

Contents

<i>Ligand Abbreviations</i>	ix
Chapter 1—Introduction	1
Stereoisomerism and Absolute Configuration	1
Geometrical Isomerism	2
Optical Isomerism and Diastereoisomerism	6
Methods of Determining Absolute Configurations	16
Chirality	16
Chapter 2—Notation of Absolute Configuration	20
Preamble	20
Notation for the Distribution of Chelate Rings	20
Notation of Conformation for Chelate Rings	28
Notation for the Distribution of Unidentate Ligands	29
Notation for the Dissymmetry from an Unsymmetrical Chelate	29
Notation for Complex Containing an Asymmetric Ligand	30
Summary of Adopted Symbolism	31
Chapter 3—Conformational Analysis	33
Introduction	33
Van der Waals Forces	34
Torsional Barriers	52
Angle-bending Energy	58
Bond-length Distortion Energy	60
Computational Methods for Conformational Analysis	61
Entropy of Ring Conformations	63
Five-membered Diamine Rings	63
Six-membered Diamine Rings	86
Five-membered Amino Acid Rings	94
Correlation of Predicted Structures with Real Structures	99
Experimental Conformational Analysis	101

Chapter 4—Absolute Configurations by X-ray Analysis	113
Normal Diffraction and Friedel's Law	113
Anomalous Dispersion and Absolute Configuration	115
Bijvoet's Method: Method A	118
Pepinsky and Okaya's Method: Method B	123
The Quadratic-equation Method: Method C	125
The Crystal-engineering Method: Method D	126
Conformations of Chelate Rings	126
Chapter 5—Circular Dichroism	148
Historical	148
Interaction of Light with an Optically Active Medium	149
Rotational Strength of Chromophores	153
The Cotton Effect	154
Absorption Spectra of Metal Complexes	157
General Theories of Optical Activity	167
Empirical Methods Based on the <i>d-d</i> Transitions	176
Nonempirical Methods	227
Chapter 6—Nuclear Magnetic Resonance	257
Theory	257
Geometrical Isomers	268
Diamine Complexes	278
Amino Acid Complexes	291
Polyaminocarboxylate Complexes	296
Pseudotetrahedral Complexes	299
Chapter 7—Miscellaneous Techniques	304
Infrared Spectroscopy	304
Delèpine's Active Racemate Method	310
Diastereoisomer Solubility Criterion	310
Chemical Correlations	313
Other Methods	315
Chapter 8—Geometrical Isomerism	318
Infrared Spectroscopy	318
Electronic Absorption Spectroscopy	327
Other Methods	332
Index	335