Computational Organometallic Chemistry

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Computational methods have become an indispensible tool for elucidating the mechanism of organometallic reactions. This snapshot of state-of-the-art computational studies provides an overview of the vast field of computational organometallic chemistry. Authors from Asia, Europe and the US have been selected to contribute a chapter on their specialist areas. Topics addressed include: DFT studies on zirconium-mediated reactions, force field methods in organometallic chemistry, hydrogenation of π-systems, oxidative functionalization of unactivated C-H bonds and olefins, the osmylation reaction, and cobalt carbonyl clusters. The breadth and depth of the contributions demonstrate not only the crucial role that computational methods play in the study of a wide range of organometallic reactions, but also attest the robust health of the field, which continues to benefit from, as well as inspire novel experimental studies.

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