عنوان مقاله:
Ab initio and DFT study of electronic effects on new (nitrenoethynyl) germylenes

محل انتشار:
چهارمین کنفرانس بین المللی نوآوری های اخیر در شیمی و مهندسی شیمی (سال: 1396)

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نویسندگان:
.Somayeh Soleimani Amiri - *Department of Chemistry, Karaj branch, Islamic Azad University, Karaj, Iran*

Sahar Badragheh - *Young researchers and elite club, Karaj branch, Islamic Azad University, Karaj, Iran*

.Behrooz Mirza - *Department of Chemistry, Karaj branch, Islamic Azad University, Karaj, Iran*

.Nasim Asadbeigi - *Department of Chemistry, Karaj branch, Islamic Azad University, Karaj, Iran*

خلاصه مقاله:
Acetylene linked reactive intermediates of (nitrenoethynyl)-X-germylenes almost are experimentally unreachable(X–Ge–C≡C–N; X = H (1), CN (2), OH (3), NH2 (4), NO2 (5), and CHO (6)). The effect of electron donating andelectron withdrawing groups compared and contrasted at B3LYP, HF, MP2, MP4, CCSD, and QCISD(T) levels with 6-311++G(d,p) basis set. All singlet (nitrenoethynyl)germylenes formed by one local closed-shell singlet germylenesubunit (δ2π0) and one local open-shell singlet nitrene subunit (π1π1). Also, one local closed-shell singlet germylenesubunit (δ2π0) and one local triplet nitrene subunit (π1π1) observed for triplet (nitrenoethynyl)germylenes. The speciesof 3s, 4s, 3t, 4t species could play a key role as an intermediate in mechanism identification of chemical reactions.Finally, one local triplet divalency subunit (π1π1) and also other local triplet nitrene subunit (π1π1) found for .quintetstates described the most unstable states

کلمات کلیدی:
Nitrenoethynyl)-X-germylene, Singlet, Triplet, Quintet, Ground state, DFT, Ab initio)

لینک ثابت مقاله در پایگاه سیویلیکا: