The Chemistry Of Organic Silicon Compounds

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The silicon atom may increase its coordination number to values greater than four, to form pentacoordinated compounds. It has been observed experimentally that, in general, pentacoordinated compounds show greater reactivity than tetracoordinated compounds. In this work, density functional theory is used to calculate the global softness and the condensed softness of the silicon atom for SiHₙF₄₋ₙ and SiHₙF₅₋ₙ. The values obtained show that the global and condensed softness are greater in the pentacoordinated compounds than in the tetracoordinated compounds, a result that explains the en