Herschel/HIFI detections of hydrides towards AFGL 2591

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Herschel/HIFI detections of hydrides towards AFGL 2591

**Envelope emission versus tenuous cloud absorption**


(Affiliations are available on page 5 of the online edition)

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ABSTRACT

The Heterodyne Instrument for the Far Infrared (HIFI) onboard the Herschel Space Observatory allows the free observations of light diatomic molecules at high spectral resolution and in multiple transitions. Here, we report deep integrations using HIFI in different lines of hydrides towards the high-mass star forming region AFGL 2591. Detected are CH, CH+, NH, OH+, H2O+, while NH+ and SH+ have not been detected. All molecules except for CH and CH+ are seen in absorption with low excitation temperatures and at velocities different from the systemic velocity of the protostellar envelope. Surprisingly, the CH(J=3/2→1/2,1/2) and CH+(J=1→0, J=2→1) lines are detected in emission at the systemic velocity. We can assign the absorption features to a foreground cloud and an outflow lobe, while the CH and CH+ molecules at high spectral resolution and in multiple transitions. Here, we report deep integrations using HIFI in different lines of hydrides towards the high-mass star forming region AFGL 2591. Detected are CH, CH+, NH, OH+, H2O+, while NH+ and SH+ have not been detected. All molecules except for CH and CH+ are seen in absorption with low excitation temperatures and at velocities different from the systemic velocity of the protostellar envelope. Surprisingly, the CH(J=3/2→1/2,1/2) and CH+(J=1→0, J=2→1) lines are detected in emission at the systemic velocity. We can assign the absorption features to a foreground cloud and an outflow lobe, while the CH and CH+ emission stems from the envelope. The observed abundance and excitation of CH and CH+ can be explained in the scenario of FUV irradiated outflow walls, where a cavity etched out by the outflow allows protostellar FUV photons to irradiate and heat the envelope at larger distances driving the chemical reactions that produce these molecules.

Key words. ISM: molecules – stars: formation – astrochemistry – ISM: individual objects: AFGL 2591

1. Introduction

The simplest constituents of interstellar chemistry, light diatomic hydrides and their ions (XH and XH+ with X = O, H, C and N), have so far not been studied thoroughly. Since their rotational ground state lines lie mostly outside atmospheric windows, they cannot be observed from ground. However, they are key-species of the chemical network. For example, most water at high temperature (T > 250 K) is formed by the reaction of OH with H2. Moreover, once their chemistry and excitation is well understood, they may be valuable tracers of warm and partly ionized gas (e.g. Sternberg & Dalgarno 1995; Bruderer et al. 2010). This is of particular interest in the context of star formation, as the radiation of the forming star may heat and ionize the envelope giving birth to it.

Herschel is an ESA space observatory with science instruments provided by European-led Principal Investigator consortia and with important participation from NASA.

** Apppendices and Table 1 (pages 6 to 7) are only available in electronic form at http://www.aanda.org

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The Heterodyne Instrument for the Far Infrared (HIFI; de Graauw et al. 2010) onboard the Herschel Space Observatory allows for the first time to carry out spectrally resolved observations of different transitions of hydrides and thus to disentangle moving regions along the line of sight and to study fine/hyperfine structure components.

AFGL 2591 is a well studied high-mass star forming region at a distance of ~1 kpc (e.g. van der Tak et al. 1999). The source is relatively nearby and its geometry thus well known (e.g. Preibisch et al. 2003). There is evidence for a cavity along the outflow that allows FUV photons to escape to longer distances and irradiate the outflow walls (Bruderer et al. 2009a,b).

