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THE DISCOVERY OF VIBRATIONALLY EXCITED H_2 IN THE MOLECULAR CLOUD NEAR GRB 080607

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ABSTRACT

GRB 080607 has provided the first observational signatures of molecular absorption bands toward any galaxy hosting a gamma-ray burst (GRB). Despite the identification of dozens of features as belonging to various atomic and molecular (H_2 and CO) carriers, many more absorption features remained unidentified. Here, we report on a search among these features for absorption from vibrationally excited H_2, a species that was predicted to be produced by the UV flash of a GRB impinging on a molecular cloud. Following a detailed comparison between our spectroscopy and static, as well as dynamic, models of H_2* absorption, we conclude that a column density of $10^{17.5\pm0.2}$ cm^{-2} of H_2* was produced along the line of sight toward GRB 080607. Depending on the assumed amount of dust extinction between the molecular cloud and the GRB, the model distance between the two is found to be in the range 230–940 pc. Such a range is consistent with a conservative lower limit of 100 pc estimated from the presence of Mg i in the same data. These distances show that substantial molecular material is found within hundreds of pc from GRB 080607, part of the distribution of clouds within the GRB host galaxy.

Key words: galaxies: ISM – gamma rays: bursts – ISM: clouds – ISM: molecules – molecular processes

1. INTRODUCTION

Long-duration gamma-ray bursts (GRBs) are currently understood to be the electromagnetic manifestation of highly beamed energy from the sites of the demise of young massive stars (see, e.g., Woosley & Bloom 2006). This implies that GRB progenitors must have formed and lived near molecular clouds in their respective host galaxies. Direct evidence for the molecular nature of their birthplace has been lacking, presumably owing to complete destruction of molecules within ∼100 pc of the GRB (Tumlinson et al. 2007; Whalen et al. 2008). Recently, Prochaska et al. (2009, hereafter P09) presented the first unambiguous spectroscopic detection of absorption bands from H_2 and CO molecules along a translucent GRB sight line (GRB 080607, $z = 3.0363$). Their initial analysis provided the first discovery of molecular gas with properties very similar to those of Galactic molecular clouds, but located in the star-forming ISM of a GRB host galaxy.

The detection by P09 of neutral species (e.g., C i, Mg i) toward GRB 080607 indicates that the bulk of the atomic gas was ⩾100 pc from the GRB, presumably beyond the photoionization sphere formed by the progenitor (Whalen et al. 2008). However, whereas Whalen et al. (2008) introduced an additional galactic-wide far-ultraviolet (FUV) field as a means to suppress the formation of unobserved H_2, the discovery of more than 10^{21} cm^{-2} of H_2 toward GRB 080607, well shielded by dust extinction (rest-frame $A_V = 3.2$ mag), raises the possibility that the molecular material could have been in close proximity to the GRB. The detection by P09 of absorption from rotationally excited CO, and the determination that atomic and molecular lines are kinematically distinguished by 30 ± 15 km s^{-1}, specifically allow for this scenario.

Excitation of fine-structure atomic lines via UV fluorescence is well attested along GRB sight lines (e.g., Fe^+; Prochaska et al. 2006). Draine (2000), followed by Draine & Hao (2002, hereafter DH02), predicted that observable quantities of vibrationally excited H_2 (from $v'' > 0$, hereafter H_2*) can be produced by UV photons in molecular gas within 100 pc from a GRB source. With an assumed model peak luminosity of $L_0 = 1/40$ of that observed for GRB 990123, DH02 produced a column density (N) of $\approx 10^{19}$ cm^{-2} of H_2* in a gas with an initial $N = 10^{21}$ cm^{-2} of cold H_2 at close proximity (⩽1 pc) to the GRB. P09 reported cold H_2 with $N \approx 10^{21.2}$ cm^{-2} toward GRB 080607, suggesting the possibility that H_2* could also have been present.

