1. INTRODUCTION

The past few years have seen a boom in studies of molecular deuteration in galactic low-mass and high-mass star-forming regions, triggered by the discovery of a large fraction of mono-, doubly, and even multiply deuterated molecules (e.g., Loren & Wootten 1985; Vrtilek et al. 1985; Walmsley et al. 1987; Mauersberger et al. 1988; Jacq et al. 1990, 1993; Gerin et al. 1992; Schilke et al. 1992; van Dishoeck et al. 1995; Ceccarelli et al. 1998; Stark et al. 1999; Roueff et al. 2000, 2005; Parise et al. 2002; Bacmann et al. 2003; Caselli et al. 2003; Vastel et al. 2004; Miettinen et al. 2009). Studying deuterium chemistry, especially in highly embedded regions, is important because in such environments, CO is depleted and deuterated species are thus driving the chemistry. In embedded regions in our Galaxy, a large deuterium fractionation is observed, well above the elemental abundance ratio D/H of $1.5 \times 10^{-5}$ (Oliveira 2003). High molecular deuteration can occur by two different mechanisms. One involves gas phase chemistry and ion–molecule deuterium exchange reactions taking place at low temperatures (Watson 1980). The second mechanism is based on grain chemistry (Tielens 1983).

In this work, we investigate deuteration in extragalactic star-forming environments, where the physical conditions can be drastically different from what we see in our own Galaxy. To date, very few detections of deuterated species have been attempted in extragalactic environments (e.g., Mauersberger et al. 1995; Martin et al. 2006). In a previous paper, Bayet et al. (2008) investigated the non-deuterated chemistry in a variety of extragalactic environments and obtained theoretical predictions for the warmer and dense gas, traced by non-deuterated species. Here we implement the mono-deuterated species (hereafter called D-species) network to our existing one used in Bayet et al. (2008), in order to investigate the differences in the D-fractionation and the D/H ratios in regions of star formation (i.e., gas with $n(H_2) \geq 10^5$ cm$^{-3}$) in various types of galaxies (i.e., starburst, cosmic-rays-enhanced environments, low-metallicity, and high-redshift). We also aim at guiding observers with potentially detectable deuterated tracers of so-called dense star-forming molecular gas in external galaxies when using Herschel or the forthcoming Atacama Large Millimeter Array (ALMA), as based on the strength of their chemical abundances.

The paper is divided in five sections; Section 2 describes the model used and presents the choice of model parameters used for mimicking various extragalactic environments. Section 3 presents the D-species fractional abundances and D/H abundance ratios obtained in the various gas components and environments investigated. Finally, in Section 4, we discuss the results and conclude.

2. MODEL DESCRIPTIONS

We have used the same chemical model as the one used in Bayet et al. (2008), but with an extended chemical network to include mono-deuterated species. The chemical code, UCL_Chem, is presented in Viti & Williams (1999) and Viti et al. (2004). We refer the reader to these papers for a full description of the code.

To summarize, the UCL_Chem model is a time- and depth-dependent chemical model. As in Bayet et al. (2008), we first model the collapse of a 10 K core (Phase I); we then follow the chemical evolution of the region once the stars are born (Phase II). The temperature in both phases is the typical average for starless and hot cores, respectively, since here we are considering an ensemble of cores within a large region of space. Bayet et al. (2010b) do in fact explore in great detail the influence of changes in temperature and density within a single hot core when subject to various environmental conditions. They find that thermal variations due to temperature structure would flatten out when averaged over a large number of cores.

The presence of an infrared source in the center or in the vicinity of the region is simulated by subjecting the gas and the dust to an increase in temperature. In our models, we have assumed equal dust and gas temperatures. This is justified since in Phase II the opacity is very high (see values listed in Table 4) and thus the thermal coupling between gas and dust is valid.

In both phases, the chemical network, now improved with D-species, is based on more than 4000 chemical reactions.
adapted from the UMIST 2006 database (Millar et al. 1997; Le Teuff et al. 2000; Woodall et al. 2007) involving about 300 species (92 of them being deuteronated) of which 62 are surface mantle species. The relevant surface reactions included in this work involve mainly simple hydrogenation, apart from the formation of CH₃CN which is believed to be formed via reactions involving HCN on grains (Garrod & Herbst 2006). We note that our approach for surface reactions is rather simplified with respect to that adopted by Garrod & Herbst (2006) and Cazaux et al. (2010). Nevertheless, a qualitative comparison of the mantle composition at the end of Phase I with the results from Cazaux et al. (2010) mantle shows good agreement (cf. H₂O and HDO abundances on grains as a function of the radiation field for example). As a first approximation and to keep the chemical network to a reasonable size, we include only the mono-D species. D₂CO and its corresponding ion are the only doubly D-species in our network.

