CHEMICAL SEGREGATION TOWARD MASSIVE HOT CORES: THE AFGL2591 STAR-FORMING REGION

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ABSTRACT

We present high angular resolution observations (0.5′′ × 0.3′′) carried out with the Submillimeter Array (SMA) toward the AFGL2591 high-mass star-forming region. Our SMA images reveal a clear chemical segregation within the AFGL2591 VLA 3 hot core, where different molecular species (Types I, II, and III) appear distributed in three concentric shells. This is the first time that such a chemical segregation is ever reported at linear scales ≤3000 AU within a hot core. While Type I species (H₂S and ¹³CS) peak at the AFGL2591 VLA 3 protostar, Type II molecules (HC₃N, OCS, SO, and SO₂) show a double-peaked structure circumventing the continuum peak. Type III species, represented by CH₃OH, form a ring-like structure surrounding the continuum emission. The excitation temperatures of SO₂, HC₃N, and CH₃OH (185 ± 11 K, 150 ± 20 K, and 124 ± 12 K, respectively) show a temperature gradient within the AFGL2591 VLA 3 envelope, consistent with previous observations and modeling of the source. By combining the H₂S, SO₂, and CH₃OH images, representative of the three concentric shells, we find that the global kinematics of the molecular gas follow Keplerian-like rotation around a 40 Mₜₙ star. The chemical segregation observed toward AFGL2591 VLA 3 is explained by the combination of molecular UV photodissociation and a high-temperature (∼1000 K) gas-phase chemistry within the low extinction innermost region in the AFGL2591 VLA 3 hot core.

Key words: ISM: individual objects (AFGL2591) – ISM: molecules – stars: formation

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1. INTRODUCTION

Hot cores are hot (∼200 K), compact (≤0.1 pc), and dense (≥10⁶ cm⁻³) condensations, which represent one of the earliest stages of massive star formation (e.g., Garay & Lizano 1999). These objects are chemically very rich and show large enhancements of S-bearing species such as H₂S, OCS, or SO₂, and of complex organic molecules (COMs) such as H₂CO, CH₃OH, or CH₃CN (Blake et al. 1987; Comito et al. 2005; Hatchell et al. 1998b). These enhancements are attributed to the thermal evaporation of the mantles of dust grains, followed by rapid photodissociation of the grain mantles and of the molecular gas within these cores. As a consequence, a chemical segregation is expected to occur by the central protostar generates a temperature gradient as a function of radius that largely affects the chemical composition of the grain mantles and of the molecular gas within these cores. The chemical segregation at the inner regions of hot molecular cores still remains to be reported.

The AFGL2591 high-mass star-forming region is located at a distance of ∼3 kpc toward the direction of the Cygnus X complex. This distance, which was substantially underestimated in the past, has been derived recently by using trigonometric parallax of the 22.2 GHz H₂O masers detected toward this region (Rygl et al. 2012). The revised mass of the large-scale AFGL2591 clump is 2 × 10⁴ Mₜₙ, and the measured total IR luminosity is ∼2 × 10² Lₜₙ (Sanna et al. 2012). AFGL2591 hosts a cluster of young stellar objects (YSOs) over scales of 0.1 pc (Campbell 1984; Trinidad et al. 2003; van der Tak & Menten 2005), where several radio continuum sources are detected (see VLA 1, VLA 2, and VLA 3 in Trinidad et al. 2003). Sanna et al. (2012) have recently reported the detection of another YSO (the NE source) at ∼0.4 (1300 AU) north the AFGL2591 VLA 3 object. From all the YSOs detected in the AFGL2591 star-forming region, AFGL2591 VLA 3 is believed to be the youngest (dynamical age of ∼2 × 10⁴ yr; Doty et al. 2002; Stauber et al. 2005) and most massive source in the cluster (estimated mass of ∼38 Mₜₙ; Sanna et al. 2012). AFGL2591 VLA 3 is very bright in the mid-IR (de Wit et al. 2009) and is responsible for most of the IR luminosity measured toward this region (Sanna et al. 2012). AFGL2591 VLA 3 is also known to power a large-scale east–west outflow detected in CO and near-IR emission (P.A. ∼28°; Mitchell et al. 1992; Preibisch et al. 2003), whose axis lies close to the direction of the line of sight (Hasegawa & Mitchell 1995; van der Tak et al. 1999). The blueshifted lobe of the outflow is detected toward the west of AFGL2591 VLA 3, while the redshifted outflowing gas is found toward the east (Mitchell et al. 1992). The AFGL2591 VLA 3 molecular envelope is seen almost pole-on and rotates in the counterclockwise direction (van der Tak et al. 2006). Van der Tak et al. (1999) have proposed that the AFGL2591 VLA 3 molecular envelope has two different physical regimes with an inner and hotter core and an outer and cooler envelope. This makes the AFGL2591 VLA 3 hot core an excellent candidate to probe for chemical segregation.

In this paper, we report the first detection of a clear chemical segregation at linear scales ≤3000 AU within the hot
core around the AFGL2591 VLA 3 high-mass protostar. The comparison of the Submillimeter Array (SMA) images with gas-grain chemical models shows that the observed chemical segregation is due to (1) a strong UV radiation field leading to molecular photodissociation and (2) a high-temperature gas-phase chemistry within the low-extinction innermost region in this core. The paper is organized as follows. The SMA observations are reported in Section 2. The images of the continuum and molecular line emission toward AFGL2591 VLA 3 are presented in Section 3. The derived excitation temperatures, column densities, and abundances of the molecular species measured toward this source are given in Section 4. The modeling of the chemical segregation detected toward this object is presented in Section 5. In Section 6, we summarize our conclusions.

