

# Theoretical Aspects and Computer Modeling of the Molecular Solid State

*EDITED BY*

*ANGELO GAVEZZOTTI*

*University of Milan, Italy*

*The Molecular Solid State Volume I*

**JOHN WILEY & SONS**

Chichester • New York • Weinheim • Brisbane • Singapore • Toronto

# Contents

<b>Contributors</b> . . . . .	vii
<b>Preface</b> . . . . .	ix
<b>1 Crystal Symmetry and Molecular Recognition</b> . . . . .	1
A. Gavezzotti	
<b>2 Intermodular Forces - from the Molecular Charge Distribution to the Molecular Packing</b> . . . . .	31
S. L. Price	
<b>3 Energetic Aspects of Crystal Packing: Experiment and Computer Simulations</b> . . . . .	61
A. Gavezzotti and G. Filippini	
<b>4 Energy Minimization and Molecular Dynamics Calculations for Molecular Crystals</b> . . . . .	99
B. P. van Eijck, L. M. J. Kroon-Batenburg and J. Kroon	
<b>5 Nucleation and Phase Transitions in Molecular Clusters: Molecular Dynamics Simulation and Experiment</b> . . . . .	147
L. S. Bartell	
<b>6 <i>Ab Initio</i> Prediction of Possible Molecular Crystal Structures</b> . . . . .	185
R. J. Gdanitz	
<b>7 The Crystal Habit of Molecular Materials: A Structural Perspective</b> . . . . .	203
G. Clydesdale, K. J. Roberts and E. M. Walker	
<b>Index</b> . . . . .	233