DISCOVERY OF MOLECULAR HYDROGEN IN SN 1987A

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ABSTRACT

Both CO and SiO have been observed at early and late phases in SN 1987A. H2 was predicted to form at roughly the same time as these molecules, but was not detected at early epochs. Here, we report the detection of NIR lines from H2 at 2.12 and 2.40 μm in VLT/SINFONI spectra obtained between days 6489 and 10,120. The emission is concentrated to the core of the SN in contrast to Hα and approximately coincides with the [Si]Ⅱ/[Fe]Ⅱ emission detected previously in the ejecta. Different excitation mechanisms and power sources of the emission are discussed. From the nearly constant H2 luminosities, we favor excitation resulting from the 44Ti decay.

Key words: molecular processes – supernovae: general – supernovae: individual (SN 1987A)

1. INTRODUCTION

Observations of molecules in supernovae (SNe) have turned out to yield important diagnostics of the conditions in the cooling ejecta. The first examples were discovered in SN 1987A shortly after explosion. CO was first detected 112 days after explosion (Spyromilio et al. 1988) and persisted to over 600 days (Bouchet & Danziger 1993). Both the fundamental and overtone bands were detected. Somewhat later, at ∼160 days, the fundamental band of SiO was also detected (Aitken et al. 1988; Roche et al. 1991). From NLTE modeling of the rovibrational lines the masses were estimated to be ~10^-3 M☉ for CO (Liu et al. 1992) and ~(4-8) x 10^-4 M☉ for SiO (Liu & Dalgarno 1994). Recently, at an age of 26 years, both these molecules have been detected in rotational transitions at <100 K with ALMA (Kamenetzky et al. 2013; Matsuura et al. 2015). The CO mass was, however, at this epoch at least an order of magnitude larger than the estimate from the NIR observations in Liu et al. (1992), indicating that most of the molecule formation may have occurred later than the last NIR observations.

In addition to these molecules, Culhane & McCray (1995, hereafter CMC) predicted that molecular hydrogen, H2, would form in the core. Their calculations showed that between 400 and 1000 days after explosion this would increase from a very low level to ∼1% of the total H abundance, where it would freeze out. Utrobin & Chugai (2005) later found that H2 could be present in the tenuous H envelope even at ∼2 weeks after explosion, with an abundance of ∼10^-4 of atomic H.

Although predicted long ago, and constituting a substantial fraction of the ejecta mass, no detection of H2 has been found in an SN. While H2 has been detected in the Crab Nebula (Graham et al. 1990) the origin of this is unknown, although Graham et al. argue for the formation in the ejecta. In this Letter, we report clear evidence of H2 from NIR rovibrational ejecta lines in SN 1987A observed with VLT/SINFONI at very late phases.

2. OBSERVATIONS

The H- and K-band observations, covering 1.45–1.80 μm and 1.95–2.45 μm, respectively, were obtained from 2004 to 2014 using the SINFONI Integral Field Spectrograph at the VLT (Eisenhauer et al. 2003; Bonnet et al. 2004). The log of the observations is given in Table 1. The data were reduced using the standard ESO pipeline (Modigliani et al. 2007) and are discussed in detail in Kjær et al. (2010), together with modeling of the atomic emission. Additional dedicated software was developed by us to combine observations spread over many epochs. The absolute reproducibility (cross calibration) of the standard stars was better than 5%. The encircled energy of the PSF for 80% of the emission is 0.150 × 0′′125 in the 2005 K-band observation (Kjær et al. 2010), which gives a good measure of the spatial resolution. The spectral resolution is 66 and 110 km s^-1 for the K- and H-band, respectively. Because of the short exposure of the 2004 observations, we do not discuss this epoch further. The observations in 2004, 2005, 2011, and 2014 are discussed in Kjær et al. (2007, 2010), Larsson et al. (2013), and J. Larsson et al. (2016, in preparation).

The Q-branch of H2 at ∼2.4 μm is awkwardly located near the end of the K-band atmospheric window and also near the rise of the thermal background from the telescope, which could give rise to the appearance of features in the spectra. We have therefore examined individually all frames to ensure that the residual thermal and atmospheric backgrounds do not create artifacts that would mimic the Q-branch emission from the SN.

