NEW CONSTRAINTS ON DIFFUSE INTERSTELLAR CLOUD MODELS. THE MODEL OF THE ζ OPHIUCHI CLOUD REVISITED.

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ABSTRACT. Using most recent observational data as well as new experimental and theoretical determinations of various reaction rate coefficients, we present a model of the ζ Ophiuchus cloud. The radiative transfer equation is solved in a plane parallel geometry taking into account absorptions by both the gas and by dust. A part certain atypical molecules (CH^+, CN) and neutral iron, we are able to reproduce the observed column densities of neutral atoms, and molecular species, including the rotational populations of molecular Hydrogen with a two shell model. The concentrations of other simple molecules are predicted.

1. INTRODUCTION

Since the pioneering work of Black and Dalgarno (1977, herafter BD) who proposed a "core enveloppe" model for the diffuse cloud ζ Oph, various observational data were reanalysed and new column densities obtained. This led Crutcher and Watson (1981, herafter CW) to propose an alternative homogeneous isothermal model for the ζ oph cloud. On the other hand, a great effort of measuring new reaction rate coefficients at the very low temperatures of the interstellar medium led to successful results which were sometimes quite unexpected and in contradiction with previous estimations. Moreover the photodissociation of some simple molecules was recently determined by ab-initio theoretical calculations. We found thus necessary to reconsider the modelling of the ζ Ophiuchus cloud with these numerous new constraints.

2. ASSUMPTIONS OF THE MODEL

We build a detailed chemical steady state model including radiative transfer and integration over the depth scale. 85 molecular species are considered containing H,D,He, C,O,N. The ionization equilibrium is treated together with the chemical balance equations by including atomic species such as Mg,Si,Fe and S. The chemical network includes 1100 chemical reactions. The radiative transfer equation is treated in a plane

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TABLE 1 : Observed and Computed Column densities (in log) with diffuse interstellar cloud ζ Ophiuchi

	Observed Column densities	ref.	Computed Column densities One layer model	Two layers model
H	20.72± 0.03	(1)	20.72	20.70
H_2	20.65 ± 0.08	(2)	20.65	20.66
H_2 J=0	20.51 ± 0.08	(2)	20.47	20.52
H_2 J=1	20.10 ± 0.08	(2)	20.19	20.09
H_2 J=2	18.56 + 0.10 − 0.19	(3)	17.40	18.49
H_2 J=3	17.07 + 0.30 − 0.39	(3)	14.96	17.11
HD	14.37 ± 0.03	(4)	15.33	15.27
	15.3 ± 0.1	(5)		
HD J=0	14.26 ± 0.03	(4)	15.33	15.25
	15.3 ± 0.1	(5)		
HD J=1	13.44 ± 0.04	(4)	13.10	13.95
HD J=2	≦ 13.41	(4)	10.16	11.11
Mg	13.93 ± 0.02	(6)	13.65	13.92
Si	≦ 12.58	(7)	12.09	12.39
Fe	≦ 11.45	(6)	11.66	11.98
S	13.65 ± 0.05	(6)	13.34	13.65
C	15.61 ± 0.10	(6)	15.64	15.60
CO	15.42 ± 0.07	(6)	15.41	15.38
CH	13.32 ± 0.02	(8)	13.31	13.34
CH^+	12.97	(7)	10.65	10.30
C_2	13.34 ± 0.07	(9)	12.66	13.47
CN	12.42 ± 0.02	(10)	10.95	11.55
OH	14.0 ± 0.1	(6)	13.91	14.03
H_2O	≦ 13.32 − 13.61	(11,12)	13.05	13.21
NO	13.42	(6)	10.49	10.64

(1) BOHLIN et al. 1978 ; (2) SAVAGE et al. 1977 ;
(3) SPITZER et al. 1974 ; (4) WRIGHT and MORTON 1979 ;
(5) CRUTCHER and WATSON 1981 ; (6) PWA and POTTASCH 1985 ;
(7) MORTON 1975 ; (8) DANKS et al. 1984 ;
(9) DANKS and LAMBERT 1983 ; (10) FEDERMAN et al. 1984 ;
(10) SNOW and SMITH 1981 ; (12) SMITH et al. 1981.

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parallel geometry with finite thickness and takes into account absorption by the dust grains and by the gas . For H_2 and HD, destruction formation reactions and excitation processes are considered simultaneously so that each rotational state of H_2 and HD is treated as a specific molecular species -6(5) rotational levels are taken into account for H_2 (HD).

We explicitly take into account collisional excitation, ultraviolet pumping and infrared cascades (quadrupolar transitions for H_2, dipolar transitions for HD) and build a cascade matrix for H_2 and HD analogous to the one calculated by Black and Dalgarno (1976). The formation of H_2 and HD in excited rotational levels through chemical reactions on grain surfaces and the gas phase reaction $D^+ + H_2 \rightarrow HD + H^+$ is also considered. Finally the uv photoabsorption rates are computed for each individual Lyman and Werner lines of H_2 and HD together with a transfer equation which takes into account all possible absorbers in the line, including line overlaps.

The density and the temperature can be taken as given parameters so that we first use constant values (one shell model). We also introduce a two shell model in order to obtain closer agreement between observations and results of our model. Nevertheless, we cannot demonstrate the uniqueness of the solution obtained.

3. RESULTS AND DISCUSSION

We give in table 1 the atomic and molecular column densities observed in the diffuse cloud ζ Ophiuchi together with the column densities computed in a one shell and two shells models. The column densities listed in table 1 are the best fits to observations. They have been obtained with the cloud parameters listed in table 2 for both models.

In a "standard" UV radiation field (Gondhalekar et al. 1980), a one shell model with $n_H = 75$ cm^{-3} and $T \cong 60$ K reproduces the observed amount of H and H_2 in its two first excited rotational levels. Our improved treatment of the H_2 photodissociation results in a very efficient self shielding and lower photodissociation rates. Due to this, the transition from H to H_2 is much more rapid than obtained in previous model calculations (BD, Federman et al. 1979). The ratio $N(H)/N(H_2)$ decreasing with increasing density, a fairly low density, an order of magnitude lower than inferred in previous models, is required to prevent this ratio to decrease below the observed value. The model gives the correct amount of C,CO and CH if the carbon abundance $\zeta_C = 2.5 \times 10^{-4}$ As is known for a long time, N(OH) scales nearly linearly with the Cosmic ray ionization rate of hydrogen and the observed amount of OH is obtained with $\xi_o = 5.1 \times 10^{-17} s^{-1}$. This relatively high value of ζ_o comes mainly from the enhanced OH photodissociation rate recently computed by Van Dishoeck and Dalgarno (1984). As for OH, the column density of HD is also proportional to ζ_o, but it also depends on another poorly known parameter : the deuterium abundance : ξ_D. With the value of ζ_o necessary to fit the observed N(OH), it is also necessary to reduce ξ_D to 2.5×10^{-6} to get the measured column density log N(HD) = 15.3 given by CW. There is some controversy about the measured N(HD) and the low value log N(HD) = 14.26 obtained by Wright and Morton (1979) would require a

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TABLE 2 : Model parameters ("one shell" and "two shells") giving the best fit to the atomic and molecular column densities observed in the diffuse cloud ζ ophiuchi.

	"One shell" cloud model	"Two shells" cloud model
		Enveloppe :
	n_H = 75 cm^{-3}	n_H = 200 cm^{-3}
	T = 60 K	T = 130 K
		A_v = 0.48 mag
		N_H = 7.1+20 cm^{-3}
		Core :
		n_H = 3000 cm^{-3}
		T = 40 K
		A_v = 0.51 mag
		N_H = 7.4+20 cm^{-2}
	f_{uv} = 1	f_{uv} = 5
	ζ_0 = 5.1 -17 s^{-1}	ζ_0 = 8.2-17 s^{-1}
	$k_{RA}(C^+ + H_2)$ = 4.5-16 cm^3 s^{-1}	$k_{RA}(C^+ + H_2)$ = 1.8-16 $cm^3 s^{-1}$
Element	Abondance (Log ξ_x) observed :	
D	-	- 5.60 - 5.30
C	-3.7 ± 0.4	- 3.60 - 4.00
N	-4.87 ± 0.23	- 4.66 - 4.66
O	-3.63 ± 0.23	- 3.46 - 3.46
Mg	-5.91 ± 0.05	- 5.89 - 5.89
Si	-5.96 ± 0.22	- 5.96 - 5.96
Fe	-6.86 ± 0.15	- 7.00 - 7.00
S	-5.11 ± 0.22	- 4.92 - 4.96

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deuterium abundance as low as $3x10^{-7}$. At the temperature of 60 K necessary to reproduce the populations of the J = 0 and J = 1 levels of H_2, the "one shell" model fails to predict the populations of the J = 2 and J = 3 levels by factors 14 and 130 respectively. Temperatures larger than ~ 100 K are necessary to populate these levels efficiently. The one shell model also predicts too few Mg,S and C_2 : higher densities are required to fit the observations of these species.

