

Contents

Declaration by Candidate	v
Certificate by the Supervisor	vii
Certificate by the Co-Supervisor	ix
Acknowledgements	xv
List of Publications	xvii
Abstract	xxvii
1 Interstellar Polycyclic Aromatic Hydrocarbon molecules	1
1.1 The Interstellar Medium	1
1.1.1 The Interstellar Molecules	3
1.1.2 The Polycyclic Aromatic Hydrocarbon Molecules in the ISM	7
1.2 Evidence of interstellar PAHs in the ISM	8
1.2.1 The mid-infrared emission bands	9
1.2.2 UV absorption bump at 217.5 nm	11
1.2.3 Diffuse Interstellar Bands	12
1.2.4 Other spectral signatures	14
1.3 Laboratory and Theoretical study on PAHs: Implications to PAH-AIB hypothesis	15
1.3.1 Experimental spectroscopy of PAHs	15

1.3.2	Theoretical spectroscopy of PAHs	18
1.4	Aim of the thesis	19
1.4.1	Theoretical methodology applied	20
1.4.2	Emission Model	22
1.5	Organization of the thesis	23
2	The Interstellar Deuterated and Deuteronated PAHs I	25
2.1	Introduction	25
2.2	Probable DPAH ⁺ formation mechanisms in the ISM	28
2.3	Molecules studied	30
2.4	Results and Discussion	31
2.4.1	Deuteronated pyrene	31
2.4.2	Deuteronated perylene	35
2.4.3	Deuteronated coronene	40
2.4.4	Theoretical spectra for deuterated-deuteronated coronene and deuteronated circumcoronene	44
2.5	DPAH ⁺ molecules as carriers of UIR emission features	46
2.6	Conclusion	49
3	The Interstellar Deuterated and Deuteronated PAHs II	51
3.1	Introduction	51
3.2	Molecules studied	52
3.3	Emission Model	53
3.4	Results and Discussion	55
3.5	Astrophysical Implications	63
3.6	Conclusion	71
4	The Interstellar PAH molecules with aliphatic side groups	73
4.1	Introduction	73
4.2	Molecules studied	74
4.3	Results and Discussion	76

4.4	Astrophysical Implications	84
4.5	Conclusion	87
5	The Interstellar Dehydrogenated PAH anions	89
5.1	Introduction	89
5.2	Molecules studied	91
5.3	Results and Discussion	92
5.3.1	Coronene	92
5.3.2	Perylene	98
5.3.3	Ovalene	98
5.4	Astrophysical implications	100
5.5	Summary	104
6	Conclusion	107
6.1	Summary of the results	107
6.2	Future Prospects	110
6.2.1	Alternative applications of PAHs	111
Bibliography		113
A Wavelengths and Relative Intensities of Vibrational Modes		141
A.1	Sample molecules studied in chapter 2	142
A.2	Sample molecules studied in chapter 3	146
A.3	Sample molecules studied in chapter 4	155
A.4	Sample molecules studied in chapter 5	160