2. OBSERVATIONS

Observations of the AFGL2591 star-forming region were carried out with the SMA\(^5\) in the very extended configuration (VEX) on 2010 February 15. The size of the synthesized beam of our VEX observations was 0′″55 × 0′″34 (see Figure 1 for the UV coverage and dirty beam of the VEX data). The phase center of the observations was set at α(J2000) = 20h29m24s90, δ(J2000) = +40°11′20″3. The zenith opacity at 225 GHz was 0.06 and the double sideband system temperatures were typically 200–280 K. The receivers were tuned to an LO frequency of 218.75 GHz and the correlator provided a uniform spectral resolution of 0.8 MHz (i.e., ~1.1 km s\(^{-1}\)). The radial velocity of the source was set at −5.5 km s\(^{-1}\) (van der Tak et al. 1999). We used 3C273 (12.5 Jy) as bandpass calibrator, and MWC349A (1.7 Jy) as flux and gain calibrator. Calibration of the raw data was carried out within the IDL MIRIAD software package, and continuum subtraction, imaging, and deconvolution was done within MIRIAD.

In order to quantitatively measure the effect of missing flux in our VEX data (see Section 3.4), we have also used unpublished data obtained by us with the SMA in Subcompact configuration (beam of 6′7 × 5′6). The central coordinates and spectral resolution of the SMA Subcompact images are the same as those of the VEX observations. However, the frequency coverage was slightly different from that of the VEX data, and the H\(_2\)S (2\(_2,0 → 21,1\)) line was not observed. A detailed analysis of the large-scale structure of the continuum and molecular line emission toward AFGL2591 VLA 3 will be presented elsewhere (I. Jiménez-Serra et al. 2012, in preparation). In the present paper, we only use the Subcompact data to demonstrate that the chemical segregation detected toward this source is not an effect of missing short spacings in the VEX observations.

3. RESULTS

3.1. Dust Continuum Emission and \(^{12}\)CO Outflowing Gas

In Figure 2, we show the \(^{12}\)CO images for the redshifted and blueshifted gas detected toward AFGL2591 VLA 3 (red and blue contours, respectively), superimposed on the 1.3 mm dust continuum emission (gray scale and black contours). The continuum emission (size of ~0′′6 × 0′′45) is associated with the brightest mid-IR source in the region (de Wit et al. 2009) and peaks at α(J2000) = 20h29m24s889, δ(J2000) = +40°11′19″51.

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kinematics of the VLA 3 molecular envelope, although the angular resolution of our observations may not be sufficient to resolve any molecular feature arising from the NE source.

From Figure 2, we find that the $^{12}$CO emission forms a bi-conical structure aligned in the east–west direction and centered at the 1.3 mm VLA 3 source. The kinematics of this structure are consistent with those of the large-scale $^{13}$CO outflow (blueshifted gas toward the west and redshifted emission toward the east; see Mitchell et al. 1992). In addition, the $^{12}$CO blue lobe detected in our VEX images matches the morphology of the bright near-IR loop detected in the K band (Preibisch et al. 2003). The opening angle of the bi-conical structure detected with the SMA is ~90°–100°, similar to that measured from H$_2$O masers (110°; Sanna et al. 2012) or from near-IR emission (>100°; Preibisch et al. 2003).

### 3.2. Differences in the Morphology of the Molecular Line Emission Toward AFGL2591 VLA 3

In Table 1, we report the molecular rotational lines measured within the 8 GHz passband of the SMA, and Figure 3 presents the integrated intensity maps for some of these lines superimposed on the 1.3 mm continuum image of the AFGL2591 VLA 3 source. From Figure 3, we find that the observed molecular species show different spatial distributions in a clear chemical segregation. According to the observed morphology, we classify these molecules into Type I, II, and III species (see Figure 3).

While Type I species (H$_2$S) have a compact structure peaking at the AFGL2591 VLA 3 continuum emission (left panels), Type II molecules (HC$_3$N, OCS, and SO$_2$) show a double-peaked morphology that circumvents the continuum peak (middle panels). For Type III species (represented by CH$_3$OH; right panels), the emission is distributed in a ring-like structure surrounding the continuum core.

### Table 1

| Molecule | Transition | Frequency (MHz) | $E_u$ (K) |
|----------|------------|----------------|-----------|
| H$_2$S   | $2_2 \rightarrow 2_1$ | 216710.44 | 84        |
| $^{13}$CS | $5_5 \rightarrow 4_4$ | 231220.99 | 33        |
| SO       | $5_6 \rightarrow 4_5$ | 191949.44 | 35        |
| OCS      | $18 \rightarrow 17$ | 218903.36 | 100       |
| SO$_2$   | $227.15 \rightarrow 226.18$ | 219275.98 | 353       |
| CH$_3$OH | $v_f = 5_4, 4_1 \rightarrow 4_2, 2_2, 2_1$ | 216945.52 | 56        |
| SO$_2$.  | $v_f = 1_6, 1_5 \rightarrow 1_4, 1_3, 1_2$ | 217299.20 | 374       |
| SO$_2$.  | $v_f = 1_3, 1_2 \rightarrow 1_1, 1_0$ | 219655.55 | 994       |
| SO$_2$.  | $v_f = 4_3, 3_2 \rightarrow 3_1, 3_0$ | 220165.26 | 893       |
| SO$_2$.  | $v_f = 7_4, 6_3 \rightarrow 6_2, 6_1$ | 229347.63 | 122       |
| SO$_2$.  | $v_f = 10_7, 9_6 \rightarrow 9_5, 9_4$ | 229854.30 | 838       |
| SO$_2$.  | $v_f = 13_10, 12_9 \rightarrow 12_8, 12_7$ | 230965.25 | 892       |
| SO$_2$.  | $v_f = 16_13, 15_12 \rightarrow 15_11, 15_10$ | 231980.53 | 865       |
| SO$_2$.  | $v_f = 19_16, 18_15 \rightarrow 18_14, 18_13$ | 235311.61 | 165       |
| SO$_2$.  | $v_f = 22_20, 21_19 \rightarrow 21_18, 21_17$ | 238940.65 | 179       |
| SO$_2$.  | $v_f = 25_17, 24_16 \rightarrow 24_15, 24_14$ | 242124.58 | 192       |

