The Astrochemical Impact of Cosmic Rays in Protoclusters. I. Molecular Cloud Chemistry

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Received 2019 March 29; revised 2019 May 7; accepted 2019 May 8; published 2019 June 19

Abstract

We present astrochemical photodissociation region models in which cosmic-ray (CR) attenuation has been fully coupled to the chemical evolution of the gas. We model the astrochemical impact of CRs, including those accelerated by protostellar accretion shocks, on molecular clouds hosting protoclusters. Our models with embedded protostars reproduce observed ionization rates. We study the imprint of CR attenuation on ions for models with different surface CR spectra and different star formation efficiencies. We find that abundances, particularly ions, are sensitive to the treatment of CRs. We show the column densities of ions are underpredicted by the “classic” treatment of CRs by an order of magnitude. We also test two common chemistry approximations used to infer ionization rates. We conclude that the approximation based on the H_3^+ abundance underpredicts the ionization rate, except in regions where the CRs dominate the chemistry. Our models suggest the chemistry in dense gas will be significantly impacted by the increased ionization rates, leading to a reduction in molecules such as NH_3 and causing H_2-rich gas to become [C II] bright.

Key words: astrochemistry – cosmic rays – ISM: clouds – ISM: molecules – methods: numerical – stars: protostars

1. Introduction

Molecular cloud dynamics and chemistry are sensitive to the ionization fraction. The chemistry of molecular clouds is dominated by ion–neutral reactions (Watson 1976) and thus controlled by the ionization fraction. The gas (kinetic) temperature of a typical molecular cloud with an average H-nucleus number density of \(n \approx 10^3\) cm\(^{-3}\) is approximately 10 K for cosmic-ray ionization rates (CRIRs) \(\zeta \lesssim 10^{-18}\) s\(^{-1}\) (Bisbas et al. 2015, 2017), thus rendering neutral–neutral reactions inefficient. Ionization in molecular clouds is produced in three difference ways: UV radiation, cosmic rays (CRs), and X-ray radiation. Ultraviolet radiation, from external O- and B-type stars and internal protostars, does not penetrate very far into the cloud due to absorption by dust. However, CRs, which are relativistic charged particles, travel much further into molecular clouds and dominate the ionization fraction when \(A_V \gtrsim 5\) mag (McKee 1989; Strong et al. 2007; Grenier et al. 2015). CR-driven chemistry is initiated by ionized molecular hydrogen, H_2^+ (Dalgarno 2006). The ion–neutral chemistry rapidly follows:

\[
\text{CR} + H_2 \rightarrow H_2^+ + e^- + \text{CR'}
\]

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

where CR’ is the same particle as CR but with a lower energy. The ejected electron from the first reaction can have an energy greater than the ionization potential of H_2 and thus cause further ionization. Once H_3^+ forms, more complex chemistry follows, thereby creating a large array of hydrogenated ions:

\[
X + H_3^+ \rightarrow [XH]^+ + H_2
\]

Both HCO^+ and N_2H^+, important molecules used to map the dense gas in molecular clouds, form this way, with X being CO and N_2, respectively. These species are also used to constrain the CRIR (i.e., Caselli et al. 1998; Ceccarelli et al. 2014). OH^+ and H_3O^+ are also formed this way through H_3^+ and H^+ (Hollenbach et al. 2012). In addition, at low column densities \((A_V < 1\) mag \)), which is typical of the boundaries of molecular clouds, the non-thermal motions between ions and neutrals may overcome the energy barrier of the reaction

\[
C^+ + H_2 \rightarrow C^+ + H_2 + \text{CR}
\]

leading to an enhancement of the CO column density (Federman et al. 1996; Visser et al. 2009) and a shift of the H_1-to-H_2 transition to higher \(A_V\) (Bisbas et al. 2019).

The ionization fraction controls the coupling of the magnetic fields to the gas, influencing non-ideal magnetohydrodynamic (MHD) effects such as ambipolar diffusion (McKee & Ostriker 2007). These non-ideal effects can play a significant role in the evolution in the cores and disks of protostars. On galactic scales, numerical simulations have shown that CRs can help drive large outflows and winds out of the galaxy (e.g., Girichidis et al. 2016). Our study focuses on the impact of CRs on Giant Molecular Cloud scales, which is typically not resolved fully in such simulations.

There have been a plethora of studies modeling the impact of CRs on chemistry and thermal balance (i.e., Caselli et al. 1998; Bell et al. 2006; Bayet et al. 2011; Meijerink et al. 2011; Clark et al. 2013; Bisbas et al. 2015). However, in these studies, and the vast majority of astrochemical models, the CRIR is held constant throughout the cloud, despite the recognition that CRs are attenuated and modulated while traveling through molecular gas (Schlickeiser 2002; Padovani et al. 2009, 2018; Schlickeiser et al. 2016). Galactic CRs, thought to be accelerated in supernova remnants or active galactic nuclei, are affected by hadronic and Coulombic energy losses and screening mechanisms that reduce the flux with increasing column density (Strong & Moskalenko 2001; Moskalenko et al. 2005; Evoli et al. 2017). The modulation of CRs has not previously been included within astrochemical models of
molecular clouds due to the difficulty of calculating the attenuation and subsequent decrease in the CRIR ( Wakelam et al. 2013; Cleeves et al. 2014).

Given that CRs are thought to be attenuated, it is expected that the ionization rate should decline within molecular clouds. However, recent observations do not universally show a lower ionization rate. Favre et al. (2017) inferred the CRIR toward 9 protostars and found a CRIR consistent with the rate inferred for galactic CRs. The OMC-2 FIR 4 protocluster, hosting a bright protostar, is observed to have a CRIR 1000 higher than the expected rate from galactic CRs (Cecarelli et al. 2014; Fontani et al. 2017; Favre et al. 2018). Gaches & Offner (2018b) showed that this system can be modeled assuming the central source is accelerating protons and electrons within the accretion shocks on the protostar’s surface. In general, accreting, embedded protostars may accelerate enough CRs to cancel the effect of the attenuation of external CRs at high column densities, producing a nearly constant ionization rate throughout the cloud (Padovani et al. 2016; Gaches & Offner 2018b).

Typical accretion shocks and shocks generated by protostellar jets satisfy the physical conditions necessary to accelerate protons and electrons (Padovani et al. 2016; Gaches & Offner 2018b). Accretion shocks in particular are a promising source of CRs because they are strong, with velocities exceeding 100 km s$^{-1}$ and temperatures of millions of degrees Kelvin (Hartmann et al. 2016). Gaches & Offner (2018b) calculated the spectrum of accelerated protons in protostellar accretion shocks and the attenuation through the natal core assuming that the CRs free-stream outwards. These models suggest that clusters of a few hundred protostars accelerate enough CRs into the surrounding cloud to exceed the ionization rate from Galactic CRs.

In this study, we explore the effects of protostellar CRs on molecular cloud chemistry by employing the model of Gaches & Offner (2018b). We implement an approximation for CR attenuation into the astrochemistry code 3D-PDR (Bisbas et al. 2012) to account for CR ionization rate gradients. We investigate the signatures of a spatially varying ionization rate. We further explore the impact of protostellar CR sources and their observable signatures.

