**SELECTED PUBLICATIONS**

1. L. Lei, **M. Kumar**, C. Zhu, J. Zhong, J. S. Francisco, X. C. Zeng, “Near Barrierless Ammonium Bisulfate Formation via a Loop-Structure Promoted Proton Transfer Mechanism on the Surface of Water Clusters”, *J. Am. Chem. Soc.* **2016**, *138*, 1816-1819 (**Highlights**: C&EN, UNL, Nebraska Center for Material Science and Nanoscience, and USTC (China)).
2. **M. Kumar**, J. S. Francisco, “Red-Light-Induced Decomposition of an Organic Peroxy Radical: A New Source of the HO2 Radical”, *Angew. Chem. Int. Ed.***2015***,* *54*, 15711-15714 (**selected for inside back cover**)**.**
3. F. Liu, Y. Fang, **M. Kumar**, W. H. Thompson, M. I. Lester, “Direct Observation of Vinyl Hydroperoxide”, *Phys. Chem. Chem. Phys.* **2015**, *17*, 20490-20494.
4. **M. Kumar**,D. H. Busch, B. Subramaniamand W. H. Thompson, “Barrierless Tautomerization of a Criegee Intermediate via Acid Catalysis, *Phys. Chem. Chem. Phys.* **2014**, *16*, 22968-22973.
5. **M. Kumar**,D. H. Busch, B. Subramaniamand W. H. Thompson, “Organic Acids Tunably Catalyze Carbonic Acid Decomposition”, *J. Phys. Chem. A* **2014**, *118*, 5020-5028; 10155-10156.
6. **M. Kumar** and P. M. Kozlowski, “Corrin Ring-Induced Redox Tuning” *ChemComm* **2012,** *48*, 4456-4458*.*
7. **M. Kumar**,H. Hirao and P. M. Kozlowski, “Co2+/Co1+ Redox Tuning in Methyltransferases Induced by a Conformational Change at the Axial Ligand”, *Inorg. Chem.* **2012,** *51*, 5533-5538.
8. P. M. Kozlowski, **M. Kumar**,P. Piecuch, W. Li, P. Lodowki,and M. Jaworska, “The Co-C Bond Dissociation in Methylcobalamin: New Benchmark Analysis Based on DFT, CASSCF/CASPT2 and Completely Renormalized Coupled-Cluster Calculations”, *J. Chem. Theory Comput.* **2012,** *8*, 1870-1894.
9. **M. Kumar** and P. M. Kozlowski, “A Biologically Relevant Co1+--H Bond: Possible Implications in the Protein-Induced Redox Tuning of Co2+/Co1+ Reduction”*, Angew. Chem. Int. Ed.***2011***,* *50*, 8702-8705.
10. P. M. Kozlowski,T. Kamachi, **M. Kumar**,T. Nakayama and K. Yoshizawa, “Theoretical Analysis of Diradical Nature of Adenosylcobalamin Cofactor–Tyrosine Complex in B12-Dependent Mutases: Inspiring PCET-driven Enzymatic Catalysis”, *J. Phys. Chem. B* **2010**, *114*, 5928-5939.
11. **M. Kumar** and P. M. Kozlowski, “Role of Tyrosine Residue in the Activation of Co-C bond in Coenzyme B12-Dependent Enzymes: Another Case of Proton-Coupled Electron Transfer?”, *J. Phys. Chem. B* **2009**, *113*, 9050-9054.