MOLECULES AND DUST IN SUPERNOVAE

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Abstract. Observations of molecules and dust in supernova SN 1987a and SN 1995ad are summarised and the inferred masses of CO and SiO are presented. The chemistry is used to argue that macroscopic mixing occurred in which the interpenetrating clumps in the ejecta retained their microscopic integrity. An explanation of the anomalous temperature structure is advanced. Molecular candidates for some of the unidentified spectral features are proposed.

1. Introduction

Emission from molecules has been observed in the late-time spectra of two supernovae, SN 1987a and SN 1995ad, both of type II. Due to the very different physical conditions of larger masses of radioactive elements, lower gas densities, and higher ionization fractions, molecules are not expected to be present in detectable amounts in supernovae of type Ia (Liu 1997).

At late times, supernova ejecta become optically thin, exposing the interior region of the object. The spectra yield reliable abundance estimates of the elements produced in the event, placing constraints on the parameters derived from explosive nucleosynthesis models. The observed, though rare, molecular emissions, give further information on the elemental abundances while the chemistry required to produce the observed molecules, or to limit the abundances of undetected molecules, places restrictions on the hydrodynamics and mixing in the ensuing expansion.

In SN1987a, carbon monoxide was seen in emission from several vibrational levels in Δv = 2 transitions at wavelengths between 2.3 μm and 2.5 μm (Spyromilio et al. 1988, Meikle et al. 1989, 1993) and Δv = 1 transitions at twice the wavelengths (Rank et al. 1988, Bouchet and Danziger 1993) and silicon monoxide was seen in emission in Δv = 1 transitions near 8 μm (Rank et al. 1988, Aitken et al. 1988, Bouchet, Danziger and Lucy 1991, Wooden et al. 1993, Roche, Aitken and Smith 1993). There is clear evidence of dust formation in the ejecta of SN 1987A (Lucy et al. 1989, 1991, Moseley et al. 1989, Danziger et al. 1991, Dwek et al. 1992). The dust may have formed in the same clumps as the molecules.

In SN1995ad, emission is detected at low resolution near 2.3 μm which is almost certainly attributable to Δv=2 transitions of carbon monoxide (Spyromilio and Leibundgut 1996). In SN 1987a, there are several unidentified features, which may be molecular in origin. Miller et al. (1992) have suggested that features at 3.41 μm and 3.53 μm may arise from H_3^+ and Petuchowski et al. (1989) that a feature at 2.26 μm may arise from CO^+.

2. Carbon Monoxide

The interpretation of the observations of CO emission requires some care because at early times the emissions are optically thick and at later times the vibrational levels fall out of thermal equilibrium (Liu, Dalgarno and Lepp 1992). The emission profiles depend on the expansion velocity and the ambient temperature and the emission intensities are a measure of the total content of CO. Analysis of the observational data indicated a uniform expansion velocity of 2000 km s^{-1}, a temperature decreasing from 1800K at day 100 to 1500K at day 400 and a total CO mass of 0.045 $M_\odot$ at day 100, diminishing to a nearly constant value of about 5×10^{-3} $M_\odot$ after day 200 (Liu and Dalgarno 1995).

The formation and destruction processes of CO in the ejecta have been explored by Petuchowski et al. (1989), Lepp, Dalgarno and McCray (1990), Rawlings and Williams (1990), and Liu, Dalgarno and Lepp (1992). The principal formation mechanism is the radiative association of C and O atoms

$$C + O \rightarrow CO + \nu \tag{1}$$

(Dalgarno, Du and You 1990). In the presence of helium, the reaction

$$He^+ + CO \rightarrow He + C^+ + O, \tag{2}$$

is a major source of destruction, so efficient that little CO exists in regions containing a significant amount of helium (Liu, Dalgarno and Lepp 1992, Liu and Dalgarno 1995). The presence of CO demonstrates that limited small scale mixing has occurred and, in the macroscopic mixing of the layers of the progenitor star that is postulated to explain the early escape of X-rays and γ -rays (McCray 1993, Woosley et al. 1995), the interpenetrating clumps of material retain their microscopic integrity.

