O2 EMISSION TOWARD ORION H2 PEAK 1 AND THE ROLE OF FUV-ILLUMINATED C-SHOCKS

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ABSTRACT

Molecular oxygen (O2) has been the target of ground-based and space-borne searches for decades. Of the thousands of lines of sight surveyed, only those toward Rho Ophiuchus and Orion H2 Peak 1 have yielded detections of any statistical significance. The detection of the O2 Nj = 3–1 and 5–3 lines at 487.249 GHz and 773.840 GHz, respectively, toward Rho Ophiuchus has been attributed to a short-lived peak in the time-dependent, cold-cloud O2 abundance, while the detection of the O2 Nj = 3–1, 5–3 lines, plus the 7–6 5–6 line at 1120.715 GHz, toward Orion has been ascribed to time-dependent preshock physical and chemical evolution and low-velocity (12 km s−1) non-dissociative C-type shocks, both of which are fully shielded from far-ultraviolet (FUV) radiation, plus a postshock region that is exposed to a FUV field. We report a re-interpretation of the Orion O2 detection based on new C-type shock models that fully incorporate the significant effects the presence of even a weak FUV field can have on the preshock gas, shock structure, and postshock chemistry. In particular, we show that a family of solutions exists, depending on the FUV intensity, that reproduces both the observed O2 intensities and O2 line ratios. The solution in closest agreement with the shock parameters inferred for H2 Peak 1 from other gas tracers assumes a 23 km s−1 shock impacting gas with a preshock density of 8 × 104 cm−3 and G0 = 1, substantially different from that inferred for the fully shielded shock case. As pointed out previously, the similarity between the LSR velocity of all three O2 lines (≈11 km s−1) and recently measured H2O5 32 44 lines at 487.249 GHz and 33 34 lines at 620.701 GHz toward H2 Peak 1 suggests that the O2 emission arises behind the same shocks responsible for the maser emission, though the O2 emission is almost certainly more extended than the localized high-density maser spots. Since maser emission arises along lines of sight of low-velocity gradient, indicating shock motion largely perpendicular to our line of sight, we note that this geometry can explain not only the narrow (≤3 km s−1) observed O2 line widths despite their excitation behind a shock but also why such O2 detections are rare.

Key words: astrochemistry – ISM: abundances – ISM: individual objects (Orion)

1. INTRODUCTION

Accounting for the low abundance of molecular oxygen (O2) in dense (n(H2) ≥ 103 cm−3) molecular clouds has long posed a challenge to both observers and theorists. For almost 30 years, the search for O2 was motivated by predictions of gas-phase chemical models that O2 was a major reservoir of elemental oxygen within dense clouds (e.g., Goldsmith & Langer 1978; Neufeld et al. 1995). However, the inability of gas-phase models to account for the observed abundance of an increasing number of species highlighted the shortcomings of such models. This became evident again following the launch of the Submillimeter Wave Astronomy Satellite (SWAS; Melnick et al. 2000) and Odin (Nordh et al. 2003), when their largely unsuccessful searches for O2 established upper limits to the O2 abundance more than 100 times below the predictions of these models (e.g., Goldsmith et al. 2000). Modified chemical models, which include the effects of dust grains as sites for molecule formation as well as freeze-out, were then invoked to explain the low O2 abundance and weak emission (see Bergin et al. 2000; Hollenbach et al. 2009). With the launch of the Herschel Space Observatory (Pilbratt et al. 2010), attention turned to using its greater sensitivity to target regions predicted by these updated chemical models to possess high columns of warm O2.

The Open Time Key Program, Herschel Oxygen Project (HOP), was proposed and selected to carry out a survey of warm molecular clouds in the following rotational transitions of O2: (N, J) = (3, 3) → (1, 2) at 487 GHz, (5, 4) → (3, 4) at 774 GHz, and (7, 6) → (5, 6) at 1121 GHz (see Goldsmith et al. 2011). Among the sources of particular interest was the Orion Molecular Cloud because of the large column densities of warm molecular gas known to exist toward several prominent components, including the Hot Core, the Orion Bar, and H2 Peaks 1 and 2. While no convincing O2 emission was detected toward the Hot Core (Goldsmith et al. 2011) or Orion Bar (Melnick et al. 2012), O2 emission has been detected toward H2 Peak 1 (Goldsmith et al. 2011; Chen et al. 2014). This detection raises two questions: (1) What plausible conditions exist at H2 Peak 1 that could produce the observed O2 line intensities and line ratios? (2) Are these conditions nonetheless sufficiently rare to explain the absence of detectable O2 emission toward most other sources searched?

