

OPTICAL EMISSION FROM SHOCK WAVES. I. ABUNDANCES IN N49

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ABSTRACT

From models of plane-parallel radiating shock waves and the observations of Osterbrock and Dufour, the abundances of oxygen, nitrogen, neon and sulfur (and indirectly, of carbon) are derived for the Large Magellanic Cloud supernova remnant N49. These are somewhat smaller than solar values, and it is concluded that the discrepancies between these and values derived for the LMC H II regions reflect the composition of "ice" grains with low sublimation temperatures which are destroyed in the supernova event.

Subject headings: galaxies: Magellanic Clouds — nebulae: abundances —
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I. INTRODUCTION

The optical filamentary nebulosity associated with supernova remnants in their later stages of evolution has long been suspected of being excited by collisions following the passage of a shock wave through the interstellar medium. This has been abundantly confirmed by increasingly sophisticated models of shock waves, of which those of Cox (1972) represent the best quantitative work so far (see this reference also for discussion of earlier work).

However, very little effort has so far been put into the question of elemental abundances in supernova remnants. This is principally because, unlike H II regions or planetary nebulae, a highly detailed dynamical model is required to interpret the line ratios which demands fairly accurate knowledge of all the atomic parameters and large amounts of computing time. As a result, little is known about the variation of line intensity ratios as a function of postshock temperature and density or other important parameters.

The aim of this paper is to produce a model which gives an optimum fit to the observed intensities in N49 taken from the very excellent work of Osterbrock and Dufour (1973) and to compare derived abundances with those obtained by Dufour (1975) for several H II regions in the Large Magellanic Cloud (LMC). In a later paper a set of diagnostic diagrams will be given for various important line ratios which will enable abundances and physical parameters to be estimated for remnants not as well observed as the one in question.

II. PRESOCK CONDITIONS

Consider a plane-parallel shock wave passing through the interstellar medium with a velocity of order 100 km s^{-1} . In the absence of a magnetic field, the presock and postshock conditions will be related

by the usual Rankine-Hugoniot conditions

$$\rho_1 v_1 = \rho_2 v_2, \quad (1)$$

$$\rho_1 \left(\frac{RT_1}{\mu_1} \right) + v_1^2 = \rho_2 \left(\frac{RT_2}{\mu_2} \right) + v_2^2, \quad (2)$$

$$\frac{\gamma_1}{\gamma_1 - 1} \frac{RT_1}{\mu_1} + \frac{v_1^2}{2} = \frac{\gamma_2}{\gamma_2 - 1} \frac{RT_2}{\mu_2} + \frac{v_2^2}{2} + Q_I + Q_c, \quad (3)$$

where v , T , ρ , μ are the gas velocity, temperature, density, and mean molecular weight, respectively, γ is the ratio of specific heats (taken as $5/3$ since we are dealing with a monatomic gas). Subscripts 1 and 2 refer to presock and postshock variables, respectively. Q_I is the heat required to ionize the gas (measured in ergs g^{-1} in cgs units), and Q_c is the net heat loss due to all the cooling processes. If x_H and x_{He} are the fractional ionizations of hydrogen and helium, respectively, then two subsidiary relations follow:

$$\mu = \frac{1 + 4.008Z(\text{He})}{(1 + x_H) + Z(\text{He})(1 + x_{He})}, \quad (4)$$

$$Q_I = \frac{h\nu_0(x_H + 1.808Z(\text{He})x_{He})}{M_H[1 + 4.008Z(\text{He})]}, \quad (5)$$

where ν_0 is the frequency of the Lyman limit, $Z(\text{He})$ is the helium abundance, and M_H is the mass of the hydrogen atom.

Provided initial conditions are defined and the coupled ionization-cooling equations can be solved, the radiative loss that produces a given postshock temperature can be easily found from equations (1)–(5).