The macroscopic mixing provides a natural explanation of the temperature inhomogeneities that are observed. In oxygen rich clumps containing helium, CO is not present and cooling occurs mostly by excitation of oxygen to the metastable ^1D level. Heating by γ-rays then yields a temperature of 3000K at day 400 (Li and McCray 1992). In the absence of helium, CO survives and excitation of its vibrational levels is a powerful cooling agent, driving the temperature down to 1500K (Liu and Dalgarno 1995).

3. Silicon Monoxide

As for CO, the level populations of SiO are far from local thermodynamic equilibrium and the equations of statistical equilibrium must be solved explicitly in order to interpret quantitatively the observed emission from SiO (Liu and Dalgarno 1994). The analysis indicates an abundance of between 10^{-3} and 10^{-4} $M_\odot$ of SiO, increasing slowly with time from day 250 to day 540.

The major source of SiO is the radiative association process

$$Si + O \rightarrow SiO + \nu \tag{3}$$

(Liu and Dalgarno 1994). Fair agreement between the SiO masses inferred from observation and predicted by chemistry is obtained with the rate coefficient for reaction (3) calculated by Andreazza, Singh and Sanzovo (1995) and loss determined by the ion-molecule charge transfer reactions

$$Ne^+ + SiO \rightarrow SiO^+ + Ne \tag{4}$$

and

$$Ar^+ + SiO \rightarrow SiO^+ + Ar \tag{5}$$

(Liu and Dalgarno 1996).

4. Candidate Molecules

There are discrepancies between the theoretical and measured SiO emission line profiles which, it appears, can only be resolved by postulating an additional source of emission or absorption. A candidate molecule is carbon monosulfide, CS, since the Δv=1 transitions lie on the long wavelength side of the SiO emissions. The Δv =2 transitions of CS would then be expected in the 3.9 μm region and indeed a feature at 3.9 μm had been previously attributed to CS by Meikle et al. (1989).

Figure 1 shows the infrared spectra from Meikle et al. (1989) along with the line positions of CS. The height of the lines is proportional to the population of the upper level at an excitation temperature of 2000K.

The difficulty with the identification lies with the chemistry of CS. It is formed by

$$\mathrm{C} + \mathrm{S} \rightarrow \mathrm{CS} + \nu \tag{6}$$

and by sequences involving negative ions, such as associative detachment

$$\mathrm{C} + \mathrm{S}^- \rightarrow \mathrm{CS} + e, \tag{7}$$

but destruction through

$$\mathrm{CS} + \mathrm{O} \rightarrow \mathrm{CO} + \mathrm{S} \tag{8}$$

is rapid at the temperatures of the ejecta. However, the abundance of CS required to explain the measured intensities may not be large. Figure 1 shows that the P branch of the 2-0 vibrational transition of CS is overlapped by the broad Brα line of atomic hydrogen in the spectrum so that the v=2 level may be efficiently populated by Brα pumping.

Other features are present in the spectrum near 3.9 μm. A possible candidate molecule is iron monoxide. As can be seen in Figure 1 the P and Q branches lie under the feature identified as CS while the R branch has a smaller feature at 3.85 μm. The explosive nucleosynthesis models (cf. Woosley 1988) predict a narrow overlap of the iron and oxygen layers of the progenitor star. The possible presence of FeO may suggest some unusual chemistry, efficient Brα pumping, or limited microscopic mixing at the interface. One intriguing possibility is that FeO is made by stimulated radiative attachment of the Fe atom

$$\mathrm{Fe} + \mathrm{e} + \nu \rightarrow \mathrm{Fe}^- + \nu + \nu, \tag{9}$$