The layout of the paper is as follows. In Section 2 we present the CR and protostellar models and describe the implementation of CR attenuation into 3D-PDR. We discuss our results in Section 3. Finally, in Section 4 we create observational predictions and compare them to observations.

2. Methods

2.1. Protocluster Model

We generate protoclusters following the method of Gaches & Offner (2018a), where the model cluster is parameterized by the number of stars and gas surface density, $N_*$ and $\Sigma_{\text{cl}}$, respectively. These parameters are connected to the star formation efficiency $\varepsilon_*=M_* / M_{\text{gas}}$, where $M_{\text{gas}}$ is related to $\Sigma_{\text{cl}}$ following McKee & Tan (2003) $\Sigma_{\text{cl}} = \frac{3 M_*}{2 \pi R_{\text{cl}}^2}$, where the cloud radius, $R_{\text{cl}}$ is determined from the density distribution (see Section 2.3). We model protoclusters with surface densities in the range $0.1 \leq \Sigma_{\text{cl}} \leq 10$ g cm$^{-2}$ and with a number of stars in the range $10^2 \leq N_* \leq 10^4$. In this parameter space, we always consider $\varepsilon_* \leq 25\%$.

We generate $N_{\text{cl}} = 20$ protoclusters for each point in the parameter space and adopt the average CR spectrum for the chemistry modeling. We use the Tapered Turbulent Core (TTC) accretion history model (McKee & Tan 2003; Offner & McKee 2011), where the protostellar core is supported by turbulent pressure and accretion is tapered to produce smaller accretion rates as the protostellar mass, $m$, approaches the final mass, $m_\star$. Gaches & Offner (2018a) showed the TTC model is able to reproduce the bolometric luminosities of observed local protoclusters.

2.2. Cosmic-Ray Model

We briefly summarize the CR acceleration and propagation model in Gaches & Offner (2018b) and refer the reader to that paper for more details. We assume CRs are accelerated in the accretion shock near the protostellar surface. Accreting gas is thought to flow along magnetic field lines in collimated flows with the shock at the termination of the flow. We assume the shock velocities are comparable to the freefall velocity at the stellar surface. Following Hartmann et al. (2016), we assume fully ionized strong shocks with the shock front perpendicular to the magnetic field lines. We adopt a mean molecular weight $\mu_\text{f} = 0.6$ and a filling fraction of accretion columns on the surface, $f = 0.1$.

We calculate the CR spectrum under the Diffusive Shock Acceleration (DSA) limit, also known as first-order Fermi acceleration (e.g., reviewed in Drury 1983; Kirk 1994; Melrose 2009). Under DSA, the CR momentum distribution is a power law, $f(p) \propto p^{-q}$, where $q$ is related to the shock properties. We attenuate the CR spectrum through the protostellar core following Padovani et al. (2009). Padovani et al. (2018) presented updated attenuation models for surface densities up to 3000 g cm$^{-2}$, but the results remain unchanged for the surface of concern in this work. The core surface density and radius for a turbulence-supported core are (McKee & Tan 2003)

\[ \Sigma_{\text{core}} = 1.22 \Sigma_{\text{cl}} = 0.122 \text{ g cm}^{-2} \left( \frac{\Sigma_{\text{cl}}}{0.1 \text{ g cm}^{-2}} \right), \] \hspace{1cm} (1a)

\[ N(H_2)_{\text{core}} = \frac{\Sigma_{\text{core}}}{\mu_{\text{M}} m_{\text{H}}} \]
\[ = 3 \times 10^{22} \text{ cm}^{-2} \left( \frac{\Sigma_{\text{core}}}{0.122 \text{ g cm}^{-2}} \right) \left( \frac{2.4}{\mu} \right), \] \hspace{1cm} (1b)

\[ R_{\text{core}} = 0.057 \Sigma_{\text{cl}} \left( \frac{m_{\text{f}}}{30 M_{\odot}} \right) \frac{1}{2} \text{ pc} \]
\[ = 0.104 \text{ pc} \left( \frac{\Sigma_{\text{cl}}}{0.1 \text{ g cm}^{-2}} \right) \left( \frac{m_{\text{f}}}{10 M_{\odot}} \right)^{1/2}, \] \hspace{1cm} (1c)

where $\mu_{\text{M}} = 2.4$ is the mean molecular weight for a molecular gas. We calculate the total protocluster CRIR by summing over the $N_*$ attenuated CR spectra.

2.3. Density Structure

We assume the molecular cloud density is described by an inverse power law

\[ n(r) = n_0 \left( \frac{R_{\text{cl}}}{r} \right)^2, \] \hspace{1cm} (2)
where $R$ is the cloud radius and $n_0$ is the number density with an inner radius of 0.1 pc. The $r^{-2}$ dependence matches the solution for isothermal collapse (Shu 1977). We take $n_0 = 100 \, \text{cm}^{-3}$, corresponding to a gas regime in which the cloud is expected to be mostly molecular under typical conditions. The radius is set by constraining the total surface density by $\Sigma_{\text{cl}}$ as defined:

$$\int_{R_i}^{R} n(r) \, dr = \frac{\Sigma_{\text{cl}}}{\mu_m m_H},$$

(3)

where $R_i$ is the inner radius delineating the transition between the molecular cloud and protostellar core. The turbulent line width, $\sigma$, of a cloud with density profile $n(r) \propto r^{-2}$ and a virial $\alpha$ parameter, is (Bertoldi & McKee 1992)

$$\sigma = \left( \frac{GM^2 \alpha}{3 \mu_m m_H \bar{n} V \nu_R} \right)^{\frac{1}{2}},$$

(4)

where $\bar{n}$ is the volume-averaged density from $n(r)$, $G$ is the gravitational constant, and $V = \frac{4}{3} \pi R^3$ is the volume of the molecular cloud. We take $\alpha = 2$ for our fiducial model (Heyer & Dame 2015).

2.4. Chemistry with Cosmic-Ray Attenuation

We use a modified version of the 3D-PDR astrochemistry code\(^5\) introduced in Bisbas et al. (2012). 3D-PDR solves the chemical abundance and thermal balance in one, two, and three dimensions for arbitrary gas distributions. The code can be applied to arbitrary three-dimensional gas distributions, such as post-processing simulations (Offner et al. 2013, 2014; Bisbas et al. 2018). Here, we use the code in one dimension to model a large parameter space. We adopt the McElroy et al. (2013) UMIST12 chemical network containing 215 species and approximately 3000 reactions. We assume the gas is initially composed of molecular H$_2$, with the rest being atomic with abundances from Sembach et al. (2000), as shown in Table 1. Cooling is included from line emission, which is mainly due to carbon monoxide at low temperatures and forbidden lines of [O I], [C I], and [C II] at higher temperatures. Heating is due to dissipation of turbulence, photoelectric heating of dust from far-ultraviolet emission, H$_2$ fluorescence, and CR heating of gas. We use a temperature floor of 10 K. Previously, 3D-PDR included CRs via a single global CRIR parameter. See Bisbas et al. (2012) for more technical details.