In these high-density PDRs, the abundances of hydrides can be enhanced by several orders of magnitude. Chemical models of these systems require a peak optical depth of $\tau_{\text{ff}} \sim 2$. Observations and data reduction

Herschel/HIFI observations of AFGL 2591 ($\alpha_{2000} = 20^h 29^m 24.87^s$, $\delta_{2000} = +40^\circ 11' 19.5''$) have been carried out as part of the Water In Star forming regions with Herschel (WISH; van Dishoeck et al., in prep.) guaranteed time key program. Target lines are given in Table 1. Molecular parameters are obtained from the CDMS (Müller et al. 2005), except for NH$^+$ (Hübbers et al. 2009) and H$_2$O$^+$ (Müritz et al. 1998). Dual beam switch mode with fast chopping was used. To disentangle lines from the upper and lower side band, the local oscillator frequency was slightly shifted after half of the integration time. Data were converted to $T_{\text{lab}}$ using a main beam efficiency of 0.74. Data from the WBS spectrometer are used and the H and V polarizations have been averaged after visual inspection. Table 1 gives the noise level of the observation $T_{\text{min}}$ for the nominal resolution of the WBS spectrometer (1.1 MHz). Data were reduced with the Herschel interactive processing environment (HIPE) package version 2.9.

2. Observations and data reduction

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3. Results

Spectra of detected target lines are given in Fig. 1, those without detection in the Appendix A. We have detected the ground state lines of CH, CH$^+$, OH$^+$, H$_2$O$^+$ and NH. The lines of OH$^+$, H$_2$O$^+$ and NH are seen in absorption without clear signs of emission on top of the absorption. The CH line is almost purely in emission. The CH$^+$(J = 1–0) line is in absorption, with emission at the systemic velocity of the envelope. The CH$^+$(J = 2–1) line is in emission. Except for CH$^+$(J = 2–1), no line between excited states is detected. Not detected are SH$^+$ and NH$^+$. While SH$^+$ has been seen in other regions (Benz et al. 2010; Menten et al. 2010), interstellar NH$^+$ has not yet been found.

By their velocity shift, the absorption lines of CH, CH$^+$, NH, OH$^+$ and H$_2$O$^+$ can be roughly classified as (i) a component around $v_{\text{lsr}} \sim 0$ km s$^{-1}$, red-shifted with respect to the systemic velocity of the envelope at $v_{\text{sys}} = -5.5$ km s$^{-1}$ (van der Tak et al. 1999) and (ii) a blue-shifted component at $\sim -11$ km s$^{-1}$ (NH) or $\sim -16$ km s$^{-1}$ (OH$^+$, H$_2$O$^+$ and CH$^+$).

The velocity integrated emission or absorption is given in Table 1. The absorption per frequency is $\tau = -\log(T_{\text{line}}/T_{\text{cont}})$, with the continuum intensity $T_{\text{cont}}$ in a single side band. The velocity integrated emission and absorption are related to the molecular column density of the upper or lower level $N_{\text{upper}}$ and $N_{\text{lower}}$ by

$$N_{\text{upper}} = \frac{8\pi k v_{\text{ul}}^2}{hc^2 A_{\text{ul}}} \int T_{\text{dv}}$$

$$N_{\text{lower}} = \frac{8\pi v_{\text{ul}}^2 g_l}{c^2 A_{\text{ul}} g_u} \int T_{\text{dv}},$$

with the Einstein-A coefficient $A_{\text{ul}}$ and the frequency $v_{\text{ul}}$ of the transition and the statistical weights $g_u$ and $g_l$ of the levels. These equations assume optically thin emission or absorption without re-emission. For Table 1, contributions of different fine/hyperfine components are summed up, weighted by their statistical weights. Detected lines together with the upper limits from higher levels yield upper limits on the excitation temperature and the column density, assuming the excitation temperature of all lines to be the same. For CH, we obtain $T_{\text{ex}} < 22.6$ K and $N$(CH) $< 1.6 \times 10^{13}$ cm$^{-2}$. OH$^+$ yields $T_{\text{ex}} < 13.2$ K and $N$(OH$^+$) $< 1.2 \times 10^{14}$ cm$^{-2}$ and H$_2$O$^+$ gives $T_{\text{ex}} < 18.5$ K and $N$(H$_2$O$^+$) $< 2.3 \times 10^{13}$ cm$^{-2}$. We refrain from deriving column densities for CH$^+$ using this method, as the molecule shows clear signs of both emission and absorption.

3.1. Modeling the line spectra

The line profile is modeled using a two-layer model (red and blue) solving the radiative transfer equation along the line of sight (Appendix B). Slab geometry is assumed and the absorbing/emitting foreground layers cover the whole background continuum. Free parameters per component are the column density, the excitation temperature and the line width and position. The intrinsic line profile is assumed to be a Gaussian. The upper limits of the OH$^+$ and H$_2$O$^+$ excitation temperature are lower than the energy of the upper level and for such low temperatures, the absorption lines do not depend much on the excitation temperature. We thus fix $T_{\text{ex}}$ at 3 K. Parameters of the best-fit model are given in Table 2. The model spectra are overlaid on the observed spectra in Fig. 1. The figure also gives only one component, showing the necessity of a second component. A good fit is obtained for the CH, NH and H$_2$O$^+$ lines. For CH and OH$^+$, further components would improve the fit. For OH$^+$, an asymmetric line would presumably be needed to fit observations. However, for the conclusions drawn here, we concentrate on the strongest components. A third component has only been added to model the emission peak of CH$^+$ at the systemic velocity of the envelope. The CH column densities derived with this method are larger compared to the calculation assuming optically thin lines. This is because the fitting of the different fine structure components requires a peak optical depth of $\tau \sim 2$.

4. Discussion

The blue-shifted component of OH$^+$, H$_2$O$^+$ and CH$^+$ suggests the association with the outflow lobe directed towards us. Mitchell et al. (1989) have detected 4.7 m$^{-1}$CO($v = 0$–1) absorption lines at $v_{\text{lsr}} \sim -28$ km s$^{-1}$. They derive a 13CO column density of $1.1 \times 10^{17}$ cm$^{-2}$ and a temperature of 200 K. With better spectral resolution, van der Tak et al. (1999) find $v_{\text{lsr}} \sim -21.5$ km s$^{-1}$, in better agreement with our observations. Their lines are broad and asymmetric, with strong wings to the blue, likely originating in winds. It is thus difficult to determine the line width and position. However, the 13CO lines reach the continuum at about $-45$ km s$^{-1}$ and are clearly broader than the OH$^+$, H$_2$O$^+$ and CH$^+$ lines. Except for CH$^+$, where the two-component model does not fit this component well, there is no evidence for asymmetric lines in this blue-shifted component. The component is not clearly detected in CH. The NH absorption is less shifted to the blue and narrower. The velocity shift
of the components, showing the relative intensity of the different hyperfine components. The spectra are corrected for the beam efficiency and the continuum level is given for one sideband (SSB).

They conclude that the absorption must take place in cold and tenuous gas, as it is not found in 12CO(J = 1–0). Where does the CH and CH⁺ emission emerge from? The line velocity suggests that the emission stems from the envelope of AFGL 2591. Abundances of CH and CH⁺ are difficult to estimate from column densities, due to the strong gradient in density in the envelope and thus the changing excitation. A spherical power-law density profile of the envelope (van der Tak et al. 1999) yields a density of n(H₂) ~ 10⁶ cm⁻³ at scales of the Herschel beam. Relative to the column density of N(H) > 10¹⁸ cm⁻² within the region with density ≥10⁵ cm⁻³, we get abundances of 4 × 10⁻⁹ (CH) and 9 × 10⁻¹¹ (CH⁺).

Notes. Fractional abundances are given relative to N(H) = N(H) + 2N(H₂). A(B) = A × 10⁶.

\(a\) Fixed at 3 K; \(b\) using \(N_{\text{H}_2} \sim 10^{23} \text{ cm}^{-2}\), see text; \(c\) using \(N_{\text{H}_2} \sim 1.2 \times 10^{23} \text{ cm}^{-2}\) (Minh & Yang 2008); \(d\) using \(N_{\text{H}_2} \sim 4.6 \times 10^{23} \text{ cm}^{-2}\) (Mitchell et al. 1989).