3. RESULTS

In Figure 1, we show a compilation of the K-band spectra of the ejecta from 2005 to 2014, days 6832, 7606, 8694, and 10,120. In order to minimize the contamination from the ring and to compare the fluxes from the same comoving region we use an expanding elliptical aperture enclosing the emitting H2 region, shown in Figure 2. Scattered light from the ring was removed as in J. Larsson et al. (2016, in preparation), using the fact that lines from the ring are much narrower (FWHM ~ 300 km s^-1) compared to the ejecta lines (FWHM ~ 2300 km s^-1). This subtraction is illustrated in the upper spectrum in Figure 1. The spectra were binned by a factor of three.
The strongest line at all epochs is the HeI 2.058 μm line. We also see a faint Brγ line at 2.166 μm. In addition to these, there is a clear line at 2.12 μm and a strong, broad feature at 2.40 μm. Based on the absence of other natural candidates (see Section 4.1), we identify the 2.12 μm line as the (1,0) S(1) transition in H2 and the feature at 2.40 μm as a blend of the (1, 0) Q(1–3) transitions at 2.406, 2.413, and 2.423 μm. We do not detect the overtone CO band, which would peak between 2.30 and 2.35 μm.

In Figure 2, we show the spatial distribution of 2005 of the 2.40 μm feature, with and without subtraction of the "continuum" in the line-free region between 2.300 and 2.345 μm, together with H2 2.12 μm, Hα from the Hubble Space Telescope (HST; Larsson et al. 2013), and HeI 2.058 μm and [Si i]/[Fe ii] from SINFONI (Kjær et al. 2010). The emission from the circumstellar ring in the 2.12 and 2.40 μm images is a result of blending with the high-velocity wing of the He I line.

4. ORIGIN OF THE H2 EMISSION

4.1. Spectral Modeling

To check that the identification of the lines with H2 is consistent with wavelengths and expected relative fluxes, as well as the presence of other lines in this spectral window, we have calculated synthetic spectra for different assumptions for the H2 excitation. Because the temperature in the H-rich gas in the SN core is \( \lesssim 200 \) K (Jerkstrand et al. 2011; Kamenetzky et al. 2013), thermal excitations of the vibrational levels are likely to be unimportant. The remaining possibilities are excitation by non-thermal electrons or, alternatively, by UV fluorescence. Both these processes can lead to ionization or photodissociation of the H2. Reformation of the molecule will then lead to vibrational–rotational excitation. Black &
Dalgarno (1976), however, argue that fluorescence should be more efficient, unless the UV flux is heavily absorbed.

There are two sources of non-thermal electrons in the ejecta. The $^{44}$Ti decay, which dominates the radioactive input (Jerkstrand et al. 2011; Boggs et al. 2015), produces positrons, which results in a cascade of non-thermal electrons with energies $\gtrsim 10$ eV. Whether the positrons will reach the H-rich blobs of the ejecta depends on the magnetic field. Coulomb collisions alone cannot trap them in the iron-rich regions where the positrons are created (Jerkstrand et al. 2011), but even a weak field decreases the mean free path dramatically. It is, however, conceivable that a fraction of the positrons may escape the $^{44}$Ti sites and may then ionize and excite the H-rich parts of the core. The other source of fast electrons may be X-rays from the interaction with the ring. The evolution of the optical flux from the ejecta is now dominated by these X-rays (Larsson et al. 2011). When absorbed, these give rise to fast electrons and a similar cascade of non-thermal electrons as the positrons (Fransson et al. 2013). A similar scenario has been advocated by Richardson et al. (2013) for the H$_2$ emission in the Crab Nebula. The presence of a pulsar generating the relativistic particles makes, however, the situation different from the ejecta in SN 1987A.

To test the non-thermal electron scenario, we use the relative fluxes calculated by Gredel & Dalgarno (1995, their Table 4). Note that the relative strengths of the lines depend on the rotational temperature of the ground state levels, as well as the degree of ionization. The calculation referred to assumes a temperature of 300 K for the ground state populations and an electron energy of 30 eV. We have then normalized the line fluxes to that of the 2.122 $\mu$m line. To approximately include the atomic lines, we have also added the $^{44}$Ti powered ejecta spectrum from Kjær et al. (2010), scaled to the extraction aperture we use (Figure 3).