followed by the reaction

$$\mathrm{Fe}^- + \mathrm{O} \rightarrow \mathrm{FeO} + \mathrm{e}. \tag{10}$$

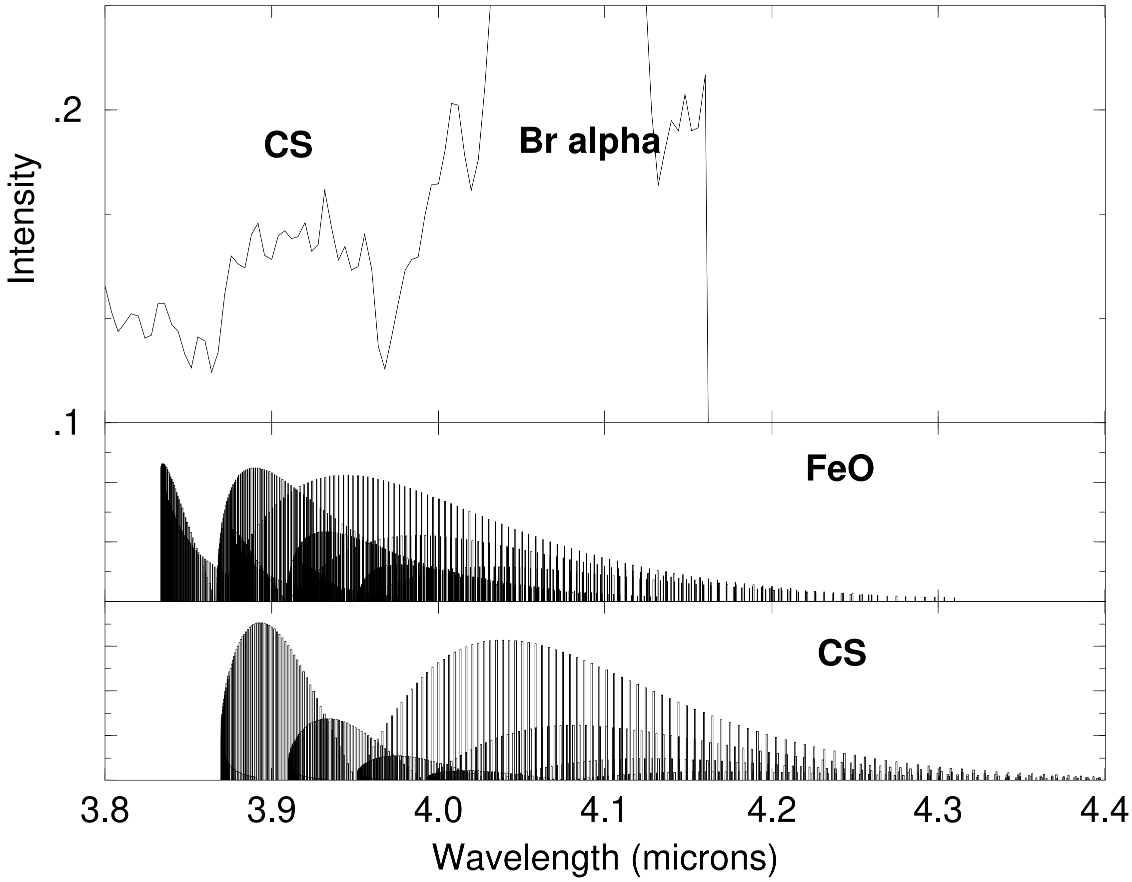

Figure 1. The infrared spectrum of SN1987A on day 192 (from Meikle et al. 1989) along with the line positions for CS and FeO. The height of the lines is proportional to the LTE population of the upper level at 2000K. The positions are for $\Delta v = 2$ transitions from upper vibrational levels of 2, 3, 4 and 5 for CS and $\Delta v = 3$ transitions from upper vibrational levels 3, 4 and 5 for FeO. The observed spectra terminates near 4.15 μm due to atmospheric absorption at longer wavelengths.