The redshifted absorption at \(v_{\text{lsr}} = -0.2\) to 2.8 km s⁻¹ is likely associated to a cold and extended foreground cloud, observed in CO (Mitchell et al. 1992; Hasegawa & Mitchell 1995). The small line width in their spectra approximately agrees with the narrow absorption lines seen in CH⁺, H₂O⁺ and NH. The broad absorption of CH⁺ is surprising: since it is only seen in CH⁺(J = 1–0), but not CH⁺(J = 2–1), the excitation temperature must be lower than 8 K, used to fit the blue shifted component. This indicates either less dense or colder gas. The ionized species OH⁺, H₂O⁺ and CH⁺ are more red-shifted and have broader lines, compared to the neutral CH and NH.

The abundances of molecules in the absorption features are roughly estimated from the total column density (\(N_{\text{H}} = N(\text{H}) + 2N(\text{H}_2)\)) obtained from ¹³CO column densities and presented in Table 2. We use a CO abundance of \(n(\text{CO})/n(\text{H}_2) = 3.7 \times 10^{-4}\) (Doty et al. 2002) and ¹²CO/¹³CO ~ 77 (Wilson & Rood 1994). Since the red component is a low-density foreground cloud, the fractional abundances of CH, H₂O⁺ and NH have been compared to a chemical model for a diffuse/translucent cloud (Le Petit et al. 2004) and found to agree within a factor of ~2. The underprediction of CH⁺ by a factor of more than 100 is well known for such models, but models of turbulent dissipation regions (Godard et al. 2009) can explain fractional abundances reached here. OH⁺ is underpredicted by a factor of 6 but the observed OH⁺/H₂O⁺ ratio of 7.3 is comparable to the value of ~4 found by Gerin et al. (2010) and explained by low density gas with a low molecular fraction.

The blue component is thought to arise in tenuous warm gas in the outflow lobes directed toward us. The observed OH⁺ and H₂O⁺ abundances are lower by factors of 7 and 16, respectively, but the OH⁺/H₂O⁺ ratio is still large, about 3. As shown in Fig. 2 of Gerin et al. (2010) such ratios are consistent with models with densities up to a few thousand cm⁻³ and enhanced radiation fields, as expected in the outflow lobe. The fractional abundances of CH⁺ and NH are similar to those found in the red component within a factor of ~2. More specific modeling of these components must await better determinations of their physical conditions.

Where does the CH and CH⁺ emission emerge from? The line velocity suggests that the emission stems from the envelope of AFGL 2591. Abundances of CH and CH⁺ are difficult to estimate from column densities, due to the strong gradient in density in the envelope and thus the changing excitation. A spherical power-law density profile of the envelope (van der Tak et al. 1999) yields a density of n(H₂) ~ 10⁶ cm⁻³ at scales of the Herschel beam. Relative to the column density of N(H) ~ 10¹⁸ cm⁻² within the region with density ≥10⁵ cm⁻³, we get abundances of 4 × 10⁻⁹ (CH) and 9 × 10⁻¹¹ (CH⁺).
Why are the hydrides mostly in the ground-state? The excitation temperature $T_{ex}$ of a species, assumed to have only two levels, is given by

$$ T_{ex} = \frac{T_{kin}}{(kT_{kin}/\Delta E) \cdot \ln (1 + \beta n_{coll}/n(H_2)) + 1}. \tag{2} $$

with the kinetic temperature of the collision partner $T_{kin}$, the energy difference between the levels $\Delta E$, the escape probability for a line photon $\beta$, the critical density $n_{crit}$ and the density of a collision partner $n(H_2)$. The observed excitation temperature of CH$^+(J = 1-0)$ of 38.4 K can be reproduced by Eq. (2) with $\beta \approx 0.04$, assuming a kinetic temperature of 500 K, necessary for the formation of the molecule, and a $H_2$ density of order $10^9$ cm$^{-3}$, typical at scales of the Herschel beam. This $\beta$ corresponds to an optical depth of a few at the line center, depending on the expression used for $\beta = \beta(\tau)$. Far infrared radiation by the dust continuum also pumps the molecule. Critical densities of other hydrides are not well known, but likely of similar order. Thus, the observed low excitation temperature found for OH$^+$ and H$_2$O can be well explained by the origin of the absorption in tenuous gas.

