2,5,8-Tri-tert-butyl-1,3,4,6,7,9-hexaazaphenalene: Synthesis, Crystal Structure and Calculation of Homolytic N–H Bond Dissociation Enthalpies

Yuqin Jiang\textsuperscript{a}, Huaqiang Zhang\textsuperscript{a}, Xiangjian Wan\textsuperscript{a}, Xiaosong Xue\textsuperscript{b}, Yuanhai Liu\textsuperscript{b}, Haibin Song\textsuperscript{c}, Ao Yu\textsuperscript{b}, and Yongsheng Chen\textsuperscript{a}

\textsuperscript{a} Key Laboratoy for Functional Polymer Materials and Center for Nanoscale Science and Technology, Institute of Polymer Chemistry, College of Chemistry, Nankai University, Tianjin 300071, China
\textsuperscript{b} Central Laboratory, College of Chemistry, Nankai University, Tianjin 300071, China
\textsuperscript{c} State Key Laboratory of Elemento-organic Chemistry, Nankai University, Tianjin 300071, China

Reprint requests to Prof. Yong Sheng Chen. Fax: +86-22-23499992. E-mail: xjwan@nankai.edu.cn


2,5,8-Tri-tert-butyl-1,3,4,6,7,9-hexaazaphenalene (6) was prepared from diethyl 2-[bis(methylsulfanyl)methylene]malonate (1) in four steps. The structure of compound 6 was confirmed by single crystal X-ray diffraction. The phenalenyl skeleton is nearly planar, and there is no $\pi-\pi$ overlap between the hexaazaphenalene rings. A calculation of the homolytic bond dissociation enthalpy (BDE) was performed for compound 6 and its analogs 7 and 8, and the results were used to explain the different reactivity for these three compounds to form the corresponding radicals.

Key words: Phenalenyl, Hexaazaphenalene, Crystal Structure, Bond Dissociation Enthalpy