CONTENTS

Foreword ................................................................. v
General Preface for Large-Scale Optimization with Applications,
Parts I, II, and III ...................................................... vii
Preface for Part III ....................................................... ix
Contents for Part I ....................................................... xi
Contents for Part II ...................................................... xiii

Large-Scale Optimization with Applications,
Part III: Molecular Structure and Optimization

CGU: An algorithm for molecular structure prediction ............... 1
   K.A. Dill, A.T. Phillips, and J.B. Rosen

Potential transformation method for global optimization ............ 23
   Robert A. Donnelly

Multispace search for protein folding ................................ 47
   Jun Gu, Bin Du, and Panos Pardalos

Modeling the structure of ice as a problem in global
minimization .................................................................. 69
   Jan Hermans

Novel Applications of Optimization to Molecule Design .......... 73
   J.C. Meza, T.D. Plantenga, and R.S. Judson

Issues in large-scale global molecular optimization ............... 99
   Jorge J. Moré and Zhijun Wu

Global minimization of Lennard-Jones functions
on transputer networks .................................................. 123
   Klaus Ritter, Stephen M. Robinson, and Stefan Schäffler

Variable-scale coarse-graining in macromolecular
global optimization ...................................................... 135
   David Shalloway

Global optimization for molecular clusters using
a new smoothing approach .......................................... 163
   C.-S. Shao, R.H. Byrd, E. Eskow, and R.B. Schnabel