Predictions for CH and CH$^+$ abundances and line fluxes can be made utilizing the photochemical and outflow model of Bruderer et al. (2009b). In a spherical envelope model, Bruderer et al. (2010) find volume averaged abundances orders of magnitude lower than observed ($\sim 6 \times 10^{-11}$ for CH and $\sim 5 \times 10^{-16}$ for CH$^+$). They present also a model including a cavity etched out by the outflow, where protostellar FUV radiation can escape and directly irradiate the outflow wall. The central protostar with a luminosity of $L_{bol} \sim 2 \times 10^4 L_\odot$ and $T_{eff} \sim 3 \times 10^4$ K can heat the gas in the outflow walls to above 1000 K at scales of the Herschel beam. Depending on the radius over which the abundance is averaged, abundances of $(0.6-2) \times 10^{-9}$ for CH and $(0.4-4) \times 10^{-9}$ for CH$^+$ are found with the outflow wall model, in acceptable agreement with the observations.

Calculating the radiative transfer in the lines for direct comparison with observations yields fluxes of $(4.3-16.1)$ K km s$^{-1}$ for CH$^+(J = 1-0)$ and $(8.9-30.8)$ K km s$^{-1}$ for CH$^+(J = 2-1)$. Note that this calculation includes the influence of the pumping by far IR radiation. In the view of uncertainties (such as distance, inclination, $T_{ex}$ of formation, and additional contribution to CH$^+$ by reactions of C$^+$ with vibrationally excited H$_2$; Agúndez et al. 2010), we consider the agreement with observations good. The abundances of OH$^+$ and H$_2$O are also enhanced in the outflow walls, but lack of collisional rate coefficients prevents us from making quantitative model results.

We conclude that the scenario of FUV irradiated outflow walls can quantitatively reproduce the abundances and fluxes observed in CH and CH$^+$ emission. This indicates the presence of a large volume/mass of hot, FUV irradiated and extended gas in the envelope of this high-mass young stellar object.

5. Conclusion

We use the new Herschel/HIFI instrument to observe light hydrides towards the high-mass star forming region AFGL 2591. Besides OH$^+$, H$_2$O$^+$ and NH detected in absorption only, we see CH and CH$^+$ in emission. The red and blue velocity shifted absorption can be assigned to a foreground cloud and an outflow lobe directed towards us, respectively. The emission of CH and CH$^+$ is at the source velocity. Its abundance and excitation can be explained in the scenario of direct FUV irradiation of the envelope through a low density cavity of the outflow region.

References

Table 1. Observed lines in AFGL 2591.