Two species, namely, $^{13}$CS and SO, have been tentatively classified as Type I and Type II species, respectively. For $^{13}$CS, although the brightest emission is detected toward the continuum peak, this molecule also presents a secondary peak toward the southwest of AFGL2591 VLA 3. This peak does not coincide with any of the sources detected in the region or with the molecular emission peaks from Type II or III species. The secondary peak could be associated with outflowing gas. However, its kinematics (at redshifted velocities) are not consistent with those of the outflow toward this position. As shown in Section 5, CS is also expected to be relatively abundant toward the regions where Type II species are detected, suggesting that the CS emission could be more extended than detected with the rarer $^{13}$CS isotopologue.

For SO, the double-peaked morphology in the SO integrated intensity map of Figure 3 is not as clearly seen as for HC$_3$N, OCS, or SO$_2$. However, a closer inspection of the position–velocity (PV) diagram of the SO emission reveals a similar kinematic structure to that of, e.g., SO$_2$ (see Figure 5 and below). Nevertheless, we cannot rule out the possibility that the emission from the low-excitation SO ($5_6 \rightarrow 4_5$) transition is affected by large optical depth effects and/or it is part of the base of the AFGL2591 VLA 3 outflow. A significant amount of SO could also be present within the same region where Type I species arise (i.e., H$_2$S and $^{13}$CS), as suggested by the modeling of the chemistry of the AFGL2591 VLA 3 source (Section 5).

We note that the double-peaked structure of Type II species such as SO$_2$ or OCS and the ring-like morphology of CH$_3$OH are not likely produced by excitation or optical depth effects since higher-excitation, optically thin transitions such as SO$_2$...
Beams are shown at the lower right corner in every panel.

and Section 3.3), suggesting that this emission likely arises from emission across the envelope is considered (see Figures 4 and 5, VLA 3 fit well with Keplerian-like rotation when all molecular gas toward AFGL2591 VLA 3 and the weaker secondary peak detected coincident with the bright 1.3 mm continuum source toward AFGL2591 VLA 3 source.

Therefore, the chemical segregation toward AFGL2591 VLA 3 has been detected (Jiménez-Serra et al. 2012), where the CH$_3$OH high-excitation, optically thin lines peak toward the hot core while the low-excitation, optically thick transitions show a double-peaked morphology across AFGL2591 VLA 3 is also evident from the PV diagrams (Figure 3). T1 and T2 are the brightest emission peaks seen in SO$_2$ and CH$_3$OH, where $T_{\text{ex}}$ has been estimated (Section 3 and Figure 7).

(A color version of this figure is available in the online journal.)

Figure 3. Integrated intensity images of several molecular species from $-8.7$ to $-2.1$ km s$^{-1}$ (thick contours), superimposed on the 1.3 mm continuum map (color scale and dashed contour). Filled star, filled square, and filled circle show, respectively, the location of the VLA 3 source (Trinidad et al. 2003), the NE source (Sanna et al. 2012), and the main 1.3 mm dust continuum peak detected with the SMA (Section 3.1). The molecular species, transition, and energy of the upper level of every transition are shown in every panel. The first contour and step levels are: 0.27 (3 $\sigma$), 0.35 Jy beam$^{-1}$ km s$^{-1}$ for $^{13}$CS (5→4), 0.20 (3 $\sigma$) and 0.35 Jy beam$^{-1}$ km s$^{-1}$ for HC$_3$N $v = 0$ (24→23), 0.21 (3 $\sigma$) and 0.21 Jy beam$^{-1}$ km s$^{-1}$ for OCS (18→17), 0.21 (3 $\sigma$) and 0.28 Jy beam$^{-1}$ km s$^{-1}$ for SO$_2$ (11→10), 0.36 (3 $\sigma$) and 0.60 Jy beam$^{-1}$ km s$^{-1}$ for SO (5→4), 0.21 (3 $\sigma$) and 0.21 Jy beam$^{-1}$ km s$^{-1}$ for CH$_3$OH $v_1 = 0$ (4→2, $v_2 = 3$), 0.18 (2 $\sigma$) and 0.18 Jy beam$^{-1}$ km s$^{-1}$ for CH$_3$OH $v_1 = 0$ (10→9, 1 $\sigma$), 0.15 (2 $\sigma$) and 0.15 Jy beam$^{-1}$ km s$^{-1}$ for CH$_3$OH $v_1 = 1$ (61→72, 0 $\sigma$), and 0.14 (2 $\sigma$) and 0.07 Jy beam$^{-1}$ km s$^{-1}$ for CH$_3$OH $v_1 = 0$ (204→19, 1 $\sigma$). Negative contours correspond to the 3 $\sigma$ level. Dashed lines show the direction of the PV cuts reported in Figure 5. T1 and T2 are the brightest emission peaks seen in SO$_2$ and CH$_3$OH, where $T_{\text{ex}}$ has been estimated (Section 3 and Figure 7)
within the envelope. As shown in Figure 5, H$_2$S (Type I) traces the regions closer to the VLA 3 protostar and is detected across a larger velocity range (from $-12$ km s$^{-1}$ to 0 km s$^{-1}$) than SO$_2$ (from $-10$ km s$^{-1}$ to $-2$ km s$^{-1}$) or CH$_3$OH (from $-8$ km s$^{-1}$ to $-3$ km s$^{-1}$). In contrast to H$_2$S, SO$_2$ (Type II species) peaks at regions further away (at $\sim0.25$ to $0.35$) from the position of the central source, while CH$_3$OH (Type III) is found at $\sim0.5$ away from VLA 3.

