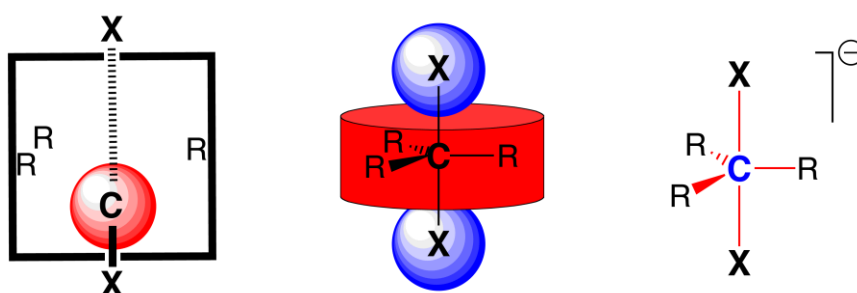


Freezing" the S_N2 Transition State: Hypervalent Silicon versus Carbon Violation of the Octet Rule: Hypervalent Carbon.

Prof. F. M. Bickelhaupt

Silicon in $[\text{Cl-SiH}_3\text{-Cl}]^-$ is hypervalent whereas carbon in $[\text{Cl-CH}_3\text{-Cl}]^-$ is not. In this talk, I show how this can be understood in terms of the ball-in-a-box model according to which silicon fits perfectly into the box that is constituted by the five substituents, while carbon is too small and, in a sense, "drops to the bottom" of the box (see illustration, left). Proceeding from this insight, I will develop a strategy for creating a stable species involving a truly hypervalent, five-coordinate carbon atom (see illustration, middle). If successful, this quest would come down to a violation of the octet rule for carbon! One might conceive this also as "freezing" the otherwise labile S_N2 transition state, turning it into a stable equilibrium structure (see illustration, right).



Literature

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