Intense H2 emission toward Peak 1 is observed in transitions with excitation energies, E/k, ranging from 1015 to 43,000 K, which has long been attributed to collisional excitations due to shock waves presumed to result from the high-velocity outflow originating ∼30″ to the SE in the BN/KL region (Gautier et al. 1976; Beckwith et al. 1978; Rosenthal et al. 2000). The Orion Molecular Cloud is also subject to strong far-ultraviolet (FUV) radiation from sources such as 6γ C Ori (see Kristensen et al. 2003). In this paper, we examine the role FUV radiation plays in altering the chemical and physical conditions in gas capable of reproducing the O2 observations reported in Chen et al. (2014). In particular, we focus on FUV-illuminated gas subject to the passage of non-dissociative C-type shocks as regions especially conducive to the production of elevated O2 abundances.
Fully shielded non-dissociative shocks are generally inefficient at producing \( \text{O}_2 \) in the postshocked gas. Even when shock velocities are sufficient to sputter material from grain surfaces, all but \( \sim 1\% \) of the gas-phase oxygen not locked in CO is rapidly processed into \( \text{H}_2\text{O} \) within the warm (\( T \gtrsim 400 \text{ K} \)) postshock gas via a set of neutral-neutral chemical reactions (\( \text{O} + \text{H}_2 \rightarrow \text{OH} + \text{H}; \text{OH} + \text{H}_2 \rightarrow \text{H}_2\text{O} + \text{H} \)). In the absence of an FUV field, the \( \text{H}_2\text{O} \) abundance is predicted to remain high throughout the postshock region, and the \( \text{O}_2 \) abundance never exceeds a few percent of that of \( \text{H}_2\text{O} \) (see Draine et al. 1983; Kaufman & Neufeld 1996a). However, the presence of an FUV field can significantly increase the postshock \( \text{O}_2 \) abundance by (1) increasing the preshock gas-phase atomic oxygen abundance through both the photodissociation of gas-phase \( \text{O} \)-bearing species and the photodesorption (from grains) and subsequent photodissociation of desorbed \( \text{O} \)-bearing species, leading to a higher postshock \( \text{H}_2\text{O} \) abundance; and (2) increasing the postshock abundance of \( \text{OH} \) and \( \text{O} \) through the photodissociation of postshock \( \text{H}_2\text{O} \), enabling increased production of \( \text{O}_2 \) via the reaction \( \text{O} + \text{OH} \rightarrow \text{O}_2 + \text{H} \).

In Chen et al. (2014), the three components necessary to model the observed \( \text{O}_2 \) emission—i.e., the preshock gas, the shock and its postshock thermal profile, and the postshock chemistry—were addressed separately. In particular, the preshock gas and shock were assumed to be fully shielded, i.e., no FUV radiation reaches these regions, while the postshock chemistry was modeled assuming various levels of FUV illumination. It is unlikely that the preshock, shock, and postshock gas, which are in close physical proximity, would experience significantly different FUV fluxes; however, the absence of a shock code that incorporates the full effects of an FUV field dictated the approach described in Chen et al. In this paper, we re-examine the results presented in Chen et al., with several important differences. The main contribution of the present work is the self-consistent treatment of the preshock, shock, and postshock regions under the influence of FUV fields common to all components. Not only can FUV radiation increase the preshock atomic oxygen abundance, as described above, but the effects of FUV radiation on the structure of C-type shocks can be significant. These effects include increased postshock temperatures at a given shock velocity, reduced velocities at which these shocks break down (and \( \text{H}_2 \) is dissociated), and the altered abundance of key postshock molecular species. We will show that (1) the thermal and chemical changes induced by the FUV radiation on the preshock, shock, and postshock gas, and including the sputtering of \( \text{H}_2\text{O} \) from grain mantles at shock velocities greater than \( \sim 20 \text{ km s}^{-1} \), yield multiple combinations of shock velocity and FUV field intensity capable of producing detectable \( \text{O}_2 \) emission; and (2) the \( \text{O}_2 \) line intensity ratios can be an important discriminator between shock models. The observed \( \text{O}_2 \) line ratios were not used as a test of the shock models presented in Chen et al.

In addition, the inclusion of an FUV field in all gas components mitigates a problem identified in Chen et al., i.e., the need in their model to assume \( \geq 10\% \) sputtering efficiency of \( \text{H}_2\text{O} \) from grain mantles behind a 12 km s\(^{-1}\) C-type shock. As will be discussed, a sputtering efficiency of 10% or greater behind a 12 km s\(^{-1}\) shock is higher than theoretical predictions, as well as recent observations.

Finally, the association between co-located \( \text{H}_2\text{O} \) maser emission and the \( \text{O}_2 \) emission noted in Chen et al. provides important clues regarding the orientation of the \( \text{H}_2\text{O} \)- and likely \( \text{O}_2 \)-producing shocks. We point out that this orientation not only justifies the assumption of relatively large column densities of \( \text{O}_2 \) along the line of sight, as discussed in Chen et al., but also provides an alternate explanation to that offered in Chen et al. for why such \( \text{O}_2 \) detections are rare.

In Section 2, we briefly review the \( \text{O}_2 \) observations upon which our analysis is based. In Section 3, we describe the modifications to the C-type shock models required when such shocks are exposed to FUV radiation. In Section 4, we describe the assumed shock geometry, the methods used to compute the \( \text{O}_2 \) line integrated intensities, and how well the results fit the observations. In Section 5, we discuss the ways in which FUV-illuminated C-type shocks and the shock geometry toward Orion \( \text{H}_2 \) Peak 1 combine to provide an explanation for the detected \( \text{O}_2 \) emission, while also accounting for the apparent rarity of such emission.

2. OBSERVATIONS AND RESULTS

The Herschel observational results considered in this paper are presented in Chen et al. (2014). The interested reader is referred to Chen et al. for details regarding the observations and data reduction; only the results we model are summarized here.

The observations were conducted in 2012 using the Heterodyne Instrument for the Far Infrared (HIFI; de Graauw et al. 2010) and were centered at J2000 coordinates R.A. = \( 5^\circ 35^\prime 14^\prime\prime 2 \) and decl. = \( -5^\circ 22^\prime 31^\prime\prime \). HIFI was used in dual-beam switch mode with the reference positions located \( 3^\prime \) on either side of the source. For each transition, eight local oscillator (LO) settings were used to allow sideband deconvolution. The integration time for each LO setting was 824 s for the 487 and 774 GHz spectra and 3477 s for the 1121 GHz spectrum. The observational results relevant to our modeling effort are presented in Table 1.

