

CONTENTS

Chapter 1. Introduction	1
A. Properties of polymers	1
B. Group contribution techniques	3
C. Topological technique	3
D. Outline of the remaining chapters of this book	12
References and notes for Chapter 1	14
Chapter 2. Topological Method for Structure-Property Correlations	16
A. Review of connectivity index calculations for simple molecules	16
B. Extension of connectivity index calculations to polymers	20
C. General forms of the correlations in terms of connectivity indices	39
D. Backbone and side group portions of the connectivity indices	44
E. Short path across the backbone of a polymeric repeat unit	45
F. Extensions for the calculation of some conformation-related properties	47
References and notes for Chapter 2	48
Chapter 3. Volumetric Properties	49
A. Background information	49
B. Correlation for the van der Waals volume	53
C. Correlation for the molar volume at room temperature	64
D. Final equations for temperature dependences of volumetric properties	72
References and notes for Chapter 3	74
Chapter 4. Thermodynamic Properties	76
A. Background information	76
B. Improvements in the ability to predict the heat capacities of polymers	81
C. Rotational degrees of freedom of the backbone and the side groups	83
D. Correlation for the heat capacity of “solid” polymers at room temperature	86
E. Correlation for the heat capacity of “liquid” polymer at room temperature	91
F. Correlation for the change in the heat capacity at the glass transition	96
References and notes for Chapter 4	101
Chapter 5. Cohesive Energy and Solubility Parameter	104
A. Background information	104
B. Correlation for the Fedors-type cohesive energy	110
C. Correlation for the van Krevelen-type cohesive energy	115
D. Correlation for the dispersion component of the molar attraction constant	122
References and notes for Chapter 5	128

Chapter 6. Glass Transition Temperature	129
A. Background information	129
B. Correlation for the glass transition temperature	133
References and notes for Chapter 6	159
Chapter 7. Surface Tension	162
A. Background information	162
B. Improvements in the ability to predict the surface tensions of polymers	165
C. Approximate “master curve” as a function of reduced temperature	165
D. Correlation for the molar parachor	167
References and notes for Chapter 7	174
Chapter 8. Optical Properties	175
A. Background information	175
B. Improvements in the ability to predict the refractive indices of polymers	178
C. Correlation for the refractive index at room temperature	179
D. Example of application: specific refractive index increments of solutions	186
E. Calculation of the molar refraction	192
References and notes for Chapter 8	197
Chapter 9. Electrical Properties	198
A. Background information	198
B. Correlation for the dielectric constant at room temperature	202
C. Calculation of the molar polarization	208
D. Calculation of the effective dipole moment	211
E. Dissipation factor	214
References and notes for Chapter 9	224
Chapter 10. Magnetic Properties	226
A. Background information	226
B. Correlation for the molar diamagnetic susceptibility	228
References and notes for Chapter 10	233
Chapter 11. Mechanical Properties	234
A. Stress-strain behavior of polymers	234
B. Small-strain behavior: moduli, compliances, and Poisson’s ratio	235
C. Large-strain behavior: failure mechanisms	245
D. Improvements in the ability to predict the mechanical properties	255
E. Correlations for the additive functions used to calculate the moduli	256
References and notes for Chapter 11	270

Chapter 12. Properties of Polymers in Dilute Solutions	273
A. Background information	273
B. Correlation for the steric hindrance parameter	278
C. Calculation of the characteristic ratio	284
D. Correlation for the molar stiffness function	287
References and notes for Chapter 12	292
Chapter 13. Melt Viscosity	294
A. Background information	294
B. Improvements in the ability to predict the zero-shear viscosity	300
C. Correlation for the molar viscosity-temperature function	301
References and notes for Chapter 13	308
Chapter 14. Thermal Conductivity	309
A. Background information	309
B. Direct correlation for the thermal conductivity at room temperature	314
References and notes for Chapter 14	317
Chapter 15. Transport of small Penetrant Molecules	318
A. Background information	318
B. Correlations for the permeability at room temperature	322
References and notes for Chapter 15	329
Chapter 16. Thermal Stability	332
A. Background information	332
B. Correlation for the molar thermal decomposition function	337
References and notes for Chapter 16	348
Chapter 17. Extensions, Generalizations, Shortcuts, and Possible Directions for Future Work	350
A. Introduction	350
B. Examples of designer correlations	351
C. Combination of new correlations and group contributions	356
D. Calculation of the properties of alternating copolymers	359
E. Calculation of the properties of random copolymers	361
F. A software package implementing the key correlations	364
G. Possible directions for future work	368
References and notes for Chapter	370

Chapter 17. Detailed Examples	372
A. Introductory remarks	372
B. Polystyrene	372
C. Random copolymers of styrene and oxytrimethylene	383
Glossary: Symbols and Abbreviations	391
Index	399