

## ON THE INITIAL EXCITATION TEMPERATURE OF INTERSTELLAR H<sub>2</sub>CO MOLECULES

T. OKA

Division of Physics, National Research Council of Canada, Ottawa

Received 1970 March 9

### ABSTRACT

The excitation temperature determined from the lowest  $K$ -type doubling line of the interstellar H<sub>2</sub>CO molecules is discussed. It is shown that, because of the rigorous dipole selection rules, the molecules are "adiabatically cooled" as they make transitions to lower levels by spontaneous emission. If a Boltzmannian rotational distribution is assumed at the time of formation, the initial excitation temperature is given by  $kT_e = 2hB$ , regardless of the temperature of formation.

Various explanations have been proposed for the observed excitation temperatures of the microwave spectra of the interstellar molecules OH (see Litvak, Zuckerman, and Dickinson 1969 for a summary) and H<sub>2</sub>CO (Townes and Cheung 1969). Optical, collisional, and chemical pumpings have been considered as possible causes for the anomalous excitation temperatures. In these discussions steady-state equations have been set up that take into account the various pumping mechanisms and radiational transitions; the solutions of these equations give molecular distributions which are "in equilibrium" with the radiation field or with the kinetic energies of the collision partners. In this paper we shall discuss the distribution of the interstellar H<sub>2</sub>CO molecules in the lowest levels of a  $K$ -type doublet shortly after they have reached these levels but before the steady state is reached. The effective temperature determined from the distribution shall be called the initial excitation temperature.

The interstellar molecules are presumably produced either by chemical reactions or by evaporation from the surface of dust grains. In both cases, the temperature at the time of formation  $T_f$  must be appreciably higher than the blackbody radiation temperature of 2.6° K; therefore,  $K$ -type doublets for relatively high  $J$ -levels are populated. Subsequently these molecules in high rotational levels make spontaneous transitions to lower levels, emitting far-infrared or millimeter-wavelength photons in a time of about  $10^4$  seconds until they reach the lowest levels of a  $K$ -type doublet,  $J = 1$  and  $K = 1$ . During this process, because of the rather rigorous dipole selection rules, molecules once formed in the upper (or lower) level of a  $K$ -type doublet stay in the upper (or lower) level of lower  $K$ -type doublets and end up in the upper (or lower) level of the lowest  $K$ -type doublet. The  $\Delta J = 0$  spontaneous transitions between the component levels of  $K$ -type doublets are much slower than the  $\Delta J = 1$  transitions and may be neglected.<sup>1</sup> In other words, the molecules move from widely split levels to narrowly split levels keeping their population ratio unchanged. This situation is analogous to adiabatic demagnetization; the molecules thus are "cooled." We thought that this "cooling" might explain the anomalously low excitation temperature of 1.8° K (Palmer *et al.* 1969); therefore, the following simple calculations were made.

<sup>1</sup> For example, the lifetime for spontaneous emission for the  $1_{10} \rightarrow 1_{11}$  transition in H<sub>2</sub>CO is  $\tau_0 = 2.8 \times 10^8$  sec whereas that for the  $2_{11} \rightarrow 1_{10}$  transition is  $\tau_1 = 1.7 \times 10^4$  sec. Therefore, even if we allow for the emission induced by the blackbody radiation and multiply  $\tau_0$  by  $h\nu/2kT$ , the former transition is still about 1000 times slower than the latter. As the value of  $J$  increases, the probability for the  $\Delta J = 0$  transition increases as  $J^4$ , whereas the probability for the  $\Delta J = 1$  transition increases as  $J^3$ . Even for  $J = 20$  the  $\Delta J = 1$  transition is still about 800 times faster than the  $\Delta J = 0$  transition.

Since the energies of interaction both in chemical reactions and in evaporation are much greater than the rotational energies of the molecule, the rotational distribution of the molecules immediately after their formation must be approximately Boltzmannian corresponding to a certain temperature of formation  $T_f$ . Thus the molecular populations in the upper and the lower levels of the  $K$ -type doublet  $J = 1, K = 1$  are

$$n_{Ju} = N(2J + 1) \exp [-h(\bar{B} + \delta)J(J + 1)/kT_f]/Z$$

and

$$n_{Jl} = N(2J + 1) \exp [-h(\bar{B} - \delta)J(J + 1)/kT_f]/Z,$$

respectively, where  $N$  is the total number of molecules in the  $K = 1$  levels,  $Z$  is the partition function

$$Z \simeq 2\sum_J(2J + 1) \exp [-h\bar{B}J(J + 1)/kT_f],$$

and  $\bar{B} = \frac{1}{2}(B + C)$  and  $\delta = \frac{1}{4}(B - C)$ , where  $B$  and  $C$  are rotational constants. In  $\sim 10^4$ – $10^5$  sec all the molecules are transferred to the lowest  $K$ -doublet. If we approximate the summations in equations (1) and (2) by integrals, we find that the resultant population  $N_u$  and  $N_l$  for the upper and the lower components, respectively, of the lowest  $K$ -type doublet are

$$N_u = \sum_J n_{Ju} \simeq N\bar{B}/2(\bar{B} + \delta); \quad N_l = \sum_J n_{Jl} \simeq N\bar{B}/2(\bar{B} - \delta).$$

These values, together with the definition of the excitation temperature  $N_u/N_l = \exp(-\Delta E/kT_e)$  and  $\Delta E = 4\delta h$ , give

$$kT_e \simeq 2h\bar{B}.$$

Thus we see that the initial excitation temperature is independent of the temperature of formation  $T_f$  but depends only on the rotational constants of the molecule. This rather unexpected result is ascribed to the fact that both the rotational energy and the splitting of the doublet levels are proportional to  $J(J + 1)$ . If the splitting depends on  $J$  as  $[J(J + 1)]^n$ , and if  $\bar{B} \gg \delta$ , a similar treatment indicates that the initial excitation temperature is, in general,

$$kT_e = kT_f(2h\bar{B}/kT_f)^n/\Gamma(n + 1).$$

The value of  $\bar{B}$  for  $\text{H}_2\text{CO}$  is  $1.2 \text{ cm}^{-1}$  or  $1.7^\circ \text{ K}$ , and equation (4) predicts the initial excitation temperature to be  $3.4^\circ \text{ K}$ . If the sums in equations (2) and (3) are numerically calculated rather than approximated by integrations, it is found that the initial excitation temperature is between  $0^\circ$  and  $3.4^\circ \text{ K}$ , depending on the temperature of formation, but is never higher than  $3.4^\circ \text{ K}$ .

