et al. 2009). For a demonstration of how α affects the cosmic-ray spectrum, and a discussion of the Monte Carlo transport we use for cosmic rays of energy < 1 GeV, see Rimmer et al. (2012) and Rimmer & Helling (2013). For ionization rate by cosmic rays of energy > 1 GeV, Q_{HECR} [$\text{cm}^{-3} \text{s}^{-1}$], we use the analytical method of Velinov & Mateev (2008).

Cosmic-ray reactions are listed in Appendix A, numbered 2694–2776, and labeled “cr.”

2.5. Test for Chemical Equilibrium

At sufficiently high temperatures and pressures, a gas should rapidly settle into chemical equilibrium. An important test for a chemical network is that its steady state solution converges to the chemical equilibrium solution. To perform this test of our network, we solve the chemical kinetics at a single (T, p) point, using the rate constants from the STAND2015 network, disabling the cosmic-ray reactions, photochemistry, and dissociative recombination. We compute a time-dependent solution of the equation

$$\frac{dn_i}{dt} = P_i - L_i. \quad (21)$$

We solve this equation for $T = 1000$ K and $p = 1$ bar, with solar abundances from Asplund et al. (2009). We compare our results to chemical equilibrium calculations using the Burcat polynomials (Burcat & Ruscic 2005), and plot our comparisons in Figure 2 and find excellent agreement. This agreement is not

⁵ http://satellite.mpic.de/spectral_atlas/index.html

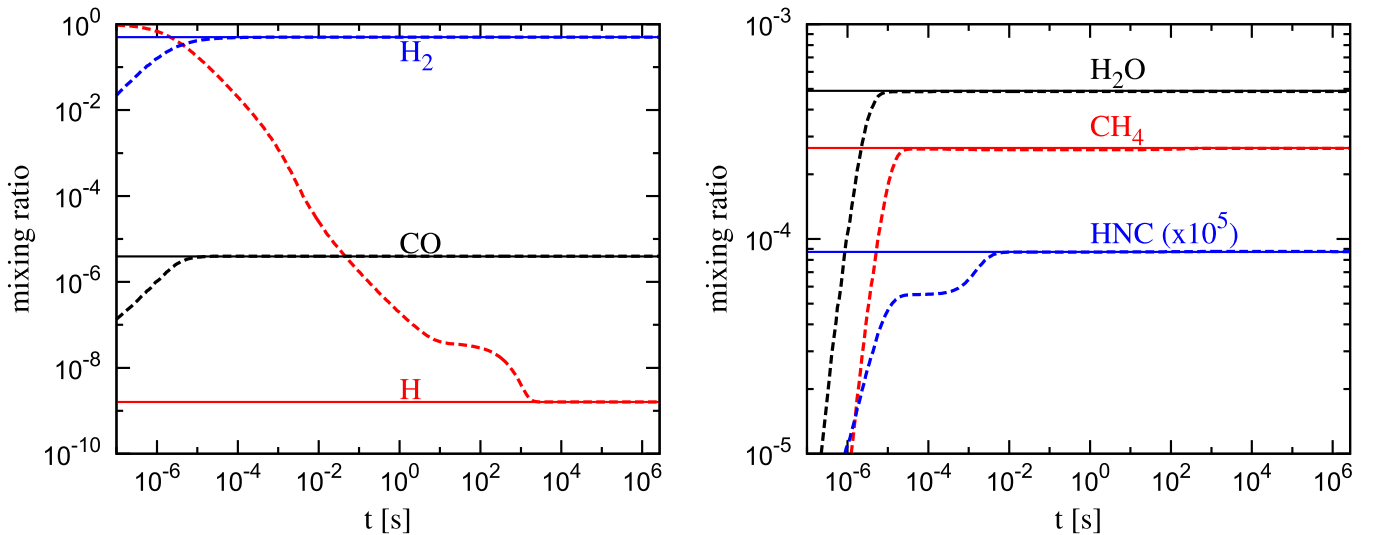


Figure 2. Mixing ratios as a function of time [s] at 1 bar and 1000 K (dashed lines) compared to chemical equilibrium (solid lines) for H_2 , H , CO , CH_4 , and H_2O .

surprising; we have used the same thermochemical data to reverse our reactions, and only include reversed reactions in this test, so once the system achieves steady state, computationally achievable at this pressure and temperature, the chemistry has effectively settled into equilibrium.

We also compare our electron number density to the electron number density achieved using the Saha equation, this time at a pressure of 10^{-4} bar and over a range of temperatures from 1000 to 10,000 K. This comparison is plotted in Figure 3. The comparison is virtually perfect when $T \gtrsim 2000$ K, unsurprising given the way the three-body recombination reactions are calculated (see Section 2.3). At ~ 1000 K, our results diverge from the Saha equation. This is because the integrator does not reliably calculate mixing ratios below $\sim 10^{-30}$. Indeed, at this stage, the electron number density achieves $\sim 10^{-300} \text{ cm}^{-3}$ while the H^+ number density rests at $\sim 10^{-60} \text{ cm}^{-3}$, producing significant charge balance errors. These large errors in the charge balance fluctuate, and only appear when the ionization fraction is $\lesssim 10^{-30}$, at which point ion-neutral chemistry is inconsequential.

3. 1D PHOTOCHEMISTRY/DIFFUSION CODE

We have developed a simple 1D photochemistry/diffusion code (ARGO) for the purposes of testing the STAND2015 network. The required inputs for ARGO are as follows.

1. (p, T) profile of the atmosphere.
2. Vertical eddy diffusion ($K_{zz} [\text{cm}^2 \text{s}^{-1}]$) profile of the atmosphere (see discussion in Lee et al. 2015).
3. Atmospheric elemental abundances.
4. Boundary conditions at top and bottom of the p, T profile.
5. Actinic flux⁶ at the top of the atmosphere.
6. Chemical Network (in our case, STAND2015).
7. Initial chemical composition.

All of these inputs except the chemical composition are fixed.

⁶ The actinic flux is the radiance integrated over all angles, expressing flow of energy through a unit sphere. There are subtle differences between the actinic flux and the spectral irradiance; see Madronich (1987).

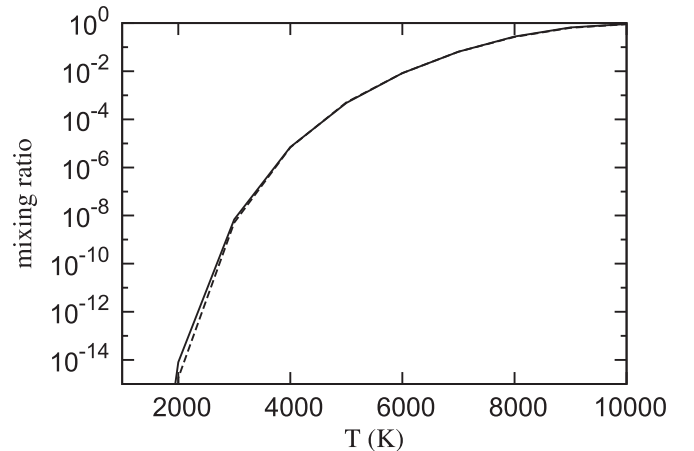


Figure 3. Mixing ratio as a function of temperature. The solid line is from the Saha equation and the dashed line is the result from our model calculation.

With these inputs, ARGO solves molecular transport in a fully Lagrangian manner, similar to Alam & Lin (2008) and Zahnle et al. (1995). The model consists of two parts: (1) A chemical transport model (Section 3.1), and (2) calculation of the photochemical and cosmic-ray chemical rate constants from cross sections and a depth-dependent actinic flux (Section 3.2). A conceptual illustration is shown in Figure 4.

3.1. The Continuity Equations for Chemical Species

The coupled 1D continuity equations describing the time-dependent vertical atmospheric chemistry are

$$\frac{\partial n_i}{\partial t} = P_i - L_i - \frac{\partial \Phi_i}{\partial z}, \quad (22)$$

where $n_i [\text{cm}^{-3}]$ is the number density of species i , and $i = 1, \dots, N_s$, and N_s is the total number of species. $P_i [\text{cm}^{-3} \text{s}^{-1}]$ is the rate of production and $L_i [\text{cm}^{-3} \text{s}^{-1}]$ is the rate of loss of species i . The rightmost term is the vertical change in flux $\Phi_i [\text{cm}^{-2} \text{s}^{-1}]$ and represents the flux due to both eddy ($K [\text{cm}^2 \text{s}^{-1}]$) and molecular diffusion ($D [\text{cm}^2 \text{s}^{-1}]$), respectively, related as (Banks & Kockarts 1973, their Equation

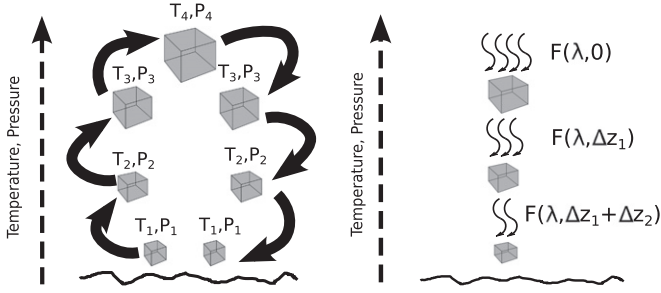


Figure 4. Illustration representation of the model. The illustration on the left represents the motion of the single parcel from the bottom of the atmosphere, T_1, P_1 , up to the top of the atmosphere, T_4, P_4 , and then back down; see Section 3.1. Once this journey is completed, we irradiate the atmosphere by stacking up the parcel at different times, when it was located at different parts of the atmosphere. The illustration on the right represents the calculation of the depth-dependent actinic flux discussed in Section 3.2. Only photons of wavelength between 1 and 10000 Å are considered. Figure 5 gives a flow chart for the calculation.

(15.14)),

$$\Phi_i = -K \left[\frac{\partial n_i}{\partial z} + n_i \left(\frac{1}{H_0} + \frac{1}{T} \frac{dT}{dz} \right) \right] - D \left[\frac{\partial n_i}{\partial z} + n_i \left(\frac{1}{H_i} + \frac{1 + \alpha_T}{T} \frac{dT}{dz} \right) \right], \quad (23)$$

where H_0 [cm] is the pressure scale height of the atmosphere at z [cm], H_i [cm] is the molecular scale height of the atmosphere for species i , and α_T is the thermal diffusion factor (Banks & Kockarts 1973; Yung & Demore 1999; Zahnle et al. 2006; Hu et al. 2012). For molecular diffusion coefficients, we adopt the Chapman–Enskog theory (Enskog 1917; Chapman & Cowling 1991). Eddy diffusion coefficients are either determined empirically, as with Earth and Jupiter, or are derived from global circulation models, as is the case for HD 209458b.

In Equation (23), the terms dealing with eddy diffusion and molecular diffusion are separated out, clarifying the four regions that Equations (22) and (23) describe. (1) Deep within the atmosphere, where pressures and temperatures are sufficiently large, the thermochemistry dominates, and the equation simplifies to Equation (21). The atmospheric chemical composition converges to chemical equilibrium or at least to some stable quasi-equilibrium. (2) Higher in the atmosphere, the eddy diffusion may dominate, and the species are quenched. Their abundance is mixed evenly over a wide range of the atmosphere at timescales shorter than the chemical timescales. (3) Above this region, molecular diffusion may dominate, and at that point, species lighter than the mean molecular mass of the atmospheric gas will rise up, and species heavier than the mean molecular mass will settle down, and the chemistry will largely be determined by the individual scale heights of the atmospheric constituents. (4) Non-equilibrium processes, such as photochemistry or cosmic-ray chemistry, may create a fourth region, the composition of which is determined by irreversible chemical reactions.

Since the purpose of this paper is to introduce a new chemical kinetics network for lightning and prebiotic processes, our focus is not on the atmospheric dynamics (for this, see Lee et al. 2015). We therefore apply a simple approximation to Equation (22), inspired by Alam & Lin (2008). We first cast Equation (22) in a Lagrangian formulation, and consider

Eddy diffusion to be moving small parcels of the gas vertically. We follow a single parcel as it moves up from the lower boundary of the temperature profile, and then returns down again. In reality, the parcel would be jostled in all three dimensions as it makes a complex journey up to the top of the atmosphere, but 1D transport models are unable to capture this effect in full.

The differential diffusion of molecules into and out of the parcel requires a different approach. The discrete formulas used by Hu et al. (2012, their Equation (9)) in the Lagrangian frame are

$$\begin{aligned} \frac{\partial n_{i,j}}{\partial t} = & P_{i,j} - L_{i,j} n_{i,j} - d_{j+1/2} \frac{n_{\text{gas},j+1/2}}{n_{\text{gas},j+1}} n_{i,j+1} \\ & - \left(d_{j+1/2} \frac{n_{\text{gas},j+1/2}}{n_{\text{gas},j}} - d_{j-1/2} \frac{n_{\text{gas},j-1/2}}{n_{\text{gas},j}} \right) n_{i,j} \\ & + d_{j-1/2} \frac{n_{\text{gas},j-1/2}}{n_{\text{gas},j-1}} n_{i,j-1}. \end{aligned} \quad (24)$$

Here, j represents the parcel being followed, $j-1$ the parcel directly beneath j , $j+1$ the parcel above j , and $j \pm 1/2$ an arithmetic average between j and $j \pm 1$. n without any i subscript represents n_{gas} at the relevant parcel, and

$$d_{j \pm 1/2} = \frac{D_{j \pm 1/2}}{2(\Delta z)^2} \left[\frac{(\bar{m} - m_i)g\Delta z}{k_B T_{j \pm 1/2}} - \frac{\alpha_T}{T_{j \pm 1/2}} (T_{j \pm 1} - T_j) \right]. \quad (25)$$

\bar{m} [g] denotes the mean molecular mass of the atmosphere at z and m_i [g] the mass of species i .

Both the third and last terms on the right-hand side of Equation (24) do not depend on n_i and can therefore be treated as source terms, P_i . The fourth term can be treated as a term in L_i , such that molecules “destroyed” by this reaction are “banked,” $A \rightarrow BA$. The “banked” molecules re-enter the parcel at a rate determined by the third and last terms on the right-hand side of the equation, thus conserving mass throughout the parcel’s travels. Violations of this conservation do not appear here, but can be accounted for via further reactions, settling, condensation and evaporation, outgassing and escape, discussed in Appendix C. Although it is straightforward to handle atmospheric escape with this method, we do not do so for any of the test cases in this paper.

Equation (24) is solved within ARGO in the same numerical manner as NAHOON (Wakelam et al. 2012) by the implicit time-dependent Gear method as incorporated by the Livermore Solver for Ordinary Differential Equations (DLSODE; Gear 1971; Brown & Hindmarsh 1989).