There may also be a weak continuum contribution. Synchrotron emission from the ring is observed at radio wavelengths with a spectrum $F_{\nu} \approx 25(\nu/100 \text{ GHz})^{-0.8}$ mJy (Indebetouw et al. 2014). Extrapolating to 2.2 $\mu$m gives a flux of $\sim 4.8 \times 10^{-18}$ erg s$^{-1}$ cm$^{-2}$ $\lambda^{-1}$. A minor fraction from high-latitude emission above the ring plane could therefore contribute to the NIR continuum, unless synchrotron cooling would steepen the spectrum. Dust emission from ultra-small grains could also contribute. From ALMA observations, we know there is a strong source of dust emission in the core of the SN (Matsuura et al. 2015) with a temperature of $\sim 24$ K. Sarangi & Cherchneff (2015) find that the size distribution of grains ranges from $\sim 10$ Å to micron-sized grains. Ultra-small grains will be transiently heated by UV photons to very high temperatures (e.g., Draine 2011) and emit their radiation in the mid- to NIR. While the absolute line fluxes depend on the continuum level, our qualitative results for the spectral models are not sensitive to these assumptions. Because of the uncertainty, we have not included this component.

The line profiles are assumed to be Gaussian with FWHM = 2300 km s$^{-1}$, the same as that found for the CO lines (Kamenetzky et al. 2013). We concentrate here on the coadded H- and K-band spectra from 2005 and 2007, which have the best signal-to-noise ratio (S/N). In the lower panel of Figure 3, we show these spectra together with the synthetic spectrum.

UV fluorescence from the H$_2$ ground state requires photons between 912 and 1108 Å, which may be created internally in the ejecta (Section 5) or, alternatively, from the ring collision. Ly$\alpha$ is strong from the ring (France et al. 2011), and resonance fluorescence from the H$_2$ v = 2 levels (Shull 1978) may be possible. This process, however, requires either a temperature of $\gtrsim 1000$ K or a sufficiently strong UV field for a significant population of this level. Between 912 Å and $\sim 1150$ Å little is known about the flux from the ring.

For the UV fluorescence model, we have taken the relative H$_2$ line strengths from Model 14 of Black & van Dishoeck (1987) and again scaled this to the 2.122 $\mu$m flux. The relative line strengths are not very sensitive to the specific shape of the spectrum in the far-UV or to the density as long as this is $\lesssim 10^{14}$ cm$^{-3}$.

Comparing the two models, the relative flux of the 2.122 $\mu$m and the 2.40 $\mu$m lines is similar and close to the observed ratio, especially considering the uncertain continuum level. This, together with the good fit of the line profiles, confirms the H$_2$ line identifications. Note also the absence of atomic lines at both these wavelengths.

The main difference between the two models is the near absence of excitation to v $\geq$ 2 in the non-thermal model. In the K-band, Gredel & Dalgarno (1995) find the (2, 1)$S(1)$ 2.248 $\mu$m/(1, 0)$S(1)$ 2.122 $\mu$m ratio to be 0.54 the UV-dominated case, compared to 0.06 in the non-thermal electron case. From Figure 3, we see that the 2.248 and 2.223 $\mu$m lines give a better fit to the feature at $\sim 2.25$ $\mu$m for the UV fluorescence model. According to this model, weaker lines at 1.953, 2.034, 2.071, and 2.351 $\mu$m may also be present in the observations. Although the H-band is more crowded, we note that in the UV model there is a line feature at 1.74 $\mu$m that does not coincide with any line included in the atomic model and coincides with a blend of comparatively strong H$_2$ lines between 1.73 and 1.75 $\mu$m. Also, H$_2$ lines at 1.50 and 1.62 $\mu$m may possibly be present. The models in Figure 3 therefore favor the UV excitation model. This conclusion is, however, fairly marginal, given the S/N level of the spectrum and uncertainties in both the H$_2$ and atomic line fluxes.

