

Contents

Preface

1. Introduction

1.1	Catalysis and Catalysts	1
1.2	Heterogeneous and Homogeneous Catalysis	3
1.3	Production of Ammonia	7
1.3.1	Kinetics and Thermodynamics	8
1.3.2	Activity, Selectivity and Stability	11
1.3.3	H ₂ Synthesis	14
1.3.4	Ammonia Synthesis	18
1.4	Relevance of Catalysis	22
	References	22
	Questions	23

2. Adsorption

2.1	Physisorption	25
2.1.1	Adsorption on Surfaces	28
2.1.2	Adsorption Isotherms	30
2.1.3	Multilayer Adsorption, BET	33
2.2	Surface Diffusion	39
2.3	Chemisorption	42
2.3.1	Chemical Bonding	42
2.3.2	Dissociative Chemisorption	50
	References	53
	Questions	54

3. Catalyst Characterisation	55
3.1 Crystal Structures	55
3.2 X-Ray Diffraction	62
3.3 Electron Microscopy	66
3.4 Scanning Tunnelling Microscopy and Atomic Force Microscopy	71
3.5 Infrared and Raman Spectroscopy	73
3.6 Nuclear Magnetic Resonance	81
3.7 Thermal Techniques	85
References	88
Questions	90
4. Catalyst Preparation	91
4.1 Heterogeneous Catalysts	91
4.2 Aluminas	94
4.2.1 Aluminium Hydroxides, Oxyhydroxides and Oxides	95
4.2.2 α -Al ₂ O ₃	100
4.2.3 γ -Al ₂ O ₃ , η -Al ₂ O ₃ and χ -Al ₂ O ₃	101
4.2.4 θ -Al ₂ O ₃ and κ -Al ₂ O ₃	105
4.3 Surface of γ -Al ₂ O ₃	106
4.4 Silica	111
4.5 Zeolites	113
4.6 Preparation of Supported Catalysts	122
References	127
Questions	129
5. Kinetics	131
5.1 Langmuir–Hinshelwood Model	131
5.2 Monomolecular Reaction	133
5.2.1 Surface Reaction is Rate-Determining	134
5.2.2 Adsorption of the Reactant or Product is Rate-Determining	137
5.3 Bimolecular Reaction	137
5.4 Influence of Diffusion	139
Questions	148

6. Metal Surfaces	149
6.1 Surface Structures	149
6.2 Surface Analysis	152
6.2.1 X-ray Photoelectron Spectroscopy	153
6.2.2 Auger Electron Spectroscopy	156
6.2.3 Surface Sensitivity	157
6.3 Surface Enrichment	159
6.4 Metal Binding	164
References	169
Questions	171
7. Metal Catalysis	173
7.1 Dissociation of H ₂	174
7.2 Hydrogenation of Ethene	177
7.3 Synthesis of CO and H ₂	181
7.3.1 Bergius, Fischer–Tropsch and Methanation Reactions	181
7.3.2 Production of CO and H ₂	183
7.4 Hydrogenation of CO	185
7.4.1 Fischer–Tropsch and Methanation	185
7.4.1.1 CO dissociation	185
7.4.1.2 Methanation	190
7.4.1.3 Fischer–Tropsch reaction	193
7.4.2 Methanol Synthesis	197
7.5 Hydrogenation of N ₂ to Ammonia	201
7.5.1 Fe Catalyst	201
7.5.2 Ru Catalyst	203
7.6 Volcano Curves	207
References	211
Questions	214
8. Catalysis by Acids	215
8.1 Reactions Catalysed by Solid Acids	215
8.2 Reactions of Carbenium Ions	217
8.3 Isomerisation of C ₅ , C ₆ and C ₄ ⁼	224
8.4 Alcohols from Alkenes	231

8.5	Alkylation of Aromatics	233
8.5.1	Ethylation and Propylation of Benzene	233
8.5.2	Methylation of Toluene	238
8.5.3	Isomerisation, Disproportionation, Transalkylation	242
8.6	Methanol to Hydrocarbons	247
8.7	Bifunctional Catalysis	253
8.7.1	Principles	253
8.7.2	Industrially Relevant Bifunctional Catalysis	262
	References	264
	Questions	267
9.	Oxidation Catalysis	269
9.1	CO Oxidation	269
9.1.1	Mechanism	269
9.1.2	Three-Way Catalysis	276
9.2	Production of Sulphuric and Nitric Acid	279
9.2.1	Sulphuric Acid	279
9.2.2	Nitric Acid	281
9.3	Oxidation of Hydrocarbons	284
9.3.1	Oxidation by Oxygen	287
9.3.2	Oxidation by Hydroperoxide	291
9.3.3	Selective Partial Oxidation of Hydrocarbons	295
9.3.3.1	Oxidation of propene to acrylic acid and acrylonitrile	295
9.3.3.2	Oxidation of C ₄ and C ₆ molecules	299
	References	300
	Questions	303
	Answers	305
	Index	321