Atomic and molecular supernovae

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Abstract. Atomic and molecular physics of supernovae is discussed with an emphasis on the importance of detailed treatments of the critical atomic and molecular processes with the best available atomic and molecular data. The observations of molecules in SN 1987A are interpreted through a combination of spectral and chemical modelings, leading to strong constraints on the mixing and nucleosynthesis of the supernova. The non-equilibrium chemistry is used to argue that carbon dust can form in the oxygen-rich clumps where the efficient molecular cooling makes the nucleation of dust grains possible. For Type Ia supernovae, the analyses of their nebular spectra lead to strong constraints on the supernova explosion models.

1. Introduction

Supernovae, the violent stellar explosions, are classified according to their spectroscopic characteristics near maximum optical light. Depending on its spectrum showing evidence of hydrogen or not, a supernova is classified as Type II or Type I. A Type I supernova is further classified as Type Ia or Type Ib/c depending on the presence or absence of a strong silicon feature. The spectrum of a Type Ib supernova shows strong helium lines while that of a Type Ic supernova does not. Physically, Type II and Type Ib/c supernovae are explosions of massive stars produced by core collapse following late stages of nuclear burning, while a Type Ia supernova is believed to result from the thermonuclear runaway burning of an accreting white dwarf in a binary system.

Interpretations of the observations of molecular emissions from Type II supernova 1987A and atomic emissions from Type Ia supernovae are summarized here. The relevant physics and chemistry are discussed with an emphasis on the important atomic and molecular processes in the expanding ejecta during the nebular phase which begins several months after the explosion. Late-time nebular spectra offer significant advantages over early-time photospheric spectra as diagnostics of the supernova physics and chemistry.

DISCLAIMER

During the nebular phase, the supernova ejecta are optically thin at least at optical and infrared wavelengths, while during the photospheric phase, the radiative diffusion time scale in the ejecta is longer than the evolution time scale. As a result, the nebular spectra are dominated by emission lines produced following collisional excitation of atoms and molecules, while the photospheric spectra consist of both emission and absorption lines produced after complicated multiple absorption and scattering processes. Thus the nebular spectra provide more powerful and reliable diagnostics of the physical conditions and chemical structures of the supernovae and yield better constraints on the explosion mechanisms, nucleosynthesis, and hydrodynamics of the supernovae.

2. Type II supernova 1987A

2.1. Carbon monoxide

Type II supernova 1987A is the brightest supernova to be observed since SN 1604 observed by Kepler, the first to be observed in every band of the electromagnetic spectrum and in neutrino, and the first in which molecules have been observed, including CO, SiO and H_3^+.
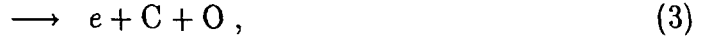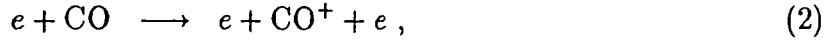
The first overtone band ($\Delta v = 2$) emission of CO in SN 1987A was detected from several vibrational levels at wavelengths between 2.3μm and 2.5μm as early as 110 days after the explosion (Meikle et al. 1989) and as late as 574 days (Meikle et al. 1993). This identification is supported by the presence of the fundamental band ($\Delta v = 1$) emission at about 4.6μm from 157 days to 532 days (Bouchet and Danziger 1993). The subsequent disappearance of the CO emission may be caused by the decrease in temperature and density rather than the change in CO mass (Liu and Dalgarno 1995). The emission detected in another Type II supernova, SN 1995ad, at low sensitivity and resolution near 2.3μm (Spyromilio and Leibundgut 1996) is very likely due to CO.

Interpretations of the first overtone spectra of CO in SN 1987A require detailed modeling of the excitation of its vibrational levels by thermal electron impact. The observed spectra differ significantly from the synthetic spectra at late times obtained by assuming that the rovibrational level populations are in local thermodynamic equilibrium (LTE) and the emission lines are optically thin (Spyromilio et al. 1988). But a remarkable agreement between the observed and synthetic spectra has been achieved by Liu et al. (1992) and Liu and Dalgarno (1995) by taking into account the effects of the departure from LTE and the finite optical depths. Their spectral analyses indicate an expansion velocity of 2000 km s^{-1}, a temperature decreasing from 1800 K at 100 days to 1500 K at 400 days and to 1000 K at 600 days, and a mass decreasing from 4×10^{-2} M$_\odot$ at 100 days quickly to 3×10^{-3} M$_\odot$ at 350 days and then increasing slowly to 5×10^{-3} M$_\odot$ at 600 days.