3.2. Calculating the XUV and Cosmic-ray Flux

Once the fluid parcel has completed the atmospheric profile, the solar XUV actinic flux from 1 to 10000 Å as a function of depth, z [cm],⁷ and wavelength λ [Å] is calculated. We consider both the direct and approximate diffusive actinic flux. The local height-dependent actinic flux is calculated without any iteration on the local temperature. The cross sections for various photochemical reactions (Section 2.4) are multiplied by each vertical step (Δz_j [cm], where $(\Delta z)_j$ is the size of the step

⁷ The depth for this model extends from $z = 0$, the bottom of the temperature profile for the planet in question, to $z = z_{\text{top}}$, the top of the profile.

at height z_j . The total optical depth as a function of the wavelength takes the form

$$\tau(\lambda, z) = \sum_j [(\Delta z)_j \sum_i \sigma_i n_{ij}] + \tau_s, \quad (26)$$

where i is summed over all species for which photoabsorption is considered (see Section 2.4 for a list of these species). τ_s is the optical depth due to Rayleigh scattering, and the actinic flux as a function of depth is defined as (Hu et al. 2012)

$$F(\lambda, z) = F(\lambda, z_{\text{top}}) e^{-\tau(\lambda, z)/\mu_0} + F_{\text{diff}}, \quad (27)$$

where $\mu_0 = \cos \theta$, where θ is the stellar zenith angle; we set $\mu_0 = 1/2$ for all calculations within this paper (see Hu et al. 2012, their Figure 7). F_{diff} denotes the actinic flux of the diffusive radiation, determined using the δ -Eddington two-stream method (Toon et al. 1989). Once the actinic flux is calculated, the photochemical rates are determined as in Section 2.4. Once the depth-dependent flux, $F(z, \lambda)$ [$\text{cm}^{-2} \text{s}^{-1} \text{\AA}^{-1}$], is determined for all layers, the parcel's path through the atmospheric profile is repeated, now accounting for the photochemistry. The cosmic-ray ionization rate, $\zeta(z)$ [s^{-1}], is likewise calculated in a depth-dependent manner following Rimmer & Helling (2013) and incorporated into the chemistry (Section 2.4).

A new depth-dependent composition is constructed, then applied to Equation (26) to solve again for $F(z, \lambda)$. The value of $\zeta(z)$ does not change significantly between iterations. This process is repeated until the results converge; i.e., until the profile from the previous global calculation (transport + depth-dependent flux) agrees to within 1% the profile from the current global calculation. The number of repetitions depends on the parameters, but is typically between 5 and 12 global iterations. This iterative process is represented as a flow chart in Figure 5.

This method is both simple and functional, requiring relatively little computational resources. It is also straightforward to adapt to diverse chemical environments, since it does not require the selection of “fast” and “slow” chemistry to ease computational speed. These strengths do not come without a cost: the simplistic dynamics does not transition as smoothly from the eddy diffusion regime to the molecular diffusion regime as the Eulerian formulation, and can result in steep changes over a handful of height steps.

3.3. Testing the Atmospheric Transport Model for Molecular Diffusion

In order to benchmark the STAND2015 chemical network in different planetary atmospheres, we test the molecular diffusion within ARGO. We consider a 1D isothermal gas under a constant surface gravity, $g = 10^3 \text{ cm s}^{-2}$, with temperature $T = 300 \text{ K}$, at hydrostatic equilibrium. The gas is initially composed of carbon and hydrogen atoms, each with a mixing ratio of $X_0(\text{C}) = n(\text{C})/n_{\text{gas}} = 0.5$ and $X_0(\text{O}) = 0.5$ throughout. All chemistry is disabled. It is expected that the heavier species, carbon, will settle into the atmosphere, and the lighter species, hydrogen, will rise up, until they stratify. The analytic solution to this system is well known. The mixing ratio should be determined by the scale heights of the individual species such that, for the carbon abundance,

$$X(\text{C}) = \frac{X_0(\text{C}) e^{-z/H_c}}{X_0(\text{H}) e^{-z/H_H} + X_0(\text{C}) e^{-z/H_c}}, \quad (28)$$

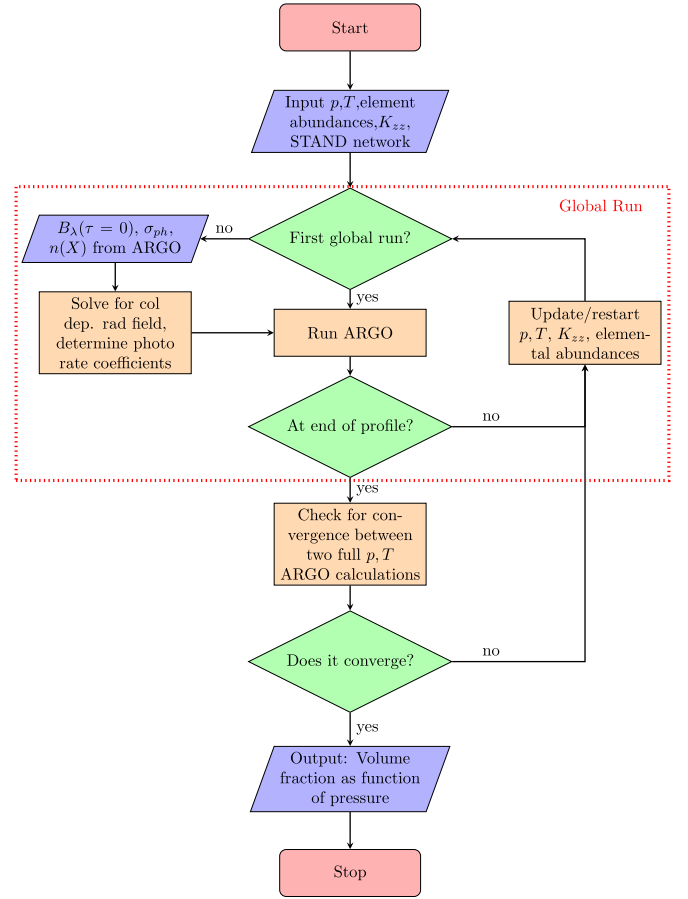


Figure 5. Flow chart representation for the program.

where $X(\text{C})$ is the final steady state carbon mixing ratio, and H_H [cm] and H_C [cm] are the atmospheric scale heights for the hydrogen and carbon.

The code is run until steady state is achieved, when the carbon in the very upper atmosphere diffuses into the lower atmosphere. The steady state mixing ratio, as a function of height is compared the analytic mixing ratio, Equation (28), in Figure 6. The comparison is reasonable through the extent of the atmosphere.

4. TESTING THE NETWORK FOR PLANETARY ENVIRONMENTS

The STAND2015 network contains chemical reactions for an H/C/N/O gas, and including both highly reducing to highly oxidizing atmospheres, and for a temperature range of 100–30,000 K. The network should then be tested for a variety of planetary atmospheres with different chemical compositions, from the (probably) oxidizing atmosphere of the early Earth to the highly reducing atmosphere of Jupiter. The large range of temperatures is tested for the irradiated exoplanet HD 209458b. We also test our model against the height-dependent measurements of select trace species within the atmosphere of the present-day Earth. It would be interesting to apply our model to Titan, due to its rich nitrile and organic chemistry. Titan's atmosphere is a very rich and complex environment, and it is important to account for these complexities when modeling Titan. Titan has upper atmospheric hazes, temperatures low enough to condense several molecular species, and ionization

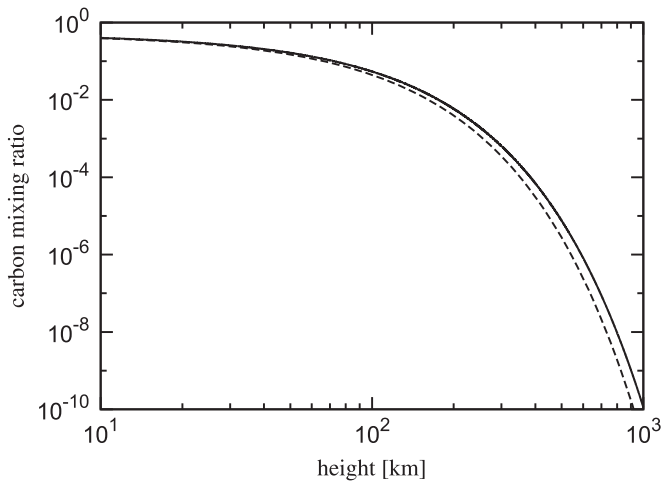


Figure 6. Carbon mixing ratio as a function of atmospheric height [km]. We test for diffusion, with chemistry turned off, for carbon atoms and hydrogen atoms in a gas at hydrostatic equilibrium for an isothermal gas ($g = 10^3 \text{ cm s}^{-2}$, $T = 300 \text{ K}$). The solid line is the result from ARGO and the dashed line is the analytic result (Equation (28)).

and dissociation by energetic particles including cosmic rays, Saturn magnetospheric particles, solar wind protons, and interplanetary electrons. As useful as a study of the atmosphere of Titan would be for exploring Miller–Urey-like chemistry (Waite et al. 2007), though such a model is beyond the scope of this paper. The boundary conditions for these various objects are given in Section 4.1. We then compare our results to the results from other chemical kinetics models and, where possible, with observations, for HD 209458b (Section 4.2), Jupiter (Section 4.3), and the Earth (Section 4.4).

4.1. Boundary Conditions for Three Test Cases: HD 209458b, Jupiter, and the Earth

Below, we compare the results of our chemical kinetics to other results for HD 209458b and also for Jupiter and the Earth. Each of these objects has different boundary conditions and parameters. These conditions and parameters include the temperature profile of the object’s atmosphere, the eddy diffusion profile, the elemental abundances, the initial composition at the lower boundary of the atmospheric profile, and the unattenuated UV flux. For HD 209458b, the conditions at the lower boundary of the atmospheric profile rapidly develop from the prescribed initial conditions toward chemical equilibrium. For Jupiter and the early Earth, the composition at the lower boundary is stable over the dynamical timescale ($dn_i(z=0)/dt \approx 0$), and so the initial composition effectively acts as a lower boundary condition. The assumed elemental abundances and initial conditions at the lower boundary of the atmospheric profile are given in Table 1.

We take HD 209458b to have solar elemental abundances throughout its atmosphere, and set the initial conditions at the lower boundary of the atmosphere to be entirely atomic. The initial composition hardly matters here, since the composition quickly settles to chemical equilibrium at such a high temperature and pressure. The temperature profile and eddy diffusion profile for HD 209458b are both taken from Moses et al. (2011) so we can directly compare results.

Since HD 209458 is a G0 star, we use the solar UV flux. The unattenuated solar UV flux at 1 au is obtained from the SORCE data (Rottman et al. 2006) for 1–350 Å and 1150–10000 Å with

Table 1
Initial Conditions for the Chemistry at the Lower Boundary
in Terms of $n(X)/n_{\text{gas}}$

Species	HD 209458b ^a	Earth ^b	Early Earth ^c	Jupiter ^d
H	9.2092(−1)
He	7.8383(−2)	1.3600(−1)
C	2.4787(−4)
N	6.2262(−5)
O	4.5105(−4)
Ar	2.3133(−6)	...	9.1150(−3)	...
K	9.8766(−8)
Cl	2.9122(−7)
Fe	2.9122(−5)
Mg	3.6663(−5)
Na	1.6004(−6)
Si	2.9800(−5)
Ti	8.2077(−8)
CO	...	1.1300(−7)	4.9005(−5)	8.0000(−10)
H ₂	...	1.0000(−6)	9.8010(−4)	8.6219(−1)
N ₂	...	7.9172(−1)	7.8408(−1)	...
NO	...	2.4000(−11)
O ₂	...	1.9793(−1)
CO ₂	...	3.5000(−4)	1.9602(−1)	...
H ₂ O	...	1.0000(−2)	9.8010(−3)	...
N ₂ O	...	3.0200(−7)
NH ₃	...	2.4000(−10)
CH ₄	...	1.9390(−6)	...	1.8100(−3)

Notes.

^a Solar metallicity from Asplund et al. (2009).

^b Surface mixing ratios based on the US Standard Atmosphere 1976.

^c Based on early Earth models (Kasting 1993).

^d Moses et al. (2005).

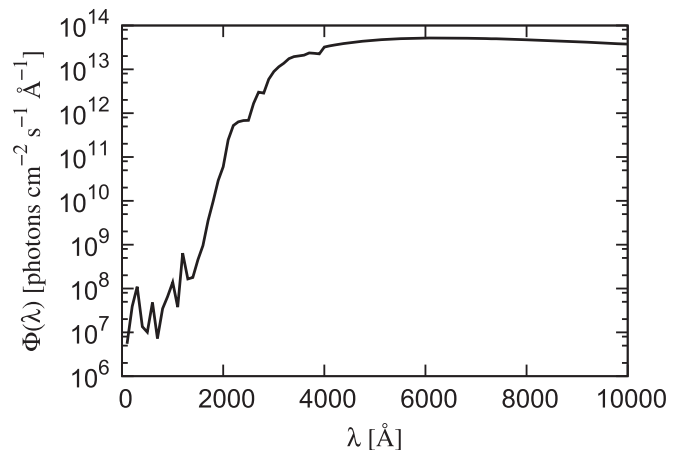


Figure 7. Solar flux used in our model [photons $\text{cm}^{-2} \text{s}^{-1} \text{Å}^{-1}$], as a function of wavelength, λ [Å], taken from Huebner & Carpenter (1979), Huebner et al. (1992), and Huebner & Mukherjee (2015). Weighted versions of this flux are used for HD 209458b and Jupiter. This flux is used, unadjusted, for the early Earth.

data from PHIDRATES for the 350–1150 Å range. The binned flux we use is plotted in Figure 7. This flux is adapted to HD 209458b by multiplying the solar UV flux by a factor of $(d_{\oplus}/d_p)^2$, where d_{\oplus} [au] is the distance from the Earth to the Sun and $d_p \approx 0.047 \text{ au}$ is the approximate distance between HD 209458b and its host star. This may not be the most accurate approximation to the UV behavior of HD 209458, since it might have quite different activity from our Sun (Tu et al. 2015).

For Jupiter, we use the temperature and eddy profiles from Moses et al. (2005). For consistency, we set the initial conditions at the lower boundary of Jupiter’s atmosphere to be the same as Moses et al. (2005); see Table 1. The solar UV spectrum at 1 au is used for Jupiter, although multiplied by a factor of $(d_{\oplus}/d_J)^{-2}$, where $d_J \approx 4.5$ au is the square of the distance between the sun and Jupiter.

For the present-day Earth, we use the measured surface mixing ratios from the US Standard Atmosphere 1976 (see Table 1) and the temperature profile from Hedin (1987, 1991), Figure 13. We use the present-day solar flux at 1 au as our incident UV flux.

We use the same chemical lower boundary conditions as from Kasting (1993) for the atmosphere of the early Earth (Table 1). The temperature profile for the early Earth is assumed to be the same as that of the present Earth (Hedin 1987, 1991), Figure 13. The UV field used for this model is that of the young Sun calculated using the scaling relationships of Ribas et al. (2005) for wavelengths between 1 and 1200 Å and the UV field of the solar analogue κ^1 Cet above 1200 Å (Ribas et al. 2010).

