

# Calculations on Tunneling by Carbon Tell Experimentalists Where to Look and What to Look For

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In organic rearrangements, which have energy barriers that are both low and narrow, tunneling by carbon can cause such reactions to occur at appreciable rates, even at very low temperatures. In order to make experimentally testable predictions about the rates of such reactions and about the effects of isotopes on the rates, small-curvature tunneling (SCT) calculations have been performed. The results of these calculations will be described and discussed for three reactions – the carbene ring expansion in eq. 1, the ring opening of cyclopropylcarbinyl radical in eq. 2, and the degenerate rearrangement of semibullvalene in eq. 3. The use of isotope effects as a probe to diagnose tunneling by carbon will also be discussed.

