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2.3.1 High Pressure, High Temperature NMR Probes2.3.2 Toroid Probes for High Pressure NMR; 2.4 High Pressure NMR of Gases Dissolved in Liquids; 2.4.1 Sapphire Tubes; 2.4.2 High Pressure Probes for Pressurized Gases; 2.5 Conclusions, Perspectives; Acknowledgments; References; 3 The Use of High Pressure Infrared Spectroscopy to Study Catalytic Mechanisms; 3.1 Introduction; 3.2 Cell Design; 3.2.1 Transmission Cells; 3.2.1.1 Amsterdam Flow Cell; 3.2.1.2 Low-temperature HP IR Cells; 3.2.1.3 HP IR Cells for Flash Photolysis; 3.2.2 Reflectance Cells
3.3 Mechanistic Studies using High Pressure IR Spectroscopy3.3.1 In situ Studies under Catalytic Conditions; 3.3.1.1 Methanol Carbonylation; 3.3.1.2 Hydroformylation; 3.3.1.3 Other Reactions of Carbon Monoxide; 3.3.2 Kinetic and Mechanistic Studies of Stoichiometric Reaction Steps; 3.3.2.1 Migratory CO Insertion Reactions of Metal Alkyls; 3.3.2.2 Substitution and Exchange Reactions of CO Ligands; 3.3.2.3 Exchange between Rh-D and H(2); 3.3.2.4 Hydrogenolysis of M-C Bonds; 3.3.2.5 Mechanistic Studies in Polymer Matrices; 3.3.2.6 Noble Gas and H(2) Complexes
3.3.2.7 Alkane Complexes and C-H Activation Reactions3.4 Conclusions; References; 4 Processing Spectroscopic Data; 4.1 Introduction; 4.2 The Catalytic System; 4.2.1 Recycle CSTR with Analytics; 4.2.2 Physical System; 4.2.3 Chemical Description; 4.3 Experimental Design; 4.3.1 Transport Time-scales; 4.3.2 Reaction Time-scales; 4.3.2.1 Spectroscopic Measurements; 4.3.2.2 Time-scales for Spectroscopic Measurements; 4.3.3 The Meaning of "In Situ" Studies; 4.3.4 The Planning of Experiments; 4.3.4.1 Batch and Semi-batch; 4.3.4.2 Choice of Spectrometers; 4.3.4.3 Groups of Experiments 4.3.4.4 Range of Experiments

Sommario/riassunto

While chemists using spectroscopic methods need to learn from the specialists, they do not normally read the spectroscopists' original papers. This book provides this very information -- summarizing some recent advances in the mechanistic understanding of metallocene polymerization catalysts and the role of NMR spectroscopy in these endeavors.Adopting a real practice-oriented approach, the authors focus on two of the most important spectroscopic techniques with two parts devoted to each of NMR and IR spectroscopy - as well as on important industrial applications with regard to the reaction