The observed CO masses agree well with those predicted by the chemistry (Liu and Dalgarno 1995). The CO is formed via radiative association

$$C + O \longrightarrow CO + h\nu \,, \tag{1}$$

and it is destroyed by the fast electrons produced by the γ-rays released from the decay of ^{56}Co,

$$e + CO \longrightarrow e + CO^+ + e \,, \tag{2}$$
$$\longrightarrow e + C + O \,, \tag{3}$$
$$\longrightarrow e + C^+ + O + e \,, \tag{4}$$
$$\longrightarrow e + O^+ + C + e \,. \tag{5}$$

The rapid decline of the CO mass at early times is caused by the increasing destruction rate by the fast electrons resulting from the enhancing energy deposition rate in the region. For any significant microscopic mixing of helium in the CO gas, charge transfer

$$He^+ + CO \longrightarrow C^+ + O + He \,, \tag{6}$$
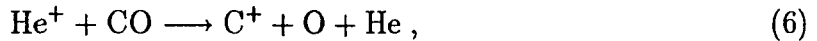
would be so efficient that little CO could survive in the ejecta. The presence of CO in the supernova indicates that the mixing, which was brought about by dynamical instabilities and caused an interpenetration of different layers, must be on a macroscopic scale rather than the microscopic scale.

Although the CO mass in SN 1987A is less than 10^{-3} of the ejecta mass, the CO emission accounts for more than 10^{-2} of the total emission from the supernova. As the dominant coolant in the carbon-oxygen region, the CO emission should follow the ^{56}Co decay rate if the energy deposition in the ejecta is uniform. However, the CO emission intensity actually increases at early times until about 200 days. Similar behaviors were also observed for many strong atomic emission lines other than those of the iron group species. The non-uniform energy deposition at the early times is a natural result of the large optical depth of the γ-rays in the iron core. As the ejecta expand and the optical depth decreases, the fraction of energy deposition in the iron core declines, while the fractions in other regions including the carbon-oxygen region rise. As the energy deposition becomes more uniform later, the CO light curve does follow the ^{56}Co decay rate closely (Liu and Dalgarno 1995).

The gradual increase in the energy deposition in the CO gas accounts partly for the roughly constant CO temperature observed during the first year (Liu and Dalgarno 1995). The decline in temperature at later times is caused by the increasing cooling by CO, due to the increasing departure from LTE, as well as by the decrease in heating rate. Extra heat to the CO gas is provided by the C and O atoms whose metastable ^{1}D states are superthermal due to excitation by the fast electrons. On the other hand, the O atoms provide the major but relatively less efficient cooling in the molecule-deficient oxygen gas whose temperature is higher at ~ 3000 K at 400 days (Li and McCray 1992; Liu and Dalgarno 1995).
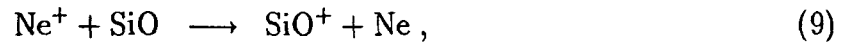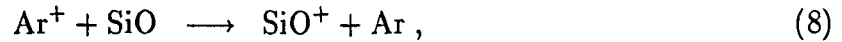
2.2. Silicon monoxide

The fundamental band emission of SiO at about 8μm was detected in SN 1987A between 160 days and 519 days (Aitken et al. 1988; Bouchet et al. 1991). Its first overtone band

emission at about 4μm should be overwhelmed by the much stronger broad Brα line of atomic hydrogen. The disappearance of the SiO emission later was accompanied by the onset of dust formation in the ejecta around 530 days (Lucy et al. 1989; Danziger et al. 1991), suggesting that the SiO may have provided the seed for grain nucleation. There are detailed differences between the observed and calculated fundamental SiO spectra, and they may be caused by other emission or absorption (Liu and Dalgarno 1994).