Here, we report on our successful search for absorption from H_2* toward GRB 080607. Previously, one Galactic sight line was shown to have ∼500 absorption lines associated with H_2* (Meyer et al. 2001, toward HD 37903), while the sample of low-redshift galaxies, meanwhile, that are found to emit rovibrational H_2* lines near 2.1 μm has been increasing steadily, albeit mostly attributed to shocked gas (Thompson et al. 1978; Jaffe & Bremer 1997; Donahue et al. 2000; Dale et al. 2009). Our sight line toward GRB 080607 at the redshift of $z = 3.0363$ is thus the most distant detection of H_2*, as well as the first extragalactic detection of H_2* via absorption: this was made possible thanks to an extremely bright GRB, an extremely capable optical system (the LRIS spectrometer on the Keck I telescope), and a rapid response to the GRB alert from *Swift*. We also show, by a comparison with theoretical predictions, that this detection serves to confirm the general picture of the interaction between a GRB and its immediate galactic environment.

2. OBSERVATIONS AND MODELING

The acquisition of the spectroscopic data analyzed here was described by P09. Here, we recap some essential information relating to the sequence of events in the rest frame of the GRB, owing to the predicted temporal evolution of the H_2* abundance (DH02).

GRB 080607 triggered the *Swift* detector at 06:07:27 UT on 2008 June 7 (Mangano et al. 2008), here defined as $t = 0$ s. A first series of three Keck/LRIS exposures was taken by us (D.A.P. and J.S.B.) with the B600 and R400 gratings, simultaneously

Table 1
H_2* Features Identified Toward GRB 080607

λ_{obs} (Å)	W_λ[a] (Å)	ID in P09[b]	λ_{rest} (Å)	ID in DH02[c]	New ID[d] (v''; J'')
5762.6	0.8	···	1427.1	···	(6; 0,1)
5783.5	1.1	···	1432.3	···	(6; 2)
5789.7	0.6	···	1433.8	···	(6; 4)
5797.4	1.4	···	1435.7	P1+R1	(8; 0)
5988.6	1.0	···	1483.1	···	(10; 2)
6002.3	2.6	···	1486.5	R0+R1	(7; 0,1)
6012.5	1.9	···	1489.0	···	(7; 1,2)
6115.3	1.1	UID	1514.5	···	(8; 0,1)
6124.8	1.5	UID	1516.8	R1+P1	(7; 2)
6130.3	1.3	UID	1518.2	P1	(11; 0,1)
6135.6	0.9	···	1519.5	···	(8; 2)
6156.6	0.9	Included in Si II	1524.7	···	(7; 3)
6179.2	0.6	···	1530.3	···	(10; 1)
6205.8	0.6	···	1536.9	···	(10; 3)
6213.8	0.6	···	1538.9	···	(9; 0,1)
6263.7	1.4	Included in C IV	1551.2	···	(12; 1,2)
6269.1	0.6	UID	1552.6	···	(13; 1)
6318.8	0.7	UID	1564.9	···	(13; 1)
6414.3	0.9	Included in Si I	1588.6	R0+R1	(10; 0,1)
6432.1	0.7	UID	1593.0	···	(10; 2)
6477.4	1.6	UID	1604.2	···	(9; 1)
6489.1	1.5	Included in Fe II	1607.1	P1+R3	(9; 2)
6525.8	0.6	···	1616.2	···	(12; 5)
6604.4	0.7	Included in Fe II	1635.7	···	(9; 1)
6614.6	1.6	Included in Fe II	1638.2	R1+R2	(11; 2)

Notes.
[a] Detections with $W_\lambda \geqslant 0.6$ Å ($\geqslant 4\sigma$).
[b] UID: listed in P09 without ID. Otherwise, was included in a stronger atomic feature.
[c] Strongest transitions within 1.0 Å of λ_{rest} for $R = 350$.
[d] Strongest contributing ro-vibrational levels for $R = 4000$.

employing the blue and red cameras. These exposures were 75, 150, and 300 co-moving seconds long, centered on rest-frame times $t = 340$, 490, and 730 s. A second series of two exposures was taken with the B600 and R1200 gratings, both 370 s long, and centered on the post-trigger times $t = 1230$ and 1640 s in the rest frame of the GRB. In terms of spectral resolution, the subarcsecond seeing resulted in $\lambda/\Delta\lambda = R \sim 4000$, 2000, and 1000, for gratings R1200, B600, and R400, respectively.