3. MODIFIED SHOCK MODELS

3.1. FUV-illuminated C-type Shocks

Within interstellar shocks possessing low fractional ionization and a strong magnetic field, the flow variables may remain continuous, i.e., the neutral and ionized gases do not experience discontinuities and the gas remains relatively cool and molecular. The physics of C-type shocks in well-shielded gas has been studied extensively (e.g., Draine 1983; Draine et al. 1983; Kaufman & Neufeld 1996b; Flower & Pineau des Forêts 2010); however, it is increasingly evident that FUV radiation from nearby stars plays a role in the physics of molecular outflows (e.g.., Kristensen et al. 2012; van Kempen et al. 2010). In order to assess the role of FUV radiation, we have made several modifications to the Kaufman & Neufeld (1996b) model. These modifications affect the abundances of important species in the preshock gas, the shock length scale, and the abundances of oxygen-bearing species in the postshock gas. We briefly describe the effects below; a more detailed description will be included in a forthcoming paper.

3.2. Preshock Conditions

To determine the conditions in the preshock molecular gas, we use the detailed photodissociation region (PDR) model of Hollenbach et al. (2009). This model computes the abundances

\( \text{O}_2 \) abundances...
of numerous atomic and molecular species, as well as those of charged and neutral dust grains and polycyclic aromatic hydrocarbons, as a function of extinction into a cloud, given the input parameters of gas density, $n$, and FUV radiation field strength, $G_0$ (scaling factor in multiples of the average Habing local interstellar radiation field; Habing 1968). In order to model a shock propagating through such gas, the important outputs of the PDR model are (i) the types and abundances of charge carriers, which determine how well the ionized species couple to the magnetic field and (ii) the abundances of gas-phase species, especially oxygen- and carbon-bearing species that become incorporated into important gas coolants. It is the interplay between momentum transfer (moderated by the coupling length) and the efficiency of gas cooling (which limits the gas temperature) that determines the final shock structure. As shown by Hollenbach et al. (2009), significant fractions of oxygen and carbon nuclei can be locked up on the surfaces of dust grains in molecular gas exposed to moderate FUV fields at extinctions $A_V \sim 1$. Based on the same PDR model described in detail in Hollenbach et al. (2009), Figure 1 shows the preshock gas-phase abundances of $H_2O$ and atomic O as functions of density and $G_0$. To first order, the length scale depends only on the ionization fraction and the strength of the magnetic field. In gas fully shielded from FUV radiation, the fractional ionization is set by the cosmic-ray ionization rate and is low, resulting in a relatively long ion–neutral coupling length scale and C-shocks that can be supported up to velocities of $\sim 40$ km s$^{-1}$. In unshielded gas, the fractional ionization reaches its maximum value of $\sim 10^{-4}$, set by the carbon abundance, and results in the shortest possible length scale. In gas at $A_V = 1$, the length scale is between these two extremes and depends sensitively on the gas density and grain properties. An important point arising from these calculations is that, because the length scale is shorter than in fully shielded gas, the maximum C-shock velocity is generally less than 40 km s$^{-1}$.

### 3.3. Postshock Chemistry

Within the shock, the abundances of gas-phase O-bearing species are set by competition between neutral-neutral reactions, which tend to drive O nuclei into $O_2$, OH, and $H_2O$, and photodissociation, which destroys these molecules. Studies of C-type shocks in fully shielded gas show that O nuclei are efficiently driven into $H_2O$ once the gas temperature exceeds $\sim 400$ K, at shock velocities $\geq 10$–15 km s$^{-1}$; in the absence of photodissociation, the $H_2O$ abundance remains high in the postshock gas. The presence of FUV radiation has two effects. First, it shortens the length scale and thus lowers the shock velocity at which the gas reaches 400 K. Second, it destroys molecules in the cooling postshock gas; to account for this, we have added photodissociation reactions to the shock chemical scheme, including dissociation of $H_2O$, OH, and $O_2$. Under these conditions, the gas has higher abundances of O and OH than without photodissociation. The O and OH are driven into molecular oxygen by the reaction $O + OH \rightarrow O_2 + H$, which has a reaction rate that is within a factor of two of $3 \times 10^{-11}$ cm$^3$ s$^{-1}$ over the range 10–500 K (McElroy et al. 2013). This is in contrast with the neutral-neutral reactions that drive O into OH and $H_2O$, each of which has barriers of $>1000$ K. We find that the postshock $O_2$ abundance is directly correlated with the postshock gas-phase O-nuclei abundance; more O nuclei in the preshock gas lead to more $H_2O$ in the warm gas, followed by more $O_2$ in the cooler gas.

In addition to increases in the postshock gas-phase O-nuclei abundance caused by FUV radiation, $H_2O$ can be removed from ice mantles by the shocks themselves. Ice mantles on grains are sputtered by ion–neutral collisions in shocked regions where there is substantial relative velocity between

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**Table 1**

Summary of $O_2$ Observations toward Orion $H_2$ Peak 1

| Rest Frequency (GHz) | Transition ($N, J \rightarrow N', J'$) | Energy above Ground State ($E_{i/k}$) (K) | Integrated$^a$ Intensity (K km s$^{-1}$) | Line$^a$ Width (km s$^{-1}$) | LSR Velocity (km s$^{-1}$) | HIFI Beam$^a$ Diameter (arcseconds) |
|---------------------|--------------------------------------|-------------------------------------------|--------------------------------------|----------------------------|----------------------------|-----------------------------------|
| 487.249             | 3, 3–1, 2                            | 26 K                                      | 0.081                                | 3.1                       | 10.2                      | 44.7                              |
| 773.840             | 5, 4–3, 4                            | 61 K                                      | 0.154                                | 1.7                       | 11.0                      | 28.2                              |
| 1120.715            | 7, 6–5, 6                            | 115 K                                     | 0.043                                | 0.8                       | 11.0                      | 18.9                              |

*Note.*

$^a$ Chen et al. (2014).

