Group 15 and 16 nitrene-like pnictinidenes

Erica C. Mitchell, Mark E. Wolf, Justin M. Turney, and Henry F. Schaefer III*

University of Georgia, Athens, GA

E-mail: ccq@uga.edu

Abstract

Pnictinidenes are an increasingly important species in main group chemistry with a general proclivity for the triplet electronic ground state. However, the elusive singlet electronic states are often desired for particular applications. We predict the singlet-triplet energy differences ($\Delta E_{\mathrm{ST}} = E_{\mathrm{singlet}} - E_{\mathrm{triplet}}$) of simple group 15 and 16 substituted pnictinidenes (Pn-R; Pn = P, As, Sb, or Bi) with highly reliable focal-point analyses, including up to the CCSDTQ formalism. ΔE_{ST} trends are discussed in light of the geometric predictions as well as qualitative natural bond order analysis to elucidate some of the electronic structure features. This work provides a rigorous benchmark for the ΔE_{ST} of Pn-R moieties and provides a firm foundation for the continued study of heavier pnictinidenes.