Since every species probes a particular region within the AFGL2591 VLA 3 hot core, the global gas kinematics of the envelope can be obtained by combining the data from Type I, Type II, and Type III species. For this, we have used the molecular line transitions H$_2$S ($2_{2,0} \rightarrow 2_{1,1}$), SO$_2$ ($11_{5,7} \rightarrow 12_{4,8}$), and CH$_3$OH $v_1 = 0$ ($4_{2,2} \rightarrow 3_{1,1}$ E). The combined image is generated by normalizing the individual line datacubes to their measured peak intensities and, after normalization, the individual images are added by considering that each of them accounts for 1/3 of the final image. The combined image is shown in panel (h) of Figure 5. We note that if H$_2$S were not included in the combined image, the final PV diagram would show a central hole in its distribution preventing us to characterize the very inner regions with the most blueshifted and redshifted velocities toward the AFGL2591 VLA 3 hot core.

In Figure 5 (panel (h)), we also compare the combined map with the expected PV diagrams from a rotating envelope that follows a Keplerian law around a central source with a mass of 10 $M_\odot$, 40 $M_\odot$, and 100 $M_\odot$ (see dashed, solid, and dotted lines, respectively). The kinematics of the molecular gas toward the AFGL2591 VLA 3 envelope can be explained by Keplerian-like rotation around a 40 $M_\odot$ source. The derived envelope size is 5400 AU, and the inclination angle is $i = 20^\circ$. This angle is consistent with that proposed by van der Tak et al. (1999) and van der Wiel et al. (2011) for this source. The derived mass of the central object, 40 $M_\odot$, is consistent with that estimated by Sanna et al. (2012, of $\sim38 M_\odot$), and corresponds to an O6 star on the zero-age main sequence (ZAMS). Previous estimates of the mass of the AFGL2591 VLA 3 source were underestimated due to the closer distance considered (of $\sim1$ kpc; see, e.g., van der Tak et al. 1999; Trinidad et al. 2003).

3.4. UV Coverage and Missing Flux in the VEX Images

The differences in the morphology between Type I, II, and III species toward AFGL2591 cannot be attributed to differences in the UV plane coverage, because all molecular lines were observed simultaneously within the same track (see Figure 1).

Alternatively, one may think that the observed morphological differences are due to missing flux in the VEX observations. In Figure 6, we compare the combined images of the 1.3 mm continuum, SO$_2$ (Type II) and CH$_3$OH emission (Type III species) obtained with the VEX + Subcompact data, with those generated with the VEX data only. From Figure 6, we find that the combined VEX + Subcompact maps provide a very similar spatial distribution to that reported in the VEX images. This demonstrates that the observed differences in the morphology...
of Type I, II, and III species are not produced by missing short spacings, but due to a real chemical segregation within the AFGL2591 VLA 3 hot core. We note that in Figure 6 we do not include the combined image of the H$_2$S($2_{20} → 2_{11}$) transition, because this line was not covered within the Subcompact observations (see Section 2).

4. EXCITATION TEMPERATURE, COLUMN DENSITIES, AND MOLECULAR ABUNDANCES TOWARD AFGL2591

From the integrated intensities of the SO$_2$, CH$_3$OH, and HCN lines measured toward single beams across the AFGL2591 VLA 3 hot core, we can estimate the excitation temperature of the gas across the envelope, $T_{\text{exc}}$, by means of the population diagram method that assumes optically thin emission and LTE (Goldsmith & Langer 1999). We select the Continuum Peak position, and the emission peaks T1 and T2 because they show the brightest molecular emission for Type I, II, and III species, respectively (see Figure 3). In Table 2, we report the observed parameters of the single beam lines measured toward the Continuum Peak for H$_2$S and $^{13}$CS, and toward emission peaks T1 for SO, OCS, HCN, and SO$_2$, and T2 for CH$_3$OH (see Figure 3) and this table for the exact coordinates of these positions. The derived central radial velocities, $v_{\text{LSR}}$, and linewidths, $\Delta v$, typically range from $-5.5$ to $-6.5$ km s$^{-1}$, and from $\sim 2.5$ to $4$ km s$^{-1}$, respectively, although significant discrepancies in $v_{\text{LSR}}$ and $\Delta v$ are found for some of the species within the same type (see, e.g., SO for Type II or the low-excitation lines CH$_3$OH $v_i = 0 (5_{1,4} → 4_{2,2})$ E and CH$_3$OH $v_i = 0 (3_{2,2} → 4_{1,1})$ E for Type III; Table 2). These discrepancies could be due to large optical depths associated with these low-excitation lines ($E_u < 100$ K; see Table 1).

In Figure 7, we show the population diagrams of SO$_2$ and HC$_3$N derived toward position T1, and the population diagram of CH$_3$OH from position T2. The derived $T_{\text{ex}}$ are $185 \pm 11$ K for SO$_2$, $150 \pm 20$ K for HC$_3$N, and $124 \pm 12$ K for CH$_3$OH, suggesting a temperature gradient within the envelope. The derived column densities of SO$_2$, HC$_3$N, and CH$_3$OH are $2 \times 10^{17}$ cm$^{-2}$, $8 \times 10^{15}$ cm$^{-2}$, and $4 \times 10^{17}$ cm$^{-2}$, respectively. In the case of CH$_3$OH, $T_{\text{ex}}$ was derived from lines with $E_u > 300$ K because its lower-excitation transitions are likely optically thick. As shown by Girart et al. (2002), large optical depths indeed lead to the underestimation of the measured column densities of the low-excitation transitions of CH$_3$OH, clearly deviating from the optically thin solution provided by the population diagram method.