From the line fits, we estimate the total luminosity in the 2014 (day 10,120) spectrum of the 2.40 $\mu$m H$_2$ lines to $\sim 6.2 \times 10^{32}$ erg s$^{-1}$ and of the 2.122 $\mu$m line to $\sim 2.4 \times 10^{32}$ erg s$^{-1}$. This should be compared to the total input from positrons that is $\sim 10^{36}$ erg s$^{-1}$, or $\sim 1/3$ of the bolometric luminosity (Larsson et al. 2011). For the non-thermal electron case, Gredel & Dalgarno (1995) find that 46% of the H$_2$ emission is in the 1.95–2.45 $\mu$m range, while in the UV fluorescence case, 15% is in this range. The total energy required for the IR H$_2$ lines is therefore $\sim 2 \times 10^{33}$ erg s$^{-1}$ and $\sim 6 \times 10^{33}$ erg s$^{-1}$, respectively.

4.2. Time Evolution

A distinguishing factor between the two different sources of energy for the H$_2$ emission, either from the radioactive decay of $^{44}$Ti in the ejecta or from an external UV or X-ray flux from the ring collision, is the time evolution. From day 6500 to 9200, both the soft and hard X-ray flux from the ring increased by a factor of $\sim 4.4$ (Helder et al. 2013). If the excitation is connected to the external X-ray or UV flux, we expect the H$_2$ emission to increase by a substantial factor, while the energy input by $^{44}$Ti is expected to decrease slowly.

A complication when measuring the flux evolution is the strong and wavelength-dependent "continuum" level, which most likely is a blend of weak lines and true continuum (e.g.,
This makes absolute measurements of the fluxes difficult and prone to systematic errors. Using the same prescription for the continuum level, the trends should, however, not be affected. For the “continuum” we use the average flux between 2.09 and 2.11 µm for the HeI and the H2 2.122 µm lines and the –2.30 2.35 µm range for the H2 2.40 µm blend, which are chosen to be reasonably free of other emission lines. To minimize any remaining contribution from scattered emission from the ring to the HeI line, we exclude for this line the central part within ±700 km s⁻¹ in the flux measurement.

From Table 2, we conclude that the H2 2.40 µm luminosity is nearly constant within the statistical errors, which we estimate to 0.15 × 10^{32} erg s⁻¹, while the HeI line shows an increase by a factor of ~2.3 from day 6832 to 10,120. The low H2 2.122 µm flux makes it difficult to draw any firm conclusion from this, although it is consistent with a constant flux within the errors. Note that these luminosities are likely to be systematically underestimated by a considerable factor, as is, e.g., seen from the models in Figure 3. The absolute luminosities given in Section 3 are probably more accurate. Here, we are more concerned with the time evolution, without making assumptions about the excitation mechanism.

The nearly constant H2 luminosities indicate that these lines are powered by the ^{44}Ti decay, either through the UV generated in the ejecta or possibly through leaking positrons.

5. DISCUSSION AND CONCLUSIONS

Summarizing, we find that the spectrum marginally favors the UV fluorescence model and that it is powered by the ^{44}Ti decay. These may together be realized if the excitation is dominated by diffuse internal UV radiation in the ejecta.

The H2 emission is concentrated to the core, as is the case for the [Si I]/[Fe II] 1.644 µm line (Figure 2). This result is consistent with the absence of time evolution. The presence of H2 in the core is also consistent with the Hα profile from Gamma-rays from the ^{44}Ti decay give an input decreasing with time as τ = t/τ decay. They, however, only contribute marginally to the H2 luminosity.

Table 2: H2 and HeI Luminosities

| Epoch | H2 2.122 µm | H2 2.40 µm | He I 2.058 µm |
|-------|-------------|-------------|--------------|
| 6832  | 0.37        | 3.11        | 1.10         |
| 7606  | 0.45        | 2.88        | 1.35         |
| 8694  | 0.57        | 3.32        | 1.59         |
| 10120 | 0.64        | 3.45        | 2.54         |

**Notes.** See the text for errors.

* In units of 10^{32} erg s⁻¹.