We modify 3D-PDR to account for CR attenuation through the cloud. Currently, our implementation is restricted to one-dimensional models where we assume spherical symmetry. 3D-PDR calculates the CRIR from $N_{\text{SRC}}$ CR sources. The user provides a CR spectrum for any number of sources and whether it is external (incident at the surface) or internal (originating at the cloud center). In 1D, the fluxes are defined on either surface of the domain. The flux due to external sources is attenuated, while the point sources are assumed to radiate isotropically; both are attenuated and spatially diluted. The spectra are attenuated after every update of the molecular abundances to keep the amount of H$_2$ for interaction losses self-consistent. 3D-PDR stores the initial CR flux in $N_{\text{one}}$ bins and self-consistently calculates $\zeta$ from all sources across the domain. Point sources require a user-set radial scaling factor, $r_s$, and a transport parameter, $a$. For our model results, we set $r_s = R_C$ to represent the core radius. Point-source CR spectra, $j(E, r)$, are attenuated by the H$_2$ column density (Padovani et al. 2009) and diluted by the radial distance following

$$j(r) \propto \left( \frac{r_i}{r + r_i} \right)^a,$$

(5)

to approximate the effects of transport. Solving the transport equations for Galactic transport problems has been done with specialized codes, such as GALPROP (Moskalenko & Strong 1998) and DRAGON2 (Evoli et al. 2017). Fully solving the steady-state transport equations is beyond the scope of this work but will be investigated in the future.

In our study, we include two CR flux sources. First, we include the internal protostellar clusters discussed above. We set the radial scaling $r_i = R_C = 0.1 \, \text{pc}$, which is approximately the size of a protostellar core. Second, we include an external isotropic CR flux to model interstellar CRs. We follow Ivlev et al. (2015) and parameterize the external flux as

$$\dot{J}_{\text{ext}} = C \frac{E^\alpha}{(E + E_0)^{\beta}} \text{(particles eV}^{-1} \text{cm}^{-2} \text{s}^{-1} \text{sr}^{-1}).$$

(6)

We use their “low” model ($L$), with $C = 2.4 \times 10^{15}$, $E_0 = 650 \, \text{MeV}$, $\alpha = 0.1$, and $\beta = 2.8$ and their “high” model ($H$), with $C = 2.4 \times 10^{15}$, $E_0 = 650 \, \text{MeV}$, $\alpha = -0.8$, and $\beta = 1.9$. The $L$ model is a direct extrapolation of the Voyager-1 data (Stone et al. 2013), while the $H$ one is a maximal model to correct for any possible effects of the solar magnetic field. The CRIR is calculated by integrating the spectrum multiplied by the H$_2$ cross section:

$$\zeta_p = 2\pi \int j(E) \sigma_i(E) \, dE,$$

(7)

where the factor of $2\pi$ accounts for irradiating the 1D surface on one side and $\sigma_i(E)$ is the H$_2$ ionization cross section with relativistic corrections (Krause et al. 2015). The code allows for an arbitrary number of energy bins, $N_{\text{bins}}$, for input CR spectrum. We compared the CRIR for bin sizes ranging from $N_{\text{bin}} = 4$ to 1000 and found that $N_{\text{bins}} > 40$ only produces changes in the CRIR at the 1% level. We do not fully solve for primary or secondary electrons. Therefore, we multiply the proton CRIR by $5/3$ to account for the electron population (Dalgarno & Griffin 1958; Takayanagi 1973).

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\(^5\) The code can be downloaded from https://uc1chem.github.io, including the new modifications presented in this paper.
Our fiducial parameters for the study are shown in Table 2. Table 3 shows the full suite of models we adopt. The model names describe the included physics: L/H denotes using the L/H (low/high) external spectrum, NI denotes no internal sources, DI denotes internal sources with $a = 1$ (diffusive transport), RI denotes internal sources with $a = 2$ (rectilinear transport), and NA denotes no internal sources or CR attenuation. We study the impact of these parameters in Section 3.

### 3. Results

#### 3.1. Cosmic-Ray Spectrum

Our modified 3D-PDR code requires as an input the flux of CR protons for any number of sources. As a result, the CR proton flux and CRIR throughout the spatial domain become outputs rather than inputs. Figure 1 shows an example CR spectrum for a molecular cloud with $\Sigma_{\text{cl}} = 0.75 \text{ g cm}^{-2}$ and $N_e = 750$ using the LDI model. The CR proton flux increases inside the cloud because of the embedded sources. The double-peaked shape of the spectrum is due to peaks in the loss function from ionization and Coulomb losses. The inset shows the CRIR as a function of the position within the cloud. In this model, the ionization rate climbs nearly two orders of magnitude throughout the cloud with increasing proximity to the protostellar cluster.

#### 3.2. Cosmic-Ray Ionization Rate Models

A number of prescriptions have been used to calculate the CRIR from observed column densities of various tracer species (Caselli et al. 1998; Indriolo & McCall 2012). The inclusion of CR attenuation allows us to directly test the accuracy of these approximations. Our astrochemical models provide the abundances throughout the cloud and the local CRIR in situ. We test two different prescriptions that are typically used for diffuse and dense gas, respectively, from Indriolo & McCall (2012).

The first, and simplest, denoted “Simple Electron Balance” (SEB), estimates the CRIR using only the abundance of $\text{H}_2^+$ and $e^-$:

$$\zeta = k_n n(e^-) \frac{n(H_2)}{n(H_2^+)}$$

where $k_n$ is the $\text{H}_2^+$ electron-recombination rate and $n(e^-)$, $n(H_2)$, and $n(H_2^+)$ are the densities of electrons, molecular hydrogen, and $\text{H}_2^+$, respectively. The second approximation includes the destruction of $\text{H}_2^+$ with CO and O, which we denote the “Reduced Analytic” (RA) model:

$$\zeta = \frac{x(H_2^+)}{x(H_2)} n_H [k_r x(e^-) + k_{CO} x(CO) + k_O x(O)]$$

$$\times \left[ 1 + \frac{2k_3 x(e^-)}{k_2 f(H_2)} + \frac{2k_4}{k_2} \left( \frac{1}{f(H_2)} - 1 \right) \right],$$

where $k_i$ are the reaction rate coefficients for the reactions in Table from Indriolo & McCall (2012) (repeated in Table 4 below), $x_i$ is the abundance of species $i$ with respect to total hydrogen nuclei, and $f(H_2) = 2n(H_2)/n_H$ is the molecular hydrogen fraction.

