The Mechanism of Methanol Decomposition. A Theoretical Study Based on the Reaction Force Analysis

María Luisa Cerón[†,‡], Barbara Herrera[‡], Paulo Araya[†], Francisco Gracia[†] and Alejandro Toro-Labbé[‡].

[†]Laboratorio de Catálisis, Falcultad de Ciencias Físicas y Matemáticas, Universidad de Chile,

[‡]Laboratorio de Química Teórica Computacional (QTC), Facultad de Química, Pontificia Universidad Católica de Chile, Casilla 306, Correo 22, Santiago, Chile. CIMAT

Abstract.

A theoretical study of methanol decomposition using a model system that represents the initial step of the reaction $CH_3OH + CuO \rightarrow CH_2O + H_2O + Cu$ is presented. Theoretical calculations using B3LYP/6-21G along with Lanl2DZ pseudopotentials on metallic centers were performed and discussed within the framework of the reaction force analysis. It has been found that the reaction takes place following a stepwise mechanism, in which electron transfer effects are predominant at the initial step of the reaction, whereas polarization effects takes over in the second step to promote a proton transfer that leads to the product formation.

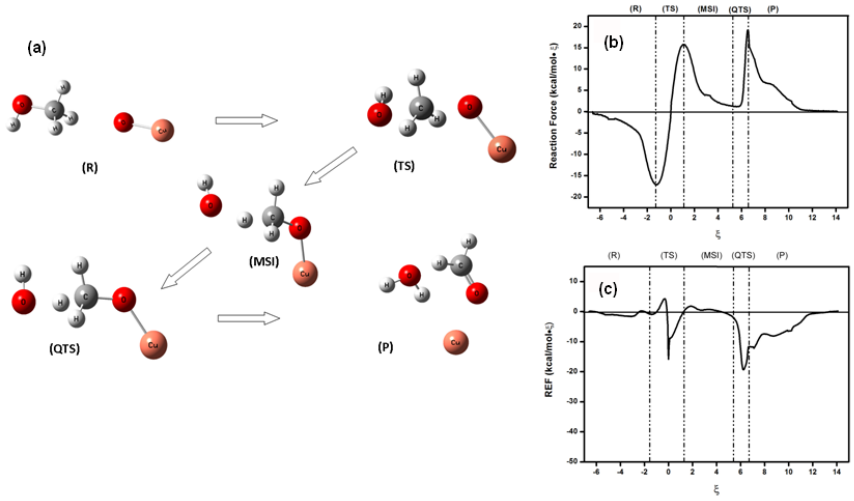

Figure 1: *(a) Methanol Decomposition Reaction. (b) Reaction Force. (c) Reaction Electronic Flux*

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