4.2. HD 209458b

HD 209458b was first observed by Henry et al. (2000), and is one of a growing number of Hot Jupiters to have a measured spectrum, via transit (e.g., Queloz et al. 2000), and also in emission (e.g., Knutson et al. 2008). Various molecular species have been tentatively identified in the spectrum, such as TiO (Désert et al. 2008), water (Madhusudhan & Seager 2009; Swain et al. 2009; Beaulieu et al. 2010), CO, CO₂, and methane features (Madhusudhan & Seager 2009; Swain et al. 2009). HD 209458b has been extensively modeled with retrieval modeling (Madhusudhan & Seager 2009) and with hydrodynamic global circulation models (Showman et al. 2008). This planet has also been a popular target for non-equilibrium chemistry models such as those of Liang et al. (2003), Zahnle et al. (2009), Moses et al. (2011), Venot et al. (2012), Agúndez et al. (2014), and Lavvas et al. (2014).

We have chosen the atmosphere of HD 209458b as one candidate for benchmarking our results because it is well characterized and has been the subject of several non-equilibrium chemistry models, and it has a very high temperature even among Hot Jupiters. An additional benefit to HD 209458b is its suspected temperature inversion (Knutson et al. 2008, although this is debated; see also Schwarz et al. 2015), which allows us to test our chemistry at very high temperatures both at both high and low pressures. The thermal profile of HD 209458b from Moses et al. (2011) is shown in Figure 8. The local gas-phase temperature $T > 2000$ K both when $p > 100$ bar and when the gas-phase pressure, $p < 10^{-4}$ bar. This is a wide parameter space relevant for ion–neutral chemistry initiated via thermal ionization.

We compare our results to the predictions of two different chemical kinetics models. (1) We compare our results to the results of Moses et al. (2011) with the ion–neutral chemistry disabled. (2) We compare the ionic abundances for our most abundant ions to the results of Lavvas et al. (2014). Also in this case, we disable cosmic-ray chemistry in order to draw a better comparison to the ion–neutral chemistry.

We compare our network and transport model to Moses et al. (2011) by examining the volume mixing ratios of major neutral species: H, H₂, He (hydrogen/helium chemistry), OH, H₂O, O,

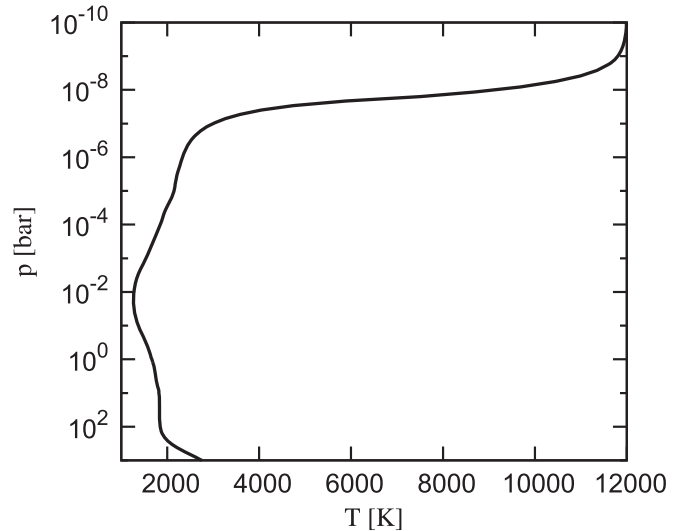


Figure 8. Temperature profile for HD 209458b, T [K], as a function of p [bar], as used by Moses et al. (2011).

and O₂ (oxygen/water chemistry), N₂ and NH₃ (nitrogen chemistry), and CO, CH₄, and CO₂ (carbon chemistry). See Figure 9. These species were chosen because they are abundant and, in the case of H₂ and N₂, play an important role in the non-equilibrium chemistry. N₂ provides the reservoir for the transition between N₂ \rightleftharpoons NH₃. Other species were chosen because they contribute to features observed in transit spectroscopy (e.g., CO₂). The molecules CO and H₂O do both. Helium was chosen because its mixing ratio is not significantly affected by the chemistry. It changes with pressure due to molecular diffusion, and so it provides a useful comparison between our dynamical calculations and those of Moses et al. (2011).

The transition of carbon between CO and CH₄, and nitrogen between N₂ and NH₃ is very sensitive to non-equilibrium chemistry, as CH₄ \approx CO when $p \sim 100$ bar and $T \sim 2000$ K. As the pressure decreases rapidly while the temperature remains relatively high ($T > 1000$ K), the thermochemical equilibrium ratio for CH₄/CO plummets, approaching 10^{-7} at 0.1 bar in the HD 209458b atmosphere. The time it takes the carbon to meander from CH₄ to CO, however, becomes significantly longer than the relevant dynamical timescales (for HD 209458b, this timescale is prescribed by the eddy diffusion coefficient; see Bilger et al. 2013), and the CH₄ and CO abundances are quenched. The same sort of process governs the transition of nitrogen from N₂ to NH₃.

The pathways for both CH₄ \rightleftharpoons CO and N₂ \rightleftharpoons NH₃ interconversions are not well understood. In both cases, the paths competing with one another are often circuitous, and tend to be regulated by one of several reactions encountered along the journey, a slow rate-limiting step (Moses 2014). The timescale of the transition between species is almost entirely set by the rate by which that single reaction proceeds. As discussed in Section 2, rate coefficients can be frustratingly uncertain, with different estimations sometimes varying by more than an order of magnitude. For example, compare the rate experimental and theoretical rate constants for C₂H₆ \rightarrow CH₃ + CH₃ (Yang et al. 2009 and Kiefer et al. 2005, respectively). The path that one believes regulates these central transitions can be very different depending on what rate coefficients are used.

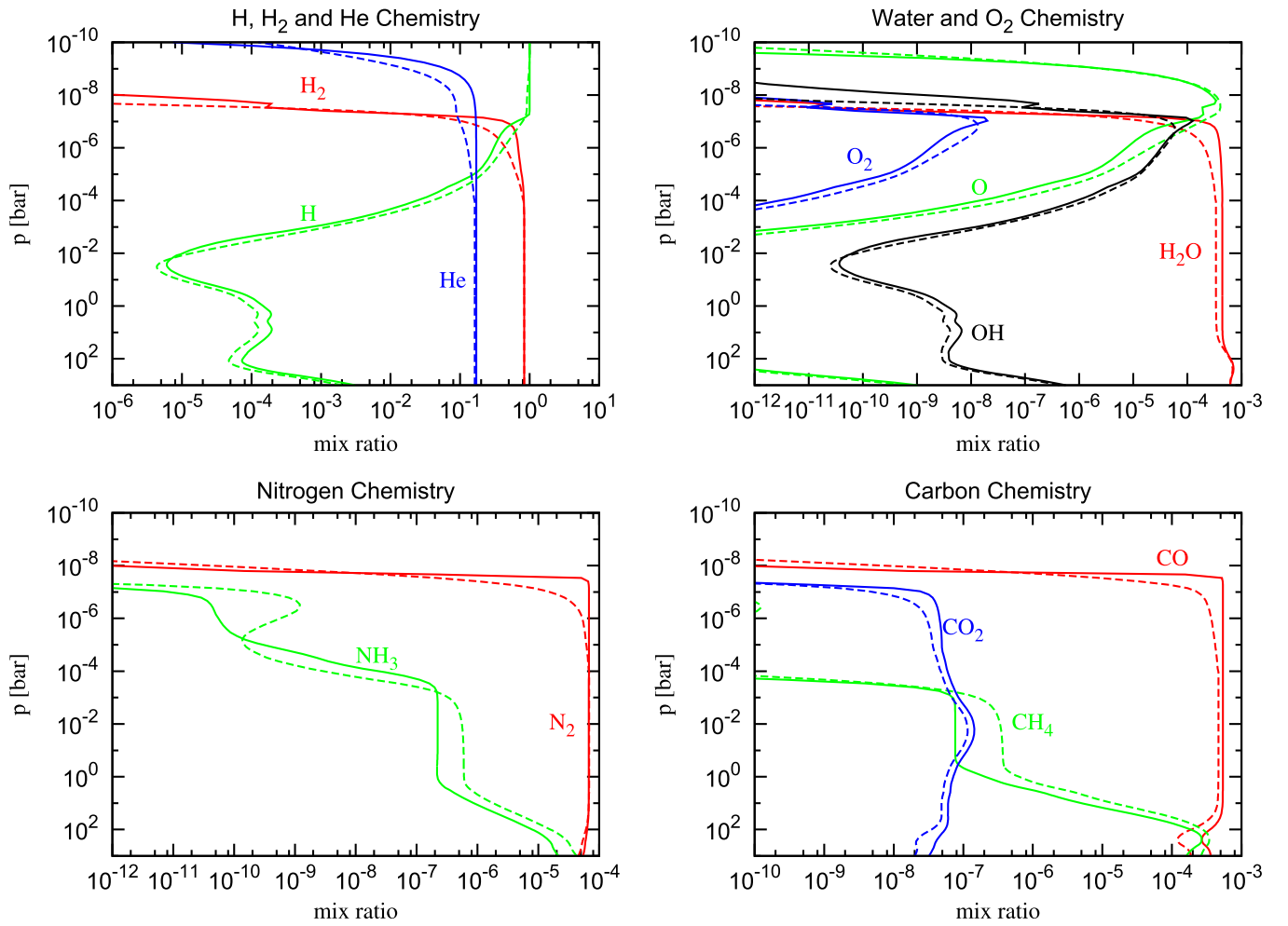
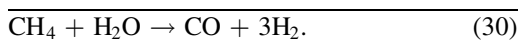
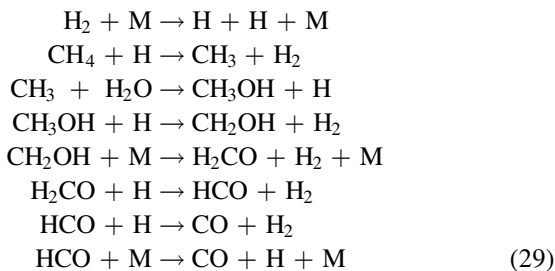
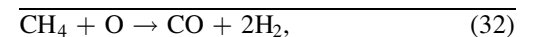
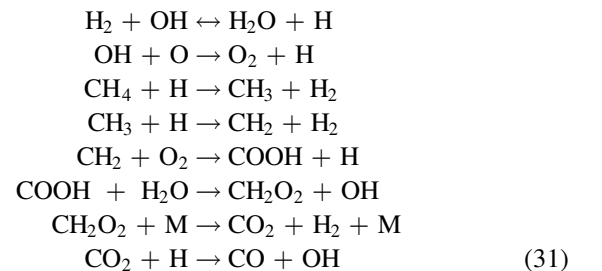


Figure 9. Mixing ratios for various chemical species as a function of pressure, p [bar]. A comparison between our model (solid lines) and that of Moses et al. (2011, dashed lines) is shown for H/H₂ chemistry, water and O₂ chemistry, nitrogen chemistry, and carbon chemistry in the atmosphere of HD 209458b.

An illustrative example is the reaction $\text{CH}_3 + \text{H}_2\text{O} \rightarrow \text{CH}_3\text{OH} + \text{H}$. Hidaka et al. (1989) has determined the rate for $\text{CH}_3 + \text{H}_2\text{O} \rightarrow \text{Products}$, Reaction (29), proceeds with a barrier of ≈ 2670 K (see Visscher et al. 2010 for a discussion on this reaction). With reasonable assumptions of the branching ratios for this reaction, namely that the branching ratios do not change much with temperature, one would set the same barrier to $\text{CH}_3 + \text{H}_2\text{O} \rightarrow \text{CH}_3\text{OH} + \text{H}$, as done by Venot et al. (2012). However, Moses et al. (2011) carried out quantum chemical calculations for this reaction using MOLPRO and estimate a barrier for this particular branch of ≈ 10380 K, much larger than the activation energies of the other branches. With the smaller barrier, the path carbon takes from CH₄ to CO proceeds as



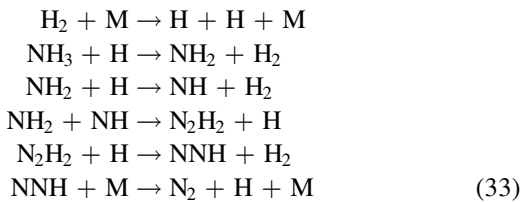
We adopt the rates of Moses et al. (2011) for this pathway, as well as the smaller rate coefficient for the three-body reaction $\text{H}_2\text{O} + \text{CH}_2 + \text{M} \rightarrow \text{CH}_3\text{OH}$. An examination of our results would reveal that, as with Venot et al. (2012), the transition of carbon from CH₄ to CO is much more efficient than with Moses et al. (2011). We have examined the rates at which reactions proceed in our network and find *another* formation pathway:



The atomic oxygen arises from thermal dissociation of OH or photodissociation of H₂O followed by diffusion downward. This pathway is critically dependent on Reaction (31). To our knowledge, the three-body rate coefficient for this reaction has

not been determined. This reaction has instead appeared in our network as the reverse reaction of $\text{CH}_2\text{O}_2 + \text{OH} \rightarrow \text{COOH} + \text{H}_2\text{O}$, for which we use an estimate based on reaction energetics (Mansergas & Anglada 2006). This pathway is highly uncertain, and removing it makes up the majority of the difference between our results and those of Moses et al. (2011) for methane between $1\text{--}10^{-4}$ bar. We suspect further differences owe to our different thermochemical constants and the use of slightly different solar abundances.

The path of nitrogen from NH_3 to N_2 is considerably more uncertain. The path is believed to roughly follow from NH_3 to NH via hydrogen abstraction, which will in turn react with another NH_x species to form N_2H_y . This species will be destroyed either by reacting with hydrogen or via thermal decomposition, to form N_2 . The reactions $\text{N}_2\text{H}_{x+2} \rightarrow \text{NH}_2 + \text{NH}_x$ involve large uncertainties, which result in variations of the NH_3 quenched abundance by an order of magnitude. We find, similar to Moses et al. (2011), that



with Reaction (33) as the rate-limiting step. The profile we have for NH_3 deviates considerably from the results of Moses et al. (2011), but this is in large part due to a difference in the nitrogen thermochemistry and initial abundances at high pressures propagating up through the atmosphere. Figure 9 shows that our quenching height is, in both cases, higher than for Moses et al. (2011), suggesting that the nitrogen in NH_3 migrates to N_2 more slowly in our network, even overtaking Moses et al. (2011) at $\sim 10^{-4}$ bar, but that we start with less NH_3 than Moses et al. (2011). The increase in NH_3 abundance at $\sim 5 \times 10^{-6}$ bar is due to a formation path for NH_3 in Moses et al. (2011) that is less efficient in our network.

