

SpringerBriefs in Molecular Science

Electrical and Magnetic Properties of Atoms,
Molecules, and Clusters

Series editor

George Maroulis

For further volumes:
<http://www.springer.com/series/11647>

Sven Heiles · Rolf Schäfer

Dielectric Properties of Isolated Clusters

Beam Deflection Studies

 Springer

Sven Heiles
Rolf Schäfer
Eduard-Zintl Institut für Anorganische und
Physikalische Chemie
Technische Universität Darmstadt
Alarich-Weiss-Straße 8, 64287
Darmstadt
Germany

ISSN 2191-5407 ISSN 2191-5415 (electronic)
ISBN 978-94-007-7865-8 ISBN 978-94-007-7866-5 (eBook)
DOI 10.1007/978-94-007-7866-5
Springer Dordrecht Heidelberg New York London

Library of Congress Control Number: 2013951802

© The Author(s) 2014

This work is subject to copyright. All rights are reserved by the Publisher, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, reuse of illustrations, recitation, broadcasting, reproduction on microfilms or in any other physical way, and transmission or information storage and retrieval, electronic adaptation, computer software, or by similar or dissimilar methodology now known or hereafter developed. Exempted from this legal reservation are brief excerpts in connection with reviews or scholarly analysis or material supplied specifically for the purpose of being entered and executed on a computer system, for exclusive use by the purchaser of the work. Duplication of this publication or parts thereof is permitted only under the provisions of the Copyright Law of the Publisher's location, in its current version, and permission for use must always be obtained from Springer. Permissions for use may be obtained through RightsLink at the Copyright Clearance Center. Violations are liable to prosecution under the respective Copyright Law. The use of general descriptive names, registered names, trademarks, service marks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

While the advice and information in this book are believed to be true and accurate at the date of publication, neither the authors nor the editors nor the publisher can accept any legal responsibility for any errors or omissions that may be made. The publisher makes no warranty, express or implied, with respect to the material contained herein.

Printed on acid-free paper

Springer is part of Springer Science+Business Media (www.springer.com)

Contents

1 Introduction	1
References	5
2 Molecular Beam Electric Field Deflection:	
Experimental Considerations	7
2.1 Experimental Setup and Measurement Principle	7
2.2 Vacuum System	10
2.3 Cluster Source Design	11
2.4 Deflection Unit	13
2.5 Position-Sensitive Mass Spectrometry	15
References	16
3 Molecular Beam Electric Field Deflection:	
Theoretical Description	17
3.1 Particles in an Inhomogeneous Electric Field: Force and Deflection	17
3.2 Quantum Chemical Prediction of Cluster Structures and Dielectric Properties	22
3.2.1 Predicting Cluster Structures Using Global Optimization Techniques	22
3.2.2 Quantum Chemical Predictions of the Dielectric Properties.	26
3.3 Rigid Rotor in a Weak Electric Field: Beam Deflection and Distribution Function	32
3.4 Classical Rigid Rotor in an External Field	38
3.5 Quantum Mechanical Rigid Rotor in an External Field	46
3.6 Floppy Clusters	54
References	56

4 Case Studies	61
4.1 Molecular Clusters and Complexes	62
4.2 Metal and Semiconductor Clusters (Group 14)	66
4.3 Core-Shell Clusters and Nanoalloys	73
References	78
5 Novel Experimental Tools	81
5.1 Light Force and Near Field Interferometry	82
5.2 Stark-Modulation of Neutral Molecule Trajectories	87
References	93
6 Summary	95
References	96
Index	99