It can be seen in table 1 that a two shell model, as suggested by BD, gives a better fit to observational data : the correct amount of H and H_2 is predicted as well as the populations of the four first rotational levels of H_2. This however requires that the UV radiation field is enhanced with respect to its mean interstellar value by at least a factor 5. It can also be seen from table 2 that our model has a hotter and denser core and a hotter and more diffuse enveloppe than those obtained by BD (enveloppe n_H = 500 cm^{-3}, T = 110K. ; core n_H = 2500 cm^{-3}, T = 22 K). The diffuse enveloppe is necessary to maintain a substantial fraction of hydrogen in atomic form and contains half of H_2 J = 1 and most of H_2 J = 2,3, OH and H_2O. All other species are concentrated in the core for which a rather high density is required to reproduce the abundances of C,Mg, Si and S which are entirely governed by the ionization balance. Our model as all other previous ones, predicts too much neutral iron, despite the fact that the iron elemental abundance is much lower than previous determinations indicated. It seems that an efficient destruction processes of Fe has been up to now omitted in all chemical models. A larger value $\zeta_o = 8.2x10^{-17}\ s^{-1}$ than in the one shell model is required to fit N(OH), note however that N(HD) is correctly predicted with a deuterium abundance of $5x10^{-6}$, in good agreement with the determination by Vidal-Madjar et al. (1983). Finally the model predicts the correct amount of C,CO, CH and C_2 with a carbon abundance of only 10^{-4} (more depleted than in the one shell model) and a rate of the radiative association between C^+ and H_2 of $1.8 \times 10^{-16} cm^{-3} s^{-1}$ at the temperature of the core of 40 K where CH and C_2 are more abundant : this is a factor 4 below the rate computed by Herbst (1982). The model reproduces to few CH^+, CN and NO. The CH^+ problem is known since a long time and cannot apparently be solved without including hot chemistry behind a shock front . The low CN abundance results from the large photodissociation cross sections computed by Lavendy et al.(1984) it seems that the cross sections have been over estimated and new calculations are being undertaken. The discrepancy for NO, about 3 orders of magnitude, is much more serious and it seems that the interstellar chemistry of this species needs to be reconsidered. In our model, HD J=1 is produced by collisonal excitation of level J = 0 and is mainly concentrated in the core. The model predicts 3 times more HD J=1 than is observed ; a more precise measurement of the amount of HD J = 0 as well as the deuterium abundance would be very useful to assess whether or not the population of HD in level J = 1 can be reproduced by model calculations.

To conclude we give some column densities for the most abundant unobserved species predicted in our two component models : log N(D) = 15.72, log N(CH_2) = 13.00, log N(C_2H) = 12.42, log N(NH) = 11.67,

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log $N(O_2)$ = 11.60, log $N(HCO^+)$ = 11.45. Among these species, C_2H stands the best chance of discovery through its fine structure emission lines at mm wavelength.

References

Black, J.H., Dalgarno, A. : 1976, Astrophys.J. 203, 132.

Black, J.H., Dalgarno, A. : 1977, Astrophys.J.Suppl.Ser. 34, 405.

Bohlin, R.C., Savage, B.D., Drake, J.F.: 1978, Astrophys.J. 224, 132.

Crutcher, R.M., Watson, W.D. : 1981, Astrophys.J. 244, 855.

Danks, A.C., Federman, S.R., Lambert, D.L. : 1984, Astron.Astrophys. 130, 62.

Danks, A.C., Lambert, D.L. : 1983, Astron.Astrophys. 124, 188.

Federman, S.R., Danks, A.C., Lambert, D.L. : 1984 Astrophys.J. 287, 219.

Federman, S.R., Glassgold, A.E., Kwan, J. : 1979, Astrophys.J. 27, 466.

Gondhalekar, P.M., Phillips, A.P., Wilson, R. : 1980, Astron. Astrophys. 85, 272.

Herbst, E. : 1982, Astronhys.J. 252, 810.

Lavendy, H., Gandara, G., Robbe, J.M. : 1984, J.Molec.Spectrosc.106,395.

Morton, D.C. : 1975, Astrophys.J. 197, 85.

Pwa, T.H., Pottasch, S.R. : 1985, in press in Astron.Astrophys.Suppl.Ser.

Savage, B.D., Bohlin, R.C., Drake, J.F., Bulich, W. : 1977, Astrophys. J. 216, 291.

Smith,P.L., Yoshino,K., Griesinger, H.E., Black,J.H. : 1981, Astrophys. J. 250, 174.

Snow,T.P.Jr, Smith, W.H. : 1981, Astrophys.J. 250, 163.

Spitzer,. Jr, Cochran, W.D., Hirshfeld, A. : 1974, Astrophys.J.Suppl. Ser. 28, 373.

Vidal-Madjar,A.,Laurent,C., Gry,C., Bruston,P., Ferlet,R., York,D.G. : 1983, Astron. Astrophys. 120, 58.

Wright, E.L., Morton,D.C. : 1979, Astrophys.J. 227, 483.

DISCUSSION

GLASSGOLD: What photodissociation rate did you use in your model for CO?
VIALA: We considered dissociation by absorption of photons from the ground state towards the predissociated states $C^1\Sigma^+$ (v' = 1) and $E\ ^1\Sigma^+$ (v' = 1) with a dissociation probability of 0.1. We also took into account a continuum dissociation in the range 912-960 Å using the absorption cross sections of Cook et al. (1965) and again assuming a dissociation field of 0.1.

PANDE: When you take grains and gas as sources of continuous opacity do you expect polarisation? What would be its wavelength dependence in ζ Ophiuci in your models?
VIALA: We did not consider this effect in our model.

VAN DISHOECK: How do you reconcile the dense core in your model with the observed C_2 rotational population which indicates a density of a few hundred cm^{-3}? The observed atomic column densities for the molecular component towards ζ Oph, on which you base your dense core, are very uncertain.
VIALA: Rotational excitation of C_2 has not yet been introduced in the model. It is planned for the near future. This requires rotational excitation cross sections of C_2 by H_2 which are presently being undertaken.

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