Time-dependent chemical modeling of H/H$_2$ and C$^+$/C/CO transitions in the Orion Bar

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The Orion A complex

M43

M42

Trapezium cluster: 560 stars in pc^{-3}

4 massive stars $\theta^1$ Ori C

spec. class O7V

80% of the ionizing photons

The nearest site of massive star formation ($\sim 414 \pm 7$ pc)

Robberto et al., 2013
Principal nebular features of the Orion A

Robberto et al., 2013
Basic model of photodissociation regions

- Photodissociation regions are regions where FUV (6-13.6 eV) photons dominate the energy balance and/or chemistry.

Tielens and Hollenbach, 1985
Success of the steady-state model

Tielens et al., 1993

PAH 3.3 mum
1-0 S(1) H2
CO(1-0)
New ALMA observations of HCO$^+$(4-3)

Goicoechea et al., 2016
Goicoechea et al., 2016

Gap between $\text{H}_2$ and CO peak emission

$\text{H}_2$ and CO diss. fronts are closer to each other ($5''$) compared to the equilibrium model predictions ($10''$)
We make dynamical calculations of the PDR to reproduce:

- the gap ≤ 5''
- CO(3-2) peak ≈ 160 K
- HCO⁺(4-3) integrated intensity ≈ 70 K km s⁻¹

Goicoechea et al., 2016
Dynamical PDR models

Storzer & Hollenbach, 1998, analytical approach:

– C⁺/C/CO transition layer is closer to the dissociation front (DF) of H₂ compared to the equilibrium model

– nonequilibrium effects in the Orion Bar are probably small

Hosokawa & Inutsuka, 2005:

1D numerical model of an expanding HII region
MARION code

- 1D gas dynamics based on the ZEUS-2D code (Stone&Norman, 2002)
- dynamics of charged dust, dust size distribution
- ionization, dissociation, gas phase chemistry + accretion and desorption
- essential heating and cooling processes

Kirsanova et al., 2009
Pavlyuchenkov et al., 2013
Akimkin et al., 2015
Akimkin et al., 2017
MARION code: study of dust and PAHs dynamics in expanding HII regions

Kirsanova et al., 2009
Pavlyuchenkov et al., 2013
Akimkin et al., 2015
Akimkin et al., 2017
Model setup

plane-parallel slab

only gas-phase chemistry

chemical network from the PDR benchmarking workshop (Rollig et al., 2007) + photo-reactions cross-sections from the Leiden photo site (van Dishoeck et al, 2006)

31 species: H, H⁺, H₂, H₂⁺, H₃⁺, O, O⁺, OH⁺, OH, O₂, O₂⁺, H₂O, H₂O⁺, H₃O⁺, C, C⁺, CH, CH⁺, CH₂, CH₂⁺, CH₃, CH₃⁺, CH₄, CH₄⁺, CH₅⁺, CO, CO⁺, HCO⁺, He, He⁺, e⁻

<table>
<thead>
<tr>
<th>Energy intensity of the Draine field ( \chi ) at surface</th>
<th>4\times10^4</th>
</tr>
</thead>
<tbody>
<tr>
<td>( n_{\text{gas}} )</td>
<td>5\times10^4 \text{ cm}^{-3}</td>
</tr>
<tr>
<td>( T_{\text{gas}} )</td>
<td>10K</td>
</tr>
<tr>
<td>Dust model</td>
<td>MRN WD07 ( R_v=3.1 ) WD16 ( R_v=5.5 )</td>
</tr>
<tr>
<td>H₂</td>
<td>0.5</td>
</tr>
<tr>
<td>He</td>
<td>0.1</td>
</tr>
<tr>
<td>CO</td>
<td>3\times10^{-4}</td>
</tr>
<tr>
<td>O₂</td>
<td>5\times10^{-5}</td>
</tr>
</tbody>
</table>
Static model

- RADEX setup: $T_{bg} = 2.7\text{K}$
- linewidth = 2 km s$^{-1}$
- line of sight depth = 0.12 pc
Dynamical model: 3 moments of time

Distance from the beginning of the first cell (arcsec)
Dynamical model – moment 1

MRN
- $t=1000 \text{ years}$
- the gap $\approx 5''$
Dynamical model – moment 2

- MRN
- \( t = 2900 \) years
- the gap \( \approx 2'' \)
Dynamical model – moment 3

- MRN
  - $t=2900$ years
  - the gap $\approx 1''$
WD 07 model with \( R_v = 3.1 \): even brighter \( \text{HCO}^+ (4-3) \) emission

**WD07**
- \( t = 2900 \) years
- the gap \( \approx 4'' \)
WD07 model with $R_v=3.1$: good agreement with observations

- $t=3000$ years
- the gap $\approx 4''$
WD16 model with Rv=5.5: brighter HCO⁺(4-3)

- t=4600 years
- the gap ≈ 5'', but H₂ and CO DF are too far away ≈ 8''
- HCO⁺(4-3) is brighter than with WD07 and MRN dust
WD 16 model with $R_v=5.5$: brighter HCO$^+(4-3)$ and CO(3-2)

WD16

- $t=6300$ years
- the gap $\approx 1''$

HCO$^+(4-3)$ and CO(3-2) are brighter than with WD07 and MRN dust and than in observations
Conclusion

• Using MARION model we reproduce ALMA observations of CO(3-2) and HCO\textsuperscript{+}(4-3) in the Orion Bar:
  – the gap between HCO\textsuperscript{+}(4-3) and CO(3-2) peaks \(\approx 4''\)
  – CO(3-2) peak intensity \(\approx 160 \text{ K}\)
  – HCO\textsuperscript{+}(4-3) integrated intensity \(\approx 70 \text{ K km s}^{-1}\)

• bright HCO\textsuperscript{+}(4-3) appears just beyond the H\textsubscript{2} dissociation front toward the density enhancement.