<table>
<thead>
<tr>
<th>Species/Transition/Electronic state/Line components</th>
<th>Frequency [GHz]</th>
<th>$E_u$ [K]</th>
<th>$A_{ul}$ [s$^{-1}$]</th>
<th>$T_{obs}$ [min]</th>
<th>$T_dv$ [K km s$^{-1}$]</th>
<th>$T_{vd}$ [km s$^{-1}$]</th>
<th>$T_{max}$ [mK]</th>
<th>$N_{mol}^i(X) [cm^{-2}]$</th>
<th>$N_{mol}^f(X) [cm^{-2}]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH $J=3/2_2-1/2_1$</td>
<td>536.9611</td>
<td>25.76</td>
<td>6.4(6)</td>
<td>4.2</td>
<td>3.46 ± 0.00</td>
<td>...</td>
<td>16</td>
<td>3.0(12)</td>
<td>0.04</td>
</tr>
<tr>
<td>CH $J=5/2_2-3/2_1$</td>
<td>1661.1074</td>
<td>105.48</td>
<td>3.8(2)</td>
<td>20.2</td>
<td>&lt;0.93</td>
<td>&lt;0.34$^c$</td>
<td>220</td>
<td>1.13(11)</td>
<td>2.6(12)</td>
</tr>
<tr>
<td>CH$^+$ $J = 1-0$</td>
<td>835.1375</td>
<td>40.08</td>
<td>6.4(2)</td>
<td>40.4</td>
<td>0.91 ± 0.03</td>
<td>32.63 ± 0.06</td>
<td>16</td>
<td>1.9(11)$^d$</td>
<td>9.3(13)$^d$</td>
</tr>
<tr>
<td>CH$^+$ $J = 2-1$</td>
<td>1669.2813</td>
<td>120.19</td>
<td>6.1(2)</td>
<td>40.4</td>
<td>3.7 ± 0.2</td>
<td>...</td>
<td>115</td>
<td>3.3(11)</td>
<td>...</td>
</tr>
<tr>
<td>o-H$<em>2$O$^+$ $N</em>{o-H_2O}$ $J = 11/2-00, 01/2$</td>
<td>1115.2041</td>
<td>53.51</td>
<td>3.1(2)</td>
<td>39.2</td>
<td>...</td>
<td>7.65 ± 0.05</td>
<td>33</td>
<td>...</td>
<td>1.6(13)</td>
</tr>
<tr>
<td>o-H$<em>2$O$^+$ $N</em>{o-H_2O}$ $J = 12/2-11, 13/2$</td>
<td>746.26</td>
<td>89.33</td>
<td>5.5(4)</td>
<td>40.6</td>
<td>&lt;0.16</td>
<td>&lt;0.52</td>
<td>25</td>
<td>&lt;2.6(11)</td>
<td>&lt;3.0(13)</td>
</tr>
<tr>
<td>OH$^+$ $N_{OH}$ $J = 12/2-00, 12$</td>
<td>1033.1186</td>
<td>49.58</td>
<td>1.8(2)</td>
<td>40.6</td>
<td>...</td>
<td>21.98 ± 0.06</td>
<td>32</td>
<td>...</td>
<td>1.1(14)</td>
</tr>
<tr>
<td>OH$^+$ $N_{OH}$ $J = 21/2-19, 23/2$</td>
<td>1892.2271</td>
<td>140.39</td>
<td>5.9(2)</td>
<td>21.0</td>
<td>&lt;0.83</td>
<td>&lt;0.28</td>
<td>210</td>
<td>&lt;8.2(10)</td>
<td>&lt;2.5(12)</td>
</tr>
<tr>
<td>NH $N_{NH}$ $J = 12/2-10, 13/2$</td>
<td>974.4784</td>
<td>46.77</td>
<td>6.9(5)</td>
<td>7.0</td>
<td>...</td>
<td>3.90 ± 0.09</td>
<td>43</td>
<td>...</td>
<td>2.9(13)</td>
</tr>
<tr>
<td>NH $N_{NH}$ $J = 13/2-11, 13/2$</td>
<td>999.9734</td>
<td>47.99</td>
<td>5.2(3)</td>
<td>38.8</td>
<td>...</td>
<td>3.99 ± 0.05</td>
<td>29</td>
<td>...</td>
<td>5.0(13)</td>
</tr>
<tr>
<td>NH$^+$ $Jp = 3/2-1/2$</td>
<td>1012.5400</td>
<td>48.59</td>
<td>5.4(2)</td>
<td>38.8</td>
<td>&lt;0.16</td>
<td>&lt;0.19</td>
<td>30</td>
<td>&lt;5.9(9)</td>
<td>&lt;1.7(10)</td>
</tr>
<tr>
<td>NH$^+$ $Jp = 3/2-1/2$</td>
<td>1019.2107</td>
<td>48.91</td>
<td>5.5(2)</td>
<td>40.6</td>
<td>&lt;0.12</td>
<td>&lt;0.13</td>
<td>22</td>
<td>&lt;4.4(9)</td>
<td>&lt;1.2(10)</td>
</tr>
<tr>
<td>SH$^+$ $N_{SH}$ $J = 13/2-00, 13/2$</td>
<td>526.0479</td>
<td>25.25</td>
<td>9.6(4)</td>
<td>4.2</td>
<td>&lt;0.083</td>
<td>&lt;0.53</td>
<td>11</td>
<td>&lt;4.7(10)</td>
<td>&lt;4.5(12)</td>
</tr>
</tbody>
</table>

Notes. The frequency is given for the strongest fine/hyperfine component. The velocity integrated intensity or absorption is summed over all fine/hyperfine components. $A(B) = A \times 10^8$.