Though both oxygen and iron are cosmically abundant, searches for FeO in other astronomical environments have been unsuccessful (Merer, Walmsley and Churchwell 1982), possibly due to iron depletion onto grains.

Two pronounced features at 3.41 μm and 3.53 μm have been tentatively attributed to H_3^+ (Miller et al. 1992) but calculations of Culhane and McCray (1995) yield abundances of H_3^+ that are much too small to explain the measured intensities. The model of Culhane and McCray (1995) assumes the temperature in the hydrogen envelope to be characterized by [CaII] emission ($T > 4000$K) and H and He 2-photon UV continua efficiently photodissociate H_2. Without significant quantities of H_2, the abundance of H_3^+ is negligible because it is produced by reaction with H_2 of H_2^+

$$H_2^+ + H_2 \rightarrow H_3^+ + H, \tag{11}$$

and of excited atomic hydrogen H^*

$$H^* + H_2 \rightarrow H_3^+ + e, \tag{12}$$

However, macroscopic mixing can produce cooler hydrogen rich clumps in which H_2 can be self-shielded from photodestruction and an alternative model developed by Yan and Dalgarno (1997) may be more successful.

There is a pronounced feature at 2.26 μm which increases in strength relative to the CO emission as time progresses. It happens to match the 2-0 vibrational transition of CO^+ (Petuchowski et al. 1989). Because dissociative recombination

$$CO^+ + e \rightarrow C + O \tag{13}$$

is so rapid, it seems unlikely that a sufficient abundance of CO^+ can exist in the ejecta. The unidentified emission feature is also present in the spectra of Nova Cassiopeia 1993 (Evans et al. 1996).

The presence of SiO suggests that moderate abundances of SO and SiS may exist in the ejecta. Unfortunately, the location of their emission bands are either overwhelmed by the CO bands or strong atomic lines or are coincident with gaps in the observed spectra. However, SO may contribute to the emission attributed to the SiO near 8.8 μm.

Because of the paucity of hydrogen in the inner ejecta, hydride molecules are not expected in the core. The outer envelope is composed primarily of hydrogen and helium, and Miller et al. (1992) have tentatively assigned weak features at 3.364 μm and 3.607 μm to HeH^+.

5. Dust

Clear evidence was found of dust formation at day 450 when the temperature in the molecular clumps was 1500K and the density of order 10^{10} cm^{-3}. Blue shifts were observed in the emission lines between 370 nm and

1 μm and attributed to the attenuation by dust of emission from the receding side of the ejecta (Lucy et al. 1991). An infrared brightening occurred suggesting thermal emission from dust (Roche et al. 1989, Wooden et al. 1993, Bouchet and Danziger 1993, Colgan et al. 1994). This increase in the IR luminosity was accompanied by a larger than expected decrease in the optical light curve, with the sum of the visible and dust IR luminosities equaling that expected from thermalized γ-rays. An IR excess is also present prior to day 450, but it is probably circumstellar in origin. The intensity of the blend of SiI at 1.645 μm and FeII at 1.644 μm diminished relative to the adjacent continuum and Lucy et al. (1991) suggested that the gas phase silicon and iron were depleted to form dust grains. The composition of the dust has been discussed by Lucy et al. (1991), Dwek et al. (1992), Wooden et al. (1993), and Colgan et al. (1994). It does not appear to be characteristic of interstellar silicates or polycyclic aromatic hydrocarbons, but the dust probably formed in the cool molecular rich clumps. There is evidence that the dust condensation moved closer to the ejecta core with time (Wooden et al. 1993), indicating that graphite grains may have formed first, followed by silicates and then metallics. Colgan et al. (1994) suggested that the dust formed in the iron core may be made of FeS grains, since some sulfur is mixed in the iron layer of the progenitor. The total mass of dust is estimated at 10^{-4} $M_{\odot}$, somewhat less than the mass of SiO.

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