TAREK TRABELSI

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EDUCATION

July 2018-present **Post-Doc**, **Computational Atmospheric Chemistry, University of Pennsylvania**
August, 2016-July 2018 **Post-Doc**, **Computational Atmospheric Chemistry, University of Nebraska-Lincoln, Lincoln, NE, USA**
Project title: "Electronic and ro-vibrational spectroscopy of small molecular system of atmospheric and astrophysics interest." (with Prof. Joseph S. Francisco)

2012-2016 **University of Paris-Est Marne-la-Vallée & University of Tunis-El Manar.**
PhD in Physics
Subject:" Spectroscopic and structural study of non-rigid molecules". under the supervision of Prof. Nejm-Eddine Jaidane (Faculty of Sciences of Tunis) and Prof. Majdi Hochlaf (University of Paris-Est Marne-la-Vallée).

RESEARCH INTEREST

Molecular systems of small and medium size of astrochemical, atmospheric, environmental or biological interests

- The generation of accurate multidimensional potential surfaces for spectroscopy and dynamics
- Molecular systems of small and medium size in their ground and electronically excited states and the treatment of nuclear motions using perturbation or variational theory (Electronic and Ro-vibrational spectroscopy)

PRESENTATIONS

- "Accurate Spectroscopy of small molecular system of astrophysics interest " ACS meeting New-Orleans March (**2018**)
- "On the role of HNS and HSN as light-sensitive NO-donors for delivery in biological media". *Quantum dynamics in molecular systems: theory, modelling, simulation* 9-13 November **2015** (Sousse)

- "Characterization and reactivity of the weakly bound complexes of the [H, N, S]$^-$ anionic system with astrophysical and biological implications". *MOLIM 1st General Meeting* (France) 27-29 August **2015**(Poster)

- Études théoriques des états excités des systèmes HNS^q/HSN^q (q=-1,0,+1)". Ecole de corrosion : *Etude Expérimentale et Approche Quantique EC2EAQ* Fès (Morocco) 17-19 Décember -**2014**.(Poster)

Full list of publications

25. **T. Trabelsi**, K.Mahjoubi, M.Hochlaf and J.S. Francisco "Spectroscopy and Stability of AlPO molecule : A Possible Progenitor of Interstellar Metal" ***J. Phys. Chem. A*** (Submitted).

24. **T. Trabelsi** and J.S. Francisco"Is AlOH the astrochemical reservoir molecule of AlO? Insights from excited electronic states" **The Astrophysical journal** (863:139 (6pp)2018).

23. W., Zhuang, C. Song, J. Liu, B. Lu, Y. Lu, **T. Trabelsi**, J. S. Francisco, and X. Zeng "Photochemistry of OPN: Formation of Cyclic PON and Reversible Combination with Carbon Monoxide" **Chem. Eur. J.** (*2018*).

22. T. Stoecklin, P. Halvick, M.d.J.Lara-Moreno, **T. Trabelsi** and M. Hochlaf "On the gas-phase formation of the HCO^- anion: Accurate quantum study of the H^-+CO radiative association and HCO radiative electron attachment" Faraday Discussion **Faraday Discussion** (*July,2018*) 10.1039/C8FD00103K.

21. **T.Trabelsi**, Y. Ajili, K. Hammami, M. Hochlaf and J.S. Francisco "The rotational excitation of $SN^+(X^1\Sigma^+)$ by collision with H_e at low temperature" **MNRAS** (July,2018).

20. J. Xu, Z. Wu, H. Wan, G. Deng,[1] B. Lu, A. K. Eckhardt, P. R. Schreiner, **T. Trabelsi**, J. S. Francisco, and X. Zeng "Phenylsulfinyl Radical: Gas-phase Generation, Photoisomerization, and Oxidation" **J. Am. Chem. Soc**. (2018).

19. **T. Trabelsi**, M.M. Al-Mogren, M. Hochlaf and J.S. Francisco "Mechanistic study of the photoexcitation, photoconversion and photodissociation of CS_2" **J. Chem. Phys.** J. Chem. Phys. **149**,64304, (2018).

18. **T. Trabelsi**, M. Hochlaf and J.S. Francisco "Toward the detection of the triatomic negative ion SPN^-: Spectroscopy and potential energy surface. " **J. Chem. Phys** 148,164305(2018).

17. R. Fortenberry, **T. Trabelsi** and J.S. Francisco "Hydrogen sulfide as a scavenger of sulfur atomic cation" **J. Phys. Chem. A** 122,4983(2018).

16. X. Dong, G. Deng, J. Xu, B. Lu, Z. Wu, **T. Trabelsi**, J. S. Francisco, X. Zeng " Generation and Spectroscopic Identification of H_2NSO and HNSOH" **Angew. Chem. Int. Ed** DOI:10.1002/anie.201802738 (2018).

