DFT study on the mechanism of site-selective acetate assisted C-H activation.

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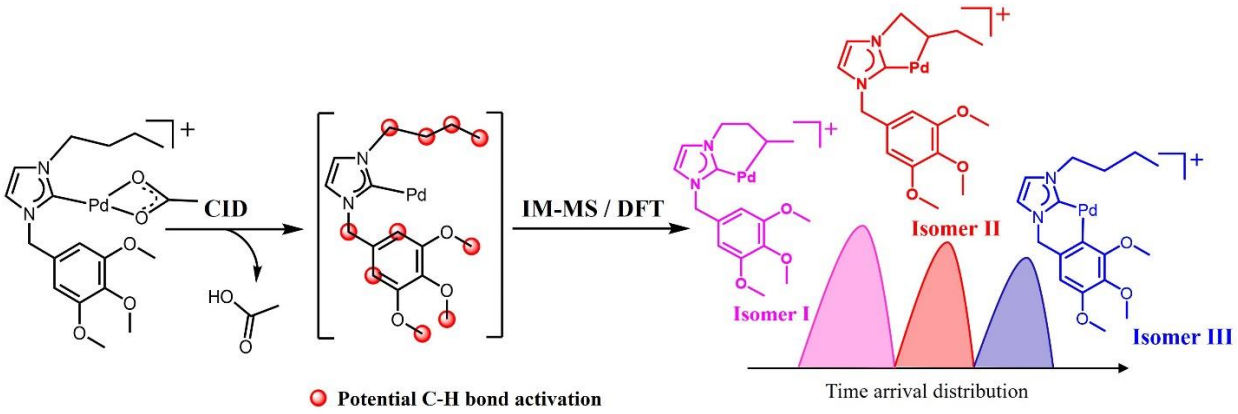
ABSTRACT

When it comes to identifying C-H bond activation, the analytical instruments do not provide sufficient discrimination between C-H bond regioisomers. Herein, we employ DFT to unveil site-selective C-H bond activation of carboxylate-assisted Pd-catalyzed reaction. Preliminary work has been investigated by experimentalists. The cation $[NHC)PdOAc]^+$ is produced in the gas phase by electrospray ionization (ESI-MS), and experiments involving collision-induced dissociation (CID) were carried out to study the potential C-H bond activation. Ion mobility mass-spectrometry (IM-MS) was introduced to explore and assign the site-selective C-H bond activation with a unique regioisomer. Afterwards, collision cross section value was computed using the optimized geometry and compared to the experimental one. [1-2]



References

[1] Mollar-Cuni, A.; Ibáñez-Ibáñez, L.; Guisado-Barrios, G.; Mata, J.A.; Vincent, C. Introducing ion mobility mass spectrometry to identify site-selective C-H bond activation in N-Heterocyclic carbene metal complexes. *J.Am .Soc.Mass Spectrom.* **2022**, *33*, 2291-2300.

[2] Ibáñez-Ibáñez, L.; Mollar-Cuni, A.; Apaloo-Messan E.; Sharma A. K.; Mata, J.A.; Maseras, F.; Vincent, C. Ion mobility mass spectrometry uncovers regioselectivity in the carboxylate-assisted C-H activation of palladium N-heterocyclic carbene complexes. *Dalton Trans.* **2024**, *53*, 656-665.