

CHAPTERS	CONTENTS	PAGE NO
1	INTRODUCTION	1
	1.1. Supramolecular Chemistry	1
	1.2. Molecular Recognition	2
	1.3. Self Assembly	3
	1.4. Hydrogen Bonding	3
	1.5. π - π Stacking	4
	1.6. Solid-State Self-Assembly	4
	1.7. Crystal Engineering	4
	1.8. Supramolecular Synthons	5
	1.9. Applications of Crystal Engineering	6
	1.10. Solid State Chemistry	7
	1.11. Crystallization	7
	1.12. Crystal Growth Techniques	7
	1.13. Organic acid-Base Crystals	8
2	EXPERIMENTAL PROCEDURE	10
	2.1. Materials	10
	2.2. Preparation of 2-Amino-5-Bromopyridinium Picrate (ABPP) Single Crystals	10
3	CHARACTERISATION OF 2-AMINO-5-BROMOPYRIDINIUM PICRATE (ABPP) CRYSTALS	12
	3.1. Elemental Analysis	12
	3.2. FTIR Spectral Analysis	12
	3.3. NMR Spectral Analysis	14
	3.3.1. ^1H NMR Spectral Analysis	14
	3.3.2. ^{13}C NMR Spectral Analysis	14
	3.4. Single Crystal X-ray Diffraction Analysis	15
	3.5. Hirshfeld Surface Analysis	19
	3.6. Optimized Geometry	21

3.7. Molecular Electrostatic Potential (MEP) and Contour Mapping	23
3.8. Mulliken Atomic Charges	24
3.9. NBO Analysis	25
3.10. Electronic Spectral Analysis	32
3.11. Thermal Analysis	33
3.12. Hyperpolarizability Calculations	34
3.13. Conclusions	36