



Computational Modeling of Homogeneous Catalysis (Catalysis by Metal Complexes)

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Computational Modeling of Homogeneous Catalysis (Catalysis by Metal Complexes) Computational Modelling of Homogeneous Catalysis is an extensive collection of recent results on a wide array of catalytic processes. The chapters are, in most cases, authored by the researchers who have performed the calculations. The book illustrates the importance of computational modelling in homogeneous catalysis by providing up-to-date reviews of its application to a variety of reactions of

industrial interest, including:

- -olefin polymerization;
- -hydrogenation;
- -alkene/alkyne isomerization;
- -hydroformylation;
- -hydroboration; hydrosylation;
- -dihydroxylation;
- -benzannulation;
- -epoxidation;
- -N-N triple bond activation.

This book facilitates understanding by experimental chemists in the field on what has already been accomplished and what can be expected from calculations in the near future. In addition, the book provides computational chemists with a first-hand knowledge on the state of the art in this exciting field.



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