



Why Are N₂ and O₂ Unreactive?

Speaker:

Prof. Weston Thatcher Borden

Department of Chemistry,
University of North Texas

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Venue: B301 room, School of Science



Experimental heats of formation and enthalpies obtained from G4 calculations both find that the resonance stabilization of the two unpaired electrons in triplet O₂, relative to the unpaired electrons in two hydroxyl radicals, amounts to 100 kcal/mol. The origin of this huge stabilization energy is described within the contexts of both molecular orbital (MO) and valence-bond (VB) theory. Although O₂ is a triplet diradical, the thermodynamic unfavorability of both its hydrogen atom abstraction and oligomerization reactions can be attributed to its very large resonance stabilization energy. The unreactivity of O₂ toward both these modes of self-destruction maintains its abundance in the ecosphere and thus its availability to support aerobic life. However, despite the resonance stabilization of the π system of triplet O₂, the weakness of the O–O σ bond makes reactions of O₂, which eventually lead to cleavage of this bond, very favorable thermodynamically.

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Manabu Abe (7432)