For H$_2$S, $^{13}$CS, OCS, and SO, the molecular column densities are estimated from single transitions by considering optically thin emission and LTE conditions. The assumed excitation temperature for all these lines is $T_{\text{ex}} = 185$ K, the excitation temperature found for SO$_2$ toward T1. For $^{13}$CS, we have also considered an isotopic ratio $^{12}$C/$^{13}$C = 60 (Wilson & Rood 1994). The derived column densities are $7 \times 10^{16}$ cm$^{-2}$ for H$_2$S, $4 \times 10^{15}$ cm$^{-2}$ for $^{13}$CS, $2 \times 10^{16}$ cm$^{-2}$ for OCS, and $3 \times 10^{16}$ cm$^{-2}$ for SO.

Since H$_2$S and $^{13}$CS are mainly detected toward the Continuum Peak, it is possible that their excitation temperature is higher than assumed here, as suggested by our modeling of the
Figure 6. Comparison of the combined (VEX + Subcompact) image of the 1.3 mm continuum emission, and of the integrated intensity maps of the SO$_2$ (11$_{5,7}$$\rightarrow$12$_{4,8}$) and CH$_3$OH $v_t=0$ (4$_{4,2}$$\rightarrow$3$_{1,2}$ E) lines, with those obtained by using the VEX data only. The velocity range considered to generate the SO$_2$ and CH$_3$OH images goes from $-8.7$ to $-2.1$ km s$^{-1}$. For the 1.3 mm images (color and thin contours in left panels), the contour levels are 6.0 (4$\sigma$), 7.5, 10.5, 25.5, 40.5, and 55.5 mJy beam$^{-1}$ for the VEX + Subcompact data, and 3.2 (4$\sigma$), 4.0, 5.6, 17.6, 29.6, 41.6, and 53.6 mJy beam$^{-1}$ for the VEX map. The SO$_2$ and CH$_3$OH emission maps (thick contours in central and right panels) appear superimposed on the 1.3 mm continuum images (color scale and dashed contour). For the SO$_2$ and CH$_3$OH line data, the first contour and step levels are, respectively, 0.5 (5$\sigma$) and 0.3 Jy beam$^{-1}$ km s$^{-1}$ for the combined VEX + Subcompact images, and 0.35 (5$\sigma$) and 0.21 Jy beam$^{-1}$ km s$^{-1}$ for the VEX maps. Symbols are as in Figures 3 and 4. Beams are shown at the lower right corner in every panel. (A color version of this figure is available in the online journal.)

Figure 7. Population diagrams for SO$_2$, HCN, and CH$_3$OH derived from the line spectra extracted from positions T1 and T2 toward AFGL2591 VLA 3 (see Table 2). The derived $T_{ex}$ are shown in the upper right corner of every panel. Error bars correspond to 1$\sigma$ uncertainties and vertical arrows indicate upper limits.

Chemical segregation toward AFGL2591 VLA 3 (see Section 5). In case $T_{ex}$ were $\sim$1000 K (as measured by Carr et al. 1995 from ro-vibrational absorption lines of HCN), the column densities derived for H$_2$S and $^{13}$CS would be factors $\sim$5–8 higher than those reported above.

To estimate the molecular abundances across the AFGL2591 VLA 3 envelope, we used the 1.3 mm continuum flux toward the Continuum Peak (68 mJy beam$^{-1}$), toward T1 (19 mJy beam$^{-1}$), and toward T2 (8 mJy beam$^{-1}$), to derive the H$_2$ column densities at these positions. From Equation (2) in Enoch et al. (2006), and by considering dust opacities of 0.01 cm$^2$ g$^{-1}$ (Ossenkopf & Henning 1994), we estimate H$_2$ column densities of $2 \times 10^{24}$ cm$^{-2}$, $4 \times 10^{23}$ cm$^{-2}$, and $3 \times 10^{23}$ cm$^{-2}$ toward the Continuum Peak, T1, and T2, respectively. We have assumed dust temperatures of $\sim$200 K toward the Continuum Peak, of $\sim$200 K toward T1, and of $\sim$120 K toward T2, following the gas excitation temperatures derived from SO$_2$ and CH$_3$OH (see above). However, we note that these H$_2$ column densities are subject to uncertainties since the dust temperature cannot be constrained from our observations. If the temperature of the dust were higher than 200 K toward the Continuum Peak as suggested by the modeling of van der Tak et al. (1999, $\sim$500–800 K for angular scales $\lesssim$0.2), the derived H$_2$ column densities would be decreased to $\sim$(3–5) $\times 10^{23}$ cm$^{-2}$.

The derived molecular abundances are presented in Columns 2 and 4 of Table 3. In this table, we also include the HCN abundances measured toward AFGL2591 and reported by Doty et al. (2002). HCN is detected in absorption in the IR toward this source (Carr et al. 1995); and since absorption is restricted to the direction of the line of sight toward the source, the bulk of the HCN gas is likely associated with the innermost regions of the AFGL2591 VLA 3 envelope. We do not include the abundance from other molecular species reported in Doty et al. (2002), because they are mainly obtained from emission
measurements toward this source, which likely probe gas at all scales throughout the envelope.

From Table 3, we find that the derived abundances decrease with increasing radius from the position of the Continuum peak to positions T1 and T2 by factors of ≳5–10 for H2S and CS, and by two orders of magnitude for HCN. For HC3N, SO2, OCS, and SO, however, their derived abundances are factors ≳6 larger toward position T1 than toward the Continuum Peak. Following a similar trend, the derived abundance of CH3OH is a factor of ≳100 larger toward position T2 than toward the Continuum Peak.

We note that, if the assumed excitation temperature of the gas were ∼800 K toward the continuum peak, the measured molecular abundances toward this position (see Column 2 in Table 3) would be increased by factors of ∼2–40. This implies that the increasing abundance trend measured for Type II species (i.e., HC3N, SO2, OCS, and SO) across AFGL2591 VLA 3 would become non-existent. However, in the case of CH3OH (Type III species), the derived upper limit to its abundance (≪2 × 10⁻⁷) would still be one order of magnitude lower than the CH3OH abundance measured toward position T2 (Table 3); and for Type I species (H2S and CS), their decreasing abundance trend with larger radii would be even stronger than reported in Table 3 (the H2S and CS abundances measured toward the Continuum Peak would be factors of ∼100–500 higher than toward T2).