$^a$ 1σ $= \sqrt{\Delta V \Delta t_m}$, with $\Delta V \sim 10$ km s$^{-1}$ (expected line width) and the channel width $\Delta v$ (corresponding to 1.1 MHz); $^b$ 1σ $= \sqrt{\Delta V \Delta t_m}$; $^c$ non-detections are given by the 3σ value; $^d$ emitting or absorbing part only; $^e$ total integration time (on+off); $^f$ hyperfine or fine structure.

Appendix A: Spectra of non-detections

Figure A.1 presents spectra without detected target lines, given in Table 1. For clarity, the spectra of CH(S/5_2_2−3/2_2−) and OH$^+$ (21/2−11, 13/2) have been scaled by a factor of 0.1. In the spectrum of CH(S/5_2_2−3/2_2−), the $H_2O(23/2−23/2−)$ line is detected, which was presented in an upcoming paper (van der Tak et al., in preparation). The H$_2$O$^+(20/2, 21/2−11, 13/2)$ spectrum contains a SO$_2$ line with upper level energy similar to the lines detected by van der Tak et al. (2003) in the same source. In the other sideband of the NH$^+(3/2, −1/2)$ spectrum, the OH$^+(2, 3/2−1, 13/2)$ line is seen. In the upper side band of the SH$^+(13/2, 2−0, 13/2)$ line, the HCO$^+$(6−5) line has been detected. The velocity range of ±40 km s$^{-1}$ corresponds to a frequency range of ±67 MHz at 500 GHz and ±253 MHz at 1900 GHz. Thus, the lines should be seen in the spectra, even if the predicted rest frequency is grossly wrong.

Appendix B: Modeling the line spectra

This Appendix gives the equations used to model the line spectra. The intensity $T_{model}(\nu) [K]$ at frequency $\nu$ for a slab of $N$ emitting or absorbing layers in front of a continuum source is obtained from

$$T_{model}(\nu) = T_{continuum}(\nu) e^{-\sum_i \Delta \nu_i} + \sum_{i=1}^{N} \frac{C_i}{2v_i^2} B_{0i}(T_{eq}) e^{-\sum \Delta \nu_i} \left(1 - e^{-\Delta \nu_i} \right),$$

with the (background) continuum intensity $T_{continuum}(\nu)$, the opacity per layer $\Delta \nu_i$, the frequency of the component $\nu_0$ with the largest Einstein-A coefficient and the Planck function $B(T)$. Note that this equation assumes a covering factor of 100% for each layer and the same excitation temperature for all hyperfine/fine components. The line opacity is calculated from the sum over the $M$ fine/hyperfine components of the transition, $\Delta \nu_i$

$$\nu' = (\nu_0 + \frac{M}{2}\nu_0) e^{-\sum \Delta \nu_i} \left(x_i^u \frac{A_{ul}}{g_i} - x_i^l \frac{A_{lu}}{g_i} \right) \phi(\nu)$$

with the column density per layer $N_{mol}^i$, the Einstein-A coefficient $A_{ul}$, the normalized line profile function $\phi(\nu)$, the normalized level population per layer $x_i^u$ and $x_i^l$, respectively) and the statistical weights ($g_i$ and $g_l$, respectively). The normalized level population per layer is a Boltzmann distribution for the temperature $T_{eq}$. The line profile function $\phi(\nu)$ is assumed to be a Gaussian with width $\Delta \nu$ (FWHM) centered.

Fig. A.1. Spectra observed towards AFGL 2591 without detection of target lines. The velocity is given relative to the systemic velocity $\nu_{sys} = −5.5$ km s$^{-1}$. Page 6 of 7
at the frequency of the component minus the velocity \( v_{lsr} \) of the layer.

