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Theoretical Study of HCO + O Reactions

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Abstract: The HCO species is important in combustion, atmospheric chemistry and planetary science, but to our acknowledgments there is not results regards the reaction HCO + O. There is extensively studied by both experimental and theoretical on CO + OH = CO_2 + H [1,2] reaction and few studies of CH + O_2 = CO_2 + H and CH + O_2 = CO + OH, with the O_2 in the triplet ground state [3]. In this work, we present a complete potential energy surface (PES) for reaction HCO + O with different products, as:

$$HCO + O = H + COO \quad (R1)$$
$$HCO + O = HOC + O \quad (R2)$$
$$HCO + O = CO_2 + H \quad (R3)$$
$$HCO + O = CO + OH \quad (R4)$$

and also, for reactions:

$$CO + OH = CO_2 + H \quad (R5)$$
$$CO + OH = CH + O_2 \quad (R6)$$
$$CH + O_2 = CO_2 + H \quad (R7)$$

Figure 1 present the complete PES for the HCO+O reaction.

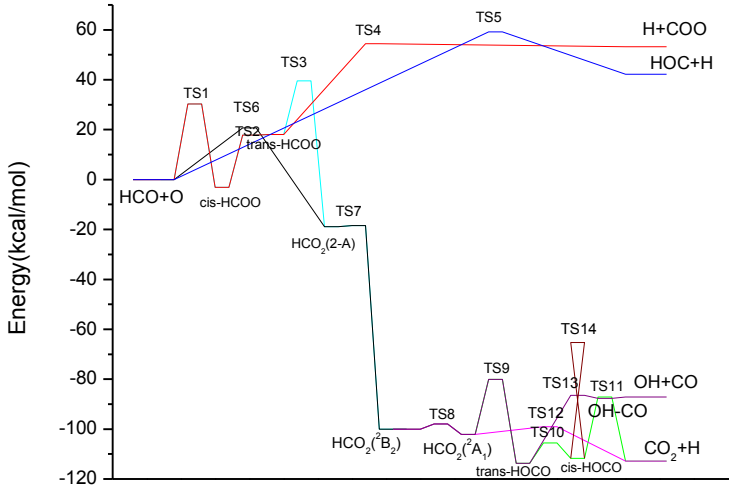

Figure 1: Complete PES for the HCO+O reaction

Figure 2 present the PES for the CO + OH and $CH+O_2$ reaction.

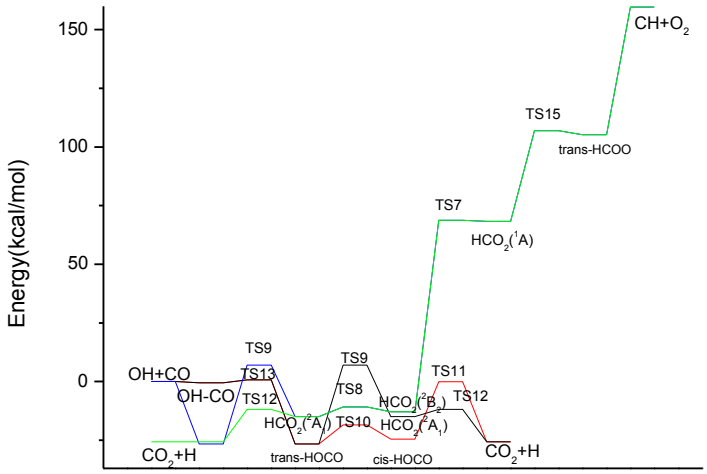

Figure 2: Complete PES for the CO+OH and $CH+O_2$ reaction

Fifteen transition state were determined and the rate constant were calculated using transition state theory and master equation software package MESMER [4], at low pressure written in the Arrhenius and alternatives forms.

The CBS-QB3 Method, in Gaussian 09 program, was employed to optimize the geometries, vibrational frequencies and energies of the reactant, intermediate complexes, transition states, and products of the H + HCO, CO+OH and $CH+O_2$ reactive process. To confirm that the transition state really connects to designated intermediates along the reaction path, the intrinsic reaction coordinate (IRC) calculations were performed. Also the IRC calculations were used to confirm the connection between the designated transition states and the reactants or products.

Key-words: Mesmer, reaction rate, H+HCO
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