

SELECTIVE WACKER OXIDATION OF A MACROCYCLIC DIENE TO A MONOUNSATURATED CARBONYL COMPOUND USED FOR THE FRAGRANCE INDUSTRY IN ONE STEP

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Ketones are ubiquitous in nature and play an important role as synthetic intermediates in organic synthesis and for the manufacture of bulk chemicals. While the palladium-catalyzed oxidation of terminal olefins to their corresponding methyl ketones, known as the Wacker oxidation, can be achieved efficiently in just one step, the oxidation of internal olefins is still challenging not least of its lower selectivity and reactivity. Multi-step synthesis and drastic reaction conditions have been used conventionally to overcome the lack of an efficient transformation of ketones from internal olefins. Regarding the increasing demand for greener and efficient processes, simplified methods are highly desirable. The Wacker oxidation was investigated to produce a monounsaturated ketone from a macrocyclic diene for a compound used in the fragrance industry. The most challenging step besides overcoming the low reactivity of internal olefin oxidation is to prevent substrate isomerization and formation of the diketone. Thus, the aim of the study was to find a catalytic system which could increase the conversion of the starting material and provide the desired monoketone with high selectivity. Different systems facing the aspects of green chemistry were investigated. Furthermore, parameters such as reaction temperature, time, concentration of catalyst precursors and co-catalyst/oxidant, solvent system, etc. were optimized. Especially in situ formed cationic PdII-salts introduced by Grubbs et al. have shown promising results. More detailed information will be given at the conference.

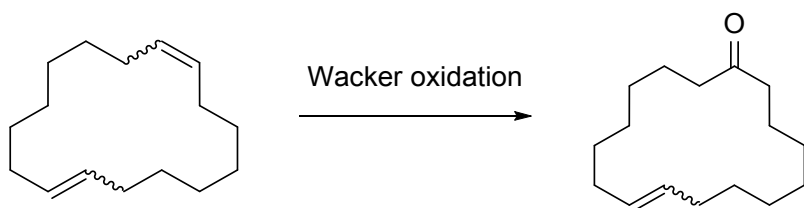


Figure. Wacker oxidation of cyclohexadecadiene to cyclohexadec-8-enone.

BIOGRAPHY

Tom Brunzel is a PhD student at the University of Rostock, Germany. As a member of the department for heterogeneous catalytic processes at the associated Leibniz Institute for Catalysis, he focuses his work on selective liquid phase oxidation reactions. His research interests center around process optimization in laboratory scale, reactor techniques and transition metal catalyzed oxidation reactions of macrocyclic olefins. Tom Brunzel received his undergraduate degree in chemistry at the University of Rostock, where he focused on organic chemistry. He then moved to the Leibniz Institute for Catalysis where he got in touch with the synthesis of flavors and fragrances for the first time. Currently, he is still working on the development and synthesis of fragrance molecules for the fragrance industry.

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