Figure 2 shows the calculated CRIR using the full model and the approximations in Equations (8) and (9) as a function of the $H_2^+$ abundance. We show the cases of four different CR models: LNA, LNI, LDI, and HDI. The first model, LNA, is of particular importance, as it represents the simplest one-dimensional PDR model. Observations typically assume an 0D distribution, such that the ratio of column densities is equal

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**Table 2**

| Parameter | Definition | Fiducial Value |
|-----------|------------|----------------|
| $\rho_1$  | Reduced gas mass | 0.6 (ionized)  |
| $\rho_M$ | Reduced gas mass | 2.4 (neutral molecular) |
| $n_0$     | Density at edge of cloud | $10^{2}$ cm$^{-3}$ |
| $N_{\text{bin}}$ | Number of CR Sources | 2 |
| $N_{\text{max}}$ | Number of CR spectrum bins | 40 |
| $a$       | CR transport parameter | 1 |
| $r_s$     | Scaling radius for CR flux | 0.1 pc |
| $\alpha$ | Cloud virial parameter | 2 |

**Table 3**

| Name       | Source | Transport | Internal | External Field | Attenuation |
|------------|--------|-----------|----------|----------------|-------------|
| LDI        | $r^{-1}$ | ✓         |          |                | ✓           |
| LRI        | $r^{-2}$ | ✓         |          |                | ✓           |
| LNI        | $r^{-1}$ | ✓         |          |                | ✓           |
| LNA        | $r^{-1}$ | ✓         |          |                | ✓           |
| HNI        | $r^{-1}$ | ✓         |          |                | ✓           |
| HDI        | $r^{-1}$ | ✓         |          |                | ✓           |

Note. L/H denotes low/high external spectrum, NI denotes no internal sources, DI denotes internal sources with $a = 1$ (diffusive transport), RI denotes internal sources with $a = 2$ (rectilinear transport), and NA denotes no internal sources or CR attenuation.
to the ratio of the abundances. This makes a tacit assumption that the ionization rate is the same throughout the domain. We find that both approximations produce a large range of CRIRs—even when the input CRIR is fixed due to other effects impacting the chemistry, notably the influence of the external FUV radiation. The SEB and RA approximation models systematically underestimate the CRIR and produce an artificial spread in the inferred CRIR. When internal sources are included, we find that both approximations infer the CRIR reasonably well. When there are no internal sources, both approximations underestimate the CRIR by up to an order of magnitude and in general do not represent any real spread in the CRIR accurately.

3.3. Impact of Cosmic-Ray Sources on Cloud Chemistry

We examine in detail two different CR models: the traditional LNA and the LDI model. Figure 3 shows the column densities of different species and density-averaged temperature and CRIR for the LNA model as a function of $\Sigma_{cl}$ and $N_a$. The total column density of each species increases with the gas surface density, $\Sigma_{cl}$, and hence the total gas mass. Furthermore, we find across the whole parameter space that $N$ (CO) $>$ N(C) $>$ N(C$^+$). This qualitative behavior is to be expected with no internal sources. Figure 4 shows the abundance profiles for the LNA model as a function of $A_V$ into the cloud, $\Sigma_{cl}$, and $N_a$. Since there are no embedded sources in this model, there is no difference between models of different $N_a$. The abundance profiles for C$^+$, C, and CO exhibit the expected “layered” behavior (Draine 2011): C$^+$ is confined to the surface, C exists in a thin, warm layer, and CO asymptotically approaches an abundance of [CO/H$_2$] $\approx$ 10$^{-4}$. Similarly, the abundance of NH$_3$ steadily increases into the cloud.

The abundance ratio [HCO$^+$/N$_2$H$^+$] is sometimes used to infer the CRIR under the assumption the two molecules are cospatial (i.e., Ceccarelli et al. 2014). We find that, while they share some local maxima, they are not completely cospatial, in agreement with the turbulent cloud study of Gaches et al. (2015). Moreover, observations show that while they are not entirely cospatial, there is overlap in the emission regions (i.e., Jørgensen 2004; Ceccarelli et al. 2014; Storn et al. 2016; Favre et al. 2017; Pety et al. 2017; Pound & Yusef-Zadeh 2018). In particular, we show HCO$^+$ can exist at much lower $A_V$ than N$_2$H$^+$. Due to similar critical densities, however, the two molecules thermalize at nearly the same densities.

Figure 5 shows the column densities across the parameter space for the LDI model. Here we find a very different behavior compared to the LNA model shown in Figure 3, where the differences are especially pronounced for the more diffuse gas tracers. The column densities are no longer strictly functions of $\Sigma_{cl}$ but depend on $N_a$. For large, massive star-forming regions (upper right corner in each panel), the gas becomes CO-deficient and C-rich, while the bulk of gas remains molecular. Similarly, there is a slight increase in the column density of HCO$^+$ and N$_2$H$^+$ due to the increase in ionization. The qualitative trends exhibited by C$^+$, C, and marginally by HCO$^+$ and N$_2$H$^+$, follow that of the density-averaged CRIR, $\langle \zeta_i \rangle$.

The effect of an embedded protocluster is also visible in the abundance profiles. Figure 6 shows the abundance profiles for the LDI model. We find that CO only approaches abundances of 10$^{-4}$ for clusters with little embedded star formation. For smaller mass clouds (i.e., smaller $\Sigma_{cl}$), the C$^+$, C and CO abundance remains fairly unchanged compared to the LNA model. In the most massive clouds, the amount of CO at $A_V \leq 1$ is enhanced by an order of magnitude and reduced by an order of magnitude at $A_V \geq 5$. We further see a reduction in N$_2$H$^+$ at mid-$A_V$ with an enhancement of HCO$^+$. Likewise, the gas temperature exceeds $T > 30$ K for most of the clouds with $\Sigma_{cl} > 0.25$ g cm$^{-2}$. As $A_V \rightarrow 10^3$, the differences between the molecular ion abundances are much lower due to the greatly increased density compared to the surface of the cloud. The abundance of H$_2$ in the dense gas is unaffected by the increased CRIR.

We now statistically quantify the impact of different CR models on the six different molecules: C$^+$, C, CO, N$_2$H$^+$, HCO$^+$, and H$_2^+$. We investigate the H$_2^+$ column density because it is the simplest molecule that can be used to constrain the CRIR (Dalgarno 2006). We calculate the column density logarithmic difference:

$$\Delta_s = \log \frac{N_{s,i}}{N_{s,LNA}},$$

with $s$ representing the different species, and $i$ being the different CR models, excluding the LNA model. Figure 7 shows violin plots representing the probability distribution of $\Delta_s$ using all clouds in the ($\Sigma_{cl}$--$N_a$) space. In all cases, CO is never enhanced but rather depleted. This is because the maximum abundance [CO] = 10$^{-4}$ is set by the C/O ratio. Our models generally increase the local CRIR, thereby dissociating the CO and reducing its abundance. We find very little difference between the LNI and LNA for all molecules except for N$_2$H$^+$ and HCO$^+$, which exhibit a 25% linear dispersion. This is caused by the impact of higher ionization rates toward the surface of the clouds. The HNI model, which