We finally stress that the scope of this paper is to show the abundance trends found across the AFGL2591 VLA 3 envelope, and not to obtain the global molecular abundances measured toward this object for which observations with lower angular resolution would be required.

5. CHEMICAL MODELING OF THE AFGL2591 HOT CORE

To qualitatively explain the chemical segregation observed toward AFGL2591 VLA 3, we have used the two-phase UCL CHEM gas-grain chemical code (Viti et al. 2004). In Phase I,
this code simulates the free-fall gravitational collapse of a cloud where the mantles of dust grains form via hydrogenation reactions. The initial atomic abundances are solar (Sofia & Meyer 2001). The formation of the initial core occurs from a diffuse medium with H$_2$ densities of $\sim$100 cm$^{-3}$ at a kinetic temperature of 20 K. The core collapse is stopped when the final density is reached in the model, and it corresponds to timescales of $\sim$5 $\times$ 10$^6$ yr. In Phase 2, we calculate the time-dependent evolution of the chemistry of gas and dust once stellar activity is present. In our case, we assume that the mantles are instantaneously evaporated after the turning on of the protostar. We also assume that H$_2$S is the main reservoir of atomic sulfur on dust grains.

The detection of ro-vibrational absorption of HCN toward AFGL2591 VLA 3 (Carr et al. 1995; Lahuis & van Dishoeck 1997) suggests the presence of an inner and hotter core with relatively low extinction ($A_v < 30^m$), embedded within a more extended and cooler envelope (van der Tak et al. 1999). The AFGL2591 VLA 3 hot core has therefore been modeled, taking into account these two physical regimes (regions A and B; Table 4). Region A corresponds to the inner core where the emission from H$_2$S and $^{13}$CS peaks (i.e., toward the Continuum Peak with angular scales of $\sim$0.2" or $r = 600$ AU at a distance of 3 kpc). Region B corresponds to an intermediate position between T1 and T2 in our observations where HCN, NCS, SO$_2$, SO, and CH$_3$OH show their maximum emission (i.e., at $\sim$0.1", or $r = 11000$ AU, from the central source in our images; see Figure 3). Therefore, for simplicity, our two-region model does not discriminate between positions T1 and T2 within the AFGL2591 VLA 3 envelope. We also consider the existence of an inner cavity within the AFGL2591 VLA 3 hot core, as proposed by Preibisch et al. (2003) and de Wit et al. (2009). These authors derived a radius of 40 AU for this cavity assuming a distance of $\sim$1 kpc for the AFGL2591 VLA 3 source (van der Tak et al. 1999). Since the actual distance to this source is 3 kpc (Rygl et al. 2012), the radius of the cavity considered in our model is 120 AU, i.e., a factor of three larger than that derived by Preibisch et al. (2003) or de Wit et al. (2009). This cavity remains unresolved in our VEX images. The wall of the cavity at $r = 120$ AU is the position at which the visual extinction in our model is $A_v = 0$.

The H$_2$ densities at the end of Phase I for regions A and B are estimated by using the H$_2$ density distribution calculated by van der Tak et al. (2000a), after correcting it from the distance of 3 kpc (see discussion in Section 4.2 of van der Tak et al. 1999 on how the H$_2$ density distribution for AFGL2591 VLA 3 is affected by a larger distance to the source). The averaged H$_2$ densities for regions A and B are, respectively, 4.6 $\times$ 10$^6$ cm$^{-3}$ and 1.8 $\times$ 10$^6$ cm$^{-3}$. These densities are kept constant in Phase II of our model.

In order to compare the H$_2$ column densities expected from these H$_2$ density values with those measured toward the Continuum Peak and positions T1/T2, one needs to consider the total H$_2$ column density across the AFGL2591 VLA 3 envelope. For instance, to compare the results from region A with those observed toward the Continuum Peak, the contribution from the inner core ($\sim$5 $\times$ 10$^6$ cm$^{-3}$ $\times$ 960 AU, i.e., 2 $\times$ 480 AU, the shell size for region A; see below) must be added to that from the outer envelope [$\sim$2 $\times$ 10$^6$ cm$^{-3}$ $\times$ (5400–960) AU], where 5400 AU is the envelope size derived in Section 3.3. This gives a total H$_2$ column density of $\sim$2 $\times$ 10$^{23}$ cm$^{-2}$. For region B (or positions T1/T2), the total H$_2$ column density can be estimated simply by doing $\sim$2 $\times$ 10$^6$ cm$^{-3}$ $\times$ 5400 AU, which gives $\sim$1 $\times$ 10$^{23}$ cm$^{-2}$. For region B, the expected and observed H$_2$ column densities are within a factor of 4. However, for region A (or the Continuum Peak), the low value of the expected H$_2$ column density (2 $\times$ 10$^{23}$ cm$^{-2}$ versus 2 $\times$ 10$^{24}$ cm$^{-2}$; see Section 4) suggests that the actual temperature of the dust toward the Continuum Peak is likely higher than 200 K (Section 4).

The gas and dust temperatures assumed for regions A and B are obtained from the theoretical modeling of the core by Stäuber et al. (2004) for region A ($\sim$1000 K) and by van der Tak et al. (1999) for region B ($\sim$200 K). We stress that the dust and gas temperature profiles do not need to be corrected by the distance of 3 kpc because they are constant in terms of projected distance (i.e., in arcseconds; see Section 4.2 of van der Tak et al. 1999).