We conclude this section with a brief discussion of the most neutral ions, in comparison with Lavvas et al. (2014). We have plotted the most abundant ions in Figure 10. Note that for this paper, n_{gas} is a sum of all neutral gas particles, cations, ions, and electrons, so the mixing ratio of ions cannot increase above unity. This plot allows a direct comparison to Lavvas et al. (2014, their Figures 5 and 6). In our model, K^+ is the most abundant ion deep within the atmosphere, followed by Mg^+ and Fe^+ . Lavvas et al. (2014) does not consider these species, but they do not seem to have very much affect on the abundances of other ions deep within the atmosphere. When the pressure delves to 10^{-2} bar, K^+ deviates considerably between our results and those of Lavvas et al. (2014). This is likely due to the inclusion of several other ions in our model that become dominant charge carriers at this height, including several complex hydrocarbon ions, of the form C_nH_m^+ . This indicates that ion-neutral chemistry can be significantly influenced by the variety of ions and neutral species under consideration. This will be especially true for the potassium chemistry. Our network contains a small number of potassium-

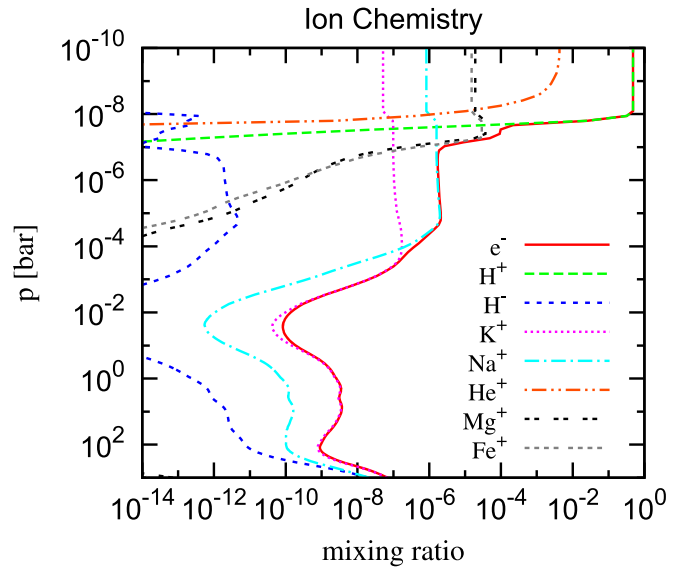


Figure 10. Mixing ratios for the dominant ionic species as a function of pressure, p [bar], for the atmosphere of HD 209458b.

bearing species. Including new species and reactions could significantly affect the degree of ionization. It will be interesting to discover how an expanded potassium and sodium chemistry affects the overall ion-neutral chemistry and the resulting abundances of trace species.

Between 10^{-3} and 10^{-4} bar, Na^+ overtakes K^+ as the dominant positive charge carrier, and remains so until $\sim 10^{-7}$ bar. This transition, the ratios between the ions, and the abundances of the ions are nearly identical between our model and that of Lavvas et al. (2014). Within the thermosphere of HD 209458b, there are some small discrepancies between our model and Lavvas et al. (2014) for He^+ , and quite large discrepancies for C^+ which we suggest are owing to the non-Alkali photochemistry that Lavvas et al. (2014) include, but that we have not included here.

4.3. Jupiter

The atmosphere of Jupiter is divided into three regions: (1) the troposphere, where the gas-phase temperature T decreases with atmospheric height, (2) the stratosphere, where T is roughly constant with increasing height, and (3) the thermosphere, where T increases with height. In this section, we consider the chemical composition of Jupiter's stratosphere. The stratosphere of Jupiter is rich in hydrocarbons, owing to its large gas-phase C/O ratio, because the majority of the oxygen is locked in water ice and then gravitationally settles to below the tropopause. This is predicted to lead to a $\text{C/O} \sim 2 \times 10^6$ (Moses et al. 2005) in the absence of external sources of H_2O and CO_2 (Feuchtgruber et al. 1997; Moses et al. 2000a, 2000b), such as Shoemaker-Levy 9 (Cavalié et al. 2012). Jupiter's stratosphere provides an extreme example of how surface deposition can radically affect the C/O ratio, an effect more recently predicted for exoplanets and brown dwarfs (Bilger et al. 2013; Helling et al. 2014). The high C/O ratio, in combination with the large abundance of hydrogen (H_2 and CH_4 are the two most abundant volatiles in the stratosphere and lower thermosphere), means that the stratosphere of Jupiter is strongly reducing (Strobel 1983).

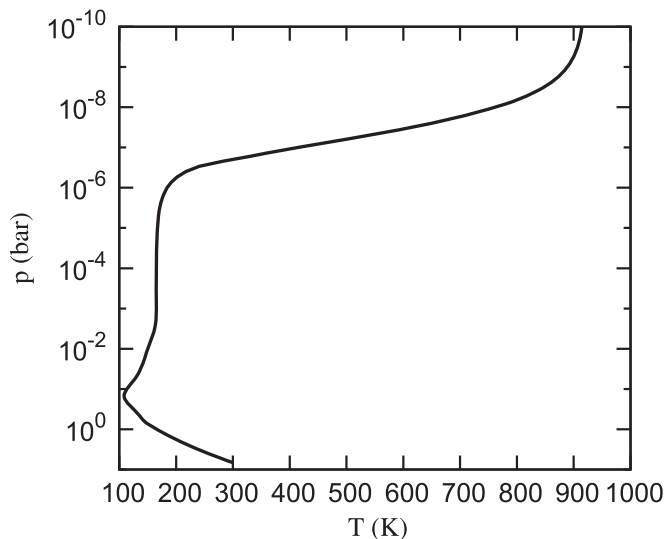


Figure 11. Temperature profile for Jupiter, T [K], as a function of p [bar] (Moses et al. 2005).

Fouchet et al. (2000) have observed ethane and acetylene in Jupiter’s stratosphere. Ethylene has also been observed by Bézard et al. (2001). The stratospheric chemistry of Jupiter has been modeled by several groups, including Gladstone et al. (1996) and Moses et al. (2005). We adopt the lower boundary conditions and temperature profile that Moses et al. (2005) used and model the carbon–oxygen chemistry in the stratosphere of Jupiter, ignoring the nitrogen chemistry (most of the nitrogen will be locked in NH_3 ice). Boundary conditions are discussed in Section 4.1.

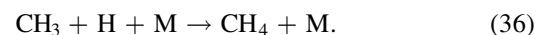
Our lower boundary is set to be identical to Moses et al. (2005). These boundary conditions are somewhat artificial; the carbon budget is controlled by the photochemistry and the dynamics. There is no effective destruction pathway for the stable hydrocarbons, but the timescale for their formation is often competing with the dynamical timescales. In the thermosphere, $\sim 10^{-7}$ – 10^{-8} bar, these hydrocarbons are lost through photodissociation and photoionization as well as molecular diffusion. At the base, the chemistry is halted once the dynamical timescale is reached, effectively treating the bottom boundary as an open boundary through which the hydrocarbons would continue to diffuse. In reality, the complex hydrocarbons are carried into Jupiter’s deep atmosphere, where the high temperatures and pressures dissociate these hydrocarbons, and force the carbon budget to return to chemical equilibrium values: CH_4 with trace amounts of CO and other species. Visscher et al. (2010, their Figure 6) demonstrate how the carbon budget is set deep within Jupiter’s atmosphere; we do not model this region.

With these reactions removed from the network, we ran the network using the temperature and $K_{z,z}$ profiles from Moses et al. (2005), shown in Figure 11. Comparisons between our results and a representative set of observations for the depth-dependent mixing ratios, for the species CH_4 , C_2H_2 , C_2H_4 , C_2H_6 , and C_4H_2 , are shown in Figure 12. The observations for CH_4 are taken from Drossart et al. (1999) and Yelle et al. (1996), C_2H_2 observations are from Fouchet et al. (2000), Moses et al. (2005), and Kim et al. (2010), C_2H_4 observations are from Romani et al. (2008) and Moses et al. (2005), C_2H_6 observations are from Fouchet et al. (2000), Moses et al.

(2005), Yelle et al. (2001) and Kim et al. (2010), and the C_4H_2 observations are from Fouchet et al. (2000) and Moses et al. (2005). We also incorporate observations for C_2H_2 , C_2H_4 , and C_2H_6 from Gladstone et al. (1996) and references therein.

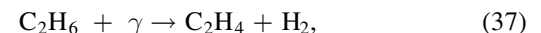
Many of the published observations do not include error bars in atmospheric pressure. Additionally, there may be seasonal changes in the pressure–temperature structure and the location of the homopause, which adds uncertainty to our predictions as a function of pressure. To account for these sources of uncertainty, we place error bars for the pressure at a factor of two above and below the published observations when errors in pressure were not given. These errors in pressure are of the same order as observations where errors in pressure are given. We do not compare our results for oxygen-bearing species, because the abundances of these species are expected to be greatly enhanced in the stratosphere by the addition of an external source of oxygen, such as Shoemaker–Levy 9.

The differences between our results and those of other models arise primarily because of different photochemistries and different rate constants, especially for the re-formation of methane after its photodissociation,

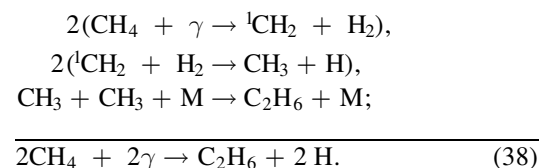


Differences between Jovian photochemical models can result in very large discrepancies between stratospheric abundances of complex hydrocarbons. The differences between Gladstone et al. (1996) and Moses et al. (2005) span several orders of magnitude in some cases (see Moses et al. 2005, their Figure 14).

Both ethane and acetylene agree reasonably well between our model and the observations, and the results for C_4H_2 lie more than a factor of five below the observational upper limits. Our predictions for the location of the methane homopause do not agree very well with observations. We use the eddy diffusion coefficient from Model C in Moses et al. (2005), and either this or the use of the Chapman–Enskog diffusion coefficient for Methane may be the source of the discrepancy. Our results are similar to the Model C results of Moses et al. (2005, their Figure 14). The molecule with the largest discrepancy between the two models is ethylene (C_2H_4), with the largest discrepancy between our predictions and the 1 millibar observations (ignoring the observation from Gladstone et al. 1996 that predicts a mixing ratio of $\sim 10^{-8}$). In our model, the primary path of formation for ethylene follows from the photodissociation of ethane (Reaction 2679 in the network),



and ethane is formed from CH_4 following paths to formation like this one:



These differences may be resolved by a more careful accounting of pressure-dependent branching ratios, such as those of



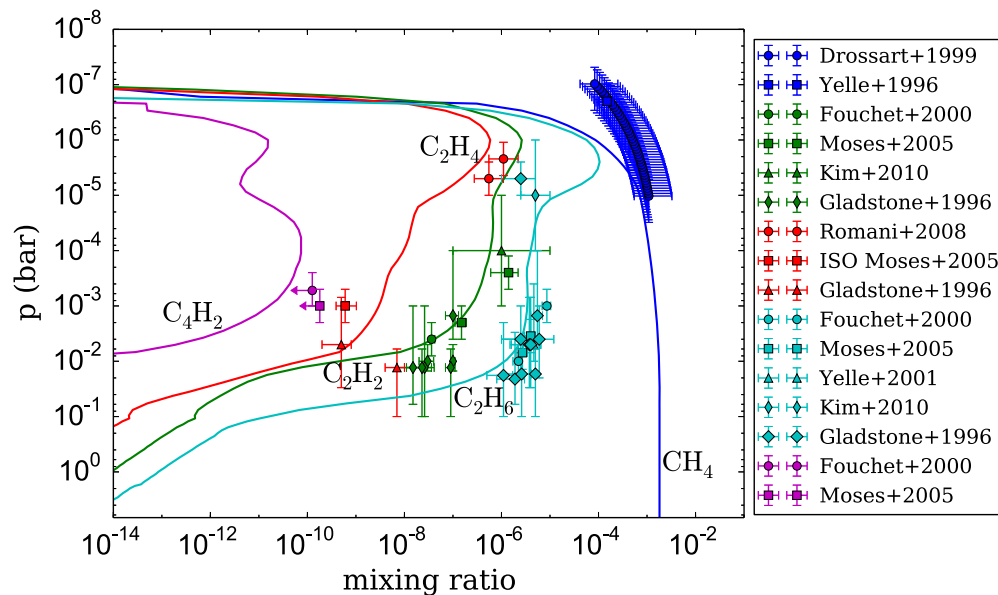
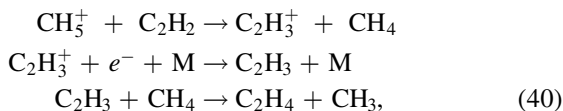


Figure 12. Mixing ratios for various chemical species as a function of pressure, p [bar]. A comparison between our model (solid lines) and that of various observations is shown for complex hydrocarbons in the stratosphere of Jupiter.

from Loison et al. (2015). We use the Kooij form for these reactions (Section 2.1), which does not account for the effect that pressure has on the rate constant.

Ion–neutral chemistry also makes a contribution, via the formation of C_2H_4 from the reaction



and CH_5^+ forms from a series of reactions starting with the photoionization of CH_3 and then a series of hydrogen abstractions, $CH_x^+ + H_2 \rightarrow CH_{x+1}^+ + H$. It should be emphasized that this is not the primary formation pathway for ethylene, but it is an important path of formation in our chemistry and makes some contribution to the mixing ratios at 1 millibar.

Finally, there is a large discrepancy for CO, but this is not due to differences in the chemistry. Rather, this results from Moses et al. (2005) injecting CO, CO_2 , and H_2O into Jupiter’s stratosphere. The inclusion of this external source of oxygen-bearing species is justified by a number of data model comparisons mentioned at the beginning of this section. We neglected to include these external sources, and therefore oxygen-bearing species, especially H_2O and CO_2 (not shown), fail to agree with observations. Our results therefore suggest that some external source of oxygen-bearing species is necessary to explain the H_2O and CO_2 observations in Jupiter’s stratosphere.

4.4. The Earth

The Earth’s atmosphere is well studied, and the profiles of trace species are well constrained, and the formation and destruction of these species is controlled by photochemistry and deposition. Comparing our results to the present-day Earth atmosphere therefore provides a comprehensive test of our

chemical network (Section 4.4.1). Additionally, the connection between lightning-driven and NO_x chemistry⁸ has been extensively studied with experiments, observations, and models, and provides a useful regime in which to compare the results of STAND2015 applied to a lightning shock model (Section 4.4.2). It is important to find out what our model predicts in habitable environments before the onset of life, and so we apply our model to the early Earth (Section 4.4.3).

4.4.1. Present-day Earth Atmosphere

The best understood planetary atmosphere, in terms of both models and observations, is the atmosphere of the present-day Earth. Earth’s atmosphere has been studied in situ, with the use of countless balloon experiments used to measure various trace elements, and remotely, with satellite measurements. Models of Earth’s atmosphere range from simple to complex, both dynamically (1D diffusion to 3D global circulation models) and chemically (from treating only oxygen and hydrogen chemistry to modeling the transport and chemistry of chlorofluorocarbons and biological aerosols). Seinfeld & Pandis (2006) provide a useful introduction and review to the subject.

Our interest is in validating our photochemical network to the present-day Earth, and not in coupling Earth’s geochemistry to its atmospheric chemistry. We therefore make some simplifying assumptions when we set our boundary conditions. We compare our model to the contemporary Earth by setting the lower boundary conditions, temperature profile, and external UV field as given in Section 4.1. We present these comparisons for O_3 , CH_4 , and N_2O (Figure 14), NO and NO_2 (Figure 15), and OH and H_2O (Figure 16).