However, the choice of presock conditions depends on whether the presock gas is ionized or not. Pre-ionization could occur in two ways. First, the shock

could be moving into a relict H II region produced by ultraviolet photons from the initial explosion. This point of view is emphasized by, for example, Brandt (1971), who considers the Gum Nebula to be an archetype. However, this point of view is challenged on theoretical grounds by Kahn (1974), who shows that the color temperature of the initial fireball is far too low to give sufficient ionizing radiation. Instead, he suggests that radiation from any pulsar produced as a result of the supernova could supply the necessary energy.

A second reason for supposing the preshock gas to be ionized was put forward by Cox (1972), who points out that in the radiative region of the shock, recombination of hydrogen to the ground state and also collisional excitation of certain ultraviolet resonance lines of heavy elements can produce photons which ionize hydrogen. These photons are unlikely to be absorbed in the cooling region of the shock and so can preionize the gas ahead.

The minimum postshock temperature that can possibly induce preionization can be estimated from the following argument.

The one-dimensional equation of transfer of the ionizing photons N_* is given by

$$\frac{dN_*}{dx} = 0.378\alpha N(H^+)N_e - \sigma N(H^0)N_*, \quad (6)$$

where 0.378α is the hydrogenic recombination rate to the ground state and σ is the photoionization cross section which will be close to the threshold value. Hence N_* must be given by the inequality

$$\frac{N_*}{N(H)} \leq 0.378 \frac{\alpha N(H)^+}{\sigma N(H^0)}, \quad (7)$$

where $N(H)$ is postshock density which approximately equals 4 times preshock density. If collisional ionization equilibrium applies in the postshock region, then

$$\frac{N_*}{N(H)} \leq 0.378 \frac{\epsilon}{\sigma}, \quad (8)$$

where ϵ is the collisional ionization rate which (derived from Canto and Daltabuit 1974) is

$$\epsilon = 1.01 \times 10^{-10} T^{1/2} (1 + 1.268 \times 10^{-5} T) \times \exp(-157800/T). \quad (9)$$

However, for preionization, the number of ionizing photons per atom emerging from the leading edge of the front must be greater than of the order unity, so

$$\frac{v_1}{4} \approx \left(\frac{R}{3}\right)^{1/2} T^{1/2} \leq \frac{N_*}{N(H)} \leq 0.378 \frac{\epsilon}{\alpha}, \quad (10)$$

which yields

$$T \geq 19,000 \text{ K}.$$

This is sufficiently low that preionization can be assumed for supernova remnants.

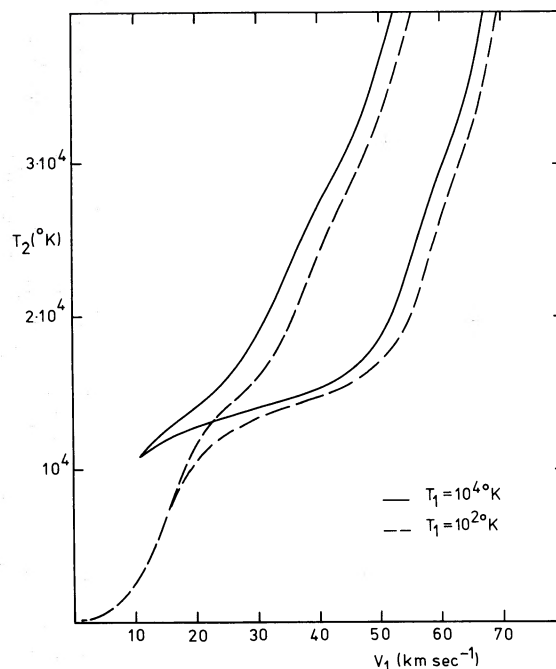


FIG. 1.—The relation between shock velocity and postshock temperature. Permitted values lie between the pairs of lines for each preshock temperature.