Our initial search for possible H_2* features involved spectral syntheses of relevant transitions with the Y.S. code Ismod.f, and comparisons with the highest-R data from the R1200 grating. Each transition was modeled with a single Voigt profile, employing as fixed parameters the resolution R, transition rest wavelength (λ_{rest}) and oscillator strength (f-value), the Doppler parameter b, and a radial velocity of +30 km s^{-1} relative to the atomic gas (P09). Both the λ_{rest} and f-values for B–X and C–X transitions of H_2* were downloaded from the MOLAT Web site[6] (E. Roueff 2009, private communication). Table 1 lists our H_2* identifications for 25 absorption features detected at the $\geqslant 4\sigma$ level in the R1200 spectrum.

Once we were convinced of the presence of (static) H_2* absorption in the data toward GRB 080607, we shifted to full dynamic modeling, with photoexcitation, photodissociation, and photoionization of the gas treated following DH02. The UV and X-ray emission from GRB 080607 was assumed to be

[6] http://molat.obspm.fr/

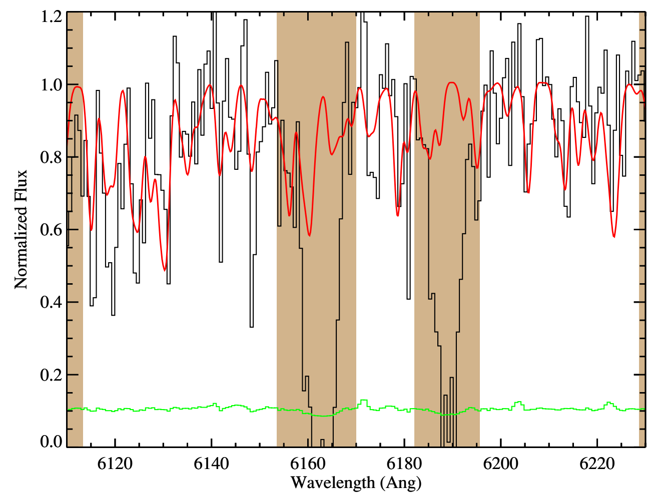

Figure 1. Zoomed comparison between the Keck/LRIS R1200 data (black histogram) and the H_2* dynamic model (smooth red line). Brown masking designates absorption from other identified species (e.g., Si II at 6163 and 6189 Å), where the detection of H_2* would be compromised by blending. The agreement is very good between stronger H_2* absorption features and equally strong, hitherto unidentified "lines" in the spectrum. The noise level is denoted by the green line at the bottom.

described by

$$\nu L_\nu = L_0 \left(\frac{h\nu}{13.6\,\mathrm{eV}}\right)^{1+\beta} \frac{4(t/t_0)^2}{[1+(t/t_0)^2]^2}, \tag{1}$$

where $L_0 = 5 \times 10^{50}$ erg s^{-1}, $\beta = -0.5$, and $t_0 = 10$ s. With $A_V = 3.2$ mag (P09), this reproduces the observed K-band flux density at $t_{obs} = 300$ s. The value of L_0 is 200 times higher than that adopted in DH02. Indeed, GRB 080607 ranks among the most powerful to date, an equal to GRB 990123 in γ luminosity (Golenetskii et al. 2008).

Total line-of-sight abundances for H and H_2 were taken from P09, with the H nucleon density (n_H) taken to be 10^3 cm^{-3}. The dust/gas ratio in the pre-GRB gas was assumed to be $\sim$10% of the local Milky Way value (P09). For photoexcitation of the H_2 and photoionization of H and H_2, we were primarily interested in the dust extinction cross section per H nucleon at $\lambda < 1110$ Å, which we take to be $\sigma = 2 \times 10^{-22}$ cm^{-2}, so that $A_{1000\,Å} = 5.33 \times 10^{22} \times 2 \times 10^{-22}/1.086 = 9.8$ mag, or $A_{1000\,Å}/A_V = 3.1$.