The data for O_3 , CH_4 , and N_2O is taken from the globally averaged mixing ratios from Massie & Hunten (1981). Following Hu et al. (2012), we apply error bars spanning an order of magnitude in mixing ratio to reflect the temporal and spatial variations. Our model fits the measured CH_4 to within the error bars throughout the atmosphere. The O_3 predicted by the model deviates from the data with errors at 15 km, and the

⁸ Referring primarily to NO and NO_2 chemistry.

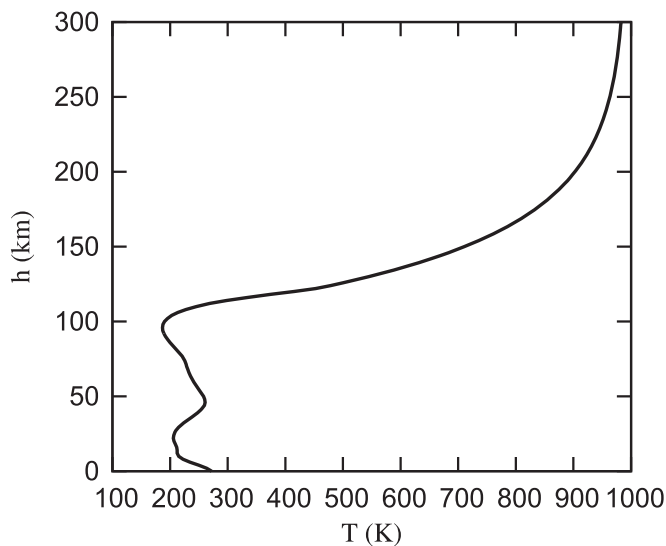


Figure 13. Temperature profile used for the early Earth chemistry, temperature [K] vs. height [km]. This profile is a synthetic profile for the Earth's atmosphere generated with the MSIS-E-90 model for the date 2000/1/1 (Hedin 1987, 1991).

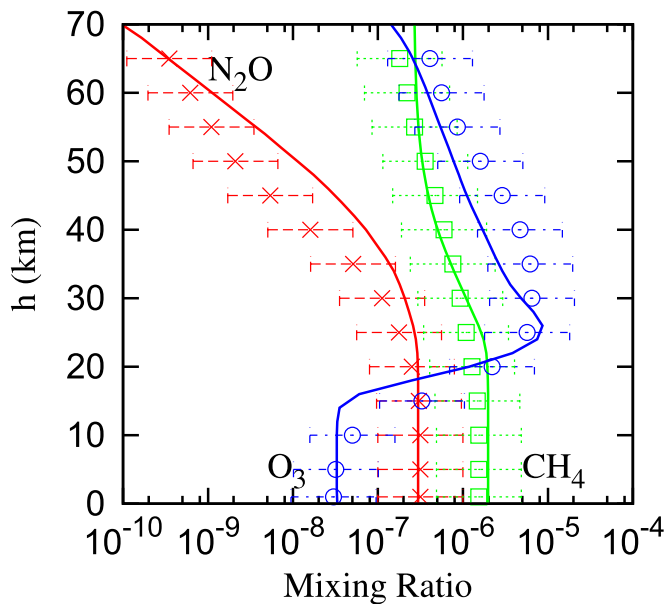


Figure 14. Mixing ratios of ozone, methane, and nitrous oxide as a function of atmospheric height [km] for the atmosphere of the present-day Earth. The lines are produced by our model and the points are taken from globally averaged measurements (Massie & Hunten 1981). Errors are set to an order of magnitude to account for diurnal and latitudinal variations.

N_2O deviates from the data with errors between 40 and 55 km. This may be due to an overestimation of the optical depth. If more UV photons in the model penetrated through to ~ 10 km, the O_3 mixing ratios would be enhanced at 15 km, and the N_2O mixing ratios would be destroyed more efficiently deeper in the atmosphere.

The data for NO and NO_2 is taken from balloon observations at 35 deg N in 1993 (Sen et al. 1998), and here also we apply error bars spanning an order of magnitude to reflect spatial and temporal variations. As with Hu et al. (2012), we seem to overpredict the abundance of NO in the upper atmosphere (30–40 km). We find that this overprediction is due to Reaction

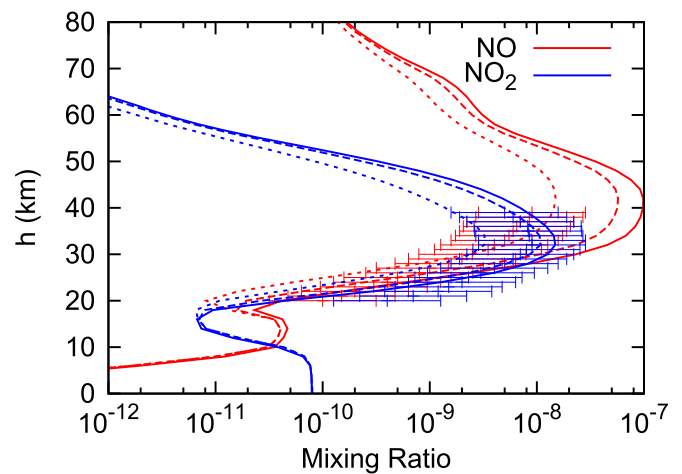


Figure 15. Mixing ratios of NO and NO_2 as a function of atmospheric height [km] for the atmosphere of the present-day Earth. The lines are produced by our model and the points are taken from balloon measurements (Sen et al. 1998). Errors are set to an order of magnitude to account for diurnal and latitudinal variations. We also show the results from suppressing the rate constant for Reaction 1300 in the network by a factor of 2 (dashed) and a factor of 10 (dotted).

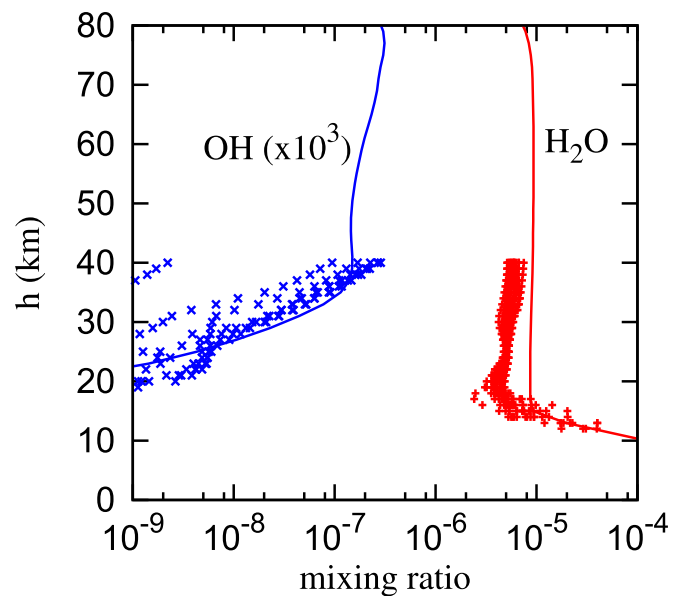
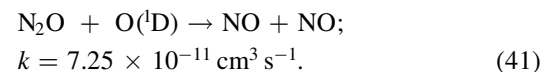


Figure 16. Mixing ratios of OH and H_2O as a function of atmospheric height [km] for the atmosphere of the present-day Earth. The lines are produced by our model and the points are taken from balloon measurements at various latitudes, heights, and times (Kovalenko et al. 2007).

1300 in the network:



We use the rate suggested by the JPL Chemical Kinetics and Photochemical Data for Use in Atmospheric Studies (Sander et al. 2011). If the rate constant for this reaction is decreased by a factor somewhere between 2 and 10, we come into much better agreement at 30–40 km, and worse agreement between 20–30 km (see Figure 15).

Finally, the data from OH and H_2O was taken from balloon measurements at various latitudes and heights in 2005 (Kovalenko et al. 2007). We plot each individual data point

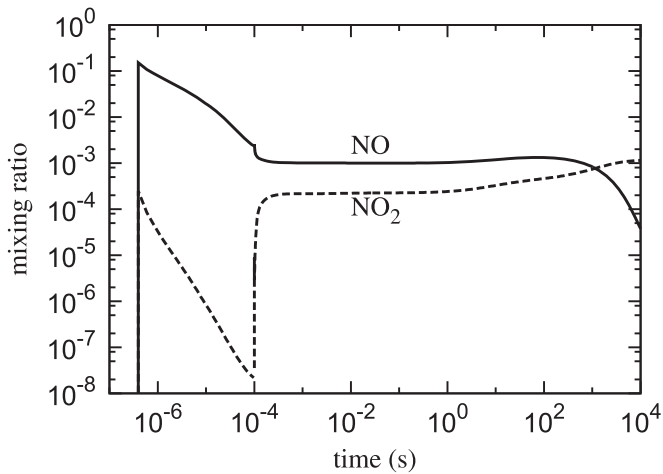


Figure 17. Mixing ratios of NO (solid) and NO₂ (dashed) vs. time [s] in a simulation of a lightning shock on a parcel of gas with an Earth-like atmospheric composition, initially at 300 K and 1 bar. The temperature and pressure vary as a function of time as described by Orville (1968), until 10⁻⁴ s, at which time conditions are returned to 300 K and 1 bar, and the system is allowed to further evolve.

without error bars in order to represent the observed variations; changes at other points of the globe or at other times of the year or day may lead to more significant variations in the abundances. The H₂O predictions are within a factor of five of the observed water abundance, and our OH predictions lie within the measurements, indicating that the model correctly reproduces the water and OH mixing ratios.

4.4.2. Lightning Shock Model and NO_x Chemistry

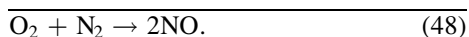
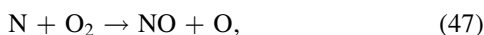
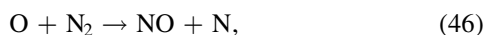
It is also useful to the model’s NO_x lightning-driven chemistry in the present-day atmosphere. For this purpose, we apply a simple shock model in order to explore the formation of NO_x species due to lightning at a single small region in the atmosphere. We employ the temperature and pressure calculations of Orville (1968, his Figures 1 and 3) and the timescaled results of Jebens et al. (1992, their Figures 2 and 3), fitting these to an exponential function. We use the following functions of temperature and pressure:

$$T(t) = 300 \text{ K} + (29800.0 \text{ K}) e^{-t/(55.56\mu\text{s})}; \quad (42)$$

$$P(t) = 1.0 \text{ bar} + (7.0 \text{ bar}) e^{-t/(5.88\mu\text{s})}. \quad (43)$$

We start with present-day atmospheric chemistry at the base of the troposphere, except without the N₂O, NO, and NO₂ species, and with $T = 300 \text{ K}$ and $p = 1 \text{ bar}$. The shock occurs at 1 ns, and is allowed to evolve until 0.1 ms. At this point the calculation is terminated, and another calculation initiated using for its initial conditions the final conditions of the shock model, except with temperature and pressure returned to 300 K and 1 bar, respectively. This model is run until 10⁴ s and results are shown in Figure 17.

We find that the NO_x species are formed in our model thermally by the Zel’dovich mechanism (Zel’dovich & Raizer 1996):



We compare our NO yield to the lightning discharge experiments performed by Navarro-González et al. (2001). We use for our NO mixing ratio the values found before the end of the shock (10⁻⁴ s in Figure 17), between 10⁻² and 10⁻³, to (Navarro-González et al. 2001, their Equation (4)). We find that

$$P(\text{NO}) \approx (2.4 \times 10^{22} \text{ K/J}) \frac{X(\text{NO})}{T_f} \\ \approx 2 - 20 \times 10^{16} \text{ molecules J}^{-1}, \quad (49)$$

where $T_f [\text{K}]$ is the “freeze-out” temperature after which the NO mixing ratio does not change appreciably over the timescale of the experiment, which we set to 1000 K (the approximate temperature of our model at $t \approx 10^{-4}$ s). This is consistent with the production of NO in the “hot core” region of the experiment. This is also roughly consistent with the literature values for NO production of 10¹⁷ molecules J⁻¹ (Borucki et al. 1984; Price et al. 1997).

This is an order of magnitude comparison between the code and lightning experiments and models, and for a more complete comparison will need to be applied to a model atmosphere, where diffusion and photochemistry together will further process the NO_x species. We plan to do this in a future paper.

4.4.3. The Early Earth

The presence of life and the evolution of the Sun both have radically altered Earth’s atmospheric chemistry. Oparin (1957) and Miller & Urey (1959) thought that the atmosphere of the early Earth⁹ was largely reducing, dominated by methane, ammonia, and molecular hydrogen. Kasting (1993) made a compelling case that prebiotic formation of hydrogen would be too slow to allow for much molecular hydrogen in the atmosphere of the early Earth. Furthermore, a major constituent in the early Earth atmosphere needs to be a strong greenhouse gas, in order to compensate for the cooler young Sun. The atmospheric chemistry of the early Earth is difficult to determine, and a severe lack of data results in many possible early Earth chemistries. As an illustrative example, Tian et al. (2005) argue that hydrogen escape was less efficient during the first 1 Gyr as was previously thought.¹⁰ If Tian et al. (2005) are correct, then Earth’s early atmospheric composition could have been reducing.

We present a model of the atmosphere of the early Earth, using the same lower boundary conditions as shown in Kasting (1993, his Figure 1), and a temperature profile for the present Earth (Hedin 1987, 1991)¹¹, shown in Figure 13. The lower boundary conditions used for the early Earth are given in Section 4.1. We treat outgassing using the deposition method (Appendix C).

We compare our results to those of Kasting (1993, see his Figure 1). Our results are presented in Figure 18. The results compare reasonably well for CO and O₂, but not for H₂O and O. The CO abundance begins to increase at 30 km, 10 km higher than for Kasting (1993), and achieves a mixing ratio of $\approx 5 \times 10^{-3}$ at 60 km, which is within a factor of 2 of Kasting (1993). The O₂ likewise begins to rise above a mixing ratio of

⁹ “Early Earth” in this context means the Earth in its first 1 Gyr.

¹⁰ The debate is ongoing (Catling 2006; Claire et al. 2006).

¹¹ <http://omniweb.sci.gsfc.nasa.gov/vitmo/>

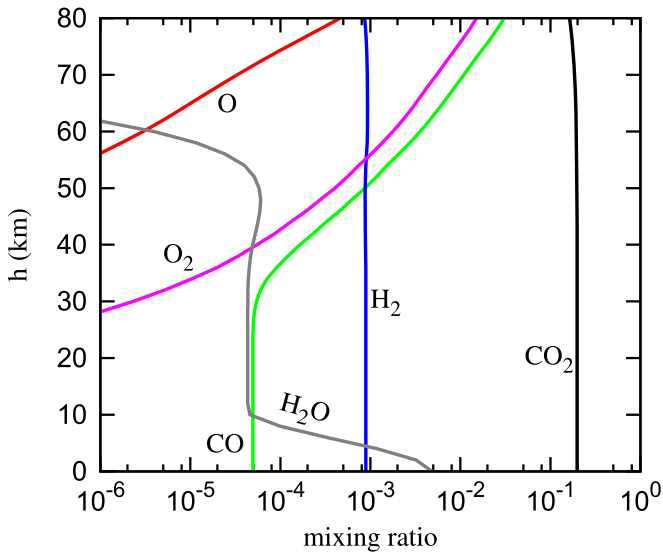


Figure 18. Mixing ratios for O, H₂, CO, O₂, H₂O, and CO₂, as a function of height [km], for early Earth photochemistry. These results can be compared to the results of Kasting (1993, his Figure 1).