The allowed values of postshock temperature and shock velocity for arbitrary preionization are in fact confined to fairly narrow limits. Figure 1 represents the relation obtained from solution of equations (1)–(5) setting Q_R equal to zero. This is a good approximation across the shock discontinuity because the collisional rate is very much higher than the cooling rate. Cases are shown for two assumed initial temperatures, 10^4 K and 10^2 K, indicated by the solid and dashed lines, respectively. The allowed values lie between the pair of lines drawn for each temperature, the right-hand boundary corresponding to zero preionization and the left-hand boundary corresponding to maximum preionization (equal to the collisional ionization equilibrium value in the postshock gas). All curves approach each other asymptotically at high temperature.

Real shocks probably evolve down close to the full-preionization, 10^4 K line until they overtake their own ionization fronts, at which point they rapidly evolve onto the zero-preionization, 10^2 K curve. Since hot gas ahead produces a counter pressure, such a transition will be associated with a slight increase in shock velocity, of order 3 km s^{-1} .

III. THE RECOMBINATION-COOLING PROBLEM

If helium is neglected, the ionization balance equation for hydrogen is

$$\frac{dx}{dt} = -N(H)(\epsilon + \alpha)x^2 + \epsilon N(H)x + \frac{P}{N(H)}, \quad (11)$$

where x is the fractional ionization and P is the number of ionizing photons absorbed $\text{cm}^{-3} \text{s}^{-1}$. In order to obtain a solution of this equation, with appropriate small corrections to allow for helium, cooling rates must be computed for each ion to obtain the net cooling rate. Since equations (1)–(5) give a net heat loss that will produce a given postshock temperature, we used a set of postshock temperatures, computed the distance between the flow points that is implied by the cooling rates, and hence derived improved values of the ionization balance which in turn led to improved cooling rates. This process was repeated until a stability in degree of ionization of better than one part in 10^4 was achieved, generally after only three iterations in the early part of the flow but as many as six later on.

The photon flux was treated as being composed of two streams, an upstream and a downstream component. The downstream component was solved from equation (6) at the same time as the initial solution proceeded, the upstream component being found afterward. If necessary, this component could then be added to the P in equation (11) and an improved solution obtained. In practice this was not generally necessary because the majority of this ionizing radiation is absorbed not in the shock but in the preshock region, so the ionization balance is only slightly affected. However, in the recombination region heating by photoionizations becomes important, especially when the recombination photons from helium are considered. A fraction about 0.65 of these recombinations produce photons able to ionize hydrogen (Hummer and Seaton 1964), and the electrons so produced have mean energies well in excess of the thermal energy in the recombination zone (T of order 7000 K).

As far as the ionic balance is concerned, consider an ion I , and the two adjacent stages of ionization $I - 1$ and $I + 1$; then the ionization equation can be written

$$\frac{1}{N_e} \frac{dN_I}{dt} = \epsilon_{I-1} N_{I-1} - (\epsilon_I + \alpha_I) N_I + \alpha_{I+1} N_{I+1}. \quad (12)$$

The ϵ represent rates for collisional excitation, and these have been derived from the semiempirical formulae given by Canto and Daltabuit (1974). In cgs units

$$\epsilon = 2.484 \times 10^6 \frac{\sigma_m}{(E_m/I - 1)} \left(1 + 2 \frac{kT}{I} \right) \times \exp \left(\frac{-I}{kT} \right), \quad (13)$$

where σ_m is the maximum collisional ionization cross section (cm^2), E_m is the energy at which this occurs, and I is the ionization potential of the ion considered. Canto and Daltabuit give a relationship between σ_m and I , but a corresponding relationship between E_m

and I does not exist. Where experimental information is lacking, we have assumed E_m to be 4 times I . This will make little difference to the ionization balance since the exponential term is by far the most important.

The α in equation (12) represent the recombination coefficients which, since such high temperatures are involved, must include both radiative and dielectronic contributions. These have been taken from Aldrovandi and Péquignot (1973), who give parametric forms for all the ions of interest here.