The deuterium chemical network is similar to that of Roberts & Millar (2000a, 2000b) and Roberts et al. (2004). We assume that D atoms react in the same way as H atoms when reacting with other atoms and molecules.

One of the outputs of UCL_Chem is the fractional abundance (with respect to the total number of hydrogen nuclei and as a function of time) of gas and surface species from which we calculate the D/H ratios.

The above assumptions (i.e., no doubly D-species except D₂CO formed on grain nor triply D-species included in the code) do affect the reliability of the predictions for a couple of species, namely D₂CO, H₂D⁺, and N₂D⁺ (see Roberts et al. 2003). On the other hand, only mono-D-species have been observed so far in extragalactic environments, and the relative doubly D/mono-D or triply D/mono-D species abundance ratios seen in galactic sources are small (see, e.g., CD₃OH/CH₂DOH = 0.46 and CHD₂OH/CH₂DOH = 0.2 from Parise et al. 2004, ND₃H/ND₂D = 0.05 from Roueff et al. 2005, and D₂CO/HDCO = 0.02–0.33 from Roueff & Gerin 2003).

To investigate the deuterium chemistry in high-mass star-forming regions in various extragalactic environments, we have run a grid of 15 chemical models (see Tables 1, 2, and 3). For each type of galaxy (see below), we have studied the deuterium chemistry coming from a moderately dense gas:

### Table 1

| Parameter | Symbol | Typical Milky Way values |
|-----------|--------|--------------------------|
| Collapse Mode | B | 0.1 |
| Initial number density (phase 1) | n₀ | 300 H cm⁻³ |
| Final number density (phase 1 and 2) | n₁ | 1 × 10⁷ cm⁻³ |
| Temperature (phase 1) | T₁ | 10 K |
| Temperature (phase 2) | T₂ | 300 K |
| External UV radiation intensity | I | 1 Habing |
| Cosmic-ray ionization rate | ζ | 1.3 × 10⁻¹⁷ s⁻¹ |
| Visual extinction | Aᵥ | 580.6 mag |
| Gas:dust ratio | d | 100 |
| H₂ formation rate coefficient | R | 1.0 × 10⁻¹⁷ × √T cm⁻³ s⁻¹ |
| Metallicity | z⊙ | solar values, see Table 3 |

Note. The collapse is treated as a "modified free-fall," as defined by Rawlings et al. (1992), and the parameter B is introduced to allow for collapse in free-fall B = 1.0, or somewhat more slowly (B < 1.0) if gas or magnetic pressure resists the collapse.

### Table 2

| Parameter | Typical Value |
|-----------|---------------|
| C/H | 1.4 × 10⁻⁴ |
| S/H | 1.4 × 10⁻⁶ |
| O/H | 3.2 × 10⁻⁴ |
| N/H | 6.5 × 10⁻⁵ |
| He/H | 7.5 × 10⁻² |
| Mg/H | 5.1 × 10⁻⁶ |

Note. The initial elemental abundance ratios correspond here to a compilation of values from Sembach & Savage (1996), Sofia et al. (1997), Meyer et al. (1998), Snow et al. (2002), and Knauth et al. (2003).

