Interpretation of the level population distribution of highly rotationally excited H_2 molecules in diffuse clouds

R WAGENBLAST
Department of Mathematics, UMIST, PO Box 88, Manchester M60 1QD, UK

September 13, 1991

The observed H_2 level population distribution of the rotational levels $J = 5, 6$ and 7 in the ground electronic and vibrational state $X(v = 0)$ is analysed using available Copernicus data (Spitzer and Morton, 1976) for the diffuse clouds toward the stars ζ Oph, δ Per and ξ Per. The abundances of H_2 in these high purely rotationally excited energy levels are due to the influence of one or more of three possible excitation mechanisms: collisions with abundant particles (e.g. H atoms and H_2 molecules), UV-photoexcitation and H_2 formation.

The UV-photoexcitation process on its own produces an occupation of the $J = 5$ level which is about 40 times bigger than that of the $J = 7$ level; the population of the $J = 6$ and $J = 7$ level of H_2 in diffuse clouds is dependent on the para-ortho ratio of molecular hydrogen. The observations show that the column density of H_2 in the $J = 7$ level is about 3 times higher than expected if UV pumping was the main excitation mechanism. Furthermore, the observed column density ratio of H_2 in the $J = 6$ and 7 level is found to be independent of the measured para-ortho of H_2. Therefore the UV pumping process cannot be the primary excitation mechanism for H_2 in these high J levels.

In contrast to UV pumping, collisional excitation of H_2 molecules could be the predominant action responsible for the observed column density distribution between the high J levels. However, the physical conditions needed to generate this distribution are quite special; the kinetic gas temperature would need to be about 2000K and the excitation of the H_2 molecules would have to be caused by H atoms at a density of about 300 cm^{-3} in quite efficient collisions. Collisions with other H_2 molecules are much less effective and so the density required would be much higher. While such a solution is possible, it is quite inconsistent with other determinations of these parameters.

We have investigated the alternative explanation of the J level population distribution which is based on the H_2 formation process. Assuming that the internal energy distribution of newly formed H_2 molecules is narrow, the observed column density distribution of H_2 in the $J = 5$, 6 and 7 level can be reproduced if H_2 molecules are initially in one of two neighbouring rovibrational levels (one for ortho-H_2, one for para-H_2) following: ($v = 1$; $J = 7, 8$), ($v = 4,...11$; $J = 9, 10$) or ($v = 10, 11$; $J = 11, 12$); this choice is

P. D. Singh (ed.), Astrochemistry of Cosmic Phenomena, 157–158.

consistent with the H_2 formation model of Hunter and Watson (1978).

If the population of high J levels is mainly due to H_2 formation, a simple estimate for the evolution time t of a diffuse cloud can be made supposing the cloud contained at the beginning of its development virtually only atomic hydrogen and there is still plenty of it available

$$t = \frac{N(\mathrm{H}_2)}{N(\mathrm{H}_2|J=5)} \times 1.5\mathrm{yr}. \tag{1}$$

The typical 'age' of diffuse clouds is within 5×10^5 to 1×10^6 yr for this kind of estimate. This is another reason why the formation of H_2 on grains is the most favourable process which can explain the observed J level population distribution of H_2.

Chemical models of diffuse clouds are strongly affected by the assumption that H_2 formation rather than UV pumping is the vital process for the population of high J levels in H_2 molecules, because there is no need any more for a strong UV field to explain why these levels are so heavily populated. A (non-equilibrium) model for the diffuse cloud toward ζ Oph was made which reproduces not only the H to H_2 ratio and the measured H_2 (J) column density distribution but also very satisfactorily the abundances of all observed chemical species (except CH^+), especially the high amount of CO. The model assumes that the cloud has a plane-parallel structure and a uniform density ($n_H = 240$ cm^{-3}). The cloud is subdivided in two parts with different kinetic temperatures (30 K and 140 K). The UV field which irradiates the cloud from the warm side has an intensity which is only a fifth of the standard value for the interstellar UV field. The cosmic ray ionization rate is 2×10^{-17} s^{-1}. The evolution time for the ζ Oph cloud is 1×10^6 yr.

Additional observations of H_2 in high rotational levels are needed to find out more about their main excitation mechanism. A far-UV spectrometer with high sensitivity and resolution is required for these observations (Lyman-FUSE in 1997). The detection of water in ζ Oph which is predicted by the model could give additional support for the theory that H_2 formation (or collisional excitation) rather than UV pumping is the vital excitation process for high J levels in H_2.

References

HUNTER, D A and WATSON, W D: 1978, *Astrophys. J.* **226**, 477
SPITZER, L and MORTON, W A: 1976, *Astrophys. J.* **204**, 731