In these models we have considered the following ions: O I, O II, O III, O IV, N I, N II, N III, N IV, S II, S III, S IV, Ne I, Ne II, and Ne III. The cases of the O I/O II and the N I/N II ionization balance are special, since charge-exchange reactions with hydrogen dominate over recombinations and collisional ionizations. The nitrogen and oxygen ionization is locked to that of hydrogen very closely because of this (Field and Steigman 1971; Steigman, Werner, and Geldon 1971). Because the oxygen reaction is very near resonance, the ratio of the singly ionized species to the neutral will be simply 8/9 of the ratio of ionized hydrogen to neutral hydrogen. However, nitrogen is not quite in resonance, and the charge-exchange equilibrium gives

$$\frac{N(N^+)}{N(N^0)} = 4.5 \exp \left(-\frac{10860}{T} \right) \frac{N(H^+)}{N(H^0)}. \quad (14)$$

We do not consider S I, because its ionization potential is well below that of hydrogen, so sulfur is likely to be ionized if only by ultraviolet starlight. Apart from this, no assumptions are made about the initial ionization, and we follow the ionization through its very rapid initial adjustment with only the implicit assumption that there is always equipartition between protons and electrons.

Forbidden line cooling is computed by calculating statistical equilibrium of all metastable states using parameters listed in Osterbrock (1975) and the references therein, supplemented by very recent data by Eissner and Seaton (1974) for O III, Seaton (1975) for N II and Ne II, and Dopita, Mason, and Robb (1976) for N I. Variation of collision strengths with temperature are included.

Other cooling processes included in the solution are ultraviolet resonance line cooling, free-free emission, and spin change scattering. The first of these (Cox and Daltabuit 1971) is virtually entirely due to carbon below about 10^5 K and depends essentially on the third power of temperature. Its effect, therefore, is to preferentially weaken visible lines of high ionization potential.

Spin change scattering (Wofsy, Reid, and Dalgarno 1971) is important in the region where the gas is predominantly neutral, and indeed is the major cooling process at low temperature.

Hydrogen line intensities are computed using effective recombination coefficients of Brocklehurst (1971) and integrating along the flow direction, and intensities of other lines are given with respect to $H\beta = 100$.

TABLE 1
EMISSION LINES IN N49

Wavelength (Å)	Ion	Measured Intensity*	Computed Intensity
3726.1.....	[O II]	{ 648	{ 356 } 670
3728.8.....	[O II]		{ 314 }
3868.0.....	[Ne III]	45	45
3967.5.....	[Ne III]	{ 41	{ 13.5
3970.1.....	H ϵ		{ ...
4068.6.....	[S II]	{ 36.1	{ 32.4 } 43
4076.4.....	[S II]		{ 10.6 }
4340.5.....	H γ	51.5	46.0
4363.2.....	[O III]	7	8.4
4861.3.....	H β	100	100
4958.9.....	[O III]	39.8	32.3
5006.8.....	[O III]	95.5	92.6
5197.9.....	[N I]	{ 8.3	3.1
5200.4.....	[N I]		
6300.3.....	[O I]	123.7	50.6
6363.8.....	[O I]	43.5	15.7
6548.1.....	[N II]	30.6	28.6
6562.8.....	[H α]	295.8	296
6583.4.....	[N II]	77.1	84.2
6716.4.....	[S II]	172	152
6730.....	[S II]	190	170

* Osterbrock and Dufour 1973.

IV. DERIVED ABUNDANCES IN N49

In order to produce a "best" fit with the observations of the LMC supernova remnant N49 the preshock density and the postshock temperature were varied until models gave the closest correspondence to the [O III] $\lambda 5007$ to [O II] $\lambda 3727 + \lambda 3729$ ratio and the [S II] $\lambda 6731$ to $\lambda 6717$ ratio observed by Osterbrock and Dufour (1973). These quantities were then kept fixed and the N, O, S, Ne, and C abundances adjusted until a synthetic spectrum was produced which showed the closest agreement with observations. The details of this "best fit" model are shown in Figures