Finally, the evolution of the irradiated dust was followed with the same assumptions as in DH02. Initial grain size was $a = 0.04$ μm, which could decrease by thermal sublimation if the grains became hot enough. For calculating UV extinction we used $Q_{ext} = 2$, where Q_{ext} is the ratio of the extinction cross section to the geometric cross section, πa^2.

3. RESULTS AND DISCUSSION

3.1. H_2* Column Density

Figure 1 shows a small portion of the R1200 data, superposed by 336 modeled transitions of H_2*. This region includes five absorption "lines" that were listed, but not identified, in P09, four of them as a group between $\lambda_{obs} = 6115$–6130 Å. However, each H_2* "line" is a blended feature that includes several strong transitions. It is evident that the four observed features near 6120 Å are too strong to be attributed to noise: their equivalent width (W_λ) values listed in P09 range over 1.1–2.3 Å, or 7–15 times the 1σ detection limit. Since these "lines" cannot be identified with any other plausible atomic or molecular species, at the redshift of either GRB 080607 or the two intervening

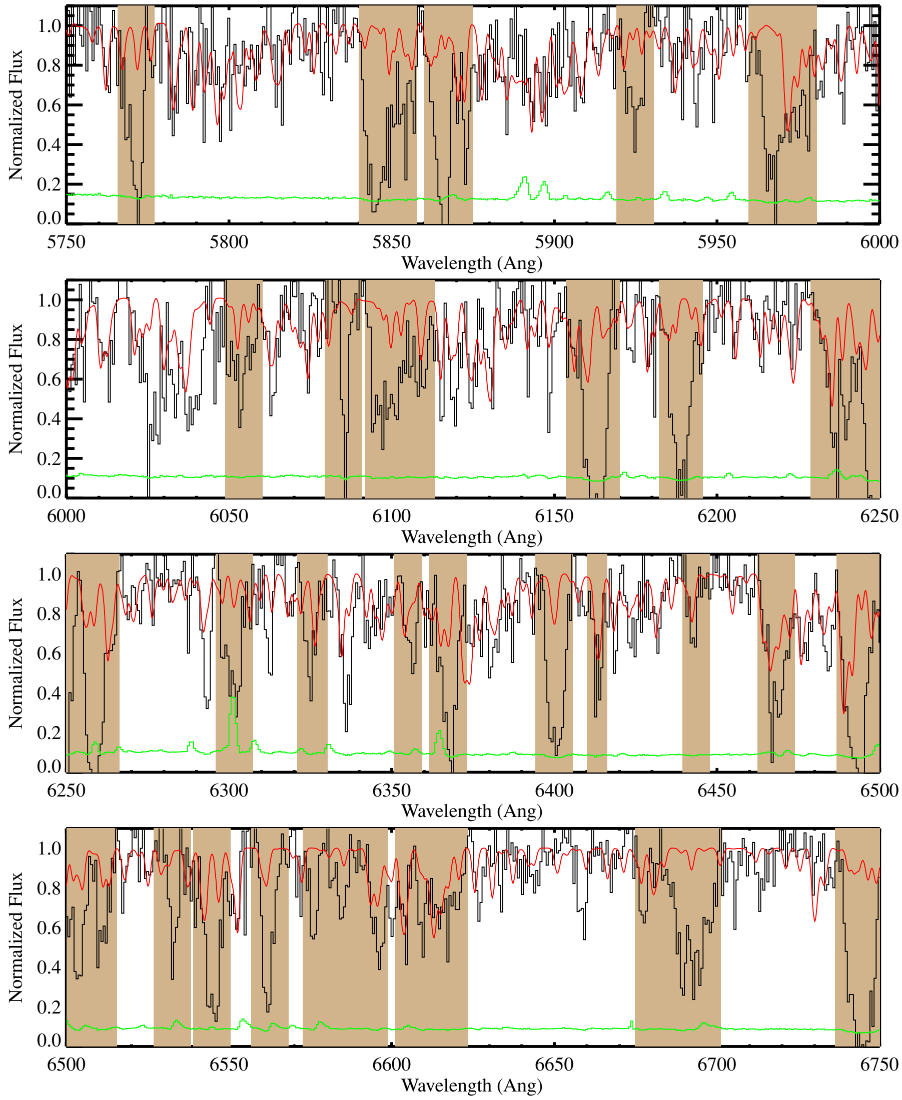

Figure 2. Same as Figure 1, but showing 1000 Å of the R1200 data and the model of H_2*. Dozens of narrow H_2* and observed features appear to agree with each other. The global pattern of variable $v' - v''$ band strength is also matched.

absorption systems, we are confident that H_2* provides the only viable model for their presence in our data. For the best match with the data, the static modeling with Ismod.f returned $\log N(H_2*) = 17.7 \pm 0.3$, using $b = 2$ km s^{-1}, a value taken from the CO analysis of P09. Our full dynamic modeling with the DH02 code, computing H_2 excitation for 10^3 s in the GRB time frame and using $b = 3$ km s^{-1}, returned $\log N(H_2*) = 17.5 \pm 0.2$, in good agreement with the static model. This served to confirm that the first case of H_2* excitation by GRB photon pumping has been identified.

