Enhanced cosmic-ray ionization rate is needed to account for the molecular chemistry towards supernova remnant 3C391

A Yebes W band Line Survey towards an Unshocked Molecular Cloud of Supernova Remnant 3C391: Evidence of Cosmic-Ray-Induced Chemistry Tianyu Tu¹, Prathap Rayalacheruvu^{2,3}, Liton Majundar^{2,3}, Yang Chen¹, Ping Zhou¹, Miguel Santander-García⁴

Cosmic-ray chemistry in molecular clouds

Cosmic rays (CRs) accelerated by supernova remnants (SNRs) have a strong influence on the chemistry in molecular clouds (MCs). The ionization process of H₂ by low-energy CR protons:

 $H_2 \rightarrow H_2^+ + e^-$ followed by $H_2^+ + H_2 \rightarrow H_3^+ + H_2$

produces the H₃⁺ ion which starts the formation of poly-atomic molecular

CR ionization rate with analytic method

The abundance ratios $R_{\rm D} = N(\rm DCO^+)/N(\rm HCO^+)$ and $R_{\rm H} = N(\rm HCO^+)/N(\rm CO)$ can be used to estimate the CR ionization rate, ζ :

$$\frac{\zeta}{n_{\rm H}} = \frac{\beta'}{k_{\rm H}} \left(2\beta x_{\rm e} + \delta\right) R_{\rm H} x_{\rm e}, \quad \text{and} \quad x_{\rm e} = \left(\frac{k_{\rm f} x({\rm HD})}{3R_{\rm D}} - \delta\right) \frac{1}{k_{\rm e}}$$

We obtained a lower limit: $\zeta \gtrsim 2.7 \times 10^{-14} \text{ s}^{-1}$, higher than typical values in

species in MCs. Other chemical effects of CRs include the transition of CO \rightarrow $C \rightarrow C^+$, non-thermal desorption, CR-induced UV photons, etc. To study the detailed chemical effects of enhanced CR ionization rate in **MCs**, we conducted a W band (71.5 – 90 GHz) molecular line survey with Yebes 40m radio telescope towards 3C391:NML, an unshocked MC.



Integrated intensity map of the ¹²CO J = 3 – 2 line between +100 and +110 km/s towards the south-western part of SNR 3C391, overlaid with contours of radio continuum. The red cross shows the 1720 MHz OH maser, while the dashed white circle delineates the 3C391:NML region we observed.

MCs by 3 orders of magnitude.

However, we estimated that the timescale of CR-induced non-thermal desorption for CO ice is \sim 3 kyr, which is comparable to the age of 3C391 (4 – 19 kyr). Therefore, the chemistry may be highly dynamic around 3C391, and the analytic method may not give a robust estimation of the CR ionization rate because of the deviation from chemical equilibrium.

Chemical simulation of unusual abundance (ratios)

We discovered two abundance ratios and one abundance different from typical values found in dense MCs:

Abundance (ratios)	Observed	Typical
N(HCO ⁺)/N(HOC ⁺)	~ 160 – 180	~ 10 ³
N(HCS ⁺)/N(CS)	~ 0.14 – 0.18	~ 10 ⁻²
$X(C_3H^+)$	$\sim 2.9 - 6.0 \times 10^{-11}$	~ 10 ⁻¹²

All of these unusual values can be qualitatively attributed to the chemistry induced by enhanced CR ionization rate.

We present a chemical simulation using the DNautilus 2.0 chemical code. The simulation consists of two steps: Step 1: evolution of a MC before SN explosion for $t_1 = 0.1$ and 1 Myr.

Results of the observation

In total, we detected transitions from 18 molecular species (including isotopes). A selection of the target transitions (among which DCO⁺ is not detected) are shown below. All of the detected species show narrow line emission centered at $V_{ISR} \approx 105.4 - 105.6$ km/s.



A selection of the target transitions. The CO lines are obtained from archival data. Spectra with lighter color shows the observed spectra, while the dashed lines show the results of (multi-)Gaussian fitting. For the spectrum of HCO+, the blue lines show the three velocity components.

Step 2: model of the impact of CRs after the SN explosion.

Two combinations of parameters can reproduce the other observed values $(N(HCS^+)/N(CS))$ cannot be explained by any models.): (a) $t_1 = 0.1$ Myr, $n_H \sim 10^4$ cm⁻³, $T \sim 32$ K, and $\zeta \sim 10^{-16}$ s⁻¹, (b) arbitrary t_1 , $n_H \sim 10^4$ cm⁻³, $T \sim 19$ K, and $\zeta \sim 10^{-14}$ s⁻¹. Combination (a) is not valid for $t_1 = 1$ Myr, while (b) fails to reproduce the $N(HCO^{+})/N(HOC^{+})$ unless higher density (~ 10^{5.5} cm⁻³) is adopted, and the temperature for (b) is too low to be compatible with the heating of CR. However, in either case, an enhanced cosmic-ray ionization rate is needed to account for the molecular chemistry towards 3C391:NML.



Estimation of molecular column density

We used the RADEX code to estimate the column densities of CO, CS and $o-c-C_3H_2$, of which multiple transitions are available (the data of CS are taken from reference). For other species, the column densities are estimated based on the assumption of LTE and $T_{ex} = 5$ K or 10 K.

Species	Column density (cm ⁻²)	Density (cm ⁻³)
CO (20 K)	~ 3.7 × 10 ¹⁷	~ 1.4 × 10 ³
<i>о-с-</i> С ₃ Н ₂ (20 К)	$\sim 2.0 \times 10^{12}$	~ 2.4 × 10 ⁵
CS (20 K)	~ 3.9 × 10 ¹²	~ 1.9 × 10 ⁵
CS (40 K)	~ 3.9 × 10 ¹²	~ 1.0 × 10 ⁵

Results of the RADEX analysis.

The adopted temperatures in the analysis are shown in the parentheses in the first column.

Grid map of the chemical simulation results with $t_1 = 1$ Myr (please refer to the original paper for the results with $t_1 = 1$ 0.1 Myr). The colorbars are adjusted to have whiter colors with the simulated values closer to the observed ones. The black contours show 2 \times the maximum observed values and 0.5 \times the minimum observed values as a rough estimate of the uncertainty.

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