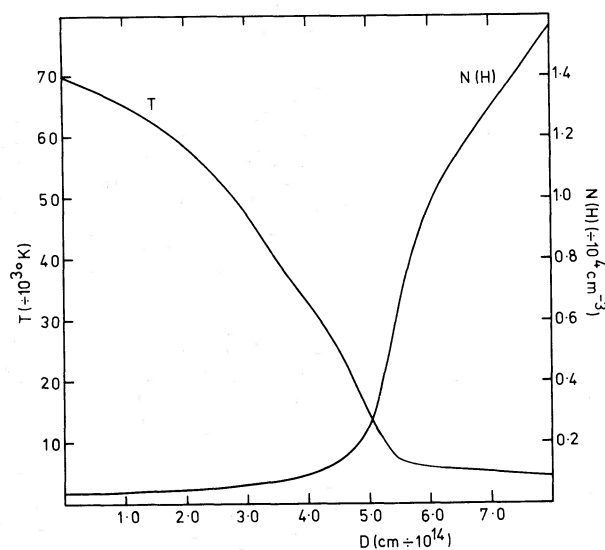


FIG. 2.—Postshock density and temperature profiles for the "best fit" model of N49.

2 and 3, and the parameters characterizing the model are preshock density N_1 , 100 cm^{-3} , immediate postshock temperature $7 \times 10^4 \text{ K}$, and shock velocity (on the assumption of full preionization), 67.5 km s^{-1} .

The shock velocity and the preshock density would be higher and lower, respectively, if the gas ahead were not preionized. Observations of the velocity ellipsoid for N49 by Mathewson and Clarke (1973) indicate an expansion velocity of close to 200 km s^{-1} , so this may well be true. However, provided the postshock temperature and density at which the gas is fully ionized remain as computed, the output spectrum will remain unchanged.

There are several points worthy of comparison between this model and the fairly closely similar Cox (1972) model (shock velocity 71 km s^{-1} , preshock density 4 cm^{-3}).

The scales of the two shocks are in very good agreement. Since ionization rates, recombination rates, and cooling rates scale as the density, the basic structure of a shock remains essentially density independent but scales as the reciprocal of the preshock density. (Of course, at very high density, when collisional de-excitation of the [O II] and [S II] lines becomes large enough to significantly affect the cooling rate, this approximation breaks down.) Thus, scaling the model shown here down to a density of 6 cm^{-3} gives a cooling scale of $12 \times 10^{15} \text{ cm}$ compared with Cox's value of $6 \times 10^{15} \text{ cm}$. The larger value found here is a consequence of the lower abundance of cooling agents used.

The notable difference between the models occurs in the ionization structure in the early part of the postshock flow. This model shows concentrations of S^+ , O^+ , N^+ , etc., to be high in the immediate postshock zone, but they fall very quickly as collisional ionization has time in which to work. The state of ionization is therefore much lower than that predicted by collisional ionization equilibrium in the early part of the postshock flow. This feature is not brought out in the Cox models because he assumes the gas to come into collisional ionization equilibrium immediately after the shock passes, although he remarks that the assumption is of "somewhat marginal" validity.

In the latter parts of the shock structure, the two models are in good agreement, but one should note that appreciable concentrations of N^{+++} and O^{+++} never have time to be built up.

From comparing this and other models, an interesting effect is shown which is of great importance in abundance determinations. The shock structure can be said to "build up" upstream as the postshock temperature is increased. Essentially all the hydrogen emission comes from the very cool recombination region. Hence the intensity of lines of any particular ion with respect to hydrogen will increase until the zone of the shock structure containing the ion considered is essentially complete. For postshock temperatures higher than this, the line intensities remain almost independent of postshock temperature; and if collisional de-excitation is unimportant, they are also independent of the preshock density. (For

