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Journal of Organometallic Chemistry Modern Computational

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Computational Organometallic Chemistry Olaf Wiest Springer

Computational methods have become an indispensable 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.

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Computational methods have become an indispensable 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

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Computational Organometallic Chemistry Taylor Francis

This work provides a how-to approach to the fundamentals, methodologies and dynamics of computational organometallic chemistry, including classical and molecular mechanics (MM), quantum mechanics (QM), and hybrid MM/QM techniques. It demonstrates applications in actinide chemistry, catalysis, main group chemistry, medicine, and organic synthesis.

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Computational chemistry Wikipedia

Computational chemistry is a branch of chemistry that uses computer simulation to assist in solving chemical problems. It uses methods of theoretical chemistry, incorporated into efficient computer programs, to calculate the structures and properties of molecules and solids.

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