| Reaction | Rate Coefficient (cm$^3$ s$^{-1}$) | Reference |
|----------|---------------------------------|-----------|
| H$^+_2$ + H$_2$ $\rightarrow$ H$_2^+$ + H | $k_2 = 2.09 \times 10^{-9}$ | Heard & Huntress (1974) |
| H$^+_2$ + e$^-$ $\rightarrow$ H + H | $k_3 = 1.6 \times 10^{-3} (T/300)^{-0.43}$ | Mitchell (1990) |
| H$^+_2$ + H $\rightarrow$ H$_2^+$ + H | $k_4 = 6.4 \times 10^{-10}$ | Karpas et al. (1979) |
| H$^+_2$ + e$^-$ $\rightarrow$ products | $k_5 = k_e = -1.3 \times 10^{-3} + 1.27 \times 10^{-5} T^{-0.48}$ | McCall et al. (2004) |
| H$^+_2$ + CO $\rightarrow$ H$_2^+$ + HCO$^+$ | $k_6 = 1.36 \times 10^{-3} (T/300)^{-0.142} \exp(3.41/T)$ | Klippstein et al. (2010) |
| H$^+_2$ + CO $\rightarrow$ H$_2^+$ + HCO$^+$ | $k_7 = 8.49 \times 10^{-3} (T/300)^{-0.066} \exp(-5.21/T)$ | Klippstein et al. (2010) |
| H$^+_2$ + O $\rightarrow$ H$_2^+$ + OH$^+$ | $k_8 = k_O = 1.14 \times 10^{-3} (T/300)^{-0.159} \exp(-1.41/T)$ | Klippstein et al. (2010) |

Note. In the Equation (8) and (9) reaction rates, $k_{CO} = k_e + k_5$ as in Equation 9.
Figure 2. Left: cosmic-ray ionization rate as a function of H$_3^+$ abundance using the full astrochemical model results. Middle: relative logarithmic error in $\zeta$, $\Delta \log \zeta$, calculated using the electron-balance approximation (Equation (8)) and full astrochemical model. Right: same as the middle row but using the reduced analytic approximation (Equation (9)). Color: gas surface density, $\Sigma_{cl}$ in g cm$^{-2}$. In descending order from the top, the models are LNA, LNI, LDI, HDI.
has the highest overall CRIR at the surface, shows a clear offset for the atomic and ionic species and a slight deficit for CO. In models LRI, LDI, and HDI there is a significant dispersion in the column density difference, $\Delta s$, in all species. Figure 7 demonstrates that considerable care must be taken when modeling observed column densities of atomic or ionic species: the possible error, $\Delta s$, in the modeled column densities may be off by an order of magnitude depending on the transport of the CRs and the amount of ongoing embedded star formation. The CRIR is not the only factor that leads to the creation of molecular ions, as typically assumed in observational studies.

The abundances are influenced by the FUV flux, which is also enhanced by a central protocluster (Gaches & Offner 2018a).

### 3.4. Abundance Ratio Diagnostics for the Cosmic-Ray Ionization Rate

Line and abundance ratios of various tracers are often used to constrain the CRIR in dense gas. The species are typically assumed to be cospatial (although as demonstrated in Section 3.3 that is not typically the case). We examine two different ratio diagnostics: global diagnostics using column

- **Figure 3.** Column density of different molecular species as a function of the number of stars in the protocluster, $N_*$, and the mass surface density, $\Sigma_{cl}$, for the LNA model. The last three panels on the far right show the density-averaged temperature, CRIR, and the total gas column density.
densities and local diagnostics using the local abundance ratios and CRIRs.

Figure 8 shows three different column density ratios for the LNA, LNI, and HNI models: \( \frac{\text{HCO}^+}{\text{N}_2\text{H}^+} \), \( \frac{\text{CO}}{\text{C}^+} \), and \( \frac{\text{CC}}{\text{C}^+} \). We find that the column density ratios in these cases increase monotonically with \( \Sigma_{cl} \). The ratio of \( \frac{\text{HCO}^+}{\text{N}_2\text{H}^+} \) is nearly constant, changing by less than a factor of two across two dex of \( \Sigma_{cl} \). The HNI case shows a slightly different behavior with a slight local minimum in \( \frac{\text{HCO}^+}{\text{N}_2\text{H}^+} \) at \( \Sigma_{cl} = 6 \text{ g cm}^{-2} \). The trends in these models are not due to changes in the CRIR but rather in the total amount of gas column. The \( \frac{\text{CO}}{\text{C}^+} \) ratio shows a buildup of CO compared to \( \text{C}^+ \). This is to be expected in an externally irradiated model: \( \text{C}^+ \) remains consistently on the surface, while the amount of CO continues to build with \( \Sigma_{cl} \) with a proportional increase in the amount of dense gas. Similarly, the \( \frac{\text{C}}{\text{C}^+} \) remains fairly constant because these species exist only in limited areas of \( A_V \).

Figure 9 shows the same column density ratios for three models including the embedded protoclusters: LRI, LDI, and HDI. Here the trends are significantly more complicated. The \( \frac{\text{HCO}^+}{\text{N}_2\text{H}^+} \) ratio still only varies by a factor of two throughout the parameter space, but it exhibits more complex

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**Figure 4.** Abundances, \([X]\), for various molecular species, as a function of the visual extinction into the cloud, \(A_V\), for the LNA model. The top two panels of the right column show the temperature and CRIR as a function of the \(A_V\). The color bar indicates the gas surface density, \(\Sigma_{cl}\). The line width indicates the number of protostars in the cluster with “Small”=10^2, “Medium”=10^3, and “Large”=10^4 protostars.
behavior. The ratio decreases with $\Sigma_{cl}$ and rises with $N_*$ up to some maximum, with an additional increase in $[\text{HCO}^+/\text{N}_2\text{H}^+]$ for $N_* \approx 10^4$ for the LDI and HDI model. To understand this, we can look at the abundance profiles of the LDI model in detail in Figure 6. The abundance of HCO$^+$ increases both with $\Sigma_{cl}$ and $N_*$, with the abundance profile flattening as a function of $A_V$ for $\Sigma_{cl} > 1$ g cm$^{-2}$. For $N_2\text{H}^+$, the trends are separated by an $A_V$ threshold at $A_V = 1$. At $A_V < 1$, the abundance of $N_2\text{H}^+$ increases like HCO$^+$, with $\Sigma_{cl}$ and $N_*$. For $1 < A_V < 100$, the abundance of $N_2\text{H}^+$ is sensitive primarily to $N_*$. In high ionization environments, CO will be destroyed in the creation of HCO$^+$ due to interactions with H$_3^+$. These environments will also produce $N_2\text{H}^+$, which destroys CO to create HCO$^+$. This is likely the main driving cause in the abundance profiles: there is a reduction of CO and $N_2\text{H}^+$ in the dense more ionized gas, and a systematic increase in HCO$^+$. The [CO/C$^+$] ratio increases monotonically across two orders of magnitude toward high $\Sigma_{cl}$ and low $N_*$; cold gas is less ionized (lower right corner), so the amount of CO increases with respect to C$^+$. [C/C$^+$] shows a different trend compared to [CO/C$^+$]. High ionization rates, in both the LDI and HDI models, have an increased [C/C$^+$] in lower-mass clouds hosting smaller clusters and a decreased [C/C$^+$] at high $\Sigma_{cl}$ compared to the LRI model. The [C/C$^+$] ratio is nearly flat across the $\Sigma_{cl}$-$N_*$.
parameter space in the HDI model. Clouds with fewer CRs and more gas shielding to the incident FUV radiation have more C compared to C$^+$.

