XIX SBQT
Simpósio Brasileiro de Química Teórica 2017
12 a 17/Nov, 2017, Águas de Lindóia/SP, Brasil

Reaction Rate of $H_2CO = H_2+CO$

H. O. Euclides, P. R. P. Barreto

Instituto Nacional de Pesquisas Espaciais (INPE/MCT), Laboratório Associado de Plasma (LAP), São José dos Campos, SP, CEP 12247-970, CP515, Brasil

Abstract: In this work, we study the dissociation of formaldehyde, H_2CO, which is a stable molecule in the singlet carbenes [1]. There is two possible pathways, the first one the dissociation reaction to H_2+CO:

$$H_2CO \rightleftarrows H_2+CO \quad (R1)$$

and second one, via the isomerization of hydroxycarbene, HCOH [2]:

$$\begin{aligned} H_2CO &\rightleftarrows^{k_1}_{k_{-1}} trans-HCOH \\ trans-HCOH &\rightleftarrows^{k_2}_{k_{-2}} cis-HCOH \\ cis-HCOH &\rightarrow^{k_3} H_2+CO \end{aligned} \quad (R2)$$

According to the mechanism the global rate is given by:

$$k = \frac{k_1 k_2 k_3}{k_{-1}k_{-2}+k_{-1}k_3+k_2 k_3} \quad (1)$$

The optimize the geometry and frequencies where determine at B3LYP/6-311g(2d,d,p) internal to CBS-QB3 methods, calculated using GAUSSIAN09 program. The reaction rate are determined using the APUAMA code [3], applying the tunneling correction of Wigner, Eckart and small curvature transmission coefficient [4,5], which is presented in the Arrhenius' form. Figure 1 below shows the rate for the dissociation reaction, and figure 2 the rate according equation (1).

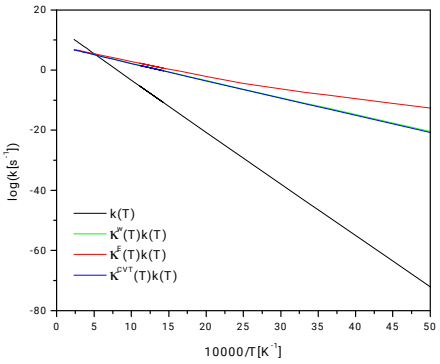

Fig.1 Dissociation reaction path

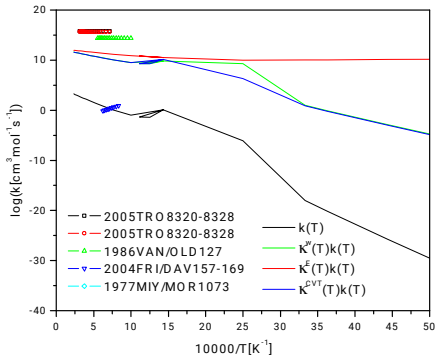

Fig. 2: Isomerization reaction path

Key-words: Rate constant; Quantum chemistry; Thermodynamic properties, H2CO.

Support: This work has been supported by CAPES.

References:

[1] Nufida Dwi Aisyah et al., Procedia Engineering, 170, 119 (2017).
[2] M. Elango, G. S. Maciel, A. Lombardi, S. Cavalli, V. Aquilanti, Int. J. Quantum Chem., 111, 1784 (2011).
[3] H.O. Euclides, P.R.P. Barreto, J Mol Model, 23, 176 (2017).
[4] Gonzalez-Lafont A., Truong T. N., Truhlar D. G., J. Chem. Phys. 95, 8875 (1991).
[5] Duncan W. T., Bell R. L., Truong T. N. J. Comput. Chem. 19, 1038 (1998).