

CONTENTS

<i>Preface</i>	xi
1 An introduction to models	
1.1 Why the book was written	1
1.2 What is a model?	5
1.3 Types of model	7
1.4 Models and problem recognition	12
1.5 The gas law as a model	17
1.6 Environments	18
1.7 Why model?	22
2 Making models	
2.1 A modelling process	26
2.2 Recognise the existence of a problem and decide to tackle it	26
2.3 Delineate the system to be studied	29
2.4 Formulate questions to be asked of the model	36
2.5 Constructing the model	41
2.6 Run the model, analyse the results and their implications	53
2.7 Doubts and pitfalls	55
3 Conceptual models in chemistry	
3.1 Introduction	64
3.2 Classes of model	64
3.3 Modelling in physical chemistry	89
3.4 The conceptual model in inorganic chemistry	92
4 Models of reacting systems	
4.1 Introduction	98
4.2 Describing reactions through models	98
4.3 Structural formulae	108

4.4	Solvation, solvent effects and salt effects	121
4.5	Catalysis as an environmental effect	127
4.6	Models of transition states	130
4.7	Models of reactions describing the relationship between reactants and products	141
4.8	Conclusion – hypothetical descriptions of reactions	147
5	Modelling in synthesis, spectroscopy, and structure determination	
5.1	Introduction	149
5.2	What constitutes a viable model, and how can we construct it?	149
5.3	Organic synthesis	152
5.4	Molecular models	174
5.5	Structure determination and physical methods	180
5.6	Conclusion	189
6	Modelling of biological systems	
6.1	Introduction	191
6.2	Modelling and biosynthesis	203
6.3	Model studies of hydrolytic enzymes (without metal cofactors)	210
6.4	Model studies of haemoproteins	217
6.5	Model studies of enzymes containing functional metal ions	225
6.6	Simulations of the origin of life on earth	231
6.7	Model studies of coenzymes	233
6.8	Models relating to the nature of enzymic catalysis	238
6.9	Conclusion	244
7	Designing chemical plant	
7.1	The business as environment	245
7.2	Problems of process design	249
7.3	Process diagrams	256
7.4	Mathematical models	260
7.5	The development of the use of mathematical models in process design	263

8	Innovation	
8.1	The nature of innovation	267
8.2	Constraints on innovation	271
8.3	Economic and technological forecasting	274
8.4	Economic models	276
8.5	Forecasting technological change	281
8.6	Project evaluation	284
8.7	Product evaluation	288
8.8	Some case histories	291
 <i>References</i>		
<i>Index</i>		302
		317