SHOCKED MOLECULAR GAS IN THE SUPERNOVA REMNANT IC 443: MODELS WITH AN ENHANCED IONIZATION RATE

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Abstract: The high molecular abundances seen in IC443 may be due to hot chemistry in shocked gas or to an increase in the cosmic ray ionization rate. New calculations reported here show that shock chemistry dominates over the relevant short time scale.

1. INTRODUCTION: IC 443 is the only supernova remnant which we know to be interacting with interstellar molecular gas. Evidence for an encounter of the remnant IC 443 with molecular material is various: (1) Emission from vibrationally excited molecular hydrogen indicates hot postshock gas (Treffers 1979; Burton et al. 1987). (2) The species HI, CO, OH, CS, HCN, and HCO^+ have extremely broad linewidths, typically 30-40 km s^{-1} (DeNoyer 1979a,1979b; Dickenson et al. 1980; Fesen and Kirschner 1980; DeNoyer and Frerking 1981; White et al. 1987). Such broad lines may indicate shock acceleration. (3) The abundances of OH, CS, HCN, and HCO^+ derived from the observations are anomalously high (DeNoyer and Frerking 1981; White et al. 1987).

Mitchell and Deveau (1983) showed that the high abundances of OH and HCO^+ could be explained by chemical processes in shocked gas. Elitzur (1983), on the other hand, suggested that the high observed HCO^+ abundance could be due to an increase in the ionization rate from cosmic rays trapped in the supernova remnant. The suggestion of Elitzur is plausible, but has not been tested by a detailed calculation. The purpose of the present work is to see whether shock models are consistent with recent molecular observations and to assess the effects of an increased cosmic ray ionization rate on molecular abundances. New calculations of molecular abundances behind shocks have been carried out using improved chemistry and using a range of ionization rates.

2. THE OBSERVATIONS: The extraction of a column density from a line intensity requires the excitation temperature, a quantity whose value is often not known. The dependence of abundances on excitation temperature can be partially removed by taking an abundance ratio. Abundances relative to CO, N(X)/N(CO), are often used. Table 1 lists abundances relative to CO for twelve species at four different positions in IC 443. The positions are given in a footnote to Table 1. The abundances at position 1 are from DeNoyer and Frerking (1981) for an excitation temperature of 100 K. All other abundances in Table 1 are from White et al. (1987). A Large Velocity Gradient (LVG) model has been applied by White et al. to their observations at positions 2 and 4 of Table 1. The LVG entries in Table 1 were obtained using a kinetic temperature of 100 K. A comparison of the optically thin and LVG abundances of HCO^+, HCN, and CS for position 2 is instructive: The LVG abundance ratios for these species are 10 to 50 times larger than the abundance ratios for optically thin transitions. White et al. (1987) conclude that the assumption of optical thinness is incorrect. There are, of course, large uncertainties in the LVG abundances themselves. For example, the shocked gas is found to be clumpy on very small scales (Burton et al. 1987), so that the use of a single density is an oversimplification. Also, the deduced LVG abundances are quite sensitive to the kinetic temperature.

3. MODEL ABUNDANCES COMPARED TO OBSERVATIONS: Table 2 gives shocked column densities relative to CO for a model in which a shock of 10 km s^{-1} propagates into gas with an initial density of 100 cm^{-3}. The cosmic ray ionization rate, ζ_0, is 10^{-17} s^{-1}. Abundances are given for species which have been detected in IC 443 and for species with observational upper limits to abundances. Column density ratios are tabulated for three postshock times, 100 years, 400 years, and 1200 years. These numbers represent possible times since the observed gas was shocked. For IC 443, we do not know the time since the remnant overtook the molecular cloud. A recent estimate of the age of IC 443, 5000 years (Mufson et al. 1986), puts an upper limit on the postshock time.

A comparison of Tables 1 and 2 shows that the model for a 400 year old shock gives the best overall agreement with observations. In particular, the model abundances for HCO^+ and CS are remarkably close to the LVG abundances of White et al. (1987). The model ratio, OH/CO = 0.24, is

https://doi.org/10.1017/S0252921100102313 Published online by Cambridge University Press

very close to the observed ratio, 0.32, at position 1. For HCN, the model ratio at 400 years is somewhat high, being four times higher than the LVG ratio at position 4 and ten times higher than the LVG ratio at position 2. The model is consistent with the observational upper limits for CH_3OH, N_2H^+, SO, SO_2, OCS, and HCS^+. The model is in disagreement with observed upper limits to H_2CO and H_2CS: The model produces too much H_2CO (by a factor of 50) and too much H_2CS (by a factor of 60).