The spectral analyses yield an SiO mass of several times 10^{-4} $M_\odot$ in SN 1987A (Liu and Dalgarno 1994), consistent with the prediction by the chemistry (Liu and Dalgarno 1996). Similar to CO, the major source for SiO is radiative association

$$Si + O \longrightarrow SiO + h\nu \, , \tag{7}$$

but different from CO, the leading sink of SiO is charge transfer

$$Ar^+ + SiO \longrightarrow SiO^+ + Ar \, , \tag{8}$$
$$Ne^+ + SiO \longrightarrow SiO^+ + Ne \, , \tag{9}$$
$$\longrightarrow Si^+ + O + Ne \, . \tag{10}$$

Because the calculated SiO mass depends on the composition adopted in the chemical model, comparison of the measured and calculated SiO masses put constraints on the supernova nucleosynthesis models. The observations are more consistent with the composition predicted by Woosley et al. (1988) than by Thielemann et al. (1990).

2.3. Carbon sulfide

The late-time infrared spectra of SN 1987A (Meikle et al. 1989, 1993) contain a broad-hump feature at about 3.9μm which coincides in wavelength with the first overtone emission of carbon sulfide. The emission around 8μm may have significant contribution from CS in addition to SiO (Lepp et al. 1998). The identification of CS would require a large mass of CS of order 10^{-3} $M_\odot$ if its vibrational levels are excited mainly by thermal electron impact (Liu 1998). This mass is roughly comparable to the masses of CO and SiO in the supernova.

However, the identification of CS is difficult because the chemistry produces a much lower CS mass of order 10^{-11} $M_\odot$ (Liu 1998). The formation efficiency is much lower for CS than CO and SiO because the mixing between C and S is much lower than between C and O and between Si and O. More importantly, the destruction efficiency is much higher for CS than CO and SiO because the CS is rapidly removed in reaction

$$O + CS \longrightarrow CO + S \, , \tag{11}$$

by atomic oxygen which is the most abundant species everywhere carbon and sulfur overlap.

The difficulty could be eased if more efficient excitation mechanisms exist. Since the P branch of the $2 - 0$ band of CS coincides in wavelength with the broad Brα line of

atomic hydrogen, the $v = 2$ level of CS can be populated by the Brα pumping (Dalgarno et al. 1998; Liu 1998). However, this introduces more difficulties, as detailed by Liu (1998). First of all, the pumping of CS is overwhelmed by the pumping of the much more abundant SiO. Secondly, the emission intensity of the first overtone bands of SiO is consistent with the thermal electron impact as the major excitation mechanism. Finally, the SiO mass would have been overestimated previously if the pumping is important, and if so, the stable SiO molecules would have to be removed by mechanisms more efficient than charge transfer reactions (8)-(10).

2.4. H_3^+

Two emission features at 3.41μm and 3.53μm in the infrared spectrum of SN 1987A at 192 days (Meikle et al. 1989) has been attributed by Miller et al. (1992) to H_3^+ with a mass of order 10^{-8} M$_\odot$ in the hydrogen envelope. But a detailed chemical model constructed by Culhane and McCray (1995) yields a much lower H_3^+ mass of order 10^{-12} M$_\odot$ due to the lack of H_2 which is the major source of H_3^+.

Culhane and McCray (1995) argued that the H_2 in the supernova is rapidly photodissociated and collisionally dissociated. But the photodissociation should not be very important because of the low abundances of metastable H and He. Also, the collisional dissociation would be much less important in the H_2 clumps because cooling by CO could lead to a temperature much lower than 7000 K which is adopted in the model and characterized by the measured [CaII] emission (Li and McCray 1993).

A successful model of H_3^+ has recently been advanced by Yan and Dalgarno (1998). Their calculations result in two steady-state solutions with very different temperatures. In the warm region where the temperature is high at 7000 K and the Ca$^+$ emits, H_2 and H_3^+ are deficient. But in the cooler region where the temperature falls below 3000 K due to the efficient cooling by CO, there exist abundant H_2 and H_3^+. Their calculated H_3^+ abundance of 10^{-8} M$_\odot$ is consistent with the observations.

