

**Lecture Notes in
Chemistry**

69

W. Kliesch

**A Mechanical
String Model
of Adiabatic Chemical
Reactions**

541-45-1



Springer

Contents

Table of Notations	V
1 Introduction	1
2 Molecular Systems	7
2.1 Translation and Rotation of Nuclear Ensembles	10
2.2 Configuration Space	15
2.3 Energy Function	21
2.4 A Modified Energy Function	35
3 Reaction Path Concept	39
4 A Mechanical String Model of Chemical Reactions	45
4.1 Molecular Dynamics	45
4.2 A Model of Chemical Reactions	50
4.3 Equilibrial Reaction Paths	64
4.4 Summary	75
5 Equilibrial Path Tracing	79
5.1 A Predictor–Corrector Method	79
5.2 Update Methods	82
5.3 Steplength Determination	94
5.4 A Path Tracing Procedure	95
6 Applications	99
6.1 Hydrocyanic Acid PES	100
6.2 Formaldehyde PES	104
6.3 Formic Acid PES	113
Bibliography	123
Index	127