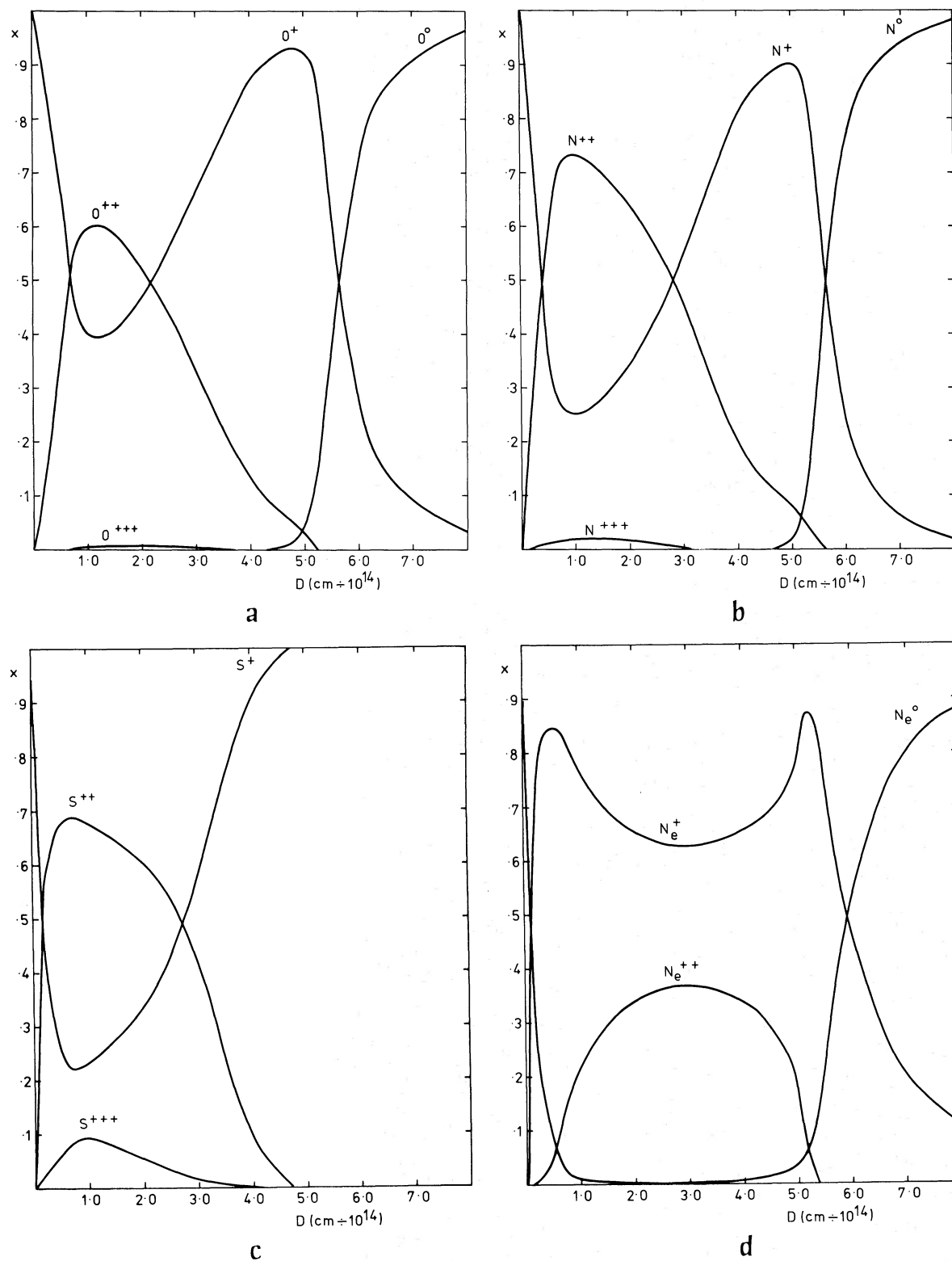


FIG. 3(a-d).—"Best-fit" postshock ionic balance for the ions considered

example, the intensity of the [N II] lines changes with respect to hydrogen by less than 20 percent when the postshock temperature is varied in the range 30,000 K–150,000 K and the preshock density in the range 1 cm^{-3} to 1000 cm^{-3} for fixed abundances.)