1. The normal spiral (NS) case assumes standard parameter values (symbol "ST") similarly as previously performed by Bayet et al. (2008, see their Tables 1 and 2).
2. For the starburst (SB) case, we have used an FUV radiation field of 1000 times the standard value, and a temperature of 500 K, in Phase II, instead of 300 K. These models aim at mimicking environments such as NGC 253 or M 82.
3. The cosmic-ray-enhanced environments (SB+) case is represented in our models by a cosmic-ray ionization rate of 100 times the standard value. This type of models aims at reproducing supernovae and massive star formation as seen in galaxies such as Arp 220 (supernovae rate of 4 year⁻¹; see, e.g., Purra et al. 2007).
4. The low-metallicity (Low-met) case is represented, in our models, by a decrease in the metallicity to a fifth of the solar value coupled with an increase of the gas-to-dust mass ratio by a factor of five. Indeed, in the code, quantities such as metallicity, optical depth (Aᵥ), and the H₂ formation rate coefficient are coupled (see values presented in Table 4 for each model). In this galaxy type, we have also assumed an increase of FUV radiation field of 1000 times the standard value, and a temperature of 500 K since we are particularly interested in sources such as IC 10, which also host a strong star formation activity.
5. Finally, the high-redshift (High-z) case is represented by models with a metallicity (and its coupled quantities) of a fifth solar as measured in IC10 (Zaritsky et al. 1994), which is a local dwarf galaxy often used as a good template for archetypical higher-z galaxy populations (e.g., Madden et al. 1997; Leroy et al. 2006; Yin et al. 2010); an increase of FUV radiation field by 1000 times the standard value; a temperature of 500 K and an increase of the cosmic-ray ionization rate by a factor of 100 times the standard value. Indeed, in distant objects (at redshifts greater than 0.1), it is expected to often have a combination of several
nuclear activities such as active galactic nuclei, SB, and supernovae (see, for instance, Seymour 2009 or the studies on the quasar APM08+279 located at z ~ 4 from Weiß et al. 2007 and Riechers et al. 2009). We note that we may indeed underestimate the metallicity at high redshift in our study since optical observations of quasars at z ~ 6 (e.g., Jiang et al. 2007; Juarez et al. 2009) recently revealed that a solar metallicity value is more likely than a subsolar one for reproducing their observations. However, we emphasize that we have not tried in our present models to match the physical conditions for any high-z source in particular, but that we model here what one can consider as an archetypical high-redshift environment. Since we know that the early universe is more populated by dwarf galaxies than any other galaxy type (e.g., White & Frenk 1991), we adopt the values for IC10 as our high redshift standard.

All the details of the parameters used in the 15 models are summarized in Tables 1–4.

3. SENSITIVITY OF DEUTERATED CHEMICAL ABUNDANCES AND D/H ABUNDANCE RATIOS TO VARIATIONS IN THE PHYSICAL AND CHEMICAL PARAMETERS

The main aim of this work is to study the sensitivity of deuterated species in models of star-forming regions to variations in physical and chemical parameters that may be characteristics of various galaxy types. A collection of likely detectable tracers as seen by the strength of their chemical abundances will be given in Subsection 3.3, but first we simply analyze the trends the deuterium chemistry follows as the environment (i.e., galaxy type) and the gas density vary. These trends are summarized in Figures 1–6.

3.1. Deuterated Fractional Abundances Sensitivity

3.1.1. Influence of the Gas Density

When the gas density increases from $n(H_2) = 10^5$ cm$^{-3}$ to $n(H_2) = 10^7$ cm$^{-3}$, regardless of the galaxy type, we can...
divide deuterated species into three categories: those which are insensitive to density changes (e.g., HDO, NH₂D, and HDCS), those that increase with density (e.g., HDS, C₂D, and CH₃OD), and those which show a decrease in their fractional abundances (e.g., DCN, DNC, and CH₂DOH). The fractional abundances of the D-species belonging to the first category actually tend to converge after ~10⁵ yr, making these species good D-tracers of dense gas (n(H₂) > 10¹⁵ cm⁻³) whatever the environments since they show abundances above 10¹⁰. In contrast, we show in Figures 1–3 that especially DCN and DNC decrease with an increase of density (e.g., compare models NS₁ and NS₃). This is no surprise since the same behavior is seen for both HCN and HNC when the density increases (Z. Awad 2010, in preparation). This phenomenon reinforces the conclusions of Bayet et al. (2009) that HCN, HNC, and their deuterated counterparts are not particularly good tracers of the very dense gas in galaxies. HDS, C₂D, and CH₃OD increase with density. The enhancements in their fractional abundance, by more than a factor of five
(Figures 1–3), are particularly interesting since observing their molecular emissions may allow us to discriminate between the different gas components in a galaxy.

