

# Photo-oxidation of Selected Carbonyl Compounds: Efficiencies of Carboxylic Acid Productions under Atmospheric Condition

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Formic acid and acetic acid are the most abundant organic carboxylic acids in the earth's atmosphere, which influence the fate of many atmospheric reactions by controlling the acidity of the atmosphere. However, the sources of these acids are yet to be understood fully, and it is assumed that photo-oxidation of VOC's play a significant role in atmospheric acid production.<sup>1</sup> In this context we have shown recently that formic acid could be produced by atmospheric photo-oxidation of acetone and related carbonyl compounds.<sup>2</sup> In the laboratory, photo-oxidation was investigated in simulated atmosphere under exposure of 311 nm UV light. In my presentation I would also discuss photo-oxidation of two other important compounds, cyclohexanone (CH) and methacrolein (MC). Cyclohexanone has been proposed recently as a potential second generation fuel and methacrolein is one of the major reaction products in atmospheric oxidation of isoprene. Therefore, it is essential to know the fate of atmospheric degradation of those compounds. However, photo-oxidation of these compounds in atmospheric condition was never studied before. We have observed formation of formic acid in photo-oxidation of both of the compounds. Acetic acid also appears as a major photo-oxidation product in case of methacrolein. Figure 1 shows time evolution of different photo products during 10 hours of UV irradiation for MC in synthetic air condition. Quantum yields of different photoproducts have been estimated. Mechanisms for formation of different photoproducts have been proposed. Reaction modeling has been performed to show contribution of different elementary reactions in product formation and the quantum yield data obtained from reaction modeling are found to agree well with experimental data. Experimental rate data for many reactions used in reaction modeling being not available, those have been calculated by RRKM method.

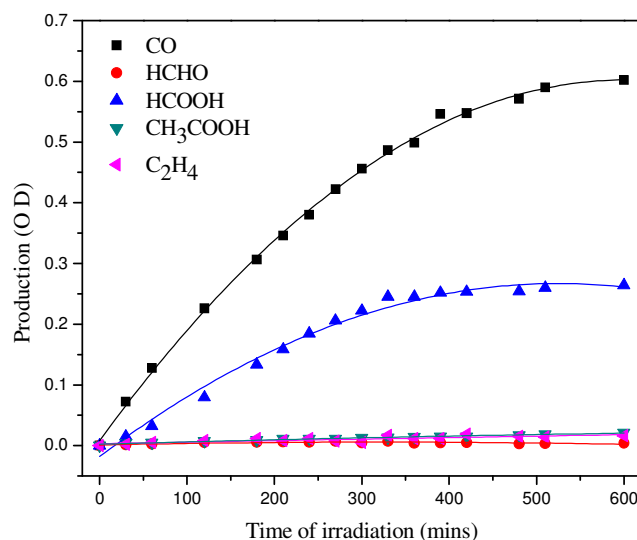


Figure1 – Change of absorbance values of different photoproducts during 10 hours of UV (311nm) irradiation of MC in synthetic air condition

## References

- (1) Millet, D. B. *Nat. Geosci.* **2012**, 5, 8–9.
- (2) Chattopadhyay, A.; Chatterjee, P.; Chakraborty, T. *J. Phys. Chem. A.* **2015**, 119, 8146–8155.