10⁻⁶ 10 km higher in the atmosphere, and also achieves a mixing ratio of $\approx 2.5 \times 10^{-3}$, again within a factor of 2 of Kasting (1993). The water vapor profile is quite different, however. Instead of falling below a mixing ratio of 10⁻⁶ at 10 km, the H₂O mixing ratio in our model levels out at 5×10^{-4} , increasing slightly at ~ 50 km before plummeting. Also, the oxygen mixing ratio only reaches $\approx 3 \times 10^{-6}$, approximately two orders of magnitude below the mixing ratio predicted by Kasting (1993). These differences may be due to the different young solar UV fields assumed between ourselves and Kasting (1993), but we suspect that the differences are more likely due either to differences in the water condensation or the temperature profiles used. This seems especially likely for atomic oxygen, which is primarily destroyed by the reaction



in spite of the sizeable 7640 K barrier. When the water vapor drops off at ~ 55 km, this destruction route becomes unviable, and the atomic oxygen mixing ratio rapidly increases.

5. GLYCINE FORMATION IN A LABORATORY ENVIRONMENT

The formation of glycine, among several other amino acids, amines, and nucleotides, has been investigated for a variety of chemical compositions, from reducing (Miller 1953) to oxidizing (Schlesinger & Miller 1983; Miyakawa et al. 2002; Cleaves et al. 2008), and exploring various energy sources (see Miller & Urey 1959, and references therein). In a recent experiment, HCN and H₂S were exposed to UV light (peak frequency 2540 Å), resulting in the formation of numerous complex prebiotic compounds (Patel et al. 2015). The techniques used in this experiment afforded the experimenters to track the pathways of formation for these various species.

Prebiotic species are produced in smaller concentrations within a more oxidizing environments (Miller & Urey 1959). Methane has been found to be important for the formation of prebiotic compounds (Schlesinger & Miller 1983; Miyakawa et al. 2002). The correlation between reducing chemistry and

the efficient production of prebiotic molecules, combined with compelling evidence that the atmosphere of the early Earth was oxidizing (Kasting 1993), would suggest that other processes were responsible for producing the prebiotic chemical inventory on Earth. This process is hypothesized to have taken place within hydrothermal vents (e.g., Ferris 1992), on the surfaces of crystals (Vijayan 1980), or possibly within the interstellar medium (e.g., Greenberg et al. 1995).

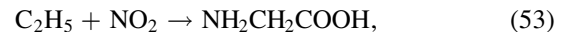
Cleaves et al. (2008) have repeated Miller’s experiment in a reducing environment, and discovered that amino acids can be efficiently produced in such environments, but that nitrites (e.g., HONO) destroy these species as quickly as they are produced. Adding ferrous iron, in the form of FeO or FeS₂ (in the form of pyrite surfaces) effectively removes the nitrites and allows the amino acids to survive.

We explore the formation of glycine in the context of a weak radiating source. An unattenuated monochromatic beam of light at $\lambda_0 = 1000$ Å is applied with an intensity of $\approx 2 \times 10^{-3}$ erg cm⁻² s⁻¹, corresponding to a flux of $F_0 = 10^8$ photons cm⁻² s⁻¹. This flux is applied to Equation (18) such that

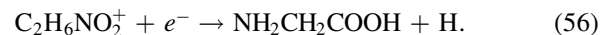
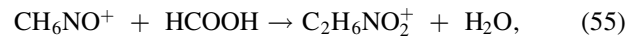
$$\begin{aligned} k_{\text{ph},i}(z) &= \int_{1 \text{ \AA}}^{10^4 \text{ \AA}} \sigma_i(\lambda) F_0 \delta(\lambda - \lambda_0) d\lambda; \\ &= F_0 \sigma_i(\lambda_0), \end{aligned} \quad (51)$$

where δ is the Dirac delta function.

The formation pathways for glycine have not been rigorously determined, although there are some proposed pathways. We include four possible pathways to glycine formation in our network. First, we include glycine formation via the three-body interaction of various species. These reactions have significant barriers, and so will only occur efficiently at rather high temperatures. The reactions are



with rate constants set equal to the three-body formation for analogous chemical species (e.g., CH₂COOH). Also included is the ion–neutral pathway proposed for interstellar formation for glycine from Charnley (1997),



Finally, the formation of glycine by a possible pathway similar to that suggested by Patel et al. (2015),



is included.

Additionally, we include FeO and reactions between FeO and nitrites. We also inject our gas with HCOOH in order to facilitate the ion–neutral formation pathway; it is likely that there are other presently unknown paths of formation for formic acid. We run this network for a set of five different initial compositions given in Table 2, labeled Model A–E. Model A is a strongly reducing environment, with only the gases NH₃, CH₄, H₂ and H₂O, FeO, and HCOOH (Model A). We transition to a more reducing environment in the successive models (Models B, C, D). Finally, for Model E, we run the experiment starting solely from CO₂, N₂, H₂O, FeO, and HCOOH. We run all models using the unattenuated UV flux, at

Table 2
Mixing Ratios for Laboratory Simulations^a

Model	H ₂ O	CH ₄	NH ₃	H ₂	CO ₂	N ₂
A	0.80	0.08	0.08	0.04	0.0	0.0
B	0.80	0.06	0.06	0.04	0.02	0.02
C	0.80	0.04	0.04	0.04	0.04	0.04
D	0.80	0.02	0.02	0.04	0.06	0.06
E	0.84	0.00	0.00	0.00	0.08	0.08

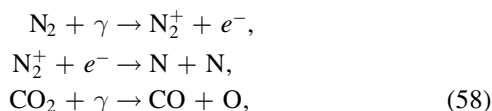
Note.

^a Not including the injected FeO and HCOOH.

1 bar pressure and 300 K temperature. The model is run to $t \approx 1$ week. Our results are plotted in Figure 19.

Moving from Model B to E, less and less glycine is formed, falling from a mixing ratio of 10^{-6} for Model B to 10^{-8} for Model E. This is what is expected from the Miller–Urey experiments performed for various chemical compositions: as the chemistry becomes less reducing, it becomes more difficult to form prebiotic molecules.

More interesting is Model A. If all N₂ and CO₂ are removed, certain formation pathways to NO₂, HNO₂, and especially H₂CO are inhibited. Additionally, HCNO forms more slowly from HCN, and especially the ionic form, CHNO⁺ (in its various permutations) is difficult to form without some excess unbonded atomic nitrogen or oxygen present in the gas. Model A produces virtually no glycine. We traced this back to the key reactions:



which is the same formation pathway for amines in the early Earth as suggested by Zahnle (1986). In our case, however, the atomic nitrogen and oxygen are both important in completing the formation of HCNO and its isomers.

6. CONCLUSION

In this paper, we have presented a gas-phase chemical network, STAND2015. The photochemistry/diffusion code, ARGO, was used to test the network. We have shown that the predictions from STAND2015 converge to chemical equilibrium under the appropriate conditions and also that the molecular diffusion modeled by ARGO makes a reasonable approximation to analytical calculations of molecular diffusion for an isothermal gas in hydrostatic equilibrium. We have compared our model results (STAND2015+ARGO) to chemical kinetics models for HD 209458b, Jupiter, and the Earth. For Jupiter, we found that ion–neutral chemistry may provide significant alternative pathways to formation of various hydrocarbons, especially ethylene (C₂H₄).

Finally, we numerically simulate a Urey–Miller-like experiment¹² under various initial chemistries. We found that, in an artificial environment, when derivatives of FeO and pyrite (FeS₂) can destroy nitrites in the presence of a reservoir of formic acid, the formation of glycine is considerable also in reducing environments, approaching a mixing ratio of $\sim 10^{-6}$. For an environment more similar to the atmosphere of the early

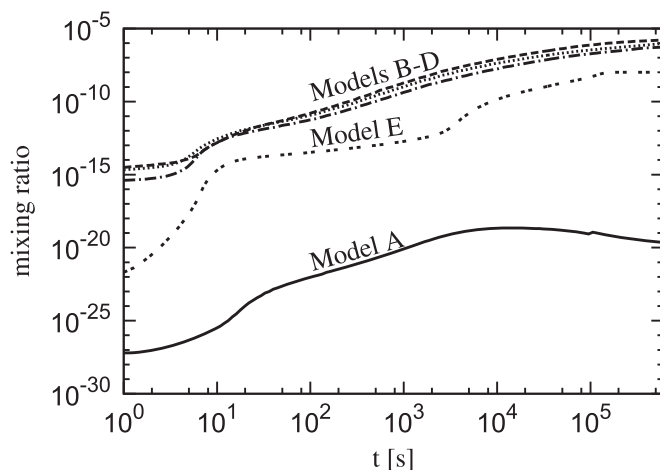


Figure 19. Mixing ratio of glycine as a function of time, for five lab simulations, labeled Models A–E, with parameters given in Table 2 and described in Section 5.

Earth, the mixing ratio drops to $\sim 10^{-8}$. Surprisingly, for a gas without any CO₂, O₂, or N₂, virtually no glycine is formed. If this result is robust for various other energy sources (shocks, thermal energy, etc.) and for other prebiotic species, this would suggest that the early Earth chemistry should not be too strongly reducing, or else the formation of glycine and other prebiotic species would be severely inhibited.

This network has limitations. It has only been tested for 1D atmosphere models, with non-self-consistent temperature profiles. Using this network within a global circulation model is presently unrealistic, but a reduced version of this network, constructed specifically for given atmospheres, could in principle be employed in 2D or 3D atmosphere simulations. Sulfur chemistry has been shown to play an important role in the formation of prebiotics, and is an essential constituent in volcano plumes. The inclusion of sulfur chemistry will be a natural next step to take the model. Additionally, the models of prebiotic chemistry should consider the formation of species other than glycine. The formation of ribose (C₅H₁₀O₅) of nucleotides, such as adenine (C₅H₅N₅), and of phosphorus-bearing species should also be included to more fully encapsulate the formation of the prebiotic chemical reservoir.

One serious problem with this network, and indeed with any chemical kinetics network, is the uncertainty in rate coefficients. The effects of this uncertainty can be estimated using sensitivity analysis (e.g., within Venot et al. 2012), but can ultimately only be resolved slowly as better experimental and theoretical determinations of the reaction rates are made available. More accurate determinations, especially of the reaction rates for the nitrogen chemistry, would be extremely helpful. This network and model provide a window into a detailed analysis of prebiotic chemistry, but much work must still be done in order to accurately predict the full budget of prebiotic molecules in the variety of environments in which they may occur.

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¹² The experiment we simulate is more like that of Patel et al. (2015).

Table 3
Bond Constants for Benson Additivity

Species	a_1	a_2	a_3	a_4	a_5	a_6	a_7
C–H							
300–1000 K	1.1E0	–3.0E-3	1.2E-5	5.8E-8	4.8E-12	–2.5E3	–2.5E-2
1000–6000 K	4.0E-1	2.3E-3	–1.9E-6	1.4E-10	–8.3E-15	–2.0E3	2.8E0
C–C							
300–1000 K	–2.4E0	1.3E-3	–1.4E-5	–2.8E-7	–5.0E-13	3.0E3	3.0E0
1000–6000 K	1.8E0	1.5E-3	5.7E-7	4.0E-11	–2.5E-15	2.5E2	–1.8E1
C–O							
300–1000 K	–6.8E-1	8.3E-3	–1.0E-5	–2.0E-7	–2.3E-12	9.0E2	4.8E-1
1000–6000 K	1.7E0	1.3E-3	8.3E-6	5.5E-11	–3.8E-15	–6.5E2	–1.1E1
O–H							
300–1000 K	5.0E-2	–7.3E-3	1.8E-5	1.2E-7	8.5E-12	–9.0E3	–4.2E0
1000–6000 K	–4.5E-1	–3.1E-3	–6.7E-6	–1.6E10	–5.4E-14	–7.5E3	5.2E0

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APPENDIX A LIST OF SPECIES, REACTIONS, AND RATES

The purpose of this appendix is to explicitly lay out the content of the chemical network itself. We list the species considered in the network and the reactions.

The species include the elements H/C/N/O, and the network includes a complete chemistry for molecules and ions of up to two carbon, six hydrogen, two nitrogen, and three oxygen atoms. The different chemical kinetics for various neutral molecular isomers is included as completely as possible, although much about branching ratios for reactions is presently not well understood. A list of all the neutral species is given in Table 4. This table lists the species considered and includes the formula as used in the network, the standard formula, the name of the molecule, and the source we used for the thermochemical data. In some cases, the chemical formula in the network is different from the standard chemical formula. This is because we incorporated our own method for distinguishing isomers in order to make sure that we did not incorporate the same molecule under two different formulas.

This list also includes some species with the elements Na, Mg, Si, Cl, K, Ti, and Fe. The chemistry attempts to include only the dominant species with these elements, in which they would be present in the gas phase. These species are generally only present in the gas phase for very high temperatures (generally >1000 K). For cooler objects, these species are typically ignored. The noble gases He and Ar are included, both for the sake of completeness and because they can play an important role in organic ion–neutral chemistry through charge-exchange reactions.

Ions are also included, and a list of the ionic species is given in Table 5. In this case, the uncertainty in reaction rates and branching ratios is much more severe, and so we made no attempt at present to distinguish isomers of ionic species.

It is difficult to determine which rate constants to use for a specific reaction, since there are often many to choose from, and they do not always agree well with each other. We employed the following method for determining which rate constant to include in our network, after plotting all the rate constants versus temperature over a range of 100–30,000 K.

1. If there exists only one published rate constant for a given reaction, we use that value.
2. Reject all rate constants that become unrealistically large at extreme temperature.
3. Choose rate constants that agree with each other over the range of validity.
4. If the most recent published rate constant disagrees with (3), and the authors give convincing arguments for why the previous rates were mistaken, we use the most recently published rate.

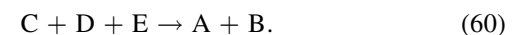
The full list of forward reactions and rate constants determined by this method comprise the STAND2015 network and are given in Table 6. Reverse reactions are not explicitly shown; when reactions are reversible, bidirectional arrows are shown. When they are irreversible, or simply not reversed in the network, only unidirectional arrows are shown. Table 6 additionally includes a full list of the references for the rate constants used for each given reaction.