3.1.2. Influence of the FUV Radiation Field and the Temperature (SB Case)

Variations in FUV or temperature do not lead to significant changes in abundances for species such as HDO, NH$_2$D, DCN, D$_2$CO, HDCS, CH$_2$DOH, and CH$_3$OD (i.e., variations in chemical abundances less than a factor of 2–3). However, HDCO and HDS abundances decrease between a factor of 5 and 15 when the FUV radiation field increases. This is due to dissociations by FUV photons. At early times ($\lesssim 10^5$ yr), and at low density ($n(H_2) = 10^5$ cm$^{-3}$), the abundance of C$_2$D increases by three orders of magnitude with the increase of both FUV radiation field and temperature. Hence, this species is likely to be a good D-tracer of excitation in galaxies since it is very sensitive to changes in both temperature and FUV radiation field. At later times, the increase of the C$_2$D abundance is less pronounced, but still significant (i.e., about two orders of magnitude). On the other hand, DNC shows the largest decrease, i.e., by more than one order of magnitude, when the FUV radiation field and the temperature are increased (linked as seen in Table 2). This may be due to cosmic-ray-induced photodissociation, which has a significant temperature dependence.

3.1.3. Influence of the Cosmic-ray Ionization Rate (SB+ Case)

Increasing the cosmic-ray ionization rate ($\zeta$) by a factor of 100 (models SB$_1$+ to SB$_3$+—see Table 3 and Figure 2) leads to most abundances been significantly reduced by several orders of magnitude (e.g., HDCS, NH$_2$D, D$_2$CO, HDCO, CH$_2$DOH, HDO, DNC). As already found by Bayet et al. (2008), by Meijerink & Spaans (2005), and Meijerink et al. (2006), the effects of increasing the cosmic-ray ionization rate are complex, and they generally lead to a chemistry that approaches steady state more quickly (see Figure 2). The general decrease of abundances seen when $\zeta$ increases is probably due to a release of reactive ions such as ionized carbon, reacting quickly with many oxygen-bearing species such as HDCO, D$_2$CO, etc. However, some species such as DCO$^+$, N$_2$D$^+$ (both at low density only), DC$_3$N, and DCN (whatever the gas component) show abundances increased by several orders of magnitude with $\zeta$. In the case of nitrogen-bearing species, we suspect that the main reservoir of nitrogen, N$_2$, becomes ionized and gives rise to N$^+$, a reactive species that promotes the formation of nitrogen-bearing species. This behavior is also found for the hydrogen counterparts (e.g., Bayet et al. 2008). What is interesting here is that D-species seem to be affected in the same way as their hydrogen counterpart. Species such as N$_2$D$^+$ and DCN are thus likely to be good D-tracers of cosmic-ray ionization-excited environments since they show high fractional abundances and are sensitive to their change. In principle, we thus can use deuterium to constrain $\zeta$ although the effects of high cosmic-rays ionization rates on the chemistry are very complex (E. Bayet et al. 2010, in preparation) and highly dependent on initial conditions as well as the available gas coolants (Bayet et al. 2010a).

3.1.4. Influence of the Metallicity (Low-met Case)

Low-metallicity environments, such as those described in Section 2 (see models Low-met$_1$ to Low-met$_3$ in Table 3), lead to few surprises for most species in that their abundance is simply reduced accordingly (see Figure 3 for HDCO, D$_2$CO, DNC, NH$_2$D, and HDS). However, some species, such as C$_2$D or DCN, show an increase in their abundances with a decrease of the metallicity, whereas other species such as HDCS, CH$_2$DOH, and CH$_3$OD do not seem sensitive to metallicity changes. Therefore these latest species (potentially) are good D-tracers of dense gas (since they have high abundances).
whatever the metallicity (especially interesting at high redshift), similarly to their hydrogen counterpart (such as CH$_3$OH) already noted by Bayet et al. (2008) and Röllig et al. (2007).