$^b$ See Roelfsema et al. (2012).
charged grains and neutral molecules. We follow the treatment of Flower & Pineau des Forêts (1994) for the removal of oxygen and water-ice mantles, but with a threshold energy for ice removal consistent with that found by Neufeld et al. (2014), i.e., complete grain mantle removal for shocks with \( v_\perp > 25 \text{ km s}^{-1} \). Note that these results are similar to those found by both Draine et al. (1983) and Jiménez-Serra et al. (2008), who find that \( \sim 10\% \) of mantles are removed in 20 km s\(^{-1}\) shocks. At velocities less than \( \sim 20 \text{ km s}^{-1} \), sputtering of grain mantles is not expected to be efficient, so the gas-phase abundances of O and C nuclei should be unchanged by the passage of the shock.

Because the O\(_2\) itself is subject to photodissociation, the O\(_2\) abundance, \( N(\text{O}_2)/N(\text{H}_2) = \chi(\text{O}_2) \), does not reach the abundance of O nuclei in the gas. An example may be seen Figure 2, in which models with \( G_0 = 0.1, 1, \) and 10 are compared. Note that the peak O\(_2\) abundance is higher in the \( G_0 = 10 \) case since the higher \( G_0 \) keeps more O in the gas phase. Moreover, the higher postshock gas temperatures when \( G_0 \) is high allow the neutral-neutral reactions to more than compensate for the photodestruction of H\(_2\)O while \( T \gtrsim 300 \text{ K} \), keeping the H\(_2\)O abundance high; however, when \( T \) drops below \( \sim 300 \text{ K} \), the H\(_2\)O photodestruction rate exceeds its formation rate and the H\(_2\)O abundance quickly drops, as shown in Figure 2.

The conditions necessary to provide a significant O\(_2\) column are (i) a large fraction of O nuclei in the preshock gas; (ii) sufficient FUV radiation to dissociate the shock-produced H\(_2\)O, but not so much that no significant O\(_2\) survives in the postshock gas; and (iii) an FUV flux that remains below the threshold at which the length scale will no longer support C-shocks.

4. MODELING APPROACH

4.1. Shock Geometry

Chen et al. (2014) have identified Orion H\(_2\) Peal 1 as the most likely source of the reported O\(_2\) emission. Peak 1 is the site where the high-velocity gas from the dynamical center of the outflow, about 30'' to the southeast in the vicinity of the BN/KL region, impacts the surrounding cloud, creating strong BN/KL region, impacts the surrounding cloud, creating strong

4.2. Shock Models and O\(_2\) Emission

A series of shock models were generated for preshock densities ranging between \( 10^3 \) and \( 10^8 \text{ cm}^{-3} \) in steps of 0.1 dex and incident FUV fluxes, \( G_0 \), of 0.1, 1, and 10. For each value of \( G_0 \) and preshock density, shock velocities ranging from \( 5 \text{ km s}^{-1} \) up to the C-shock breakdown velocity, in steps of \( 1 \text{ km s}^{-1} \), were also generated. In total, 839 shock models were computed for \( G_0 = 0.1 \), 618 models were computed for \( G_0 = 1 \), and 455 models were computed for \( G_0 = 10 \). That fewer models were generated as \( G_0 \) increases reflects the fact that as \( G_0 \) increases, C-type shocks break down at lower shock velocities. Thus, a smaller range of shock velocities—and models—are consistent with C-type shocks as \( G_0 \) rises.

For each shock model, the postshock H\(_2\) density, temperature, and H\(_2\)O, OH, and O\(_2\) abundance are computed as a function of distance behind the shock front. The range of postshock distances considered extends beyond where (1) the H\(_2\)O, OH, and O\(_2\) abundances peak and subsequently drop by at least a factor of 10; and (2) the postshock temperature drops to 10 K. Meeting these criteria ensures that our modeling captures essentially all of the O\(_2\) emission since, beyond the postshock distances we consider, the reduced O\(_2\) abundances combined with the low gas temperatures produce negligible contributions to the total O\(_2\) integrated intensity.

Within the postshock region in which the density, temperature, and O\(_2\) abundance favor non-negligible O\(_2\) emission (as defined above), the gas is divided into 1000 equally spaced zones, each characterized by an H\(_2\) density, temperature, and O\(_2\) abundance (relative to H\(_2\)) as computed by the C-shock code. To obtain the O\(_2\) line intensities from each zone, the equilibrium level populations have been calculated using an escape probability method. We use the rate coefficients for collisions between O\(_2\) and He computed by Lique (2010), multiplied by 1.37 to account for the different reduced mass when H\(_2\) is the collision partner. Since these rates were computed for gas temperatures \( \lesssim 350 \text{ K} \), extrapolation to higher temperatures was necessary for application to postshock conditions. To do this, a polynomial was fitted to the 13 computed rates between 5 and 350 K for each transition and extended to 1400 K. As presented in Section 4.3 (and figures therein), O\(_2\) is formed in the postshock gas downstream of where H\(_2\)O and OH are formed. At the postshock distance where the O\(_2\) abundance approaches its peak, gas temperatures
have typically dropped below about 500 K. Thus, rates up to 1400 K suffice.

