Downloaded from UvA-DARE, the institutional repository of the University of Amsterdam (UvA)
http://dare.uva.nl/document/68531

File ID	68531
Filename	CONTENTS

SOURCE (OR PART OF THE FOLLOWING SOURCE):

Type	Dissertation
Title	Excited state spectroscopy by ionic projection
Author	D.H.A. ter Steege
Faculty	Faculty of Science
Year	2003

FULL BIBLIOGRAPHIC DETAILS:
http://dare.uva.nl/record/129779

Copyright

It is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), other then for strictly personal, individual use.

UvA-DARE is a service provided by the library of the University of Amsterdam (http://dare.uva.nl)

CONTENTS

CHAPTER ONE: INTRODUCTION

1.1	The importance of excited states	1
1.2	Orbitals and transitions	2
1.3	Selection rules	4
1.4	Molecules with carbonyl and amide groups	5
1.5	Multiphoton absorption	7
1.6	Vibronic coupling	8
1.7	Excited state photoelectron spectroscopy	9
1.8	Rydberg states	11
1.9	Introduction in general computational methods	12
1.10	Outline of the thesis	16
References		19

CHAPTER TWO: RESONANCE-ENHANCED MULTIPHOTON IONISATION PHOTOELECTRON SPECTROSCOPY OF THE CLO RADICAL: THE $C^2\Sigma^-$ STATE

2.1	Introduction	22
2.2	Experimental setup	25
2.3	Computational details	27
2.4	Results and Discussion	28
2.5	Conclusions	39
References		40

CHAPTER THREE: VIBRONIC COUPLING IN EXCITED STATES OF ACETONE

3.1	Introduction	44
3.2	Experimental and theoretical details	49
3.3	Results and discussion	51
	3.3.1 (2+1) REMPI-PES of supersonically cooled acetone-h_6 and -d_6	51
	3.3.2 (3+1) REMPI-PES of acetone-h_6 and -d_6	66
	3.3.2.1 58500 – 64200 cm^{-1} (7.2 – 7.9 eV) spectral region	67
	3.3.2.2 65 000 – 71 000 cm^{-1} (8.0 – 8.8 eV) spectral region	72
	3.3.2.3 71 000 – 76 500 cm^{-1} (8.8 – 9.5 eV) spectral region	74
3.4	Conclusions	76
References		78

CHAPTER FOUR: EXCITED AND IONIC STATES OF FORMAMIDE: AN EXCITED-STATE PHOTOELECTRON SPECTROSCOPY AND *AB INITIO* STUDY

4.1 Introduction 82
4.2 Experimental and theoretical details 85
4.3 Results and discussion 87
4.3.1 Calculations 87
4.3.2 Ionisation energies 91
4.3.3 Excitation and excited-state photoelectron spectroscopy 95
4.4 Conclusions 106
References 108

CHAPTER FIVE: SPECTROSCOPY AND DYNAMICS OF EXCITED STATES IN MALEIMIDE AND N-METHYL MALEIMIDE: IONIC PROJECTION AND *AB INITIO* CALCULATIONS

5.1 Introduction 112
5.2 Experimental and theoretical details 116
5.3 Results and discussion 118
5.3.1 Maleimide 118
5.3.1.1 Ab initio calculations 118
5.3.1.2 Multiphoton ionisation and excited-state photoelectron spectroscopy 124
5.3.2 N-methyl maleimide 132
5.3.2.1 Ab initio calculations 132
5.3.2.2 Multiphoton ionisation and excited-state photoelectron spectroscopy 138
5.4 Conclusions 142
References 144

SAMENVATTING 147

DANKWOORD 152

Aan mijn moeder en mijn vader.
Aan Juliette, Sander en Bart.