

**INFORMATION**  
**ON THE NEW CONTRIBUTIONS OF DOCTORAL THESIS**  
(Information will be posted on the Website)

Title: *Study on stability and nature of interactions of functional organic molecules with CO<sub>2</sub> and H<sub>2</sub>O by using quantum chemical method*

Speciality: Theoretical and Physical Chemistry

Code No.: 9440119

PhD student: PHAN DANG CAM TU

Course: 5(2017-2021) .....

Advisors: Assoc. Prof. Dr. Nguyen Tien Trung

Training institution: **Quy Nhon University**

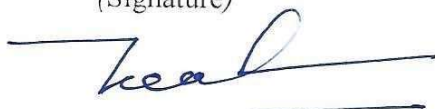
**NOVEL CONTRIBUTIONS OF THE THESIS**

1. The structure and stability of complexes between functional organic molecules including (CH<sub>3</sub>)<sub>2</sub>SO, (CH<sub>3</sub>)<sub>2</sub>CO, (CH<sub>3</sub>)<sub>2</sub>CS, CH<sub>3</sub>OCHX<sub>2</sub> (X = H, F, Cl, Br, H, CH<sub>3</sub>), (CH<sub>3</sub>)<sub>2</sub>S, CH<sub>3</sub>OH, C<sub>2</sub>H<sub>5</sub>OH, C<sub>2</sub>H<sub>5</sub>SH and CO<sub>2</sub> with/without H<sub>2</sub>O molecules are thoroughly investigated. The addition of CO<sub>2</sub> or H<sub>2</sub>O molecules into binary complexes leads to an increase in the stability of the resulting complexes, and it is significantly larger for the H<sub>2</sub>O than CO<sub>2</sub> addition. This is an important study for future experimental works aimed at developing CO<sub>2</sub>-philic materials and CO<sub>2</sub>-related applications.

2. The role and nature of noncovalent interactions to the stabilization of complexes are elucidated by high level computational chemistry methods. The complexes of organic compounds with CO<sub>2</sub> molecules prefer the formations of C···O tetrel bond, while those with the presence of H<sub>2</sub>O are stabilized by O-H···O/S hydrogen bonds. The positive cooperative effect is found in all investigated systems. A larger positive cooperativity is found in case of H<sub>2</sub>O as compared to CO<sub>2</sub> addition.

3. The obtained results in work provide a reliable data on the structure, stability, and characteristics of noncovalent interactions. Remarkably, the tendency of stable geometries of complexes between C<sub>2</sub>H<sub>5</sub>OH and 1-5 CO<sub>2</sub> molecules was found and is expected to contribute to the understanding of dissolution of ethanol in supercritical CO<sub>2</sub>.

Advisor  
(Signature)



Assoc. Prof. Dr. Nguyen Tien Trung

Binh Dinh, March 10, 2022

PhD Student  
(Signature)



Phan Dang Cam Tu