The entire range of the R1200 spectrum ($\lambda_{\rm rest}$ = 1400–1720 Å) covers the red portion of H_2* absorption, and includes 3372 transitions with J'' = 0–29, v'' = 1–14, and v' = 0–16. Figure 2 presents a global view of the H_2* model spectrum superposed over 1000 Å of the R1200 data. The overall agreement between data and model is acceptable, given that the S/N $\approx$ 10 and the presence of numerous other absorption features from, e.g., host-galaxy CO bandheads and Fe II from two foreground absorbers (P09). The few instances where the modeled absorption is significantly deeper than the data involve levels with $v'' \geqslant 9$, presumably related to our incomplete description (underestimation) of UV photoionization rates out of high-v'' levels.

We identified 25 narrow H_2* features that are the least blended with other species and list these in Table 1. Previously, P09 estimated atomic abundances in the weak limit from the measured W_λ of absorption features. Since some transitions listed in P09 are seen here (Figure 2) to be blended with some of the stronger H_2* features, certain W_λ values should be revised downward. For example, the H_2* feature at 6466 Å falls into a blend with the Ge II 1602 line, contributing 2.0 Å to the total W_λ of 5.3 Å and reducing its weak-limit abundance (estimated by P09 to be super-solar). However, only a future detailed study of sight-line saturation will be able to provide robust abundance determinations based on H_2*-corrected data.

The presence of H_2* in our R1200 spectrum is confirmed by the lower signal-to-noise ratio (S/N) exposures from the B600 grating (R = 2000). In all, the blue and red gratings provide ~500 Å of rest-frame coverage of numerous absorption features belonging to (or blended with) H_2* toward GRB 080607.

3.2. H_2* *Variability Versus Nonvariability*

The theoretical work of DH02 followed the temporal behavior of H_2* abundance in response to the initial UV flash from a GRB afterglow. Upon photoexcitation into the electronic B and C states, only ~15% of H_2 is photodissociated, with the

