Formation of H_2

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Workshop on Benchmarking PDR Models
Lorentz Center, Leiden, 2004 April 7

KEY ISSUES

- What is the H_2 formation efficiency at high dust temperatures?
- What is the rate of formation?
  Predictions of models
  Can it be determined from observations of PDRs?
- Excitation of newly formed molecules
  distribution over vibration-rotation states (v,J)
  line broadening of kinetically hot molecules?
  do these effects leave observable signatures?

BENCHMARKING RATE

Expressed as a binary rate coefficient:

$$R = 3 \times 10^{-18} T_{\rm gas}^{1/2} n({\rm H}) n_{\rm H} \quad {\rm cm}^{-3}\ {\rm s}^{-1}$$

thus, for example, $R = 2.121 \times 10^{-17} n({\rm H}) n_{\rm H}$ cm^{-3} s^{-1} at $T_{\rm gas} = 50$ K. This form of the rate follows from Hollenbach, Werner, and Salpeter (1971).

EXPERIMENTS

Pirronello and collaborators have measured association of HD and H_2 on silicate (olivine) and amorphous carbon surfaces, which were designed to be good experimental analogues of interstellar dust surfaces. Because several processes are occurring in the tranformation of H into H_2 on a surface

- H atoms collide with a surface
- H atoms bind to the surface and migrate around on it
- H atoms meet on the surface and associate to form H_2
- H-atom desorption may occur before association
- H_2 desorption releases the new molecule into the gas phase

it is necessary to construct a numerical model of the experiments. This consists mainly in a pair of coupled differential rate equations. Katz et al. (1999) presented such a model of the experiments and Biham et al. (1998) discussed the behavior of two limiting cases in the astrophysical context.

Cazaux & Tielens (2004) offered an alternative model that incorporates chemisorption and tunneling as well as the processes considered by Katz et al. Cazaux & Tielens conclude that the association efficiency can remain high even for warm surfaces ($T_{\mathrm{surface}} \geq 100$ K). Cazaux & Tielens (2002) had previously applied their model to the computation of association efficiencies that can be included in the astrophysical rate.

I have taken the model of Katz et al. and integrated the formation efficiency over the standard particle-size distribution of Mathis, Rumpl, and Nordsieck in order to express the experimentally determined rate in terms of a binary rate coefficient; i.e., a form that can be compared directly with the benchmarking rate (above). Examples are shown in the following tables. Details are explained in accompanying notes.

Effective binary rate coefficients R_{eff} [cm^3 s^{-1}]
Conditions of model F1: $T_{\mathrm{gas}} = 50$ K, $T_{\mathrm{surface}} = 20$ K, $n_{\mathrm{H}} = 10^3$ cm^{-3}

n(H)	R_{eff} silicate	R_{eff} carbon
10^3	1.5E–20	7.4E–17
10^2	1.5E–21	6.6E–17
10	1.5E–22	4.9E–17
1	1.5E–23	2.6E–17

Dependence of rate on T_{surface} at $T_{\mathrm{gas}} = 300$ K, $n(\mathrm{H}) = 10^3$

T_{surface}	R_{eff} silicate	R_{eff} carbon
12	1.7E–16	2.1E–20*
15	3.1E–17	5.6E–17*
20	8.7E–20	1.8E–16
25	9.0E–22	5.9E–17
30	4.2E–23	3.4E–18
35	4.8E–24	9.5E–20

*Note: for these conditions, H_2 formation on the surface achieves the steady-state limit only after times of the order of 10^5 s or longer.