3.1.5. Influence of the Above Parameters Coupled Together (High-$z$ Case)

In extreme conditions such as those used for mimicking high-redshift environments (see models High-$z_1$ to High-$z_3$ in Table 3 and Figure 3), most of the chemical abundances of D-species decrease; CH$_3$OD, HDS disappear completely from Figure 3 as compared to the normal spiral case (see Figure 1); NH$_3$D, D$_2$CO, DNC, and CH$_3$DOH have chemical abundances above the limit of detectability only at early time (i.e., before $(1.5-3) \times 10^4$ yr) then they drop severely at later time: HDCS, HDO, HDCO, even if still above the limit of detectability at all times, decrease by more than two orders of magnitude in high-redshift environments as compared to the normal spiral case. These species nonetheless remain the best D-tracers of dense gas components in high-redshift environments since they are very sensitive to the parameters changes. Only DCN and C$_2$D show fractional abundance either boosted by up to four orders of magnitude as compared to the models NS$_1$–NS$_3$ or
stay unchanged, respectively. In the case of the high-\(z\), the formation of DCN is dominated by the reaction D + HCN which is inefficient in our models for normal spirals because of the deficiency of atomic deuterium. In the models for normal spirals, the fractional abundance of D is indeed five orders of magnitude lower than in the models for high-\(z\) cores.

### 3.2. D/H Abundance Ratios Sensitivity

As seen in Figures 4–6, the D-fractionation calculated from the chemical abundances of all species does not show similar D/H ratio values, regardless of the environment. In protostellar galactic cores, such as IRAS 16293–2422, such behavior is already well known (e.g., van Dishoeck et al. 1995; Ceccarelli et al. 1998; Parise et al. 2004). The authors indeed observed NH\(_2\)D/NH\(_3\) = 0.1, whereas they obtained DCO\(^+\)/HCO\(^+\) = 0.009. They interpret the higher D/H ratios they obtained as coming from a cooler and more extended gas located in the envelope around the source and not coming from the hot gas in the core. In our study, we can see (Figure 4) that the highest ratios are indeed obtained, on average, for the galactic cases (i.e., models NS), for model NS\(_1\) which has got the smallest density (see Table 5).

In roughly all the models, there are three groups of molecules which converge to similar D/H values: (1) the group including DCO\(^+\)/HCO\(^+\), N\(_2\)D\(^+\)/N\(_2\)H\(^+\), and HDCO/H\(_2\)CO; (2) the group containing NH\(_2\)D/NH\(_3\) and D\(_2\)CO/H\(_2\)CO; and (3) the group containing CH\(_2\)DOH/CH\(_3\)OD, CH\(_2\)DCN/CH\(_3\)CN, and CH\(_3\)OD/CH\(_3\)OH. D/H, however, varies by several orders of magnitude among those groups. With the current limited D/H data set on galactic and extragalactic sources, confirmation of such results is not possible.

The H\(_2\)D\(^+\)/H\(_3^+\) does not vary as much as the other D/H ratios from a galaxy type to another. On average, the largest discrepancy between D/H ratios group estimates is shown to be for the SB+ case where the spread between all the D/H values is the largest (see Figure 5).

Despite these uncertainties and for providing future observers with D/H values, steady-state D/H ratios for various molecules are listed in Table 5.

### 3.3. Predictions for Observers

In Table 5, we list the D-species that should be likely detectable in external galaxies as based on the values obtained for their chemical abundance. We define the limit of detectability as \([n(X)/n_\text{H}] = 1 \times 10^{-12}\), as is typical for dense gas molecules in the Milky Way. Of course, detectability will also depend on...
the excitation conditions as well as the geometry of the source. According to the estimates of Lintott et al. (2005), however, these abundances may be sufficiently large that unresolved active galaxies should be likely detectable in these species even at high redshift.

Of particular interest are HDO, DCN, and HDCO which are very abundant \((n(X)/n(H) > 10^{-10})\) in all the investigated environments. These species are ideal molecules to be used for a first observational campaign aiming at validating the model predictions described here.

A second category of interesting species includes DCO\(^+\), DC\(_3\)N, DNC, and N\(_2\)D\(^+\) as they seem to arise only from one gas component in a single galaxy type: SB\(_3^+\) (for DCO\(^+\)), SB\(_1\) (for DC\(_3\)N), NS\(_1\) (for DNC), and SB\(_{1+}\) (for N\(_2\)D\(^+\)). In a similar vein, C\(_2\)D and HDCS are predicted to be excessively reactive to the presence of cosmic-rays ionization whereas they survive easily in FUV-enhanced environments. HDS is more sensitive to FUV changes than C\(_2\)D and HDCS and it survives to both FUV and cosmic-ray ionization as long as the gas is dense. Here, HDS may thus be a good discriminant of the different gas components in SB and SB\(_{1+}\) environments since it shows high abundances for the densest gas component. However, as soon as the metallicity drops, it becomes undetectable whereas HDCS and C\(_2\)D abundances are still high.