2.5. Dust

The formation of molecules in SN 1987A naturally leads to formation of dust in the ejecta. The evidence includes the blue shifts of many optical emission lines around 500 days likely due to attenuation by dust (Lucy et al. 1991), the more rapid decline in the line intensities than expected from thermalized γ-rays (Danziger et al. 1991), the brightening of the infrared continuum indicative of thermal emission from dust (Roche et al. 1989; Bouchet and Danziger 1993), and the diminishing of the line emissions from metals and molecules relative to the adjacent continuum (Lucy et al. 1991; Bouchet and Danziger 1993) due probably to their depletion to form dust grains. On the other hand, the infrared excess observed before 450 days is believed to be circumstellar in origin.

Although the compositions and sizes of the dust in SN 1987A are not well determined (Lucy et al. 1991; Dwek et al. 1992; Colgan et al. 1994), there seems to be a trend of condensation moving inward as the ejecta evolved (Wooden et al. 1993). If so, graphite

grains may have formed first, followed by silicates and later by metallics containing iron. Graphite grains can form in the ejecta even though carbon is less abundant than oxygen. Oxidation of the carbon is not very effective in the non-equilibrium chemistry in the supernova so that only a small fraction of the carbon is locked in CO (Liu and Dalgarno 1995). The abundant free carbon are available for condensation in the ejecta. The implications of this non-equilibrium chemistry to dust formation in supernovae have been elaborated lovely by Clayton (1998) in this symposium.

The grain condensation requires a cool environment which are achieved most likely through molecular cooling in the supernova. The atomic gas deficient in molecule is too warm to condense dust because the atomic cooling is relatively less efficient. In the oxygen core, dust may form in the clumps rich in CO or SiO with temperatures of about 1000 K at 500 days (Liu and Dalgarno 1994, 1995), while the clumps with very little molecules inside should be dust-free because the temperature is much higher at about 3000 K at 500 days (Li and McCray 1992). Colgan et al. (1994) speculated that FeS may be an important constituent of the dust in the iron core where some limited amount of sulfur exists. But the iron core may be too warm for dust condensation to occur in it according to the spectral analyses of Li et al. (1993). It would be interesting to see whether more efficient cooling can occur in the denser clumps or due to possible molecular cooling.

3. Type Ia supernovae

No observational evidence exists of molecular formation in Type Ia supernovae whose physical conditions and elemental composition differ significantly from those of Type II supernovae. With more abundant radioactive materials and lower gas densities, Type Ia supernovae are characterized by much higher ionization stages and higher temperatures. Thus they are an unfavorable environment for molecular and dust formation (Liu 1997), though Clayton et al. (1997) have suggested otherwise for dust formation.

Type Ia supernovae are very rich in iron-group elements, and their nebular spectra contain mainly broad emission lines of singly and doubly charged ions of iron and cobalt. Accurate models of the ionization and thermal structures of the iron core have now become available because of the recent improvements both in the quality of relevant atomic data and in the treatment of critical atomic processes. The ionization of the iron core is made by a combination of the fast electron impact ionization and charge transfer, while photoionization is relatively less important because it is made possible only by the recombination photons which undergo a complicated cascading process and are softened (Liu et al. 1998).

Density and composition of the iron core can be inferred through spectral analyses and they are consistent with those predicted by the sub-Chandrasekhar-mass models (Woosley and Weaver 1994b) but inconsistent with those by the Chandrasekhar-mass models (Thielemann et al. 1986; Woosley and Weaver 1994a). The Chandrasekhar-mass models predict a too dense core and too much stable nickel to match the observations

(Liu et al. 1997a,b,c, 1998). It should be noted that these conclusions are based on the best available atomic data. Future advance on the atomic data front may either reinforce or alter the assessment of the explosion models. It is interesting to mention that the spectral calculations by Ruiz-Lapuente (1996) favor the Chandrasekhar-mass models over the sub-Chandrasekhar-mass models. The discrepancy is caused mainly by the use of different atomic data and also by the different treatments of the critical atomic processes. The new results presented by Liu et al. (1997a,b,c, 1998) should be more reliable because of the better treatment of the critical atomic processes with the better quality of atomic data.

Acknowledgements

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