To derive the FUV luminosity emitted by the AFGL2591 VLA 3 source, we have used the FUV luminosity profile derived by Bruderer et al. (2009a) as a function of effective temperature, $T_{\text{eff}}$ (see Figure A.1 in their work). For an O6-type star on the ZAMS with an effective temperature of $T_{\text{eff}} \sim 4 \times 10^4$ K, the luminosity in the FUV band is $\sim 2 \times 10^{33}$ erg s$^{-1}$ per $L_{\odot}$. Considering that the AFGL2591 VLA 3 source has a total bolometric luminosity of $L_{\text{bol}} \sim 2 \times 10^5 L_{\odot}$ (Sanna et al. 2012), we obtain that the total FUV luminosity emitted by this source is $4 \times 10^{38}$ erg s$^{-1}$. This luminosity is a factor of 10 higher than that used by Bruderer et al. (2009a), because the distance assumed

\begin{table}[h]
\centering
\caption{Comparison of the Observed Molecular Abundances with Those Predicted by Our Two-point Model of the AFGL2591 VLA 3 Envelope}
\begin{tabular}{|c|c|c|c|c|}
\hline
Abundances & Observed (Continuum Peak) & Model* (Region A) & Observed (Positions T1/T2) & Model* (Region B) \\
\hline
H$_2$S & $5 \times 10^{-8}$ & $5 \times 10^{-9}$ & $\leq 4 \times 10^{-9}$ & $1 \times 10^{-10}$ \\
CS & $2 \times 10^{-8}$ & $1 \times 10^{-6}$ & $\leq 4 \times 10^{-7}$ & $1 \times 10^{-7}$ \\
HCN & $1 \times 10^{-6}$ & $4 \times 10^{-5}$ & $1 \times 10^{-8}$ & $3 \times 10^{-7}$ \\
HC$_3$N & $7 \times 10^{-9}$ & $4 \times 10^{-11}$ & $2 \times 10^{-8}$ & $3 \times 10^{-8}$ \\
OCS & $9 \times 10^{-10}$ & $1 \times 10^{-11}$ & $6 \times 10^{-8}$ & $2 \times 10^{-9}$ \\
SO$_2$ & $1 \times 10^{-7}$ & $3 \times 10^{-11}$ & $6 \times 10^{-9}$ & $1 \times 10^{-6}$ \\
SO & $1 \times 10^{-8}$ & $2 \times 10^{-9}$ & $6 \times 10^{-9}$ & $1 \times 10^{-8}$ \\
CH$_3$OH & $\leq 2 \times 10^{-8}$ & $1 \times 10^{-13}$ & $2 \times 10^{-6}$ & $5 \times 10^{-8}$ \\
\hline
\end{tabular}
\end{table}

\begin{table}[h]
\centering
\caption{Physical Parameters of the Two-point Chemical Model of the AFGL2591 VLA 3 Envelope}
\begin{tabular}{|c|c|c|}
\hline
Region & Region A & Region B \\
\hline
$\rho$(H$_2$)$^a$ & 600 AU & 1100 AU \\
$T_{\text{kin}}$$^b$ & 4.6 $\times$ 10$^3$ cm$^{-3}$ & 1.8 $\times$ 10$^3$ cm$^{-3}$ \\
$A_v$$^c$ & 1000 K & 200 K \\
\hline
\end{tabular}
\end{table}

Notes.

* Abundances predicted by the model for a dynamical age of $\sim$2 $\times$ 10$^4$ yr (Doty et al. 2002).

* Upper limits derived from the 1$\sigma$ level in the H$_2$S and $^{13}$CS spectra toward position T2.

* Lower limits derived from the population diagram shown in Figure 7 for position T2.

* Consistent with HCN line absorption data (Carr et al. 1995; van der Tak et al. 1999) and with our SO$_2$ data (Section 4).

* See the text for the derivation of $A_v$. 

References.
in their calculations was 1 kpc instead of 3 kpc. Since our model considers a cavity within the AFGL2591 VLA 3 envelope, the FUV photon flux illuminating the wall of this cavity (at 120 AU) is \( \sim 6 \times 10^6 \) hab (1 hab = 1.6 \times 10^{-3} \text{ erg s}^{-1} \text{ cm}^{-2} \); Habing 1968), as derived from geometrical dilution. We thus assume an incident FUV flux of \( \sim 6 \times 10^6 \) hab at the position with \( A_v = 0 \) in our model.

At \( r > 120 \) AU, the extinction is calculated as \( A_v = [\text{size} \times n(\text{H}_2)]/[1.6 \times 10^{21} \text{ cm}^{-2}] \). For region A (shell thickness size = 600 AU–120 AU = 480 AU), the extinction is \( \sim 20^m \). For region B, however, the individual extinction from regions A and B should be added since the FUV field from the AFGL2591 star will be attenuated as it propagates outward through the envelope. The individual extinction at \( r = 1100 \) AU (shell thickness size \( \sim 1100 \) AU–600 AU = 500 AU) is \( \sim 8^m \), leading to a total extinction of \( \sim 28^m \) (20^m+8^m) for region B.

In Figure 8, we present the abundances of H$_2$S, CS, HCN, SO, SO$_2$, H$_2$N, OCS, and CH$_3$OH, predicted for Phase 2 by our two-point model of the AFGL2591 VLA 3 envelope. Our results show that the chemical segregation observed toward this source can be explained by the combination of molecular UV photodissociation and a high-temperature gas-phase chemistry in the inner core of AFGL2591 VLA 3. In region A, H$_2$S and CH$_3$OH are initially destroyed by FUV photons (extincted FUV flux of \( \sim 7.5 \) hab for \( A_v \sim 20^m \)) after the release of the grain mantles into the gas phase (\( t < 100 \) yr). However, the high temperatures of the gas (\( T_{\text{kin}} \approx 10^4 \) K) allow the re-formation of H$_2$S via the endothermic reaction H$_2$ + HS\( \rightarrow \) H$_2$S + H (activation barrier of 8050 K), making H$_2$S abundant in the inner core (\( 5 \times 10^{-9} \) for \( t \approx 2 \times 10^5 \) yr; Figure 8). We note that these high temperatures are strictly required for region A because the H$_2$S abundance would dramatically drop otherwise, in contrast with what is observed. Like H$_2$S, HCN and CS survive the FUV photodissociation thanks to the gas-phase reactions H$_2$ + CN\( \rightarrow \) HCN + H and C$_2$ + S\( \rightarrow \) CS + C. CH$_3$OH is completely destroyed since it cannot be re-formed in the gas phase (e.g., Garrod et al. 2008).

