# Physical Chemistry Seminar

**Tuesday, October 26, 2010** | **11:00 a.m.** | **Room 1315 Chemistry Building**

# Reactions that don't Follow the Transition State Path


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In this seminar I shall explain how detailed analysis of the energy disposed in the products reveals information about the reaction mechanism. I will illustrate two unusual mechanisms discovered recently. "Roaming", first reported in 2004 in the photodissociation of $H_2CO$ [*1*], seems not to have a transition state – at least not one that TST can accommodate. It involves a long-range excursion of a H-atom in the van der Waals region of the HCO fragment, leading to self-abstraction of the other H-atom. Roaming has also been well-characterized in $CH_3CHO$, where the methyl group "roams" about the HCO core, abstracting H to produce $CH_4$ + CO. [*2*] In the intervening 6 years, at least a dozen other systems have shown roaming mechanisms, however the theoretical calculation of the kinetics of roaming remains a challenge.

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*[1] Signatures of $H_2CO$ photodissociation from two electronic states*, H.M. Yin, S. H. Kable, X. Zhang and J.M. Bowman, Science, 311, 1443 (2006).

*[2] Roaming dynamics: the dominant pathway to molecular products in acetaldehyde photodissociation*, B.R. Heazlewood, M.J.T. Jordan, S.H. Kable, T.M. Selby, D.L. Osborn, B.C. Shepler, B.J. Braams, J.M. Bowman, Proc. Nat. Acad. Sci., USA, 105, 12719 (2008)


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