Because O₂ has no dipole moment and can only emit quadrupole radiation, the line center optical depth is small under almost all circumstances. As a result, the emergent line intensity is proportional to the O₂ column density, \( N(O₂) \). The range of H₂ densities and O₂ abundances over which the postshock O₂ emission peaks is determined from the postshock densities, temperature, and abundances computed for each shock model, combined with the radiative transfer calculations; however, \( N(O₂) \) also depends on the line of sight depth of the shock, which is difficult to assess. A study of water maser emission from behind C-type shocks by Kaufman & Neufeld (1996a) suggests that the aspect ratio of the zone of H₂O abundance—i.e., the ratio of the line-of-sight shock depth to the cross-sectional width of the high-H₂O abundance zone on the plane of sky—could exceed a factor of 100. For our purposes, we assume that distance behind the shock front at which the gas temperature and H₂O, OH, and O₂ abundances peak and the length scale over which the elevated temperatures and abundances persist decrease with increasing \( G_0 \).
H2 and O2 column densities thus derived since the total integrated intensity measured for each O2 line depends not only on $N$(O2) but also on the number of shocked regions within the Herschel/HIFI beams, and hence the total spatial extent of the O2 emission within these beams. The spatial extent of the O2 emission was only weakly constrained by Chen et al. (2014), other than inferring that the O2 emission most likely did not fill the Herschel/HIFI beams at 487, 774, and 1121 GHz. Thus, we treat the spatial extent of the O2 emission as a free parameter.

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We seek to match both the absolute O2 line fluxes and the observed line ratios. We first derive the column densities and emission area needed to reproduce the measured O2 487 GHz line flux. The ratios of the accompanying line fluxes at 774 and 1121 GHz to that at 487 GHz are then compared with those observed. We assume that the H2 and O2 column densities and emission area needed to reproduce the observed 487 GHz O2 line flux are given by

$$N(H_2) = 100 \times n(H_2)d_{10} \gamma$$  \hspace{1cm} (1)
The Astrophysical Journal, 806:227 (13pp), 2015 June 20

\[ N(O_2) = N(H_2) \chi(O_2), \]

(2)

where 100 is the assumed aspect ratio, \( n(H_2) \) is the H\(_2\) postshock density in the zones where 487 GHz emission peaks, \( d_{10} \) is the postshock distance between where the gas temperature first rises above 10 K and where it first returns to 10 K, and \( \chi(O_2) \) is the O\(_2\) abundance relative to H\(_2\). Because the O\(_2\) column density required to reproduce the observed optically thin line flux is inversely proportional to the area of the emitting region, we introduce the scaling factor \( \gamma \), which is defined as

\[ \gamma = \frac{400 \text{ arcsec}^2}{A_{487}}, \]

(3)

where 400 arcsec\(^2\) is chosen to be roughly consistent with the area of the O\(_2\)-emitting region assumed by Chen et al. (2014), and \( A_{487} \) is the actual area of the O\(_2\) 487 GHz emission in arcsec\(^2\) were it known. Since we compute the 487, 774, and 1121 GHz line emission as a function of postshock depth, the area of the 774 and 1121 GHz emitting regions, relative to \( A_{487} \), is computed for each shock model and scale as

Relative area of 774 GHz emitting region = \( A_{487} \left( \frac{w_{774}}{w_{487}} \right) \)

(4)

Relative area of 1121 GHz emitting region = \( A_{487} \left( \frac{w_{1121}}{w_{487}} \right) \)

(5)

where \( w_{487} \), \( w_{774} \), and \( w_{1121} \) are the widths of the 487, 774, and 1121 GHz emitting regions behind the shock front, respectively. The width of the emitting region in each line is taken to be the range of postshock depths over which the line flux remains greater than 1% of its peak value.

Finally, we define a “goodness of line ratio fit” parameter to measure how closely each model comes to reproducing the observed 774 GHz and 1121 GHz line fluxes once the 487 GHz line flux has been matched:

\[ \text{Goodness of Line Ratio Fit} = \left| \frac{R_{774m} - R_{774o}}{R_{774o}} \right| + \left| \frac{R_{1121m} - R_{1121o}}{R_{1121o}} \right| \]

(6)

where \( R_{774m} \) is the model-predicted ratio of the 774 GHz integrated intensity to the 487 GHz integrated intensity, and \( R_{774o} \) is the observed ratio of the 774 GHz integrated intensity to the 487 GHz integrated intensity. Likewise, \( R_{1121m} \) is the model-predicted ratio of the 1121 GHz integrated intensity to the 487 GHz integrated intensity, and \( R_{1121o} \) is the observed ratio of the 1121 GHz integrated intensity to the 487 GHz integrated intensity. Chen et al. (2014) report an observed 487:774:1121 GHz integrated line intensity ratio of 1:1.90:0.53 toward Orion H\(_2\) Peak 1. As indicated by Equation (6), model-predicted line ratios that exactly match the observed ratios would result in a “goodness of line ratio fit” of zero.

4.3. Shock Model Results

The results for shock models of varying preshock density, shock velocity, and FUV field, computed for \( G_0 = 0.1 \), 1, and 10, are shown in Figures 5–7, respectively. Only those models that produce a “goodness of line ratio fit” less than 6 for \( G_0 = 0.1 \) and 1 less than 14 for \( G_0 = 10 \) are shown for clarity. The best-fit model for each value of \( G_0 \) is summarized in Table 2; the O\(_2\) line ratios produced by these best-fit models are shown in Figure 8. The profiles of postshock O\(_2\) line integrated intensity, abundance, and temperature for the best-fit \( G_0 = 0.1 \), 1, and 10 shocks models are shown in Figures 9–11, respectively. Finally, the line center optical depth, \( \tau \), in the 487, 774, and 1121 GHz transitions was evaluated for each of the best-fit results given in Table 2. In no case did \( \tau \) exceed 0.07, and in most cases it was significantly lower, thus justifying the optically thin assumptions made here.