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Figure 3. Upper panel: coadded H- and K-band spectra from 2005 to 2007 (blue), together with the synthetic spectrum (black) for the UV-dominated H2 excitation model added to the ejecta spectrum from Kjærg et al. (2010). The individual contributions from H2 (red) and the Kjærg et al. spectrum (green) are shown. Lower panel: same for the non-thermal electron excitation model. Note the absence of H2 lines in the H-band for this model.
early observations, which was seen down to \( \lesssim 700 \text{ km s}^{-1} \) (Kozma \& Fransson 1998). Outside the core, the UV and X-ray emission from the ring collision may dissociate the \( \text{H}_2 \), while these X-rays are responsible for most of the \( \text{H}_\alpha \) emission, resulting in the “horseshoe” shape in Figure 2. The core itself is largely shielded from X-rays by the high metallicity (Fransson et al. 2013). Also, the UV from the ring may be absorbed at energies higher than the C\( \text{I} \) photoelectric threshold at 11.2 eV (<1100 Å), depending on the covering factor of the C-rich regions relative to the H-rich in the core.

The UV excitation scenario requires an internally generated UV field, like the \( \text{He}\alpha \) two-photon continuum, as proposed by CMC (see also Jerkstrand et al. 2011). CMC also point out that the total opacity of the H-rich region in the range 912 < \( \lambda \) < 1400 Å should be dominated by resonance scattering in the Lyman and Werner bands of \( \text{H}_2 \), converting the radiation in this region into fluorescence lines between 1400 and \( \lambda \sim 1700 \) Å. Sternberg (1989) has calculated this in detail, based on an ISM-like UV spectrum. Of particular interest is the strong blend of lines at 1590–1610 Å, which also stands out in the simulations of CMC. In the COS spectrum by France et al. (2011), there is indeed a weak feature at this wavelength. The spectrum is, however, complex, and the significance of this feature is marginal.

Most of the \( \text{H}_2 \) formation in the CMC models took place before \( \sim 1000 \) days after explosion. NIR observations between days 377 and 1114 (Meikle et al. 1993) showed a weak feature that they proposed could be due to the \( \text{Fe}\text{II} \) 2.133 \( \mu \text{m} \) line, but noted that this could be due to \( \text{Fe}\text{II} \) 2.133 \( \mu \text{m} \). In the spectra before 600 days, this feature was much stronger than in the models. The simulations of CMC, while at later epochs it was consistent with the models. The observations of Meikle et al. (1993) did not show the 2.40 \( \mu \text{m} \) line, so no definite conclusion could be drawn.

Other \( \text{H}_2 \) lines expected in the UV case include blends at \( \sim 1.24, 1.31, \) and 1.40 \( \mu \text{m} \). The J-band is, however, more crowded than the K-band and has a lower S/N and Strehl ratio and is therefore not shown here. The lowest excitation lines of \( \text{H}_2 \) at 28.211 and 17.030 \( \mu \text{m} \) are expected to have fluxes \( \sim 1.5 \) and \( \sim 1.0 \) times the 2.122 \( \mu \text{m} \) line, respectively.

Finally, the fact that the \( \text{He}\alpha \) line shows an increase similar to \( \text{H}_\alpha \) (Fransson et al. 2013) implies that at least part of this emission should be affected by the X-ray input from the ring collision. This is somewhat surprising, given the similar distribution of this emission to that of \( \text{H}_2 \) (Figure 2). The \( \text{He}\alpha \) emission, however, has contributions both from the H, He, and Fe/He zones (Kjær et al. 2010). The Fe/He component, together with the mixed-in H- and He-rich material in the core, may therefore explain the centrally peaked \( \text{He}\alpha \) emission, while the former two components in the envelope may be responsible for the luminosity increase, which is mainly seen in the line wings, as for \( \text{H}_\alpha \) (J. Larsson et al. 2016, in preparation).

In conclusion, the discovery of \( \text{H}_2 \) in SN 1987A adds a new and important diagnostic of the conditions in the ejecta and may, together with observations with ALMA, provide new insight into the chemistry of the H-rich regions of the core (e.g., Cherchneff \& Dwek 2009).

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