APPENDIX B REVERSING REACTIONS

For reverse reactions, we follow the prescription given by Burcat & Ruscic (2005). For the reaction



there is a rate constant, k_f . We resolve to determine the reverse rate constant, k_r , for the reaction



Note that the number of species is different between the right-hand side and left-hand side of Equation (60). We denote this difference in number of reactants and products (n_{react} and n_{prod} , respectively) by $\Delta\nu$, which in our case

Table 4
Neutral Species Included in the STAND2015 Network

Network Formula	Standard Formula	Name	Thermochem Data
H	H	Atomic hydrogen	Burcat
C	C	Atomic carbon	Burcat
C(¹ D)	C(¹ D)	Singlet D carbon	Burcat
C(¹ S)	C(¹ S)	Singlet S carbon	Burcat
N	N	Atomic nitrogen	Burcat
O	O	Atomic oxygen	Burcat
O(¹ D)	O(¹ D)	Singlet D oxygen	Burcat
O(¹ S)	O(¹ S)	Singlet S oxygen	Burcat
He	He	Helium	Burcat
Na	Na	Atomic sodium	Burcat
Mg	Mg	Atomic magnesium	Burcat
Si	Si	Atomic silicon	Burcat
Cl	Cl	Atomic chlorine	Burcat
Ar	Ar	Argon	Burcat
K	K	Atomic potassium	Burcat
Ti	Ti	Atomic titanium	Burcat
Fe	Fe	Atomic iron	Burcat
H ₂	H ₂	Molecular hydrogen	Burcat
C ₂	C ₂	Dicarbon	Burcat
N ₂	N ₂	Molecular nitrogen	Burcat
O ₂	O ₂	Molecular oxygen	Burcat
O ₂ (a ¹ Δ)	O ₂ (a ¹ Δ)	Singlet oxygen	Burcat
CH	CH	Methylidyne radical	Burcat
HN	NH	Nitrogen monohydride	Burcat
HN(a ¹ Δ)	NH(a ¹ Δ)	Singlet nitrogen monohydride	Burcat
HO	OH	Hydroxyl radical	Burcat
CN	CN	Cyano radical	Burcat
CO	CO	Carbon monoxide	Burcat
KH	KH	Potassium hydride	Burcat
NO	NO	Nitric oxide	Burcat
HCl	HCl	Hydrogen chloride	Burcat
NaH	NaH	Sodium hydride	Burcat
MgO	MgO	Magnesium oxide	Burcat
SiH	SiH	Silylidyne	NASA-CEA
SiO	SiO	Silicon monoxide	NASA-CEA
KCl	KCl	Potassium chloride	Burcat
TiO	TiO	Titanium(II) oxide	NASA-CEA
FeO	FeO	Iron(II) oxide	Burcat
O ₃	O ₃	Ozone	Burcat
³ CH ₂	CH ₂ (X ³ B ₁)	Triplet methylene	Burcat
¹ CH ₂	CH ₂ (a ¹ A ₁)	Singlet methylene	Burcat
¹ CH ₂	CH ₂ (a ¹ A ₁)	Singlet methylene	Burcat
C ₂ H	CCH	Ethynyl radical	Burcat
H ₂ N	NH ₂	Amidogen	Burcat
HN ₂	N ₂ H	Amino radical	Burcat
H ₂ O	H ₂ O	Water	Burcat
HO ₂	HO ₂	Hydroperoxyl	Burcat
C ₂ N	CCN	Cyano-methylidyne	Burcat
CNC	CNC	CNC radical	Burcat
CN ₂	CNN	CNN radical	Burcat
C ₂ O	C ₂ O	Dicarbon monoxide	Burcat
CO ₂	CO ₂	Carbon dioxide	Burcat
N ₂ O	N ₂ O	Nitrous oxide	Burcat
NO ₂	NO ₂	Nitrogen dioxide	Burcat
HCN	HCN	Hydrogen cyanide	Burcat
HNC	HNC	Hydrogen isocyanide	Burcat
HNO	HNO	Nitroxyl	Burcat
NCO	NCO	Isocyanato radical	Burcat
NaOH	NaOH	Sodium hydroxide	Burcat
MgHO	MgOH	Magnesium monohydroxide	NASA-CEA

Table 4
(Continued)

Network Formula	Standard Formula	Name	Thermochem Data
NaCl	NaCl	Sodium chloride	Burcat
SiH ₂	SiH ₂	Silylene	NASA-CEA
KOH	KOH	Potassium hydroxide	Burcat
FeO ₂	FeO ₂	Iron oxide	Burcat
CH ₃	CH ₃	Methyl radical	Burcat
C ₂ H ₂	C ₂ H ₂	Acetylene	Burcat
H ₃ N	NH ₃	Ammonia	Burcat
H ₂ N ₂	N ₂ H ₂	Diimide	Burcat
HNNH	HNNH	(Z)-Diazene	Burcat
H ₂ O ₂	H ₂ O ₂	Hydrogen peroxide	Burcat
NCCN	(CN) ₂	Cyanogen	Burcat
H ₂ CN	H ₂ CN	Dihydrogen cyanide	Burcat
HCCN	HCCN	HCCN radical	Burcat
CHN ₂	HCNN	HCNN	Burcat
CH ₂ O	H ₂ CO	Formaldehyde	Burcat
HOCH	HCOH	Hydroxymethylene	Burcat
HCCO	HCCO	Ethynyloxy radical	Burcat
COOH	COOH	Hydrocarboxyl radical	Burcat
NH ₂ O	NHOH	NHOH	Burcat
HNO ₂	HNO ₂	Nitrous acid	Burcat
OCCN	NCCO	NCCO	Burcat
HCNO	HCNO	Fulminic acid	Burcat
HNCO	HNCO	Isocyanic acid	Burcat
CHNO	CHNO	Cyanic acid	Burcat
HCNO	HCNO	HCNO	Burcat
SiH ₃	SiH ₃	Silyl radical	Burcat
CH ₄	CH ₄	Methane	Burcat
C ₂ H ₃	C ₂ H ₃	Vinyl radical	Burcat
NH ₂ NH	NH ₂ NH	Hydrazinyl radical	Burcat
N ₂ O ₃	N ₂ O ₃	Nitrogen trioxide	Burcat
CH ₃ N	CH ₂ NH	Methanimine	Burcat
CH ₂ CN	CH ₂ CN	Cyanomethyl radical	Burcat
CH ₂ N ₂	CH ₂ N ₂	Diazomethane	Burcat
HC ₃ N	...	Propiolonitrile	Burcat
CH ₂ OH	CH ₂ OH	Hydroxymethyl radical	Burcat
CH ₃ O	CH ₃ O	Methoxy radical	Burcat
C ₂ H ₂ O	H ₂ CCO	Ethenone	Burcat
HCOOH	HCOOH	Formic acid	Burcat
CH ₂ O ₂	CH ₂ OO	CH ₂ OO	Burcat
HNO ₃	HNO ₃	Nitric acid	Burcat
NH ₂ OH	NH ₂ OH	Hydroxylamine	Burcat
HCOCN	HCOCN	HCOCN	Benson
MgO ₂ H ₂	H ₂ MgO ₂	Magnesium hydroxide	NASA-CEA
SiH ₄	SiH ₄	Silane	Burcat
C ₂ H ₄	C ₂ H ₄	Ethylene	Burcat
C ₃ H ₃	...	Propargyl radical	Burcat
H ₄ N ₂	N ₂ H ₄	Hydrazine	Burcat
H ₄ O ₂	H ₂ O-H ₂ O	Water dimer	Burcat
CH ₃ CN	CH ₃ CN	Acetonitrile	Burcat
C ₂ H ₃ N	CH ₂ CNH	CH ₂ =C=NH	Burcat
CH ₃ N ₂ H	CH ₃ N ₂ H	Methyl diazene	Burcat
CH ₃ OH	CH ₃ OH	Methanol	Burcat
CH ₃ O ₂	CH ₃ O ₂	CH ₃ O ₂	Burcat
C ₂ H ₃ O	CH ₃ CO	Acetyl radical	Burcat
cyc-C ₂ H ₃ O	Oxyranyl	Oxyranyl radical	Burcat
CH ₂ CHO	CH ₂ CHO	CH ₂ CHO	Burcat
C ₃ H ₂ O	...	2-Propynal	Benson
C ₂ H ₂ O ₂	(CHO) ₂	Glyoxal	Burcat
H ₂ NNO ₂	H ₂ N-NO ₂	H ₂ N-NO ₂	Burcat
CH ₃ NO	HCONH ₂	Formamide	Burcat

Table 4
(Continued)

Network Formula	Standard Formula	Name	Thermochem Data
C ₂ H ₅	C ₂ H ₅	Ethyl radical	Burcat
C ₃ H ₄	...	Propyne	Burcat
CH ₃ N	CH ₃ NH ₂	Methylamine	Burcat
C ₃ H ₃ N	...	Acrylonitrile	Burcat
C ₂ H ₄ O	CH ₃ CHO	Acetaldehyde	Burcat
H ₂ C ₂ HOH	CH ₂ CHOH	Vinyl alcohol	Burcat
Oxirane	Oxirane	Oxirane	Burcat
C ₃ H ₃ O	...	1-Oxoprop-2-ynyl	Burcat
CH ₄ O ₂	CH ₃ OOH	Methyl peroxide	Burcat
CH ₃ OCO	CH ₃ OCO	CH ₃ OC(O)	Burcat
CH ₃ NO ₂	CH ₃ NO ₂	Nitromethane	Burcat
CH ₃ ONO	CH ₃ ONO	Methyl nitrite	Burcat
C ₂ H ₆	C ₂ H ₆	Ethane	Burcat
C ₄ H ₄	...	1-Buten-3-yne	Burcat
CH ₂ NCH ₃	NH ₂ NCH ₃	N-Methyl methanimine	Benson
CH ₃ COOH	CH ₃ COOH	Acetic acid	Burcat
CH ₃ OCHO	CH ₃ OCHO	Methyl formate	Burcat
CH ₃ CHOH	CH ₃ CHOH	1-hydroxy Ethyl radical	Burcat
CH ₃ CH ₂ O	CH ₃ CH ₂ O	Ethoxy radical	Burcat
CH ₃ OCH ₂	CH ₃ OCH ₂	Methoxymethyl radical	Burcat
CH ₃ NO ₃	CH ₃ NO ₃	Methyl nitrate	Burcat
C ₂ H ₃ NO ₂	C ₂ H ₃ NO ₂	Nitroethylene	Burcat
Si ₂ H ₆	Si ₂ H ₆	Disilane	Burcat
C ₃ H ₆	...	Propene	Burcat
C ₂ H ₆ N	(CH ₃) ₂ N	Dimethyl amidogen	Burcat
C ₂ H ₅ OH	CH ₃ CH ₂ OH	Ethanol	Burcat
C ₂ H ₅ OO	C ₂ H ₅ OO	C ₂ H ₅ OO	Burcat
C ₂ H ₄ O ₃	HOCH ₂ COOH	Glycolic acid	Burcat
(CH ₃) ₂ O	(CH ₃) ₂ O	Dimethyl ether	Burcat
C ₂ H ₅ NO	C ₂ H ₅ NO	Acetaldoxime	Benson
C ₄ H ₆	...	1,3-Butadiene	Burcat
(CH ₃ N) ₂	(CH ₃ N) ₂	Dimethyl diazene	Burcat
(CH ₃ O) ₂	(CH ₃ O) ₂	Dimethyl peroxide	Burcat
(CH ₂ OH) ₂	(CH ₂ OH) ₂	1,2-Ethanediol	Burcat
(CH ₃) ₂ CO	(CH ₃) ₂ CO	Acetone	Burcat
C ₂ H ₆ O ₂	HOCH ₂ CH ₂ OH	Ethylene glycol	Burcat
C ₂ H ₅ NO ₂	NH ₂ CH ₂ COOH	Glycine	Burcat
aC ₂ H ₅ NO ₂	C ₂ H ₅ NO ₂	Nitroethane	Burcat
bC ₂ H ₅ NO ₂	C ₂ H ₅ ONO	Ethyl nitrate	Benson
C ₃ H ₈	...	Propane	Burcat
(CH ₃) ₂ N ₂ O	(CH ₃) ₂ N ₂ O	Dimethylnitrosamine	Benson
C ₄ H ₁₀	...	Butane	Burcat

(This table is available in machine-readable form.)

$= n_{\text{prod}} - n_{\text{react}} = 2 - 3 = -1$. We then solve for the reaction rate constant as (Burcat & Ruscic 2005, their Equation (6))

$$K_c = (RT)^{-\Delta\nu} \exp\left(\Delta a_1(\log T - 1) + \frac{\Delta a_2 T}{2} + \frac{\Delta a_3 T^2}{6} + \frac{\Delta a_4 T^3}{12} + \frac{\Delta a_5 T^4}{20} - \frac{\Delta a_6}{T} + \Delta a_7\right), \quad (61)$$

where $R = 8.314472 \text{ J mol}^{-1} \text{ K}^{-1}$ is the gas constant, and $\Delta a_i = a_i(C + D + E) - a_i(A + B)$ for $1 \leq i \leq 7$ are the NASA thermodynamics coefficients, which Burcat & Ruscic

(2005) describes and tabulates. It is important to emphasize here, as done by Visscher & Moses (2011), the multiplicative factor $(RT)^{-\Delta\nu}$, which in our example would be $1.38065 \times 10^{-22} T$.

The Burcat values for the NASA coefficients have been used for all possible species (see Table 4). For some species, however, the coefficients had to be obtained from other sources. For sources with elements Na, Mg, Si, Cl, K, Ti, and Fe, the Burcat values were sparse, so we made use instead of the NASA-CEA values (McBride et al. 1993; Gordon & McBride 1999), which use nine-coefficient polynomials, so we fit them to a series of seven-coefficient polynomials for various temperature ranges. We do the same for the monatomic gases and ions at high temperatures $6000 \text{ K} < T < 20,000 \text{ K}$, using fits to the polynomials provided by Gordon & McBride (1999). For some species, the thermodynamic properties have not been determined. In these cases, for neutral species we use Benson's additivity method as described by Cohen & Benson (1993).

Benson's additivity method can be naturally combined with the NASA and Burcat polynomial coefficients using the experimental values for the small alkanes listed within Cohen & Benson (1993). For the arbitrary alcohol from Cohen & Benson (1993), we use methanol, and for the arbitrary ether, we used dimethyl ether. The Benson coefficients are

$$P_i = \frac{1}{2} a_i(\text{C}_2\text{H}_6), \quad (62)$$

$$S_i = a_i(\text{C}_3\text{H}_8) - a_i(\text{C}_2\text{H}_6), \quad (63)$$

$$D_i = a_i(\text{C}_2\text{H}_6\text{O}) - a_i(\text{C}_2\text{H}_6), \quad (64)$$

$$F_i = a_i(\text{CH}_3\text{OH}) - a_i(\text{CH}_4). \quad (65)$$

Here, $a_i(X)$ denotes the seven coefficients, $i = 1, \dots, 7$ for species X . The coefficients for fundamental bonds are calculated using these coefficients as follows:

$$a_i([\text{C} - \text{H}]) = \frac{1}{2}P - \frac{1}{4}S, \quad (66)$$

$$a_i([\text{C} - \text{C}]) = \frac{3}{2}S - P, \quad (67)$$

$$a_i([\text{C} - \text{O}]) = \frac{1}{2}D + \frac{3}{4}S - \frac{1}{2}P, \quad (68)$$

$$a_i([\text{O} - \text{H}]) = F - \frac{1}{2}D - \frac{1}{2}S. \quad (69)$$

The values for these bonds are given in Table 3. The values for [N-H], [N-C], and [N-O] are similarly determined.