5. DISCUSSION

Following more than six years of observations, and more than 7000 Galactic lines of sight surveyed, the SWAS mission reported only one tentative detection of O\(_2\), toward the Rho Ophiuchi molecular cloud (Goldsmith et al. 2002). Likewise, the Odin mission reported only upper limits to the O\(_2\) line strengths (Pagani et al. 2003; Sandqvist et al. 2008), with the exception of one possible detection, also toward the Rho Ophiuchi cloud (Larsson et al. 2007). The upper limits to the O\(_2\) abundance set by SWAS and Odin are more than 100 times
the observed O₂ line ratios, with a value of zero representing a perfect region. The above plot assumes a 487 GHz O₂-emitting area of 400 arcsec² lower the value of the goodness of fit, the better the shock conditions reproduce the observed O₂ line ratios, with a value of zero representing a perfect fit. Log₁₀ of the preshock H₂ density is shown for each family of models. The required H₂ (and O₂) column density scales inversely with the area of the O₂-emitting region. The above plot assumes a 487 GHz O₂-emitting area of 400 arcsec² (see text).

Figure 6. Plot of the agreement between the predicted and observed 487, 774, and 1121 GHz O₂ line ratios produced by various shock models versus H₂ column density and shock velocity for G₀ = 1. As discussed in the text, the lower the value of the goodness of fit, the better the shock conditions reproduce the observed O₂ line ratios, with a value of zero representing a perfect fit. Log₁₀ of the preshock H₂ density is shown for each family of models. The required H₂ (and O₂) column density scales inversely with the area of the O₂-emitting region. The above plot assumes a 487 GHz O₂-emitting area of 400 arcsec² (see text).

Figure 7. Plot of the agreement between the predicted and observed 487, 774, and 1121 GHz O₂ line ratios produced by various shock models versus H₂ column density and shock velocity for G₀ = 10. As discussed in the text, the lower the value of the goodness of fit, the better the shock conditions reproduce the observed O₂ line ratios, with a value of zero representing a perfect fit. Log₁₀ of the preshock H₂ density is shown for each family of models. The required H₂ (and O₂) column density scales inversely with the area of the O₂-emitting region. The above plot assumes a 487 GHz O₂-emitting area of 400 arcsec² (see text).

lower than that predicted by equilibrium gas-phase chemical models. This discrepancy was later understood to be primarily the result of the exclusion of dust grains from these models, as these dust grains serve as important sites for both the freeze-out of H₂O and the surface formation of H₂O. This water-ice subsequently remains locked on grain surfaces until either photodesorbed by FUV or X-ray photons, sublimated at grain temperatures above ∼100 K, or sputtered by shocks with velocities >25 km s⁻¹ (Draine et al. 1983; Neufeld et al. 2014). By sequestering large amounts of elemental oxygen in water-ice, Bergin et al. (2000) and Hollenbach et al. (2009) showed that the gas-phase production of O₂ is effectively suppressed.

The Herschel Oxygen Project, guided by these updated models, used Herschel’s greater sensitivity to continue the search for O₂. To date, however, Rho Ophiuchi (Liseau et al. 2012) and Orion H₂ Peak 1 remain the only sources with statistically significant O₂ detections. It might be expected that
processes common to both sources, yet rare overall, could account for the O$_2$ emission. Unfortunately, the conditions inferred by Liseau et al. to explain the O$_2$ emission toward Rho Ophiuchi are insufficient to account for the emission toward Orion H$_2$ Peak 1. In particular, toward Rho Ophiuchi, the O$_2$ emission is attributed to a combination of two emitting regions, one with $N$(O$_2$) $>$ 6 $\times$ 10$^{15}$ cm$^{-3}$ and $T$ $<$ 30 K, and the other with $N$(O$_2$) $=$ 5.5 $\times$ 10$^{15}$ cm$^{-3}$ and $T$ $>$ 50 K. The inferred beam-averaged O$_2$ abundance is $\sim$5 $\times$ 10$^{-8}$ in the warmer component, and somewhat higher in the colder component. The successful detection of O$_2$ toward this source, among the many sources toward which no O$_2$ emission was detected, was attributed to time-dependent quiescent cloud chemistry—i.e., Rho Ophiuchi was surmised to have been observed during a relatively short period when the evolving O$_2$ abundance was near its peak.

Such a scenario is unlikely to apply to Orion H$_2$ Peak 1. First, the constraints on the spatial extent of the O$_2$ emission toward Peak 1 provided in Chen et al. (2014)—i.e., an O$_2$-emitting region less than 25" in diameter—require that the O$_2$ column density be between about 3 $\times$ 10$^{17}$ and 3 $\times$ 10$^{18}$ cm$^{-2}$ to produce the absolute O$_2$ line intensities measured. O$_2$ column densities this high are hard to produce in quiescent gas (e.g., Hollenbach et al. 2009). Second, Peak 1 is the site of intense shock, rather than quiescent cloud, emission. Third, if a component of quiescent gas close to H$_2$ Peak 1 were responsible for the O$_2$ emission, and the O$_2$ abundance were close to its quiescent cloud peak of $\sim$5 $\times$ 10$^{-8}$, as in Rho Ophiuchi, the required H$_2$ column density, $N$(H$_2$) $=$ $N$(O$_2$) / $\chi$(O$_2$), would be on the order of 10$^{25}$ cm$^{-2}$, which is much higher than observed. Thus, process(es) different from those invoked to explain the O$_2$ emission toward Rho Ophiuchi are needed to explain the detections toward Orion H$_2$ Peak 1.

