

CONTENTS

CONTRIBUTORS

xi

PREFACE

xv

PART I STRUCTURES AND DYNAMICS OF GAS-PHASE BIOMOLECULES

1

1 Spectroscopy of Neutral Peptides in the Gas Phase: Structure, Reactivity, Microsolvation, Molecular Recognition

3

Markus Gerhards

2 Probing the Electronic Structure of Fe-S Clusters: Ubiquitous Electron Transfer Centers in Metalloproteins Using Anion Photoelectron Spectroscopy in the Gas Phase

63

Xin Yang, Xue-Bin Wang, You-Jun Fu, and Lai-Sheng Wang

3 Ion-Molecule Reactions and H/D Exchange for Structural Characterization of Biomolecules

119

M. Kirk Green and Carlito B. Lebrilla

4 Understanding Protein Interactions and Their Representation in the Gas Phase of the Mass Spectrometer

147

Frank Sobott and Carol V. Robinson

5 Protein Structure and Folding in the Gas Phase: Ubiquitin and Cytochrome <i>c</i>	177
<i>Kathrin Breuker</i>	
6 Dynamical Simulations of Photoionization of Small Biological Molecules	213
<i>Dorit Shemesh and R. Benny Gerber</i>	
7 Intramolecular Vibrational Energy Redistribution and Ergodicity of Biomolecular Dissociation	239
<i>Chava Lifshitz</i>	
PART II ACTIVATION, DISSOCIATION, AND REACTIVITY	277
8 Peptide Fragmentation Overview	279
<i>Vicki H. Wysocki, Guilong Cheng, Qingfen Zhang, Kristin A. Herrmann, Richard L. Beardsley, and Amy E. Hilderbrand</i>	
9 Peptide Radical Cations	301
<i>Alan C. Hopkinson and K. W. Michael Siu</i>	
10 Photodissociation of Biomolecule Ions: Progress, Possibilities, and Perspectives Coming from Small-Ion Models	337
<i>Robert C. Dunbar</i>	
11 Chemical Dynamics Simulations of Energy Transfer and Unimolecular Decomposition in Collision-Induced Dissociation (CID) and Surface-Induced Dissociation (SID)	379
<i>Asif Rahaman, Kihyung Song, Jiangping Wang, Samy O. Meroueh, and William L. Hase</i>	
12 Ion Soft Landing: Instrumentation, Phenomena, and Applications	443
<i>Bogdan Gologan, Justin M. Wiseman, and R. Graham Cooks</i>	
13 Electron Capture Dissociation and Other Ion–Electron Fragmentation Reactions	475
<i>Roman Zubarev</i>	
14 Biomolecule Ion–Ion Reactions	519
<i>Scott A. McLuckey</i>	

PART III THERMOCHEMISTRY AND ENERGETICS	565
15 Thermochemistry Studies of Biomolecules	567
<i>Chrys Wesdemiotis and Ping Wang</i>	
16 Energy and Entropy Effects in Gas-Phase Dissociation of Peptides and Proteins	619
<i>Julia Laskin</i>	
INDEX	667