It has been suggested by Lias (1988) and Cohen & Benson (1993) that using Benson's additivity method to determine the thermodynamic properties of ions, or at least strongly of strongly polarizing groups, can lead to large errors, because the thermodynamic properties of ions do not depend linearly on their length, although Hammerum & Sølling (1999) have had some success applying Benson's method to ions.

We found, by investigating the thermodynamic properties of ionic species tabulated by Burcat & Ruscic (2005), that the thermodynamic properties of ions do depend nonlinearly but predictably based on size. We therefore placed all the known thermodynamic properties of ions into a database, and have extrapolated to calculate the thermodynamic properties for the undetermined ions.

Table 5
List of Ions Included the STAND2015 Network

e ⁻	C ⁺	C ⁻	H ⁺	H ⁻	K ⁺	N ⁺
O ⁺	O ⁺ (² D)	O ⁺ (³ P)	O ⁻	Ar ⁺	Cl ⁺	C ₂ ⁺
C ₂ ⁻	C ₃ ⁺	C ₄ ⁺	CH ⁺	CN ⁺	CN ⁻	CO ⁺
Fe ⁺	H ₂ ⁺	H ₃ ⁺	HN ⁺	HO ⁺	HO ⁻	He ⁺
Mg ⁺	Na ⁺	N ₂ ⁺	N ₃ ⁺	N ₃ ⁻	NO ⁺	NO ⁻
O ₂ ⁺	O ₂ ⁺ (X ² Π _g)	O ₂ ⁻	O ₃ ⁻	Si ⁺	Ti ⁺	Ar ₂ ⁺
ArH ⁺	C ₂ H ⁺	C ₂ H ⁻	C ₂ N ⁺	C ₂ O ⁺	C ₃ H ⁺	C ₃ N ⁺
C ₃ O ⁺	C ₄ H ⁺	C ₅ N ⁺	CH ₂ ⁺	CH ₃ ⁺	CH ₄ ⁺	CH ₅ ⁺
CHN ⁺	CHO ⁺	CN ₂ ⁺	CNO ⁺	CNO ⁻	CO ₂ ⁺	CO ₃ ⁻
CO ₄ ⁺	CO ₄ ⁻	FeO ⁺	H ₂ N ⁺	H ₂ N ⁻	H ₂ O ⁺	H ₃ N ⁺
H ₃ O ⁺	H ₄ N ⁺	HN ₂ ⁺	HN ₃ ⁺	HNO ⁺	HO ₂ ⁺	HO ₂ ⁻
HO ₄ ⁺	HSi ⁺	He ₂ ⁺	HeH ⁺	MgO ⁺	N ₂ O ⁺	NO ₂ ⁺
NO ₂ ⁻	NO ₃ ⁻	Si ₂ ⁺	SiH ⁺	SiO ⁺	TiO ⁺	Ar ₂ H ⁺
ArH ₃ ⁺	C ₂ H ₂ ⁺	C ₂ H ₂ ⁻	C ₂ H ₃ ⁺	C ₂ H ₃ ⁻	C ₂ H ₄ ⁺	C ₂ H ₅ ⁺
C ₂ H ₆ ⁺	C ₂ H ₇ ⁺	C ₂ HN ⁺	C ₂ HO ⁺	C ₂ HO ⁻	C ₂ N ₂ ⁺	C ₃ H ₂ ⁺
C ₃ H ₃ ⁺	C ₃ H ₄ ⁺	C ₃ H ₅ ⁺	C ₃ H ₆ ⁺	C ₃ H ₇ ⁺	C ₃ H ₈ ⁺	C ₃ H ₉ ⁺
C ₃ HN ⁺	C ₃ N ₂ ⁺	C ₃ N ₃ ⁺	C ₄ H ₂ ⁺	C ₄ H ₃ ⁺	C ₄ H ₄ ⁺	C ₄ H ₅ ⁺
C ₄ H ₇ ⁺	C ₄ H ₈ ⁺	C ₄ H ₉ ⁺	C ₅ HN ⁺	CH ₂ N ⁺	CH ₂ O ⁺	CH ₃ N ⁺
CH ₃ O ⁺	CH ₃ O ⁻	CH ₄ N ⁺	CH ₄ N ⁻	CH ₄ O ⁺	CH ₅ N ⁺	CH ₅ O ⁺
CH ₆ N ⁺	CHNO ⁺	CHO ₂ ⁺	CHO ₂ ⁻	FeO ₂ ⁺	H ₂ NO ⁺	H ₂ O ₂ ⁺
H ₃ O ₂ ⁺	HN ₂ O ⁺	HNO ₂ ⁺	MgHO ⁺	MgO ₂ ⁺	Si ₂ H ⁺	SiCH ⁺
SiH ₂ ⁺	SiH ₃ ⁺	SiH ₃ ⁻	SiH ₄ ⁺	SiH ₅ ⁺	SiHO ⁺	C ₂ H ₂ N ⁺
C ₂ H ₂ N ⁻	C ₂ H ₂ O ⁺	C ₂ H ₃ N ⁺	C ₂ H ₃ O ⁺	C ₂ H ₃ O ⁻	C ₂ H ₄ N ⁺	C ₂ H ₄ O ⁺
C ₂ H ₅ N ⁺	C ₂ H ₅ O ⁺	C ₂ H ₅ O ⁻	C ₂ H ₆ O ⁺	C ₂ H ₇ O ⁺	C ₂ HN ₂ ⁺	C ₃ H ₂ N ⁺
C ₃ H ₄ O ⁺	C ₃ H ₅ O ⁺	C ₃ H ₆ N ⁺	C ₃ H ₆ O ⁺	C ₃ H ₇ O ⁺	C ₃ H ₉ O ⁺	C ₃ HN ₂ ⁺
C ₄ H ₂ N ⁺	CH ₂ NO ⁺	CH ₃ NO ⁺	CH ₄ NO ⁺	CH ₅ NO ⁺	CH ₆ NO ⁺	CH ₂ O ₂ ⁺
CH ₂ OH ⁺	CH ₃ O ₂ ⁺	H ₂ NO ₂ ⁺	H ₂ NO ₃ ⁺	Si ₂ H ₂ ⁺	Si ₂ H ₃ ⁺	Si ₂ H ₄ ⁺
Si ₂ H ₃ ⁺	Si ₃ H ₂ ⁺	Si ₃ H ₃ ⁺	Si ₃ H ₄ ⁺	Si ₃ H ₅ ⁺	Si ₃ H ₆ ⁺	Si ₃ H ₇ ⁺
Si ₄ H ₂ ⁺	Si ₄ H ₃ ⁺	Si ₄ H ₄ ⁺	Si ₄ H ₅ ⁺	Si ₄ H ₆ ⁺	Si ₄ H ₇ ⁺	SiCH ₂ ⁺
SiCH ₃ ⁺	SiCH ₄ ⁺	SiCH ₅ ⁺	SiC ₂ H ⁺	SiH ₃ O ⁺	SiH ₃ O ⁻	aCHNO ⁺
C ₂ H ₄ NO ⁻	C ₂ H ₅ O ₂ ⁺	C ₄ H ₇ O ₂ ⁺	CH ₂ NO ₂ ⁻	CH ₃ NO ₂ ⁺	CH ₄ NO ₂ ⁺	MgH ₂ O ₂ ⁺
SiC ₂ H ₃ ⁺	SiC ₂ H ₄ ⁺	SiC ₂ H ₅ ⁺	SiC ₂ H ₆ ⁺	TiC ₂ H ₄ ⁺		

APPENDIX C OUTGASSING, CONDENSATION, EVAPORATION, AND ESCAPE

Boundary conditions play a key role in determining the atmospheric compositions of planets. For rocky planets, these boundary conditions are set by outgassing and escape into the exosphere. At temperatures $\lesssim 1500$ K, metals such as silicates, iron, and corundum begin to condense out of the atmospheric gas phase. At much lower temperatures, various other species (e.g., water, ammonia, methane) may also condense out. It is important for comparison to previous models to consider both the atmospheric boundary conditions and atmospheric condensation.

As discussed in Section 3.1, there exist, in addition to the STAND2015 reactions, a series of “banking” reactions for all major species, that collect particles and reintroduce them to the fluid parcel at a rate determined by the diffusion timescales. The very bottom banking reaction can be set to act effectively as an outgassing rate. Imagine a particular reservoir for a species, A. This reservoir is outgassing into the atmosphere with a flux, $\Phi(A)$ [$\text{cm}^{-2} \text{s}^{-1}$]. This can be accounted by first taking a reservoir concentration of A, which for a large reservoir will be $\gg [A](z = 0)$, the bottom of the atmosphere. For a reservoir that will not be appreciably depleted over the chemical-dynamical timescale of the

atmosphere, the rate is simply:

$$P_{\text{out}}(A) = \frac{\Phi(A)}{\Delta z}. \quad (70)$$

For a finite reservoir, we can place the reservoir concentration into the bottom “bank” for the species in question, and the $t = 0$ flux, $\Phi(A, 0)$, and concentration ($[BA]$) can be used to determine the rate of outgassing,

$$P_{\text{out}}(A) = L(BA) [BA], \quad (71)$$

where

$$L(BA) = \frac{\Phi(A, 0)}{[BA(t = 0)] \Delta z}. \quad (72)$$

These approximations are not used anywhere in this paper. For HD 209458b, we simply start with solar elemental abundances, with everything in atomic form at the bottom of the atmosphere. For both Jupiter and Earth, we start with fixed lower boundary conditions.

Condensation or evaporation of species A can be treated by the reactions (“JA” represents “A in condensate form”):

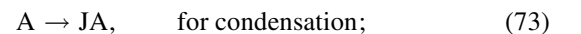


Table 6
STAND2015 Chemical Kinetics Network

#	Type	Reaction	α	β	γ	References
1	2d	$C_2 \rightleftharpoons C + C$	2.49e-08	0.00	71600	1
2	2d	$C_2 \rightleftharpoons C + C$	6.01e+11	-1.00	71600	...
3	2d	$CH \rightleftharpoons C + H$	3.16e-10	0.00	33700	2
4	2d	$CH \rightleftharpoons C + H$	7.63e+09	-1.00	33700	...
5	2d	$CN \rightleftharpoons C + N$	1.00e-09	0.00	71000	3
6	2d	$CN \rightleftharpoons C + N$	2.42e+10	0.00	71000	...
7	2d	$CO \rightleftharpoons C + O$	1.52e-04	-3.10	129000	4
8	2d	$CO \rightleftharpoons C + O$	3.67e+15	-4.10	129000	...
9	2d	$H + H \rightleftharpoons H_2$	9.13e-33	-0.60	0	30
10	2d	$H + H \rightleftharpoons H_2$	1.00e-11	0.00	0	5

Note.

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(This table is available in its entirety in machine-readable form.)

This physical process is treated in two ways in this paper for Earth and Jupiter. The first method is by considering supersaturation concentrations, above which the species in question condenses out and below which the species in question will evaporate. This method is given by Hamill et al. (1977), Toon & Farlow (1981), and (Hu et al. 2012), and has the form (for species A)

$$P = \frac{[A]}{t_c}, \quad L = \frac{[JA]}{t_c} \quad (75)$$

$$t_c = \frac{m_A v_{\text{th}} n_{\text{gas}} - n_c(T, p)}{4\rho_{\text{nuc}} a}, \quad (76)$$

where m_A [g] is the mass of the condensing species, v_{th} is the thermal velocity of the gas, ρ_{nuc} [g cm⁻³] is the material density of the condensation seed, n_{gas} [cm⁻³] is the density of the gas, and n_c [cm⁻³] is the saturation number density, at the given temperature and pressure, and a [cm] is the average radius of the nucleation site. We consider condensation only for low temperatures, so $n_c = p_v/k_B T$, where p_v [dyn cm⁻²] is the vapor pressure, and is estimated using the relatively simple Antoine equation:

$$\log p_v = A - \frac{B}{C + T}, \quad (77)$$

where A , B , and C are all parameters taken from the tabulated NIST chemistry webbook.¹³

Alternatively, one can use the method commonly used in the astrochemical context (Hasegawa et al. 1992; Caselli et al. 1998), where

$$L [\text{s}^{-1}] = \pi a^2 v_{\text{th}} n_{\text{nuc}} \quad (78)$$

and

$$P = \nu_0 [JA] e^{-E_D/k_B T}. \quad (79)$$

Here, E_D is the desorption energy, an empirically determined quantity, taken from Garrod et al. (2008). The frequency,

$$\nu_0 [\text{Hz}] = \left(\frac{2n_s E_D}{\pi^2 m_A} \right)^{1/2}, \quad (80)$$

is the characteristic frequency of the surface. The number of sites is estimated, also empirically, by the relation $n_s = 1.5 \times 10^{15} \text{ cm}^2 (a/a_0)^2$, where $a_0 = 0.1 \mu\text{m}$. The advantage of this approximation is that it is identical to the form generally used for complex surface chemistry in protoplanetary disks. This would allow one to take the results from disk chemistry and utilize them straightforwardly in atmospheric outgassing models.

¹³ <http://webbook.nist.gov/chemistry/>

It is worth pointing out that exponentiating Equation (78), dividing by k_{BT} , and then placing the resulting form of n_c into Equation (77) yields a form:

$$\frac{P}{L} \sim \frac{\text{Const.}}{v_{\text{th}}} e^{T_c/T}, \quad (81)$$

where $T_c/T = B/(C + T)$ from Equation (78). The two forms are therefore analogous parameterizations, with the same temperature dependence, but the saturation approach is dependent on the parameterized vapor pressure, and the deposition approach is parameterized by the number of nucleation sites and the binding energy of the nucleation particle.

Neither the supersaturation method nor the deposition method explain where the condensation seeds first arise. It is assumed that the condensation seeds are already present, and therefore that condensation occurs whenever the supersaturation ratio $S \gtrsim 1$. In some environments like Earth, the condensation seeds come in the form of sand or ash particles, and the supersaturation ratio for water to condense is very small, $S \approx 1.01$. If the seed particles are not already present in the atmosphere, they must form within the gas phase by the growth from small to large, complex clusters. This requires a supersaturation ratio $S \gg 100$, which only occurs when $T \ll T_c$ (Helling & Fomins 2013). Zsom et al. (2012) explore the microphysics of water condensation and cloud formation for Earth and Earth-like planets.

None of these reactions appear in the generic kinetic network, because their inclusion is atmosphere-dependent. Condensation is not considered at all for HD 209458b because it is too hot, but is considered for Earth and Jupiter for water. Ammonia and methane condensation can also be considered for Jupiter and methane and other condensation should be considered for even colder planets, such as Uranus and Neptune.

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