Observational measurements of $\zeta$ in dense gas typically use astrochemical modeling and local abundance ratios (see Section 4.2). Figure 10 plots the CRIR for models with $5\% \leq \varepsilon \leq 25\%$ as a function of different abundance ratios. A good CRIR indicator should exhibit a monotonic trend in response to changes in the CR flux. The LNI model does not exhibit much change in the CRIR, so the local trends depend on density and radiative effects. In the HNI model, only the [HCO$^+$/CO] ratio exhibits a monotonic trend.

The models with sources show completely different abundance ratios because the dense gas is warmer and the ionization rates are higher. In all of these cases, the ratios are monotonic for $\Sigma_{\text{cl}} \gtrsim 1$ g cm$^{-2}$. For $\Sigma_{\text{cl}} \lesssim 1$ g cm$^{-2}$, each exhibits a similar trend as in the NI model subsets. This demonstrates that these diagnostics only constrain regimes where the CRIR influences the chemistry more than radiative or other heating processes.

Figure 6. Same as Figure 4 but for model LDI.
4. Discussion

4.1. Model Assumptions and Caveats

Our models require a variety of assumptions. First and most importantly, the models are one-dimensional and we assume protostars are clustered in the center. In reality, protostars are distributed throughout molecular clouds. Furthermore, the density distribution of molecular clouds is set by turbulence and is not a purely radial distribution. However, our results will hold qualitatively for the molecular gas around young, dense embedded clusters in molecular clouds, such as the central cluster in $\rho$ Oph. Second, our chemical network does not include any gas-grain chemistry or freeze-out (see McElroy et al. 2013). Therefore, we over-predict the CO abundance in regions where $n > 10^4$ cm$^{-3}$ and $T \lesssim 30$ K (van Dishoeck 2014). Comparing this criteria to the temperature profiles in Figure 6 shows the models with $\Sigma_{cl} < 0.5$ g cm$^{-2}$ and where $1 \lesssim A_V \lesssim 10$ are below the freeze-out temperature. When embedded sources are included, the densest gas heats to temperatures $> 50$ K. These temperatures lead to desorption from the grains, producing gas-phase CO: any CO-ice that formed before star formation occurred would be evaporated back into the gas phase (Jørgensen et al. 2013, 2015).

We do not fully solve the CR transport equations or the acceleration dynamics of protons in protostellar accretion shocks. We use analytic approximations to describe the acceleration of CRs at the protostellar shock and the transport out of both the parent core and cloud. Gaches & Offner (2018b) explore the changes in the CRIR for different transport regimes, shock efficiencies, and magnetic fields. Differences in the protostellar magnetic field change the maximum energy of the accelerated CRs but have little effect on the CRIR. However, the CRIR scales nearly linearly with the shock efficiency. Our results assume CR transport in the rectilinear regime through the core. More diffusive transport would produce higher temperatures at the surface of the core than are observed. The details of the transport depend both on the magnetic field morphology and on the coupling between the particles and the field. In molecular clouds, turbulence is much stronger than it is in cores, allowing CRs to diffuse across magnetic field lines rather than stream along them (Schlickeiser 2002). Conversely, if the particles are well-coupled, their trajectories would follow the field lines, potentially producing asymmetries in the CR flux. The directionality imposed by the protostellar outflow could cause CR beaming in the outflow direction or simply advect the particles along with the outflow gas (Rodgers-Lee et al. 2017). We assume CRs transport from their parent cores through the clouds by parameterizing the radial scaling by either diffusive ($1/r^1$) or free-streaming ($1/r^2$). We do not fully solve the transport equations, which has yet to be done for CRs propagating out of molecular clouds from internal sources.
4.2. Comparison to Observed CRIRs

Figure 11 shows the results from the different PDR models in Table 3 compared to four different observational surveys covering a range of $1 \leq A_V \leq 10^2$. The CRIR is one of the trickier astrochemical parameters to constrain from observations. Unfortunately, no universal method is applicable to all cloud conditions. Historically, there have been two main methods: absorption measurements of simple ions, such as H$_3^+$ or OH$^+$, in the infrared; or molecular line observations using key molecules in neutral–ion pathways along with astrochemical modeling. H$_3^+$ is typically thought to be among the best tracers of the CRIR due to its simple chemistry. However, H$_3^+$ is only observed in infrared absorption, limiting its use to sightlines with bright background sources. Indriolo & McCall (2012) and Indriolo et al. (2015) used H$_3^+$, H$_2$O$^+$, and OH$^+$ absorption to trace the CRIR in diffuse gas with $A_V < 1$ and found the CRIR in low $A_V$ gas varies between $10^{-16}$ and $10^{-14}$ s$^{-1}$. The gas at low $A_V$ is particularly sensitive to external influences, motivating the need to model the chemistry with external CR spectra derived from examining the local galactic environment. The groupings of points at low $A_V$ with high CRIR ($\zeta > 10^{-14}$ s$^{-1}$) are clouds in sightlines toward the galactic center and thus in environments with extreme external particle irradiation. Caselli et al. (1998) used a combination of HCO$^+$, DCO$^+$, and CO together with analytic chemistry approximations to infer the CRIR in 24 dense cores. Their observations exhibit a nearly bimodal distribution: some are clustered at $\zeta \approx 10^{-17}$ s$^{-1}$, while the majority are at $\zeta \approx 10^{-16}$ s$^{-1}$. They infer the ionization rates using the abundance ratios of [DCO$^+$/HCO$^+$] and [HCO$^+$]/[CO] under 0D spatial assumptions and a reduced analytic chemical network. Finally, we include the CRIRs from the van der Tak & van Dishoeck (2000) survey toward single high-mass protostars with the central protostar being massive enough to provide a bright background source for H$_3^+$ absorption. They find CRIRs scattered from $10^{-17}$ to $10^{-16}$ using an assumed H$_3^+$ abundance and density distribution. They find the observed H$_3^+$ column density increases with cloud distance, which can be explained by contamination from low-density clouds along the line of sight.

Our model results show good agreement with the inferred CRIRs from Indriolo & McCall (2012), Indriolo et al. (2015), and Caselli et al. (1998). We find the LDI model is able to replicate the spread in the CRIR. There are two main controlling factors for the CRIR in the clouds: the number of embedded sources and the cloud environment. Embedded
sources create a natural dispersion in \( \zeta \) for different molecular cloud masses and star formation efficiencies. Without internal sources, there is no spread in our modeled CRIR as a function of column density. In order to represent the observations, the external CRIR must be increased instead for different regions. Local sources of CRs, such as nearby OB associations or supernova, contribute significantly to the CR flux at the cloud boundary. As the external CR flux is increased, the impact of attenuation also increases due to the rapid reduction in low-energy CRs. Figure 11 shows that the impact of attenuation is different between the HNI and LNI models. For the LNI model, \( \zeta \) changes by less than an order of magnitude across four orders of magnitude in \( AV \). Conversely, the HNI model CRIR decreases by two orders of magnitude due to an overall reduction in MeV-scale CRs. The HNI model overpredicts the CRIRs measured in diffuse gas to CRIRs measured near high-mass protostars, excluding the galactic center sightlines. However, the HDI model underpredicts the observed CRIR for all but a few sightlines. Thus, Figure 11 demonstrates that it is essential to consider the cloud environment and properly treat the CR physics and cloud density distributions. Models without attenuation only represent the CRIR within narrow ranges of \( AV \) and not in the cloud interiors. Figure 11 also underscores that the low-energy CR spectrum, which, if often adopted in astrochemical modeling, is a poor fit to the majority of the observations.

### 4.3. Challenges for Deriving the CRIR from Chemical Diagnostics

There have been numerous attempts to find chemical diagnostics that are strong tracers of the CRIR (Caselli et al. 1998; Indriolo et al. 2007, 2015; Neufeld et al. 2010; Indriolo & McCall 2012; Neufeld & Wolfe 2017; Albertsson et al. 2018). Some of these, such as \([\text{DCO}^+]/[\text{HCO}^-]\), cannot be modeled with the current 3D-PDR version due to the lack of deuterium and isotopic chemistry. Most probes of the CRIR are based on the local abundance, which is difficult to directly ascertain from observations. The use of column density ratios typically assumes the line emission observed between species is co-spatial. Figures 8 and 9 examine effects of CR physics on the \([\text{HCO}^-]/[\text{N}_2\text{H}^+]\), \([\text{CO}/\text{C}^+]\) and \([\text{C}/\text{C}^+]\) column density ratio diagnostics. However, we find that none of these ratios are monotonically sensitive to the average CRIR, shown for the LDI model in Figure 5. The \([\text{CO}/\text{C}^+]\) column density ratio is
Figure 10. Cosmic-ray ionization rate as a function of different abundance ratios. Left: $C/C^+$, middle: $\text{HCO}^+/\text{CO}$ and right: $\text{HCO}^+/\text{N}_2\text{H}^+$. The models are in descending order from the top: LNI, LDI, HNI, HDI.
Figure 11. Cosmic-ray ionization rate, $\zeta$, vs. $A_V$ for the six different models in Table 3. The filled curves represent the 1σ spread from the models covering the $(\Sigma_{cl}-N_{\text{H}2})$ parameter space. The squares represent diffuse gas measurements from Indriolo & McCall (2012) and Indriolo et al. (2015). The diamonds represent dense gas measurements from Caselli et al. (1998). The crosses represent observations toward high-mass protostars from de Boissangnet et al. (1996), and van der Tak & van Dishoeck (2000).

4.4. Impact of Cosmic-Ray Feedback on Cloud Chemistry

The Herschel Galactic Observations of Terahertz C+ (GOT C+) (Pineda et al. 2013) survey mapped [C II] 158 μm emission over the whole galactic disk, providing the best constraint on where [C II] emission originates. Pineda et al. (2013) found that nearly half of the [C II] emission originates from dense photon-dominated regions, with about another quarter of the emission from CO-dark $H_2$ gas. Clark et al. (2019) performed synthetic observations of young simulated molecular clouds and found the majority of their [C II] emission originates from atomic-hydrogen-dominated gas. This discrepancy was explained by the time evolution of molecular gas due to star formation and feedback. The results presented here provide a complementary explanation for the [C II]-bright molecular gas. When protoclusters become active, they accelerate CRs into the densest regions of molecular clouds. Figure 6 shows that high-mass protoclusters will lead to [C II]-bright $H_2$ dominated gas because CRs (i) increase the gas temperature to values closer to the [C II] excitation temperature of 91.2 K, (ii) increase the abundance of $C^+$ in dense gas due to the destruction of CO, and (iii) do not significantly alter the abundance of $H_2$.

In local star-forming regions, the lowest inversion transitions of ammonia, $NH_3$, have been widely used to map the dense gas cores within molecular clouds (i.e., Goodman et al. 1993; Jijina et al. 1999; Rosolowsky et al. 2008; Wienen et al. 2012). Ammonia remains optically thin, and while it does suffer from depletion, its formation is enhanced in regions where CO freezes out (Caselli & Ceccarelli 2012) (although this effect is not included in our models). However, this also makes ammonia much more susceptible to local variations in the FUV radiation field, temperature, and CRIR. Recently, the Green Bank Ammonia Survey (GAS) mapped all the Gould Belt clouds with $A_V > 7$ mag (Friesen et al. 2017). The DR1 data show that the line-of-sight averaged abundance, $X(NH_3) = N(NH_3)/N(H_2)$, exhibits a spread through molecular clouds. The spread could be caused by the porosity of molecular clouds, allowing more FUV radiation into regions of density, $n_{H_2}$, and the size of the cloud, $L$. Most sightlines are well fit using their method by clouds with densities $10 \leq n_{H_2} \leq 100$ cm$^{-3}$ corresponding to $5 \leq L \leq 100$ pc. Our models suggest that these length scales would incur CR screening effects that would change the CRIR. Similarly, for the high-density clouds, the energy losses will deplete MeV CRs and reduce the CRIR. In these cases, there is a further degeneracy in the $n_{H_2}-L$ plane resulting in an average decrease in the CRIR. The reduction would systematically produce model fits with lower densities to correct for the lower CRIR.

Rimmer et al. (2012) used a similar hybrid approach, adopting a prescription for $\zeta(N)$ ad-hoc with the MEUDON PDR code Le Petit et al. (2006) to model the Horsehead Nebula. They found their high $\zeta(N)$ model improved agreement over standard constant CRIR PDR prescriptions. However, their treatment of $\zeta(N)$ is static and fixed in time. The decoupling of CR attenuation and chemistry is only a good approximation if the abundance of neutral hydrogen ($H, H_2$) does not change much in time, ensuring that the CR spectrum is constant in time. The new approach presented here will allow $\zeta(N)$ to be connected to the chemical time evolution.
dense gas. However, our 1D models also exhibit a variation in this abundance measurement for the models with internal sources (LRI, LDI, and HDI). Figure 6 shows that ammonia is depleted in clusters exhibiting more embedded star formation by a couple of orders of magnitude. The abundance within the dense gas goes from \(10^{-8}\) in small clusters to \(10^{-10}\) in the largest. Furthermore, the gas also heats up, leading to stronger emission in higher transitions, such as NH$_3$(3,3).

Redaelli et al. (2017) examined the NH$_3$ GAS map of the Barnard 59 clump in more detail. They found that the abundance appears to drop dramatically in gas around the central central 0 0 0. This suggests that a smaller amount of H$_2$ and CO is created, thereby leading to recombination with HCO$^+$.

4.5. Impact of Cosmic-Ray Feedback on Chemistry in Dense Cores

Protostars are observed to be dimmer than classic collapse models predict, i.e., the “Protostellar Luminosity Problem” (Dunham et al. 2014). One possible solution is that accretion is strongly episodic (Kenyon et al. 1990; Vorobyov 2009; Offner & McKee 2011). Although our models assume steady-state accretion, we can infer the impact of large bursts of accretion on chemical equilibrium. A large accretion shock, which in turn produces higher-energy CRs and a higher CRIR. The CRIR increase in the dense gas then raises the temperature. The higher temperatures, whether caused by radiative or CR heating, lead to several different chemical effects. First, molecules frozen onto dust grains will evaporate, either by thermal desorption (Öberg 2016) or CR-induced desorption (Hasegawa & Herbst 1993), into the gas phase.