In region B, molecular photodissociation is less severe (extincted FUV flux of only \( \sim 0.003 \) hab for \( A_v \sim 28^m \)); and since the gas temperature is only 200 K, the activation barrier for the endothermic reaction to form H$_2$S cannot be overcome. As a consequence, other S-bearing products such as SO, OCS, and SO$_2$ are enhanced (Figure 8). This explains the detection of H$_2$S only toward the inner core of AFGL2591 and the double-peaked structure observed for SO, SO$_2$, and OCS (Section 3). We note that this S-bearing chemical structure was also predicted by more complex chemical modeling of the AFGL2591 VLA 3 source, which includes UV and X-ray photochemistry (Bruderer et al. 2009b).

In the case of CH$_3$OH and H$_2$N, these molecules are found to survive in region B thanks to the higher extinction. For HCN, the formation of this molecule is less efficient at lower temperatures, explaining the decrease of the HCN abundance (by a factor of \( \geq 100 \)) in region B (Figure 8). This decrease is consistent with that observed toward the AFGL2591 VLA 3 envelope (Table 3; van der Tak et al. 1999; Boonman et al. 2001).

The agreement between the predicted and measured abundances for the rest of the molecular species is within factors \( \sim 2–50 \), except for H$_2$N, OCS, and SO$_2$ for region A where the discrepancies are found to be of several orders of magnitude. This could be due to the simplistic physical structure assumed for the AFGL2591 VLA 3 envelope. Continuous variations of the density and temperature of the gas and dust with increasing radius, as derived by comprehensive radiative transfer and chemical models (see, e.g., van der Tak et al. 1999; Doty et al. 2002; Bruderer et al. 2009b), could significantly change the predicted abundances of these molecules. Indeed, the molecular abundances are very sensitive to the extinction assumed for regions A and B (\( A_v \) in Table 4), which depends on the H$_2$ density distribution of the envelope and the distance to the central protostar. If the assumed extinction is decreased by 1$m$ for regions A and B, the general trend for the molecular abundance is to decrease by factors of \( \geq 100 \) in region B (Figure 8). This decrease is consistent with that observed toward the AFGL2591 envelope (Figure 8). We note that this S-bearing chemical structure was also predicted by more complex chemical modeling of the AFGL2591 VLA 3 source, which includes UV and X-ray photochemistry (Bruderer et al. 2009b).

Alternatively, the large discrepancies in the measured and predicted abundances of H$_2$N, OCS, and SO$_2$ for region A could be due to the fact that the beam size of our VEX observations is larger (0.3 $\times$ 0.5) than the angular scale considered for region A (of only 0.2). The measured abundances for H$_2$N, OCS, and SO$_2$ could therefore have received some contribution from emission outside the inner 0.2 of the envelope, artificially increasing the abundances for these molecules toward this region.

We note that the maximum extinction allowed for region B is 28$^{m}$. If an extinction of \( A_v > 29^m \) is assumed for this region, the abundance of H$_2$S increases to \( \sim 10^{-6} \), which is several orders of magnitude higher than found from our observations.
(the upper limit to the H$_2$S abundance measured toward position T2 is of $\leq 4 \times 10^{-9}$; see Table 3).

Finally, our results do not depend on our selection of H$_2$S as the main carrier of S on the grain mantles. We have run two models with (1) 100% of S locked onto OCS, and (2) 50% of S locked on H$_2$S and 50% just as S. For region A, once OCS is released from the mantles, it is photodissociated, leading to large abundances of S. S subsequently reacts to form HS, which is rapidly converted into H$_2$S. This also applies to the case with 50% S and 50% H$_2$S, where all S is transformed into H$_2$S. For region B, the only difference is found for the 100% OCS model, where OCS is the most abundant molecule after the release of the mantles. OCS is then efficiently converted into SO and SO$_2$, showing a behavior similar to that found for our previous 100% H$_2$S model.

6. CONCLUSIONS

We report the detection of a clear chemical segregation at linear scales $\leq 3000$ AU within the massive hot core around the high-mass protostar AFGL2591 VLA3 with the SMA. The molecular gas is distributed in three concentric shells where: (1) H$_2$S and $^{13}$CS (Type I species) peak at the AFGL2591 VLA3 continuum source; (2) HC$_3$N, OCS, SO$_2$, and SO (Type II species) show a double-peaked morphology circumventing the dust continuum peak; and (3) CH$_3$OH (Type III species) is distributed in a ring-like structure that surrounds the dust continuum emission. The global kinematics of the gas, probed by the different molecules found across the envelope, are consistent with Keplerian-like rotation around a central source of $40 M$_\odot$. This mass is consistent with previous findings (Sanna et al. 2012). In addition, the molecular gas shows a temperature gradient for increasing distance to the central source, as revealed by the higher $T_{\text{ex}}$ derived for SO$_2$ (of 185 ± 11 K) than for CH$_3$OH (of 124 ± 12 K). By comparing our SMA images with gas and dust chemical modeling, we find that the chemical segregation toward the AFGL2591 VLA 3 hot core is explained by the combination of molecular UV photodissociation and a high-temperature gas-phase chemistry within the low extinction innermost region in the AFGL2591 VLA 3 massive hot core.

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