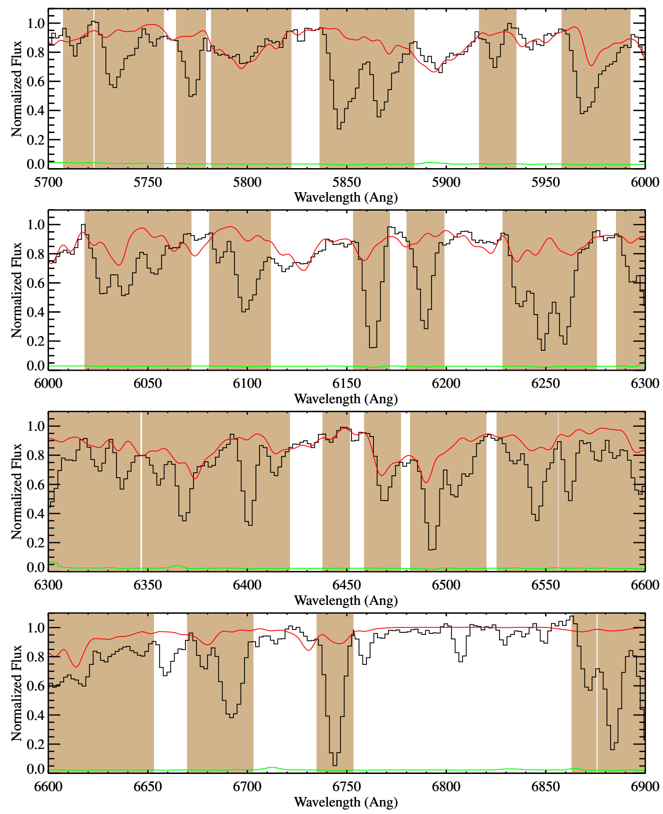

Figure 3. Same as Figure 2, but showing the lower-resolution R400 data and H_2* model. Absorption from wide features made up of numerous H_2* transitions is determining the shape of the continuum of the R400 spectrum. Some absorption features previously assigned to atomic carriers are clearly significantly blended with contribution from H_2*.

majority, therefore, decaying immediately into $v > 0$ levels of the X ground state. A very rapid rise in $N(H_2*)$ occurs over the timescale of the burst (≈10 s) as the UV photons get absorbed by the cold H_2 gas. The 10^6 s lifetime of H_2* (Draine 2000) means that it remains around for almost two months in the observer frame.

As described in Section 2, our two groups of red exposures were centered on $t \sim 500$ and 1400 s in the GRB rest frame. As shown in Figure 3, a degraded $R = 1000$ version of the H_2* model that matches the R1200 spectrum shows remarkable agreement with the upper envelope of the R400 spectrum. Thus, there is no indication of variation in $N(H_2*)$ over the $\Delta t \sim 900$ s that elapsed between the clusters of R400 and R1200 exposures. This observational result confirms the DH02 theoretical predictions that $N(H_2*)$ varies over timescales that are either significantly shorter or significantly longer than those covered by our observations.

3.3. *The Distance of H_2* from the GRB*

The value of $N(H_2*)$ detected here is only ∼3% of that produced by the models in DH02. According to DH02, the amount of H_2* produced depends on the fluence, F, of the source, and hence on the ratio L_0/D^2, where D is the distance from the GRB to the center of the initial H_2 integration zone. Owing to the much higher value of L_0 used in our modeling of GRB 080607 (Section 2), the production of an appreciably *smaller* amount of H_2* relative to DH02 would require a very large increase in D.

We employ the detailed modeling of DH02 in order to explore the dependence of $N(H_2*)$ on D. The effect of the GRB on the H_2 will depend on what fraction of the H I is located between the GRB and the H_2, because the dust in the H I gas can help shield the H_2 from photons with $\lambda < 1110$ Å, and the H I itself will help protect the H_2 from photoionization.