The detailed effect on line intensities of shock conditions and abundances will be investigated in full in the second paper of this series, in which a method for determining these quantities from observed spectra of any evolved supernova remnant will be given.

To summarize, although appreciable errors may have been made in the determination of the shock conditions (which, after all, depend essentially on just two line ratios), the errors in abundance determinations are much smaller. In particular the O, N, and S abundances (which are found from the line intensities of singly ionized species) are most accurate, limitations being principally due to the fairly low accuracy with which some of the important atomic constants are known. The estimated error in abundances of these elements is 30 percent.

The error on the neon abundance is much larger: the quoted value may be out by a factor of 2 because only two lines of one species, Ne II, are observed, and the intensity of these depends critically on the temperature and on the relative importance of ultraviolet line cooling, particularly because of carbon which dominates by very large factors over the visible lines in the high-temperature zone of the shock. The carbon abundance is little better than a guess.

The most notable failure of the model is in the predicted [N I]/[N II] and [O I]/[O II] ratios which are underestimated by very similar factors (2.6 and 2.4, respectively). This can be taken as indicating that the computed recombination temperature ($x_H = 0.5$ at $T = 6750 \text{ K}$) is too low by about 1400 K. This is probably due to the ultraviolet line heating in the recombination that would be important if we have underestimated the shock velocity.

V. THE ROLE OF INTERSTELLAR DUST

Table 2 shows that the abundances derived here differ by appreciable factors from those of the LMC H II regions. These appear to contain $1\frac{1}{2}$ times less oxygen and 5 times less nitrogen. This result is at first sight surprising, as in one case one deals with

radiatively excited interstellar gas and in the other with a shocked slab of the same medium. It seems likely that these differences are caused by volatile interstellar "ice" grain material that has been destroyed and returned to the gaseous phase in the supernova, but which still remains in the H II regions.

The problem of grain survival in H II regions and the growth of "ice" mantles in interstellar dust and gas clouds has been considered by many authors (e.g., Mathews 1967; Wickramasinghe and Williams 1968; Isobe 1971, 1972; Dopita, Isobe, and Meaburn 1975; Falk and Scalo 1975). On balance, it seems reasonable that in the interstellar cloud and intercloud region much of the oxygen and nitrogen present can condense onto graphite particles to form a complex ice with a sublimation temperature of order 90 K.

When these grains are put into a hostile high-temperature environment, they will be destroyed by sputtering caused by proton impacts (Mathews 1967). This sputtering rate depends critically on the charge that the grain acquires. If it is negative, protons will be attracted and so the cross section of the grain is increased by a factor $(1 + Ze^2/kTa)$, where Z is the charge on the grain, a is the radius of the grain, and T is the gas temperature. On the other hand, a positive charge inhibits collisions, and the effective cross section is now reduced by a factor $\exp(-Ze^2/kTa)$. In the absence of ionizing radiation the charge is negative because the electron velocity is higher than that of the protons (Moorwood and Feuerbacher 1975) and the effective cross section for collisions becomes close to $3\frac{1}{2}$ times the geometrical value. However, close to a bright star, photoelectric charging becomes predominant, and this leads to greatly reduced sputtering rates. Thus, provided that the grains are not so close to the exciting stars that photon heating raises the grain temperature to a value close to the sublimation temperature, it seems likely that grains survive for time scales of order 10^5 years in the H II region. If the radiation pressure force is sufficient to trap grains in neutral globules known to exist in H II regions, as proposed by Dopita, Isobe, and Meaburn (1975), this would provide a further reason why we would expect gas-phase abundances in H II regions to give an indication of the residue of heavy elements left after grain formation and mantle growth is essentially complete.

