

# Raman Snapshots of Ultrafast C-H Bond Activation inside a Water-soluble Nanocage

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The most fundamental detail of any chemical reaction lies in the intricate electronic and structural details of its bond-breaking and/or bond-making steps.<sup>1</sup> It has been chemist's dream to visualize the nuclear dynamics that drive product formation in well-known organic transformations. Selective C-H bond activation represents a grand chemistry challenge<sup>2</sup> as it promises to allow atom economy during synthesis.<sup>3</sup> Here we aim to probe the structural dynamics of C-H bond breaking reaction at a  $sp^3$  site to during its conversion to an intermediate  $sp^2$  hybridized C-atom. We chose to incarcerate 5-(5-methylthiophene-2-yl)-thiophene-carbaldehyde (BT-CH<sub>3</sub>) inside a water-soluble cavity Pd<sub>6</sub>L<sub>4</sub><sup>12+</sup> and generate a host-guest CT state which enabled the C-H activation step to be driven via light excitation.<sup>4,5</sup> We find that in presence of O<sub>2</sub>, BT-CH<sub>3</sub> selectively turned over to the BT-CHO product while showing a kinetic isotope effect of ~1.5 in the C-H bond breaking step. I will discuss our attempts to track the C-H bond activation reaction in BT-CH<sub>3</sub> with femtosecond stimulated Raman spectroscopy.

References:

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