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# Theoretical modeling of alkanediol decomposition via metal free organocatalysis

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Quantum chemical calculations have been carried out to investigate the gas-phase structure, stability and decomposition of the two simplest alkanediols, methanediol and 1,1-ethanediol, in the presence of various catalysts. The calculations reveal that alkanediols may not only exist as monomers, but also as dimers that have high binding energies of 7-11 kcal/mol due to hydrogen bonding among the oxygenate functionalities. Some of these dimers have high dipole moments and thus, may be more easily detected experimentally than the monomers of alkanediols. For the decomposition of alkanediols, the calculations dominantly favor dehydration over dehydrogenation. The relatively low barrier for the decomposition of 1,1-ethanediol suggests that the structure of an alkanediol plays a role in its decomposition. Though the dehydration of alkanediols with or without water catalyst involves large barriers, organic and inorganic acids, and hydroperoxy radical catalytically influence the reaction to such an extent that the dehydration reaction either involve significantly reduced barriers or essentially become barrier less. Considering that alkanediols contain hydroxyl groups and their dimers have high binding energies, the gas-phase dehydration may be self-driven. Since acids are present in significant amounts in the troposphere, results suggest that diol dehydration may be facile under atmospheric conditions.

## Biography

Manoj Kumar is a Post-doc candidate in Computational Atmospheric Chemistry, University of Nebraska-Lincoln, Lincoln, NE, USA June from 2015 to present. His project title is "Computational Modeling of Atmospheric Chemistry" (with Prof. J S Francisco). He did his Post-doctorate in Computational Organometallic Chemistry, University of Kansas, Lawrence, KS, USA May 2012 to May 2015. His project title is "Molecular Modeling of Olefin Ozonolysis" (with Prof. W H Thompson) and "Molecular Modeling of Rhodium-catalyzed Hydroformylation" (with Prof. T A Jackson). He completed his PhD in Computational Bioinorganic Chemistry, University of Louisville, Louisville, KY, USA during 2007-2012 with thesis title "Computational Modelling of Cobalamin-Dependent Enzymatic Reactions" (with Prof. P M Kozlowski). Summer Research Project, Computational Material Chemistry, Jawahar Lal Nehru Center for Advanced Scientific Research (JNCASR), Bangalore, India, May,2005-July,2005 Thesis title: "Theoretical Analysis of Gold Clusters and Their Interactions with Thiolates" (with Prof. Swapan K Pati). He completed his MSc, Computational Material Chemistry, Panjab University, Chandigarh, India during 2004-06 with the thesis title, "Theoretical Analysis of Finite-Sized Gold Clusters" (with Prof. T K Sau) and BSc, Physics, Chemistry & Mathematics, SVSD PG College, Bhatoli, Himachal Pradesh University, Shimla, India, 2001-04.

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