TABLE 2
COMPARATIVE ELEMENTAL ABUNDANCES

Element	N49 (this work)	LMC ^a	"Cosmic" ^b	Solar ^c	M42 ^{a,d}
N.....	3×10^{-5}	5.8×10^{-5}	1.08×10^{-4}	8.50×10^{-5}	3.63×10^{-5}
O.....	3×10^{-4}	2.1×10^{-4}	1.04×10^{-3}	5.88×10^{-4}	3.80×10^{-4}
S.....	1×10^{-5}	1.1×10^{-5}	2.24×10^{-5}	1.62×10^{-5}	2.63×10^{-5}
Ne.....	2×10^{-4}	3.2×10^{-5}	2.33×10^{-4}	...	6.16×10^{-5}
C.....	($\geq \times 10^{-4}$)	...	6.0×10^{-4}	3.55×10^{-4}	...

^aDufour 1975.

^bUrey 1972.

^cLambert 1968; Lambert and Warner 1968.

^dPeimbert and Costero 1969.

Now, consider the question of sputtering in the shocked region of the supernova remnant. The loss rate of lattice particles will be given by

$$\frac{dN}{dt} = 3.5\pi a^2 N_p Y (8kT/\pi m_p)^{1/2}, \quad (15)$$

where Y is the sputtering yield and N_p the proton density. Hence, if ρ is the grain density and A is the mean molecular weight of the lattice particles, the sputtering lifetime t_s of a grain of radius a is

$$t_s = \frac{0.24ap}{YA(kTm_H)^{1/2}N_p} \text{ s}. \quad (16)$$

The question of the value of Y is rather open. For a knock-on process the likely value is in the range 10^{-2} to 10^{-3} , but Wickramasinghe and Williams (1968) suggest that chemical sputtering may be important for ice grains, in which case

$$Y \approx \exp(-10650/T). \quad (17)$$

This means that Y could be as great as 0.8 in the immediate postshock environment. Putting in a T of order 10^5 K, equations (16) and (17) indicate that ice grains smaller than 3×10^{-6} cm radius could be destroyed. This is, however, an order of magnitude smaller than the probable "average" interstellar ice grain radius (Crézé and Isobe 1975). For graphite or silicate particles the size limit is two orders of magnitude smaller. Since time scales in the shock (cooling, recombination, etc.) vary inversely as the density, this means that these lower limits are independent of the preshock density selected. In conclusion then, sputtering will not be serious in the radiating region of the shock.

Also, unless the shock is very dense, grains will not be heated to their sublimation temperature. If we assume that each collision gives a heat input to the

grain of kT , and since the efficiency of emission of radiation from the grain, $\epsilon \approx 33.3aT_g$ (Greenberg 1971), it is easy to show that the equilibrium grain temperature T_g is

$$T_g = (7.5 \times 10^{-9} T^{3/2} N_p / a)^{1/5}. \quad (18)$$

Thus, an ice grain with $a = 10^{-5}$ cm in a gas at 10^5 K with a proton density $N_p = 10^3$ will reach a temperature of only 30 K.

We believe rather that it is the supernova event itself, not the passage of the subsequent shock, that destroys the volatile grains. At peak luminosity, a supernova radiates at the rate of about 4×10^{43} ergs s^{-1} (Colgate 1969). Using the relation given above for the grain emission efficiency and Stefan's law, we find that the relationship between maximum grain temperature achieved, T_g , and distance from the supernova r is

$$r^2 = 4.2 \times 10^{44} / a T_g^5. \quad (19)$$

Thus an ice grain of 10^{-5} cm radius is destroyed out to a distance of order 25 pc by the radiation pulse alone. Since the expelled gas is observed to produce X-rays, and may well be a source of suprathermal particles both of which are highly efficient in destroying grains, equation (19) may give a lower limit for the survival distance.

In conclusion, therefore, the abundance measured in the supernova remnant compared to the LMC H II regions indicates that in the LMC about 90 percent of the nitrogen and 75 percent of the oxygen present in the interstellar medium is condensed onto interstellar grains. The low carbon abundance estimated in N49 suggests that a substantial proportion of this element may also be in the form of grains, although in view of the very large uncertainties involved, this question is better left open.

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