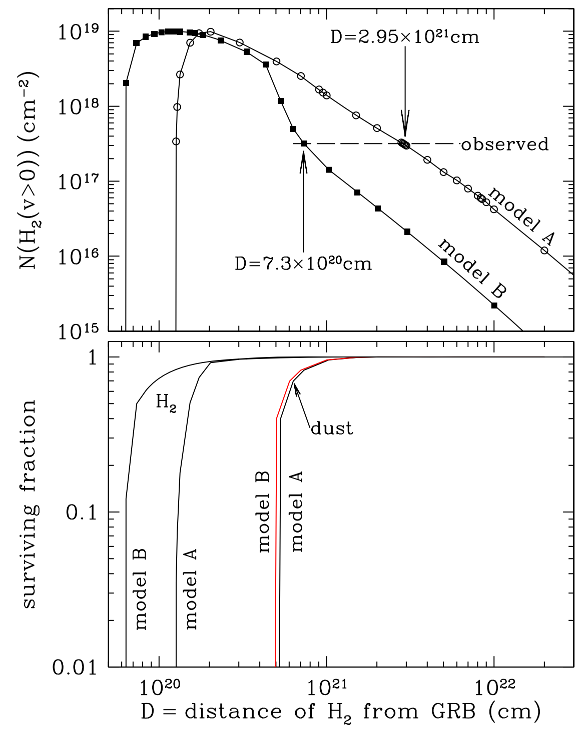

Figure 4. Column density of vibrationally excited H_2 as a function of distance from GRB 080607, for two models differing in the location of the H I relative to the H_2 (see the text).

We consider two cases. Model A has $N(H^0) = 2 \times 10^{21}$ cm^{-2} located between the GRB and the H_2, with the remainder of the H I located beyond the H_2. Model B has $N(H^0) = 5 \times 10^{22}$ cm^{-2} (i.e., *all* of the H I detected by P09) located between the GRB and the H_2. For a given large value of D, model B will have less UV-pumped H_2 than model A, because of the additional dust shielding in model B. However, for smaller values of D, reduced shielding by the destruction of dust and H I in model B may result in complete destruction of the H_2 by photodissociation or photoionization.

The upper panel of Figure 4 shows $N(H_2*)$ versus D for the two models. The observed value of $\approx 10^{17.5}$ cm^{-2} (Section 3.1) is generated for $D = 2.9 \times 10^{21}$ or 7.3×10^{20} cm for Model A or B, respectively. Thus, we conclude that the H_2 in GRB 080607 is located between 230 and 940 pc from GRB 080607, a value much larger than that used in DH02 ($D \ll 1$ pc).

The lower panel of Figure 4 shows the fraction of the initial dust and H_2 that survives after the GRB flash. For more than 50% of the initial grain mass to be sublimed, the H_2 gas would have to be within ∼190 pc, slightly closer than the location of the H_2* in model B, and substantially closer than in model A. We conclude that for these two models, the bulk of the dust survives the GRB flash, consistent with $A_V \approx 3.2$ mag observed during the afterglow phase. Substantial destruction of the H_2 by a combination of photodissociation and photoionization occurs only for $D < 2 \times 10^{20}$ cm = 65 pc. Given the observed $N(H_2*)/N(H_2) \approx 10^{-3.7}$, we conclude that there has been minimal destruction of H_2 in the cloud where the H_2* resides.

More complex models are of course possible: if more than one H_2 cloud is present, there could have near-complete destruction of the H_2 in the inner cloud, leaving only a small amount of H_2

with high levels of vibrational excitation, with the bulk of the H_2 in a more distant cloud with little vibrational excitation.

3.4. *What about CO*?*

The presence of H_2* prompted us to search for vibrationally excited CO (CO*) in our data. P09 reported the detection of log $N = 16.5 \pm 0.3$ cm^{-2} of cold ($v'' = 0$) CO, all of which was rotationally- excited (hereafter r-CO*) at $T_{ex} \sim 300$ K up to $J'' = 25$. If the vibrational excitation of CO owing to UV pumping scales with that of H_2, then we should expect log N(CO*) = log N(CO) − 3.7 ≈ 12.8 cm^{-2}. CO* transitions for $v'' > 0$ bands were taken from Kurucz line lists[7] and modeled with Ismod.f, but no match with the R1200 data was found. Based on the strongest $v'' = 1$ band at 6400 Å, a feature with N(CO*) = 1×10^{13} cm^{-2} would have a depth of 10%, comparable to the 1σ noise level in the data.