The validity of the assumption of a Boltzmannian distribution at the time of molecule formation is not certain. It is quite possible that there exists a slight preference to populate one component of the  $K$ -type doublets than the other. For example, if  $\text{H}_2\text{CO}$  is formed by the reaction of  $\text{HCO}$  with  $\text{H}$ , similar considerations of angular-momentum transfer, as Townes and Cheung (1969) used in the discussion of collisional excitation, suggest a preference for populating the lower component of the  $K$ -doublets.<sup>2</sup> A slight preference of this type can change the initial excitation temperature to a great extent. Suppose the formation of  $\text{H}_2\text{CO}$  in the lower components is preferred by  $1 + \epsilon$ , where  $\epsilon$  is a small number. Then equations (3) and (4) are modified as

$$N_u = N\bar{B}(1 - \epsilon/2)/2(\bar{B} + \delta), \quad N_l = N\bar{B}(1 + \epsilon/2)/2(\bar{B} - \delta)$$

and

$$kT_e = 2h\bar{B}/(1 + \epsilon\bar{B}/2\delta).$$

<sup>2</sup> Similar considerations will also apply for the preference of the  $6_{16}$  rotational level over the  $5_{23}$  level in  $\text{H}_2\text{O}$ .

Since  $2\delta/\bar{B}$  is about 0.03 in H<sub>2</sub>CO, a value of  $\epsilon$  as small as 3 percent is enough to reduce the excitation temperature by a factor of 2 and make the initial excitation temperature 1.7° K. Such a small preference may exist also in the evaporation processes.

It has thus been demonstrated that the initial excitation temperature of H<sub>2</sub>CO is very low even if the temperature of formation may be very high. This low temperature will last for about  $2 \times 10^7$  sec before the equilibration due to the blackbody radiation becomes appreciable. Also, if we assume the density of hydrogen molecules in the cloud to be about  $10^3 \text{ cm}^{-3}$  (Cheung *et al.* 1968), the equilibration due to collisions becomes appreciable after about  $10^7$  sec.

Therefore, if the H<sub>2</sub>CO molecules exist in interstellar space very much longer than  $10^7$  sec, the initial distribution will be unimportant. If we combine the fact that the H<sub>2</sub>CO molecules in the excited vibrational states in the lowest electronic state are predissociated (Herzberg 1966), with the observed oscillator strength of 0.0008 and the estimated amount of interstellar ultraviolet radiation at 3400 Å, we find that the H<sub>2</sub>CO molecules will survive for about  $10^{10}$  sec. This would mean that the "cooled" H<sub>2</sub>CO molecules are only about 0.001 of the total H<sub>2</sub>CO molecules, and the initial excitation temperature may play only a minor role. However, if either the collisional transitions are much slower because of lower hydrogen density or the decomposition rate is much faster because of higher ultraviolet density, the role of the initial excitation temperature will be more important; the initial excitation temperature is important where the molecules are created and destroyed rather rapidly.

In the discussions given above the  $\Delta K \neq 0$  transitions have been ignored. The transitions  $K = 1 \leftarrow 0$  or  $K = 1 \leftarrow 2$  are extremely slow since they are transitions between the ortho and the para modifications. However the  $K = 1 \leftarrow 3$  transitions are reasonably fast. For example, the spontaneous-emission time for the  $3_{30} \rightarrow 2_{11}$  transitions is about  $1.5 \times 10^5$  sec. The  $3_{30}$  level is about  $80 \text{ cm}^{-1} = 116^\circ \text{ K}$  above the  $1_{11}$  levels; therefore, if  $T_f$  is of this order or higher, the  $\Delta K \neq 0$  transitions should not be ignored. Since the  $K = 3$  levels have much smaller  $K$ -type doubling than the  $K = 1$  levels, these transitions will increase the initial excitation temperature.

An initial negative temperature may be established either when  $\epsilon$  is negative for some reason or when the order of the doublet components is inverted at some  $J$ -values. The latter is the case for the OH radical in the  ${}^2\Pi_{1/2}$  levels where the inversion occurs at  $J = \frac{9}{2}$ .

I wish to thank G. Herzberg for several stimulating discussions on this problem. I have profited from discussions with B. L. Lutz and K. O. Kutschke.

#### REFERENCES

- Cheung, A. C., Rank, D. M., Townes, C. H., Thornton, D. D., and Welch, W. J. 1968, *Phys. Rev. Letters*, **21**, 1701.  
Herzberg, G. 1966, *Electronic Spectra of Polyatomic Molecules* (New York: D. Van Nostrand Co.).  
Litvak, M. M., Zuckerman, B., and Dickinson, D. F. 1969, *A p. J.*; **156**, 875.  
Palmer, P., Zuckerman, B., Buhl, D., and Snyder, L. E. 1969, *A p. J. (Letters)*, **156**, L147.  
Townes, C. H., and Cheung, A. C. 1969, *A p. J. (Letters)*, **157**, L103.