The activation of certain hydrocarbons in the presence of metal complexes is of fundamental importance in chemical transformations and catalysis. Depending on the nature of the metal complex and the reaction conditions, different mechanisms can be operative.

In the presence of metal complexes, hydrocarbons can be activated through the breaking of C-H bonds, leading to the formation of reactive species such as radicals, cations, or anions. This activation process is crucial for many chemical reactions, including hydrogenation, oxidation, and hydrocarbon functionalization.

The mechanism of C-H bond activation by metal complexes is complex and depends on various factors such as the metal type, coordination environment, and reaction conditions. In general, metal complexes can activate C-H bonds through different routes, including the formation of metal-carbon bonds, the donation of electron density from the metal to the C-H bond, and the stabilization of reactive intermediates formed during the reaction.

The activation of hydrocarbons by metal complexes is often accompanied by the formation of new bonds with other reactants, leading to the production of functionalized products. These functionalized products can be used in a variety of applications, including the synthesis of pharmaceuticals, materials, and fine chemicals.

In conclusion, the activation of hydrocarbons by metal complexes is a critical step in many chemical reactions and catalytic processes. Understanding the mechanisms of C-H bond activation can provide insights into the design of new catalysts and the development of more efficient chemical processes.

References:


Further reading:

For a comprehensive review of C-H bond activation by metal complexes, see the following references:

density functional theory methods (DFT) to first identify relevant surface CO coverages during FTS; reaction energy profiles are then calculated using DFT to determine the most facile path for C-O bond activation on Ru cluster surfaces. Kinetic during FTS. This study is an important example of how theoretical calculations performed on relevant surfaces at relevant coverages are an invaluable compliment to experimental studies of metal-catalyzed chemical reactions.

Theoretical investigations of FTS reactions must be performed on cluster surfaces at high CO* coverages that prevail during relevant step-edge sites are larger than those on high-coordination sites because of unfavorable interactions between di-carbonyl species and vicinal C-O activation transition states. DFT results also show that C-O bond activation during FTS is non-irreversible, and any direct CO dissociation path, as a result, is much larger than the barrier for CO hydrogenation, a reaction that is consistent with observed reaction pathways. Furthermore, theoretical investigations show that CO conversion activation energies in the form of oxygen rejection selectivities (in the form of H2O/H2) are consistent with experimentally determined values for hydrogen production from CO.

This work demonstrates the ability of DFT to make important contributions to the understanding of FTS reaction pathways and mechanisms. It also highlights the importance of performing theoretical investigations at high CO* coverages to accurately model the kinetics and mechanisms of metal-catalyzed chemical reactions.

Electrochemical Activation of Ru Clusters

Catalysis by Surface Engineering

In conclusion, DFT is a powerful tool for investigating elementary reactions under conditions inaccessible to experimental techniques. Theoretical investigations of FTS reactions must be performed on cluster surfaces at high CO* coverages that prevail during relevant step-edge sites are larger than those on high-coordination sites because of unfavorable interactions between di-carbonyl species and vicinal C-O activation transition states. DFT results also show that C-O bond activation during FTS is non-irreversible, and any direct CO dissociation path, as a result, is much larger than the barrier for CO hydrogenation, a reaction that is consistent with observed reaction pathways. Furthermore, theoretical investigations show that CO conversion activation energies in the form of oxygen rejection selectivities (in the form of H2O/H2) are consistent with experimentally determined values for hydrogen production from CO.

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Activation and Catalytic Reactions of Saturated Hydrocarbons in the Presence of Metal Complexes

William B. Tolman

1990

The subject of dioxygen activation and homogeneous catalytic oxidation by metal complexes has been in the focus of attention over the last 20 years. The widespread interest is illustrated by its recurring presence among the sessions of important international conferences. The subject of dioxygen activation and homogeneous catalytic oxidation by metal complexes continues to be a fruitful and expanding area of research.

The book is divided into five parts:

1. Dioxygen activation and homogeneous catalytic oxidation by metal complexes
2. Dioxygen activation and homogeneous catalytic oxidation by metal complexes
3. Dioxygen activation and homogeneous catalytic oxidation by metal complexes
4. Dioxygen activation and homogeneous catalytic oxidation by metal complexes
5. Dioxygen activation and homogeneous catalytic oxidation by metal complexes

Each part is further divided into chapters, and each chapter is dedicated to a specific aspect of the subject. The book includes contributions from leading experts in the field, covering a wide range of topics, from the fundamental principles to the latest developments.

The book is intended for researchers, students, and practitioners in the fields of bioinorganic and organometallic chemistry, as well as those interested in catalysis and homogeneous catalytic oxidation by metal complexes.

Activation and Catalytic Reactions of Saturated Hydrocarbons in the Presence of Metal Complexes is the primary source for researchers in academia and industry working in the field of organic synthesis, catalysis, natural product synthesis, pharmaceutical chemistry, and crop protection.

These volumes comprise the proceedings of the major international meeting on catalysis which is held at 4 year intervals. The programme focussed on New Frontiers in Catalysis including nontraditional catalytic materials and environmental catalysis. The invited lectures and 433 papers included in these volumes present an update on all areas of catalysis and applications.