TABLE 1
IC 443 OBSERVATIONS: COLUMN DENSITIES RELATIVE TO CO

	N(X)/N(CO)				
SPECIES	Position 1* opt. thin	Position 2 opt. thin	Position 2 LVG	Position 3 opt. thin	Position 4 LVG
HCO^+	7.0(-4)	8.2(-4)	7.7(-3)	8.2(-4)	6.3(-3)
HCN	2.3 (-4)	<8.8(-5)	5.0(-3)	4.4(-4)	1.3(-2)
OH	0.32	-----	-----	-----	-----
H_2CO	<6.1(-5)	-----	-----	-----	-----
CH_3OH	-----	<7.0(-3)	-----	<9.0(-3)	-----
N_2H+	<1.1(-5)	-----	-----	-----	-----
CS	3.2(-4)	6.8(-5)	3.2(-3)	3.8(-5)	-----
SO	<1.2(-4)	<2.2(-4)	-----	<2.6(-4)	-----
SO_2	-----	<3.0(-3)	-----	<3.0(-3)	-----
H_2CS	-----	<8.0(-5)	-----	<1.4(-4)	-----
OCS	<7.2(-4)	-----	-----	-----	-----
HCS^+	-----	<9.4(-5)	-----	<2.0(-4)	-----

* Position 1: RA(1950) = $6^h\ 14^m\ 15^s$, Dec(1950) = 22° 27' 50"
Position 2: RA(1950) = $6^h\ 14^m\ 41.9^s$, Dec(1950) = 22° 22' 40"
Position 3: RA(1950) = $6^h\ 14^m\ 44.1^s$, Dec(1950) = 22° 23' 30"
Position 4: RA(1950) = $6^h\ 14^m\ 42.0^s$, Dec(1950) = 22°33' 40"

Formaldehyde is produced by the reactions $CH_3 + O \rightarrow H_2CO + H$ and $CH_2 + OH \rightarrow H_2CO + H$. A lower H_2CO would follow if less CH_3 and CH_2 were formed. This is not expected, however, since CH_3 and CH_2 are formed in hot gas which has *either* appreciable C *or* appreciable C^+. A low H_2CO abundance is difficult to understand since C is observed to be abundant in dense clouds and C^+ is abundant in lower density gas. Enhancement of formaldehyde is a rather robust prediction of shock models because it can be formed via C or C^+. Further observations of formaldehyde in IC 443 would be useful. Thioformaldehyde is formed in the postshock gas from methane via $S^+ + CH_4 \rightarrow H_3CS^+ + H$, followed by dissociative recombination. Less H_2CS would be produced if the preshock gas contained less S^+ (i. e. if the preshock gas were denser) or if methane did not become abundant in the postshock gas. It remains, of course, possible that one or more rapid destruction processes for H_2CO and/or H_2CS have not yet been recognized.

4. AN INCREASED COSMIC RAY IONIZATION RATE: Calculations were carried out for the shock models described above but with larger cosmic ray ionization rates. To illustrate the effect of the ionization rate on abundances, Figure 1 shows fractional abundances as a function of postshock time for the ions HCO^+ and N_2H^+ and the neutrals OH and HCN. Abundances are given for two ionization rates, the accepted mean value of $\zeta_0 = 10^{-17}\ s^{-1}$, and an enhanced ionization rate of $10^{-15}\ s^{-1}$. It can be seen from Figure 1 that abundances begin to be affected by the change in ζ_0 after several hundred years. N_2H^+ is more abundant in the high ionization case at early times, but does

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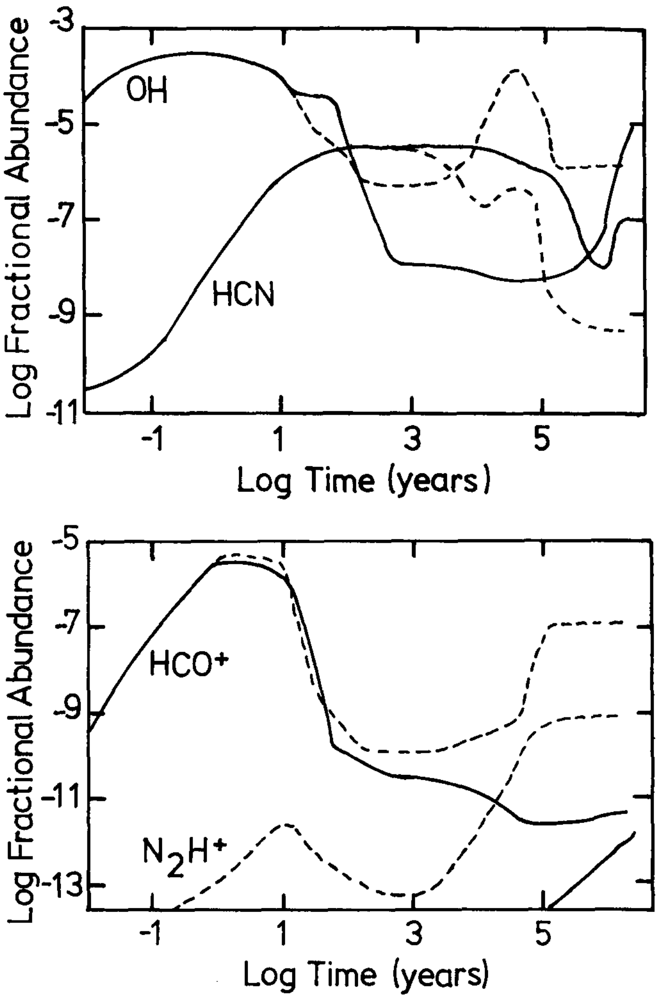

Fig. 1. Fractional abundances, n(X)/n, as a function of postshock time for several species. Solid curves represent a model with $\zeta_0 = 10^{-17}$ s^{-1} and dashed curves represent a model with $\zeta_0 = 10^{-15}$ s^{-1}. Shock speed is 15 km s^{-1} and initial gas density is 100 cm^{-3}.

not become abundant until some 10^5 years after the shock. The fractional abundance of HCO^+ is larger in the high ionization model, being about 10 times larger by 5,000 years. The shocked *column density* after 5,000 years is, however, dominated by HCO^+ near the shock front: The shocked column density of HCO^+ after 5,000 years is essentially identical for the two ionization rates. The abundance of OH becomes much larger, in the high ζ_0 model, after several hundred years. Again, however, the column density of OH is dominated by the abundant OH near the shock front (i. e. at early times in Figure 1): The shocked column density of OH is not influenced by the ionization rate until ~ 10^4 years after the shock. At 10^4 years, the column density of OH in the $\zeta_0 = 10^{-15}$ s^{-1} model is ~3 times larger than in the standard ($\zeta_0 = 10^{-17}$ s^{-1}) model. For the higher ionization model, the fractional abundance of HCN becomes *lower* after several hundred years. Again, the column density of HCN is little affected by the change in ζ_0 until several thousand years after the shock: At 5,000 years, the column density of HCN is ~3 times lower with the higher ionization rate. Because the encounter of IC 443 with the molecular gas probably began less than 5,000 years ago, any increase in the cosmic ray ionization rate has not yet had an appreciable effect on column abundances.

TABLE 2
SHOCKED COLUMN DENSITIES RELATIVE TO CO FOR A MODEL WITH AN INITIAL DENSITY OF 100 CM^{-3} AND A SHOCK SPEED OF 10 KM S^{-1}

Species	N(X)/N(CO) 100 years	400 years	1200 years
HCO^+	2.9(-2)	5.4(-3)	1.6(-3)
HCN	5.0(-2)	5.3(-2)	5.0(-2)
OH	1.2	0.24	7.1(-2)
H_2CO	2.8(-3)	3.0(-3)	2.8(-3)
CH_3OH	9.2(-6)	1.6(-5)	3.2(-5)
N_2H^+	1.8(-9)	3.6(-10)	1.2(-10)
CS	2.3(-3)	7.8(-3)	1.1(-2)
SO	7.8(-5)	1.1(-4)	6.1(-5)
SO_2	1.7(-6)	3.0(-6)	4.1(-6)
H_2CS	9.3(-4)	6.5(-3)	9.0(-3)
OCS	2.2(-6)	4.5(-6)	2.7(-6)
HCS^+	3.4(-5)	1.7(-5)	4.3(-6)

5. CONCLUSIONS: (1) The observed high abundances of HCO^+, OH, and CS in IC 443 can be explained by shock models; (2) The models produce more HCN than is observed, by factors of 4 to 10; (3) The models are consistent with observed upper limits to CH_3OH, N_2H^+, SO, SO_2, OCS, and HCS^+; (4) The models overproduce H_2CO and H_2CS by a factor of 50; (5) If the supernova event occurred about 5,000 years ago, as models suggest, any enhancement in the cosmic ray ionization rate has had a negligible effect on molecular column abundances.

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https://doi.org/10.1017/S0252921100102313 Published online by Cambridge University Press