Seminar

５研究科共同セミナー

Hiroshima Univ

Why Are N_2 and O_2 Unreactive?

Speaker:
Prof. Weston Thatcher Borden

Department of Chemistry,
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Date: Friday, March 30th, 2018
Time: 16:30–17:30
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.

J. Am. Chem. Soc. **2017**, *139*, 9010−9018

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