Effect of the Electronic Structure of Substituents at the Silicon Atom on the Structure and Bond Energies of Methylhydrosilanes and Silenes

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Abstract - *Ab initio* calculations with full geometry optimization were performed for methylhydrosilanes R_2HSiCH_3, dimethylsilanes $C_2Si(CH_3)_2$, and silenes $R_2Si{=}CH_2$ (R = H, CH_3, SiH_3, CH_3O, NH_2, Cl, F). The enthalpies of dehydrogenation methylhydrosilanes into silenes and of dehydrocondesation of methylhydrosilanes into dimethylsilanes were calculated. The enthalpies of dehydrogenation and dehydrocondensation increase with the electronegativity of substituent R. The Si–C and Si=C bond energies were calculated. As the electronegativity of the substituent increases, the Si–C bond shortens and strengthens, while the Si=C bond shortens and weakens.