In addition to the presence of shock activity, Orion is the site of O and B stars that produce strong FUV radiation. The FUV field near the Trapezium has been estimated to be $G_0$ $\gtrsim$ 10$^4$ based on the total radiation from the Trapezium stars—and the O star $\beta$ Ori C in particular. The intensity of this field is corroborated by the strength of the far-infrared [C II] and [O I] fine-structure lines mapped toward the Orion molecular ridge, the strength of several near-infrared lines whose intensities have been ascribed to recombinations to highly excited states of C I, and the strength of near-infrared N I lines excited by the fluorescence of UV lines (Herrmann et al. 1997; Marconi...
The amount by which the FUV field is attenuated between the Trapezium and H$_2$ Peak 1 due to intervening material is uncertain, as is the FUV radiation from other B stars in the Orion cloud. However, as discussed in Section 3, even modest amounts of FUV radiation (i.e., $G_0 \leq 10$) can affect both the structure of and chemistry behind C-type shocks and motivate the study here.

FUV-illuminated C-type shocks provide a natural explanation for the Orion H$_2$ Peak 1 O$_2$ emission for three reasons. First, as discussed in Sections 3.2 and 3.3, the FUV field can increase the atomic oxygen abundance in the preshock gas, which will increase the peak H$_2$O abundance in the postshock gas. Second, the postshock OH abundance (and, ultimately, the O$_2$ abundance) is increased via the photodissociation of H$_2$O, as well as OH-producing chemical reactions, some with high activation barriers, enabled by the elevated postshock gas temperatures. By raising the O$_2$ abundance above that attainable in cold quiescent gas, the implied H$_2$ column density can be brought closer to observed values. Finally, the similarity between the LSR velocities measured for the O$_2$ lines of $\sim$11 km s$^{-1}$ (see Chen et al.) and those measured for the 22 and 621 GHz H$_2$O masers of 10–13 km s$^{-1}$ suggests a possible physical connection. As discussed in Section 4.1, the maser emission indicates that some shocks are propagating in the plane of the sky, which can potentially provide a higher line-of-sight column density of O$_2$ than face-on shocks while allowing for the narrow observed O$_2$ line widths.

For these reasons, as well as the conspicuous presence of shock activity associated with H$_2$ Peak 1, both Chen et al. (2014) and we focus on shocks as the most likely source of the detected O$_2$ emission. However, three significant differences distinguish the approach previously taken by Chen et al. and that taken here. First, Chen et al. assume that the preshock gas and the shock are fully shielded from FUV radiation, with only the postshock gas subject to an FUV field. Here, we assume that the preshock, shock, and postshock gases are illuminated by a common FUV field. Given that the width of the shock front is approximately $10^{16}$ cm or less (see Figures 9–11), this approach seems well justified. In particular, the analysis presented here avoids the inconsistency in which the postshock physical conditions are determined assuming the absence of FUV radiation while the postshock chemistry, which is governed by these physical conditions (e.g., density and temperature), requires the presence of FUV radiation.

Second, the above is important since the effects of FUV radiation on the shock structure can result in substantial changes to the shock width and postshock temperature, with the latter affecting the postshock chemistry. As shown in Figure 2, for a given preshock density and shock velocity, increasing the FUV field intensity both increases the peak postshock temperature and reduces the shock width. As shown in Bergin et al. (1998), the formation rate of H$_2$O via the neutral-neutral reactions O + H$_2$ → OH + H; OH + H$_2$ → H$_2$O + H becomes important when the postshock temperature exceeds $\sim$300 K and increases rapidly with temperature. In fact, as the peak postshock temperature rises with increasing $G_0$, the H$_2$O formation rate begins to exceed the H$_2$O photodestruction rate, resulting in a net increase in the postshock H$_2$O abundance with $G_0$ (e.g., compare middle and bottom panels of Figure 2). This trend continues up to the full conversion into H$_2$O of all gas-phase O nuclei not locked in CO. Only when the postshock cooling causes the temperature to drop below about 300 K does the H$_2$O formation rate decrease significantly. When this occurs, photodestruction dominates formation and the H$_2$O abundance begins to decline, as shown in Figure 2. Ignoring the effects of FUV radiation leads to an underestimate of the postshock temperature and the postshock depth to which H$_2$O exists in high abundance, as
of $H_2O$, i.e., O and OH, $H_2O$ must be relatively abundant as well as an overestimate of the shock width, all of which affect the resulting $O_2$ emission.

Third, since $O_2$ is formed from the photo-destroyed products of $H_2O$, i.e., O and OH, $H_2O$ must be relatively abundant (i.e., $\chi(H_2O) > 10^{-5}$) in the postshock gas to produce the observed $O_2$ emission. There are two ways to achieve this: (1) by placing $H_2O$ into the gas phase directly through the sputtering of $H_2O$ from the ice-covered mantles of dust grains behind the shock, and (2) by chemically forming $H_2O$ behind the shock via the neutral-neutral reactions above. However, for process 2 to form a high $H_2O$ abundance, the preshock gas must have a high abundance of atomic oxygen. Within gas in which the $H_2O$ depletion onto grains is significant, Chen et al. require that the sputtering efficiency be $\geq 10\%$ behind a 12 km s$^{-1}$ shock. This efficiency exceeds all theoretical predictions of which we are aware, including Draine et al. (1983), Jiménez-Serra et al. (2008, see their Figure 7), and Flower & Pineau des Forêts (2010). Recently, Neufeld et al. (2014) have modeled the water abundance behind interstellar shocks based on Herschel measurements of far-infrared and submillimeter measurements of CO and $H_2O$ in combination with Spitzer measurements of mid-IR $H_2$ rotational emission. Their best-fit results are in good agreement with the prediction that only when shocks reach a velocity of $\geq 25$ km s$^{-1}$ will $H_2O$ be completely removed from grain mantles. Thus, it is not clear that sufficient $H_2O$ can be removed from grain mantles to support the model offered in Chen et al. if depletion of $H_2O$ onto dust grains is significant in the preshock gas and negligible sputtering efficiency is assumed behind a 12 km s$^{-1}$ shock.

Alternately, Chen et al. suggest that the preshock gas is sufficiently young that depletion is minimal, in which case the atomic oxygen abundance is high. However, since this model assumes that the preshock gas is collapsing from an initial density of 100 cm$^{-3}$, the time between when the density evolves to its required preshock value (i.e., $4.2 \times 10^4$ cm$^{-3}$) and when depletion becomes important is $\sim 1.7 \times 10^5$ yr. Nevertheless, invoking a short interval during which the preshock is sufficiently dense, but undepleted, could result in the high preshock O abundance needed to yield a postshock $H_2O$ abundance sufficient to produce detectable $O_2$ emission. A short-lived period in which both the preshock gas density and O abundance are high could also account for the rarity of $O_2$ detections, as discussed by Chen et al. However, this model still presumes that the preshock gas is fully shielded while the postshock gas is not, an assumption not justified in the Chen et al. model.

Introducing an FUV field to the preshock gas solves these problems. FUV photons can photodesorb $H_2O$ from grain mantles when shock velocities are too low to produce significant sputtering (i.e., $v_s \lesssim 20$ km s$^{-1}$). (When shock velocities are $\geq 25$ km s$^{-1}$, sputtering will remove any $H_2O$ not photodesorbed in the preshock gas.) Even if the FUV field results in the photodestruction of gas-phase $H_2O$ in the preshock gas, the O and OH produced will be rapidly converted to $H_2O$ in the warm postshock gas. Thus, an FUV field can eliminate the need for high assumed sputtering efficiencies at low shock velocities while relaxing the need to invoke a particular epoch in the time-dependent evolution of the preshock gas. As for time-dependent preshock evolution being the cause for the rarity of $O_2$ detections, a different explanation is suggested below.

Table 2 lists shock models considered here that reproduce both the absolute $O_2$ line intensities and line ratios for incident FUV fields having a $G_0 = 0.1$, 1, and 10. Several trends are evident. First, as discussed in Section 3, as $G_0$ increases, the ion–neutral coupling increases and the width of the shock decreases. This is evident in the scale of the $x$-axes in Figures 2, 9–11. Likewise, as $G_0$ increases, roughly the same postshock temperatures are achieved with decreasing shock velocities. Second, as $G_0$ increases, the increased photodissociation of $H_2O$ is converted to $H_2O$ in the warm postshock gas. Thus, an FUV field can eliminate the need for high assumed sputtering efficiencies at low shock velocities while relaxing the need to invoke a particular epoch in the time-dependent evolution of the preshock gas. As for time-dependent preshock evolution being the cause for the rarity of $O_2$ detections, a different explanation is suggested below.

![Figure 11](attachment:image.png)

**Figure 11.** Profiles of integrated intensity (top), abundance (middle), and gas temperature (bottom) as a function of distance behind the shock front for the best-fit shock parameters for $G_0 = 10$. 
molecules lowers the peak postshock abundance of H$_2$O, OH, and O$_2$, thus requiring greater H$_2$ column densities to produce the same optically thin O$_2$ line flux (see Table 2).

Within the observational uncertainties, all three models in Table 2 can explain both the measured O$_2$ line fluxes and line ratios; is one model preferred? One possible discriminator is the degree to which each model agrees with estimates of the total H$_2$ column density and number density toward Peak 1. Rosenthal et al. (2000) estimate the H$_2$ column density to be $\approx 2 \times 10^{22}$ cm$^{-2}$ based on the observation of 56 H$_2$ ro-vibrational and pure rotational lines toward Peak 1 using the *Infrared Space Observatory’s* Short Wavelength Spectrometer (de Graauw et al. 1996). However, because the lowest-lying H$_2$ pure rotational transition lies 510 K above the ground state, estimates based on H$_2$ lines are more sensitive to the warm and observer with a potentially large line-of-sight column of gas with this relatively high O$_2$ abundance. Of course, shocks of the sort described here would be expected to produce enhanced optically thin O$_2$ emission regardless of whether these shocks were propagating perpendicular to our line of sight or not. However, if such shocks produce O$_2$ integrated intensities comparable to what was detected toward Peak 1, but with propagation angles closer to our line of sight, the O$_2$ lines would appear broader. Thus, the same total line flux would be spread over a greater number of velocity bins with a corresponding reduction in the line center amplitude. For weak emission, such as that exhibited by the observed O$_2$ lines, narrow lines are generally much easier to detect than lower-amplitude broad lines, particularly in the presence of noise. The rarity of O$_2$ detections may therefore result from the need to simultaneously satisfy four conditions: (1) an O$_2$-emitting area that fills a non-negligible fraction of a beam, (2) the presence of C-type shocks having peak postshock temperatures sufficient to drive the efficient production of H$_2$O, (3) illumination by FUV radiation that can both enhance the preshock gas-phase O-nuclei abundance and photodissociate postshock H$_2$O, and (4) a shock propagation vector close to perpendicular to the line of sight that naturally provides narrow line profiles.

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