

# Physical Chemistry Seminar

Tuesday,  
February 19, 2013

11:00 am

Room 1315  
Chemistry Building

## Roaming in the Dark: Solving the Complex Photochemistry of the Nitrate Radical

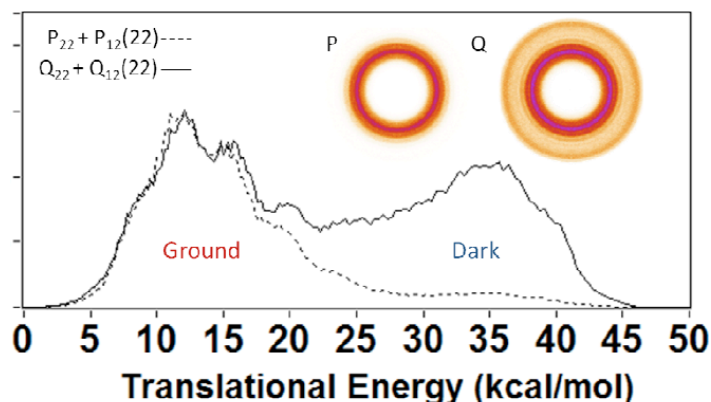


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Host: Professor Frank Keutsch

It has been over a century since the nitrate radical,  $\text{NO}_3$ , was first observed by optical absorption<sup>1</sup> but the mechanism of  $\text{NO}$  and  $\text{O}_2$  production through the visible photolysis has long proven elusive. Recent ion imaging studies and *ab initio* calculations have suggested that two distinct pathways are responsible for molecular products and that both pathways involve 'roaming dynamics' on the 'dark' excited electronic state. Thus, the  $\text{NO}_3 \rightarrow \text{NO} + \text{O}_2$  reaction proceeds in the absence of a traditional transition state. New detailed vector correlation



and  $\Lambda$  doublet propensity measurements, along with *ab initio* calculations, confirm that both pathways arise from roaming-type mechanisms, but each pathway arises from roaming on a different electronic potential (*Science*, 355, 1075 (2012)). This compelling evidence opens additional questions regarding this unusual reaction mechanism and the prevalence of multistate roaming in other molecular systems. 1. J. Chappuis, *Ann. Sci. Ec. Norm. Sup.*, **1882**, 11, 137.

Refreshments will be available prior to the seminar at 10:45 a.m. outside room 1315

Graduate Students may meet with the speaker at 1:00 p.m. in Room 8335