The free parameters per layer are thus the excitation temperature \( T_{ex} \), the column density \( N_{mol} \), the width \( \Delta v \) and the velocity \( v_{lsr} \). Two layers are used for CH, \( \text{H}_2\text{O}^+ \), \( \text{OH}^+ \) and NH with a red-shifted layer in front of a blue-shifted layer. Three layers are used for \( \text{CH}^+ \) with a layer centered at the source velocity between the background continuum and the blue-shifted layer. To constrain the parameters of the layer, the least squares of the modeled to the observed spectra are minimized.

Molecular data of the individual hyperfine components of CH, \( \text{OH}^+ \), \( \text{NH} \) and \( \text{H}_2\text{O}^+ \) used to model the line spectra in Fig. 1 are given in Table B.1. The table gives the frequency, Einstein-A coefficient \( (A) \), the upper level energy \( (E_u) \) and the statistical weights of the upper and lower level of the transition \( g_u \) and \( g_l \), respectively. The third column refers to the velocity shift in km s\(^{-1}\) of the component relative to the one with the largest Einstein-A coefficient. The component with the largest Einstein-A coefficient is marked by \(^*\).

### Table B.1. Hyperfine components used to model the spectra.

<table>
<thead>
<tr>
<th>Species</th>
<th>Frequency</th>
<th>Shift to (^*)</th>
<th>( E_u )</th>
<th>( A_u )</th>
<th>( g_u )</th>
<th>( g_l )</th>
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<tbody>
<tr>
<td>CH (^*)</td>
<td>536.7611</td>
<td>0.0</td>
<td>25.76</td>
<td>6.4 \times 10^{-4}</td>
<td>5</td>
<td>3</td>
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<td>CH</td>
<td>536.7820</td>
<td>-11.6</td>
<td>25.76</td>
<td>2.1 \times 10^{-4}</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>CH</td>
<td>536.7957</td>
<td>-19.3</td>
<td>25.76</td>
<td>4.3 \times 10^{-4}</td>
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<td>1</td>
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<tr>
<td>( \text{H}_2\text{O}^+ )</td>
<td>1115.1505</td>
<td>14.4</td>
<td>53.51</td>
<td>1.7 \times 10^{-2}</td>
<td>6</td>
<td>4</td>
</tr>
<tr>
<td>( \text{H}_2\text{O}^+ )</td>
<td>1115.1862</td>
<td>4.8</td>
<td>53.51</td>
<td>2.8 \times 10^{-2}</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>( \text{H}_2\text{O}^+ ) (^*)</td>
<td>1115.2041</td>
<td>0.0</td>
<td>53.51</td>
<td>3.1 \times 10^{-2}</td>
<td>6</td>
<td>4</td>
</tr>
<tr>
<td>( \text{H}_2\text{O}^+ )</td>
<td>1115.2632</td>
<td>-15.9</td>
<td>53.51</td>
<td>1.4 \times 10^{-2}</td>
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<td>4</td>
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<tr>
<td>( \text{H}_2\text{O}^+ )</td>
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<td>53.51</td>
<td>3.5 \times 10^{-3}</td>
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<td>4</td>
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<tr>
<td>( \text{OH}^+ )</td>
<td>1032.9979</td>
<td>35.0</td>
<td>49.58</td>
<td>1.4 \times 10^{-2}</td>
<td>3</td>
<td>2</td>
</tr>
<tr>
<td>( \text{OH}^+ )</td>
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<td>33.1</td>
<td>49.58</td>
<td>3.5 \times 10^{-3}</td>
<td>4</td>
<td>2</td>
</tr>
<tr>
<td>( \text{OH}^+ )</td>
<td>1033.1186</td>
<td>0.0</td>
<td>49.58</td>
<td>1.8 \times 10^{-2}</td>
<td>4</td>
<td>4</td>
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</table>

**Notes.** \( (A)_B \equiv A \times 10^B \).