

Contents

Part I Jahn-Teller Effect and Vibronic Interactions: General Theory

Recent Developments in the Jahn-Teller Effect Theory	3
Isaac B. Bersuker	

Electronic Degeneracy and Vibrational Degrees of Freedom: The Permutational Proof of the Jahn-Teller Theorem	25
Arnout Ceulemans and Erwin Lijnen	

Group-Theoretical Analysis of Jahn-Teller Systems	51
Martin Breza	

Spin-Orbit Vibronic Coupling in Jahn-Teller and Renner Systems	77
Leonid V. Poluyanov and Wolfgang Domcke	

Vibronic Coupling Constant and Vibronic Coupling Density	99
Tohru Sato, Ken Tokunaga, Naoya Iwahara, Katsuyuki Shizu, and Kazuyoshi Tanaka	

A New Method to Describe the Multimode Jahn-Teller Effect Using Density Functional Theory	131
Matija Zlatar, Carl-Wilhelm Schl�pfer, and Claude Daul	

Part II Conical Intersections and Nonadiabatic Dynamics in Molecular Processes

Second-Order Analysis of Conical Intersections: Applications to Photochemistry and Photophysics of Organic Molecules	169
Llu�s Blancafort, Benjamin Lasorne, Michael J. Bearpark, Graham A. Worth, and Michael A. Robb	

Influence of the Geometric Phase and Non-Adiabatic Couplings on the Dynamics of the $H+H_2$ Molecular System	201
Foudhil Bouakline, Bruno Lepetit, Stuart C. Althorpe, and Aron Kuppermann	
Multi-Mode Jahn–Teller and Pseudo-Jahn–Teller Effects in Benzenoid Cations	239
Shirin Faraji, Etienne Gindensperger, and Horst Köppel	
On the Vibronic Interactions in Aromatic Hydrocarbon Radicals and Radical Cations	277
V. Sivaranjana Reddy and S. Mahapatra	
The Jahn–Teller Effect in Binary Transition Metal Carbonyl Complexes	311
Russell G. McKinlay and Martin J. Paterson	
 Part III Impurities; Spectroscopy of Transition Metal Complexes	
Jahn–Teller Effect for the 3d Ions (Orbital Triplets in a Cubic Crystal Field)	347
M.G. Brik, N.M. Avram, and C.N. Avram	
Constructing, Solving and Applying the Vibronic Hamiltonian	371
Philip L.W. Tregenna-Piggott and Mark J. Riley	
Instabilities in Doped Materials Driven by Pseudo Jahn–Teller Mechanisms	415
P. García-Fernández, A. Trueba, J.M. García-Lastra, M.T. Barriuso, M. Moreno, and J.A. Aramburu	
The Influence of Jahn–Teller Coupling on the High-Spin/Low-Spin Equilibria of Octahedral $M^{III}L_6$ Polyhedra ($M^{III} : Mn - Cu$), with NiF_6^{3-} as the Model Example	451
D. Reinen and M. Atanasov	
 Part IV Fullerenes and Fullerides	
Following Jahn–Teller Distortions in Fulleride Salts by Optical Spectroscopy	489
G. Klupp and K. Kamarás	

Jahn–Teller Effects in Molecules on Surfaces with Specific Application to C₆₀	517
Ian D. Hands and Janette L. Dunn, Catherine S.A. Rawlinson, and Colin A. Bates	

Part V Jahn-Teller Effect and Molecular Magnetism

Jahn–Teller Effect in Molecular Magnetism: An Overview	555
Boris Tsukerblat, Sophia Klokishner, and Andrew Palii	

The Effect of Jahn–Teller Coupling in Hexacyanometalates on the Magnetic Anisotropy in Cyanide-Bridged Single-Molecule Magnets	621
Mihail Atanasov and Peter Comba	

Part VI The Cooperative Jahn-Teller Effect and Orbital Ordering

Cooperative Jahn–Teller Effect: Fundamentals, Applications, Prospects	653
Michael Kaplan	

Orbital Ordering Versus the Traditional Approach in the Cooperative Jahn–Teller Effect: A Comparative Study	685
Victor Polinger	

Frustration Effect in Strongly Correlated Electron Systems with Orbital Degree of Freedom	727
Sumio Ishihara	

Ultrasonic Consequences of the Jahn–Teller Effect	743
Vladimir Gudkov	

Long Range Cooperative and Local Jahn-Teller Effects in Nanocrystalline Transition Metal Thin Films	767
Gerald Lucovsky	

Part VII Jahn-Teller Effect and High-Tc Superconductivity

Jahn–Teller Polarons, Bipolarons and Inhomogeneities. A Possible Scenario for Superconductivity in Cuprates	811
Joaquin Miranda Mena	

Polarons and Bipolarons in Jahn–Teller Crystals841
Chishin Hori and Yasutami Takada

**Vibronic Polarons and Electric Current Generation by a Berry
Phase in Cuprate Superconductors873**
Hiroyasu Koizumi

Index907