Second, the increase of the CRIR will increase the ionization fraction leading to a chain of ion–neutral reactions following $H_2^+$. Finally, the elevated radiative and CR flux may be strong enough to destroy some molecules. Jørgensen et al. (2015) and Frimann et al. (2016) showed that episodic accretion can cause the sublimation of CO-ice and explain the excess C$^{18}$O emission observed near protostars. Intuitively, a burst of CRs will lead to a reaction chain: H$_3^+$ is created, thereby leading to the destruction of CO to form HCO$^+$. However, the increase in CRs will provide a large population of free electrons that recombine with HCO$^+$ to form CO. HCO$^+$ also interacts with water and other dipole neutrals (in the case of water, the reaction leads to the formation of CO and protonated water).

HCO$^+$ is observed to be depleted near protostars that have undergone episodic accretion (Jørgensen et al. 2013). Ices sublimated by an accretion burst will cause a more active gas-phase chemistry and lead to an increase in carbon-chain molecules in molecular clouds as well as increase gas-phase CO in the dense gas where it would otherwise freeze-out. Overall, the addition of CRs magnifies the effect of an accretion burst. Temperatures increase beyond that expected from radiative heating alone. This suggests that a smaller change in accretion rate may be needed to produce the observed chemical changes.

4.6. Implications for Comparing Data and Models

Synthetic observations of hydrodynamic simulations are a vital tool for comparing theoretical predictions to observations. The synthetic observations may treat the chemistry in different ways: from assuming a constant abundance of some molecule to post-processing simulations with an astrochemical code or using the reduced-network chemistry from the hydrodynamic simulation (see review by Haworth et al. 2018). These synthetic observations are used to gauge how well the simulations correspond to the observed universe. As such, it is paramount to ensure that all astrochemical parameters are as accurate as possible. Radiation-MHD simulations can provide the density and temperature at every point (e.g., Offner et al. 2009). Simulations also now often include FUV radiation and optical depth calculations using packages such as FERVENT (Baczynski et al. 2015), TREERAY (Wünsch et al. 2018; used in Haid et al. 2019) and HARM$^2$ (Rosen et al. 2017). These methods can provide the FUV radiation and/or optical depth into the cloud. Our results show that the H$_2$ optical depth into the cloud should be considered when calculating the appropriate CRIR for post-processing. Typically, the CRIR is held constant throughout the entire simulation domain, which will lead to systematic differences in the simulation line emission.

5. Conclusions

We implement cosmic-ray attenuation in the public astrochemistry code 3D-PDR. The implementation uses the H$_2$ column density from the chemistry to attenuate the CR spectra. We couple the code to the protostellar CR models from Gaches & Offner (2018b), which solve for the total attenuated protocluster CR spectrum as a function of the cloud surface density, $\Sigma_{\text{cl}}$, and number of constituent protostars, $N_\ast$. An external spectrum is calculated for the solar environment using the commonly adopted spectrum with internal sources (LDI, LRI, and HDI; Offner et al. 2009) matched both the low- and mid-A_V observations of $\zeta$ and the observed spread.

1. Models with no sources or attenuation cannot explain observed CRIRs. Models with no internal sources but a higher ($H_\gamma$) external spectrum (HNI) match the observed CRIRs, although they may underpredict the CRIRs inferred for high-mass protostars. We find that a model using the commonly adopted spectrum with internal sources (LDI) matches both the low- and mid-A_V observations of $\zeta$ and the observed spread.

2. CRs accelerated by protostellar accretion shocks significantly alter the carbon chemistry in star-forming clouds. The amount of neutral and ionized Carbon increases in the dense gas as the number of protostars increases. Models with embedded sources (LDI, LRI, HDI) increase the amount of C, HCO$^+$, and NH$_3$ at lower $A_V$ and decrease the abundance of CO and NH$_3$ at higher $A_V$. Overall, models including internal sources (LDI, LRI, and HDI) exhibit a higher abundance of HCO$^+$ and H$_3^+$ with $\Sigma_{\text{cl}}$ and $N_\ast$.

3. Approximations that use H$_3^+$ and C-based tracers to estimate the CRIR systematically underpredict the CRIR unless CRs are the dominant source of ionization. The Reduced Analytic Approximation, which uses the abundances of H$_3^+$, CO, and O, always produces more accurate values of the CRIR, highlighting the importance of obtaining accurate oxygen and carbon monoxide abundances within molecular clouds.
4. Ions are systematically underproduced using the canonical CRIR, while CO is overproduced. Internal sources created a dispersion in the distribution of column densities by driving more active ion–neutral chemistry deep within molecular clouds.

5. Models using the low external CR spectrum (C) and/or no internal sources of CRs underestimate the H\textsubscript{2} column density by an order of magnitude or more.

6. Internally accelerated CRs will naturally lead to molecular gas, which become CO-deficient but [C\textsc{ii}]-bright, particularly for high-surface-density molecular clouds hosting large clusters.

7. Including CR attenuation in PDR models will help break the degeneracy in astrochemical modeling between the density, CR, and FUV radiation.

As protoclusters grow in constituent numbers, the impact on the chemistry is amplified, greatly so if CRs diffuse out of molecular clouds rather than stream. Comparison to observed CRIRs suggested the external CR spectrum, attenuation, and internal sources are important for modeling the chemistry of molecular clouds. However, the current uncertainties are large due to lack of observational data that can simultaneously constrain the density, FUV radiation, and CRIR on molecular cloud scales. Observations to constrain the CRIR within dense gas necessitate multi-line data, to independently determine the temperature as in, e.g., Ceccarelli et al. (2014), and multi-species data, to act as astrochemical diagnostics as in, e.g., Caselli et al. (1998). The 3D-PDR CR attenuation FORTRAN module can be included in any FORTRAN astrochemistry code.

S.S.R.O. and B.A.L.G. acknowledge support from the National Science Foundation (NSF) grant AST-1510021. S.S.R.O. was also supported by NSF CAREER grant AST-1650486. T.G.B. acknowledges funding by the German Science Foundation (DFG) via the Collaborative Research Center SFB 956 “Conditions and impact of star formation.” The authors are thankful for helpful discussions with Neal Evans and Nick Indriolo and the anonymous referee for their useful comments. The calculations performed for this work were done on the Massachusetts Green High Performance Computing Center (MGHPCC) in Holyoke, Massachusetts supported by the University of Massachusetts, Boston, Harvard University, MIT, Northeastern University and the Commonwealth of Massachusetts.

Software: 3D-PDR (Bisbas et al. 2012), MATPLOTLIB (Hunter 2007), NUMPY (van der Walt et al. 2011), SCIPY (Jones et al. 2001), JUPYTERLAB.
