# CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Foreword</td>
<td>xi</td>
</tr>
<tr>
<td>Preface</td>
<td>xiii</td>
</tr>
<tr>
<td><strong>1 Aluminum Oxides and Hydroxides under Environmental Conditions</strong></td>
<td>1</td>
</tr>
<tr>
<td>1.1 Introduction</td>
<td>1</td>
</tr>
<tr>
<td>1.2 Occurrence of Aluminum Oxides and Hydroxides in the Subsurface</td>
<td>2</td>
</tr>
<tr>
<td>1.3 Occurrence of Aluminum Oxides and Hydroxides in Surface Water</td>
<td>4</td>
</tr>
<tr>
<td>1.4 Use of Aluminum Hydroxide in Water Treatment</td>
<td>6</td>
</tr>
<tr>
<td>1.5 Summary</td>
<td>7</td>
</tr>
<tr>
<td><strong>2 Formation and Properties of Gibbsite and Closely Related Minerals</strong></td>
<td>9</td>
</tr>
<tr>
<td>2.1 Al Polymerization Models</td>
<td>9</td>
</tr>
<tr>
<td>2.1.1 The “Core-Links” Model</td>
<td>10</td>
</tr>
<tr>
<td>2.1.2 The “Cage-Like” (Keggin-Al_{13} Structure) Model</td>
<td>10</td>
</tr>
<tr>
<td>2.1.3 The “Continuous” Model</td>
<td>11</td>
</tr>
<tr>
<td>2.2 Formation of Gibbsite and Other Al Hydroxides and Oxyhydroxides</td>
<td>12</td>
</tr>
<tr>
<td>2.3 Aluminum Hydroxide Polymorphs: Structure and Nomenclature</td>
<td>15</td>
</tr>
<tr>
<td>2.4 Gibbsite</td>
<td>19</td>
</tr>
<tr>
<td>2.4.1 Kinetics of Precipitation and Crystal Growth</td>
<td>19</td>
</tr>
<tr>
<td>2.4.2 Structure</td>
<td>21</td>
</tr>
<tr>
<td>2.4.3 Common Techniques of Synthesis</td>
<td>21</td>
</tr>
<tr>
<td>2.4.4 Synthesized Gibbsite and Differences from Natural Gibbsite</td>
<td>24</td>
</tr>
<tr>
<td>2.5 Bayerite</td>
<td>25</td>
</tr>
<tr>
<td>2.5.1 Kinetics of Precipitation and Crystal Growth</td>
<td>25</td>
</tr>
</tbody>
</table>
2.5.2 Structure / 26
2.5.3 Differences from Gibbsite / 26
2.5.4 Synthesized Bayerite and Transformation to Gibbsite / 27
2.6 Nordstrandite / 27
2.7 Doyleite / 28
2.8 Other Forms of Aluminum Oxides and Oxyhydroxides / 28
   2.8.1 Corundum (α-Al₂O₃) / 28
   2.8.2 Boehmite (γ-AlOOH) / 29
   2.8.3 Diaspore (α-AlOOH) / 29
2.9 Other Forms Manufactured under High Temperature and Pressure / 30

3 Types of Available Data
   3.1 Gibbsite Structure Verification / 33
   3.2 Physical–Chemical Properties / 34
      3.2.1 Specific Surface Area / 34
      3.2.2 Surface Site Characterization / 35
         3.2.2.1 Hydroxyl Surface Sites / 35
         3.2.2.2 Surface Site Density / 36
   3.3 Acid–Base Titration Data / 37
   3.4 Cation and Anion-Sorption Data / 40
   3.5 Spectroscopic Data for Sorption on Gibbsite / 41
   3.6 Proton Release/Uptake Data / 43
   3.7 Electrokinetic Data / 43
   3.8 Summary / 44

4 Data Compilation and Treatment Methods
   4.1 Collection of Data / 45
   4.2 Assessment of Data Quality / 46
      4.2.1 Solid Preparation Method / 46
      4.2.2 Type of Reaction Vessel / 47
      4.2.3 Nature of Background Electrolyte / 47
      4.2.4 Sorption Kinetics / 48
         4.2.4.1 Proton Sorption Kinetics / 48
         4.2.4.2 Cation and Anion Sorption Kinetics / 49
      4.2.5 Method of Solid–Liquid Separation / 49
      4.2.6 CO₂ Exclusion / 50
      4.2.7 Experimental Temperature / 51
   4.3 Compilation of Surface Properties / 51
   4.4 Extraction of Equilibrium Sorption Constants / 51
      4.4.1 Solution Activity Coefficients / 52
4.4.2 FITEQL / 52
4.4.3 Data Grouping / 54
4.4.4 Selection of Surface Species / 54
4.4.5 Selection of Best Estimates / 55
4.5 Optimal-Fit Simulations / 56
4.6 Presentation of Results / 56

5 Surface Properties of Gibbsite

5.1 Surface Area / 59
5.2 Site Density / 62
5.3 Point of Zero Charge / 64
5.4 Surface Acid–Base Chemistry / 65
5.5 Effects of Dissolution on Gibbsite Surface Acid–Base Chemistry / 76
5.6 Summary / 80

6 Cation Sorption on Gibbsite

6.1 Modeling Methodology and Reactions / 81
6.2 Available Spectroscopic Data and Use in Modeling / 86
   6.2.1 Copper / 86
   6.2.2 Lead / 87
   6.2.3 Cobalt / 88
   6.2.4 Cadmium / 88
   6.2.5 Manganese / 88
   6.2.6 Iron(II) / 88
   6.2.7 Calcium / 88
   6.2.8 Zinc / 89
   6.2.9 Mercury / 89
   6.2.10 Uranium / 90
   6.2.11 Thorium / 91
6.3 Copper / 92
6.4 Lead / 99
6.5 Cobalt / 107
6.6 Cadmium / 117
6.7 Manganese / 126
6.8 Iron (II) / 127
6.9 Calcium / 128
6.10 Zinc / 130
6.11 Mercury / 132
6.12 Uranium / 142
6.13 Thorium / 145
7 Anion Sorption on Gibbsite

7.1 Modeling Methodology and Reactions / 149
7.2 Available Spectroscopic Data and Use in Modeling / 153
  7.2.1 Phosphate / 153
  7.2.2 Arsenate / 154
  7.2.3 Arsenite / 154
  7.2.4 Molybdate / 155
  7.2.5 Selenate / 155
  7.2.6 Chromate / 155
  7.2.7 Borate / 155
  7.2.8 Sulfate / 156
  7.2.9 Fluoride / 156
  7.2.10 Silicate / 156
7.3 Phosphate / 157
7.4 Arsenate / 164
7.5 Arsenite / 176
7.6 Molybdate / 182
7.7 Selenate / 185
7.8 Chromate / 187
7.9 Borate / 188
7.10 Sulfate / 192
7.11 Fluoride / 195
7.12 Silicate / 197

8 Coherence and Extrapolation of the Results

8.1 Cation Sorption on Gibbsite / 199
8.2 Anion Sorption on Gibbsite / 204
8.3 Comparison of Gibbsite Surface-Complexation Constants
   with Those of Goethite, Hydrous Ferric Oxide, and
   Hydrous Manganese Oxide / 208
8.4 Summary / 213

References / 219

Appendix A: Summary of Experimental Details / 241

Author Index / 283

Subject Index / 289