We note that the photophysical behavior of CO differs from that of H_2 in two important respects. First, owing to the existence of strongly predissociating Rydberg states in CO below $\lambda_{rest} =$ 1100 Å (Letzelter et al. 1987; van Dishoeck & Black 1988; Sheffer et al. 2003), CO*/CO should be much lower than H_2*/H_2. Second, CO* spontaneously decays via dipole transitions with a lifetime of ca. 10^{-2} s (Okada et al. 2002), roughly 10^8 times faster than the quadrupole transitions of H_2*. Any small amount of surviving CO* would be rapidly converted into r-CO*. However, while CO photophysics may explain the absence of CO* toward GRB 080607, the challenge of accounting for the conversion of the bulk of cold CO into r-CO* remains.

Both dust extinction and cold H_2 provide very effective UV shielding of CO below $\lambda_{rest} = 1100$ Å, allowing it to survive in deeper layers of a cloud. The nondissociating $A - X$ bands (with $v' \leqslant 8$) are significantly less shielded: the data toward GRB 080706 (Figure 1 of P09) show that the UV flux level at $\lambda_{rest} > 1322$ Å is ∼5 times higher than at $\lambda_{rest} < 1150$ Å. UV pumping into the CO A state could result in its complete conversion into CO* and then into r-CO*. However, assuming that initially the CO is cold ($T_{ex} \sim 11$ K, $J'' \leqslant 5$), the production of r-CO* that happens to maintain a quasi-thermal distribution at ∼300 K up to $J'' = 25$ must be considered a coincidence of indirect excitation.

Radio observations show that collisionally excited r-CO* can be found in Galactic photodissociation regions (PDRs; Tielens & Hollenbach 1985), with $T_{ex} \sim 100$–1000 K (van Dishoeck & Black 1988; Draine & Bertoldi 1996; Hollenbach & Tielens 1997). This range agrees with $T_{ex} \sim 300$ K for r-CO* toward GRB 080607, subject to the caveat that appreciably higher values of N(CO) and A_V are found in Galactic PDRs. We surmise that the r-CO* toward GRB 080607 could be a pre-burst observational signature of the PDR produced by the progenitor of the GRB, as it was forming a giant H II region around itself (Whalen et al. 2008). A detailed calculation of this process is clearly warranted.

4. CONCLUDING REMARKS

In addition to providing the first positive detection of H_2 bands and the first observation of CO bands in a GRB host galaxy (P09), we have shown that GRB 080607 also provides the first evidence for H_2* in a GRB host galaxy and marks the highest-redshifted H_2* detected to date.

This discovery of UV-pumped H_2* toward GRB 080607 serves to confirm the predictions for its production under precisely such circumstances (Draine 2000, DH02). Our initial static modeling with Ismod.f indicated log $N(H_2^*) < 18.0$ toward GRB 080607, significantly lower than the original predictions of DH02. We then showed that the dynamic models of DH02 can successfully reproduce observed H_2* absorption once modifications involving individual GRB luminosities and adjustable distance to the molecular cloud are incorporated. Thus, the DH02 photoexcitation code shows that the bulk of the molecular cloud harboring H_2* is located at a model distance of 230–940 pc along the line of sight from the UV afterglow. This is much farther than the original arrangement in DH02, but still in the local galactic neighborhood of GRB 080607. In the scheme of Whalen et al. (2008), a model distance of >230 pc for the molecular cloud means that it is located outside the ≈100 pc radius of H II region carved by the progenitor of GRB 080607.

One interesting result of the increased distance from the GRB to the gas is the inability of the radiation beam to destroy dust embedded in the cloud. Whereas in DH02 dust was easily destroyed at close quarters to the GRB, following its heating to 2000–3000 K, this process cannot operate at larger distances, leading to survival of the dust in the cloud. Such dust remains on the line of sight between the GRB and the H_2 destruction front, diminishing the effects of such destruction.

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[7] http://kurucz.harvard.edu/LINELISTS/LINESMOL/