Time-dependent chemical modeling of H/H₂ and C⁺/C/CO transitions in the Orion Bar

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The Orion A complex

M42

M43

The nearest site of massive star formation $(\sim414 \pm 7 \text{ pc})$

Trapezium cluster: 560 stars in pc⁻³

4 massive stars θ¹ Ori C spec. class O7V 80% of the ionizing photons

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.



Success of the steady-state model



Tielens et al., 1993

New ALMA observations of HCO⁺(4-3)



[SII] 6731 A [OI] 6300 A 1" resolution HCO⁺ (4-3)

Goicoechea et al., 2016

Gap between H₂ and CO peak emission



H₂ and CO diss. fronts are closer to each other (5") compared to the equilibrium model predictions (10")

Goicoechea et al., 2016



We make dynamical calculations of the PDR to reproduce:

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



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	energy inte of the Drai field x at si
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)	n _{gas} T _{gas} dust mode
31 species: H, H ⁺ , H ₂ , H ₂ ⁺ , H ₃ ⁺ , O, O ⁺ , OH ⁺ , OH, O ₂ , O ₂ ⁺ , H ₂ O, H ₂ O ⁺ , H ₃ O ⁺ , C, C ⁺ , CH, CH ⁺ , CH ₂ , CH ₂ ⁺ , CH ₃ , CH ₃ ⁺ , CH ₄ , CH ₄ ⁺ , CH ₅ ⁺ , CO, CO ⁺ , HCO ⁺ , He, He ⁺ , e ⁻	H ₂ He CO
,	

energy intensity of the Draine field χ at surface	4×10 ⁴
n _{gas}	5×10 ⁴ cm ⁻³
T _{gas}	10K
dust model	MRN WD07 R _v =3.1 WD16 R _v =5.5
H ₂	0.5
Не	0.1
СО	3×10 ⁻⁴
O ₂	5×10 ⁻⁵

Static model

C⁺/C/CO

- RADEX setup: $T_{bg} = 2.7K$
- 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



Dynamical model – moment 2



Dynamical model – moment 3



WD 07 model with Rv=3.1: even brighter HCO⁺(4-3) emission



WD07 model with Rv=3.1: good agreement with observations



WD16 model with Rv=5.5: brighter HCO⁺(4-3)



WD 16 model with Rv=5.5: brighter HCO⁺(4-3) and CO(3-2)



Conclusion

- Using MARION model we reproduce ALMA observations of CO(3-2) and HCO+(4-3) in the Orion Bar:
 - the gap between HCO⁺(4-3) and CO(3-2) peaks \approx 4"
 - CO(3-2) peak intensity \approx 160 K
 - HCO⁺(4-3) integrated intensity \approx 70 K km s⁻¹
- bright HCO⁺(4-3) appears just beyond the H_2 dissociation front toward the density enhancement.