15. **T. Trabelsi**, M.M. Al-Mogren, M. Hochlaf and J.S. Francisco "Electronic and spectroscopic characterizations of SNP isomers" **J. Chem. Phys**. 148,54305 (**2018**).

14. Z. Wu, R. Feng, J. Xu, Y. Lu, B. Lu, T. Yang , G. Frenking, **T. Trabelsi**, J.S. Francisco and X.Zeng "Photoinduced Sulfur-Nitrogen Bond Rotation and Thermal Nitrogen Inversion in Heterocumulene OSNSO" " **J. Am. Chem. Soc**. Doi: 10.1021/jacs.7b12622(**2018**).

13. O Denis-Alpizar, **T Trabelsi**, M. Hochlaf, T. Stoecklin "Rotational relaxation of AlO^+ ($X^1\Sigma^+$) in collision with He" **MNRAS** 2017.

12. Z. Wu, J. Xu,L. Sokolenko, Y.L. Yagupolskii, R. Feng, Q. Liu, Y. Lu, L. Zhao, I. Fernandez, G. Frenking, **T. Trabelsi**, J.S. Francisco and X.Zeng "Parent Thioketene S-Oxide H_2CCSO: Gas-Phase Generation, Structure, and Bonding Analysis" **Chem. Eur. J. 23**,1(2017) .

11. Z. Wu, J. Xu, G. Deng, X. Chu, L. Sokolenko, **T. Trabelsi**, J.S. Francisco, A.K. Eckhardt, P. R. Schreiner and X. Zeng, "The Trifluoromethyl Sulfinyl and Oxathiyl Radicals" **Chem. Eur. J.** doi:10.1002/chem.201705142. Inside Back Cover.

10. C.T. Bop, **T. Trabelsi**, K. Hammami, M. Al-Morgen, F. Lique and M. Hochlaf "Cold collision of SH^- with He: Potential energy surface and rate coefficients" **J. Chem. Phys. 147**,124301(2017).

9. **T. Trabelsi**, M.Kumar and J.S. Francisco, " Substituent effects on the spectroscopic properties of Criegee intermediates" **J. Chem. Phys. 147**,164303(2017).

8. **T. Trabelsi**, M. Kumar and J.S. Francisco, " How Does the Central Atom Substitution Impact the Properties of Criegee Intermediate? Insights from Multi-Reference Calculations. " **J. Am. Chem. Soc**. **139**,15446(2017).

7. Z. Wu, J. Xu, Q. Liu, X. Dong, D. Li, N. Holtzman, G. Frenking, **T. Trabelsi**, J.S. Francisco and X. Zeng " The hypothiocyanite radical OSCN and its isomers" **Phys. Chem. Chem. Phys**. 19,16713 (2017).

6. Z Wu, Q Liu, J Xu, H Sun, D Li, C Song, DM Andrada, G. Frenking, **T. Trabelsi**, J.S. Francisco and X.Zeng. "Heterocumulene Sulfinyl Radical OCNSO" **Angew. Chem. Int. Ed** 129, 2172(2017) Inside Back Cover.

5. Y Ajili, **T Trabelsi**, O Denis-Alpizar, T Stoecklin, AG Császár, M Mogren Al-Mogren, JS Francisco, M Hochlaf "Vibrational memory in quantum localized states" **Phys. Rev. A** 93,052514(2016).

4. **T. Trabelsi**, S. Ben Yaghlane, N.-E. Jaidane, M. Al-Mogren, J. S. Francisco and M. Hochlaf "HNS^+ and HSN^+ cations: Electronic states, spin-rovibronic spectroscopy with planetary and biological implications" **J. Chem. Phys**. 145, 084307 (2016).

3. **T. Trabelsi**, O. Yazidi, J. S. Francisco, R. Linguerri, and M. Hochlaf."Electronic structure of NSO^- and SNO^- anions: Stability, electron affinity and spectroscopic properties". The Journal of chemical physics. **J. Chem. Phys**. 143, 164301 (2015).

2. **T. Trabelsi**, R. Linguerri, S. Ben Yaghlane, N.-E. Jaidane, M. Al-Mogren, J. S. Francisco and Hochlaf. "On the Role of HNS and HSN as Light-Sensitive NO-Donors for Delivery in

Biological Media". **J. Chem. Phys**. 143, 134301 (2015).

1. **T. Trabelsi**, Y. Ajili, S. Ben Yaghlane, N.-E. Jaidane, M. Al-Mogren, J. S. Francisco and M. Hochlaf."Characterization and reactivity of the weakly bound complexes of the [H, N, S]$^-$ anionic system with astrophysical and biological implications". **J. Chem. Phys**. 143, 034303 (2015).

Inside Back Cover:
Heterocumulene Sulfinyl Radical OCNSO
(Angew. Chem. Int. Ed. 8/2017)

Cover Feature:
The Trifluoromethyl Sulfinyl and Oxathiyl Radicals
(Chem. Eur. J. 7/2018)