The third category of species contains D\(_2\)CO, CH\(_3\)DOH, and CH\(_3\)OD. These molecules do not survive in high-redshift or in low-metallicity galaxies. The fact that these species survive nonetheless in SB sources may reflect the poor influence of FUV photons on highly embedded material.

Species such as CH\(_3\)DCN and H\(_2\)D\(^+\) are likely undetectable, whatever the conditions since their chemical abundances are low.

Finally, DCN, HDO, HDCO and to a lesser extent D\(_2\)CO, DCO\(^+\), and NH\(_2\)D seem also to be good candidates, i.e., abundant enough at various redshifts.

Of course, our predictions are qualitative in nature since they are based only on an abundance criterion. For more quantitative predictions, radiative transfer models, as well as knowledge of the source geometry, are needed. DCN, HDCO, D\(_2\)CO, DCO\(^+\), and NH\(_2\)D expected line intensities cannot be derived due to the lack of collisional rates. For HDO, however, we have been able to derive very rough estimates of line intensities using RADEX\(^1\) developed by van der Tak et al. (2007) and using the collisional rates from the Leiden Atomic and Molecular Database (LAMDA\(^2\)). We have assumed a plane-parallel geometry, used model SB\(_1\) HDO fractional abundances for describing the local universe abundances, and model High-\(z\)\(_1\) HDO fractional abundances for the \(z > 1\) case. We have converted the predicted HDO fractional abundances from both models into column densities as described in Section 4 (see the footnote), using the \(A_v\) values listed in Table 4. The HDO column densities obtained have then been used in RADEX, in addition to the gas density and the kinetic temperature as listed in Table 2. A FWHM of 50 km s\(^{-1}\) has been assumed, as seen typically in extragalactic molecular line measurements (e.g., Mauersberger et al. 1995; Israel & Baas 2003; Martín et al. 2006; Bayet et al. 2009; Aladro et al. 2010). For models SB\(_1\), we have obtained values ranging from \(1.8 \times 10^{-4}\) K km s\(^{-1}\) (for the HDO(3\(_1\)\(_2\)\(_{2}\)-6\(_1\)\(_1\)) line emitting at 356 GHz) up to \(9.5 \times 10^3\) K km s\(^{-1}\) (for the HDO(2\(_{2}\)\(_2\)\(_{2}\)-1\(_{1}\)\(_1\)) transition emitting at 490 GHz). Beam and distance dilution correction factors have to be applied to these values. Following the Lintott et al. (2005) formula (see the Appendix), we have assumed a distance of 3 Mpc (such as M 82) as well as a beam size of 12 arcsec as listed for ALMA-band 8\(^3\) (i.e., at 490 GHz). With such assumptions, the HDO(2\(_{2}\)\(_2\)\(_{2}\)-1\(_{1}\)\(_1\)) line intensity can be reproduced by \(~10^{10}\)–\(10^{18}\) cores, depending on the source size considered. If we perform the same calculation but for the high redshift case (i.e., HDO fractional abundances from model High-\(z\)\(_1\)), for a galaxy located at \(z = 4.7\) (Carilli et al. 2002), and increasing the ALMA beam to 56 arcsec (since the frequency line drops to ALMA-band 1),

\[^1\] See http://www.strw.leidenuniv.nl/~vdtaek/radex/radex.php.
\[^2\] See http://www.strw.leidenuniv.nl/~moldata/.
\[^3\] See primary beam size values in http://www.eso.org/sci/facilities/alma/observing/specifications/.

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Figure 6. D/H abundance ratios as a function of time for various D-species in the low metallicity case (top three plots) and the high redshift case (bottom three plots). See the captions of Figures 1 and 4.
Deuterated Molecules Detectable in Extragalactic Star Forming Regions and their Corresponding D/H Ratios (at a time = 10^6 yr) for Five Models Representative of Five Types of Galaxies (See Section 2)

| Molecule | Normal Spiral | Starburst | Cosmic-rays Enhanced | Low metallic | High redshift |
|----------|---------------|-----------|----------------------|-------------|--------------|
|          | NS1 | NS2 | NS3 | SB1 | SB2 | SB1 | SB1+ | SB1+ | SB1+ | Low-met1 | Low-met2 | Low-met1 | High-z1 | High-z2 | High-z3 |
| HD CO    | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  |
| D2 CO    | +   | +   | +   | +   | +   | +   | +   | +   | +   | +   | +   | +   | +   | +   | +   | +   | +   |
| DCO      | ++  | +   | +   | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  |
| DCN      | +   | +   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   |
| DCN+/N   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   |
| DCO+     | +   | +   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   |
| H2 D+    | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   |
| HDO      | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  |
| C2 D     | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  |
| HCDS     | +   | +   | +   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   |
| HDS      | +   | +   | +   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   |
| NH2 D    | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  | ++  |
| N2 D+    | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   | -   |
| CH2 OD   | +   | +   | +   | +   | +   | +   | +   | +   | +   | +   | +   | +   | +   | +   | +   | +   | +   |
| CH2 DOH  | +   | +   | +   | +   | +   | +   | +   | +   | +   | +   | +   | +   | +   | +   | +   | +   | +   |
| CH2 DCO  | +   | +   | +   | +   | +   | +   | +   | +   | +   | +   | +   | +   | +   | +   | +   | +   | +   |
| CH2 DCCN| +   | +   | +   | +   | +   | +   | +   | +   | +   | +   | +   | +   | +   | +   | +   | +   | +   |

Notes. The limit of detectability has been taken to be [n[X]/nH] = 1 × 10^-12, as is typical for dense gas in the Milky Way. Below this limit, we assumed the species as not detectable (symbol "+"). Otherwise, they are marked with the symbol "+". When the fractional abundance of a deuterated species is above [n[X]/nH] = 1 × 10^-10, the symbol "++" is used.
we thus need \( \sim 10^9 \) cores to reproduce the HDO(1\( \text{0}_{1,0}\)-\( \text{0}_{0,0}\)) line emitting at 465 GHz, which shows the strongest RADEX line intensity estimate of \( 2.09 \times 10^4 \) K km s\(^{-1}\). In this case, HDO may not, of course, be detectable.

4. DISCUSSION AND CONCLUSIONS

Although we do not aim at modeling any specific source, we have qualitatively compared our models with extragalactic D-species observations published so far. Mauersberger et al. (1995) obtained upper limits for the emission of the DCN \( J = 2-1 \) line toward NGC 253 and IC 342. More recently, Martín et al. (2006) observed DCO\(^+\), DCN, DNC, and \( N_2D^+ \) in NGC 253. When we convert these observations and our predicted fractional abundances into approximate column densities,\(^4\) we find a general good agreement between the two sets within a factor of \( \leq 3 \), even if one single model is not able to reproduce consistently all the data. As already shown in Bayet et al. (2009), several gas components are needed to account for the molecular emission observed in external galaxies. More precisely, in NGC 253 (data from both Mauersberger et al. 1995 and Martín et al. 2006), the model SB\(_{1+}\) best reproduces the observed DCO\(^+\) column density (less than a factor of three). This indicates that a cosmic-ray-enhanced environment may be present in the nucleus of NGC 253. Model NS\(_{2}\) best reproduces the observed DCN column density in NGC 253, within a factor of one. Finally, all models in our grid, except model NS\(_{1}\), are able to reproduce the observation of DNC (\( N(DNC)^+ < 9.4 \times 10^{10} \) cm\(^{-2}\)) reported in Martín et al. (2006). For IC 342, only one D-species has been observed (i.e., DCN) and model NS\(_{2}\) gives the closest predicted column densities to the observed values (factor of 11). This factor is higher than that in the case of NGC 253 because the DCN detection suffers from larger uncertainties in IC 342 (see Mauersberger et al. 1995) as compared to the detection obtained in NGC 253.

Due to the lack of additional observations in extragalactic environments, we are not able to further refine our predictions. Nevertheless, our simple approach offers some significant insights on the major trends of the deuteron chemistry when subject to various physical conditions. Our models can also potentially help discriminate cold and dense star-forming gas between SB, SB\(_{+}\), low-metallicity, etc., activity. These predictions may be of particular interest when looking at extragalactic very dense high-mass star-forming regions where CO is expected to be depleted onto grains (similarly to what it is seen in our own Galaxy), and where thus D-species drive the chemistry.

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\(^4\) We performed such conversion by simply multiplying our predicted fractional abundance by the column density of hydrogen at the relevant visual extinction.

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