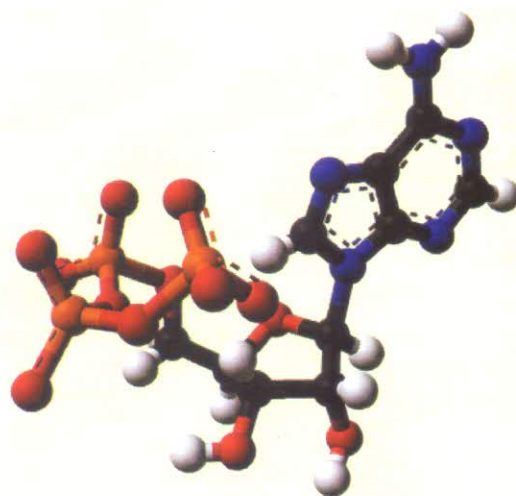


**SINGLE CRYSTAL STRUCTURE
DETERMINATION
OF ORGANIC COMPOUNDS AND
METAL-ORGANIC COMPLEXES
BY X-RAY DIFFRACTION**

**FINAL REPORT SUBMITTED
FOR
MINOR RESEARCH PROJECT IN PHYSICS
[F. No. PSW-134/13-14(ERO) dated: 18-03-2014]
UNIVERSITY GRANTS COMMISSION,
NEW DELHI-11002**

**BY
ARPITA DAS**



**DEPARTMENT OF PHYSICS
MUGBERIA GANGADHAR MAHAVIDYALAYA
BHUPATINAGAR, PURBA MEDINIPUR
WEST BENGAL – 721425, INDIA**



Estd. 1964



**Single crystal structure
determination
of organic compounds and
metal-organic complexes
by X-ray diffraction**

**FINAL REPORT SUBMITTED
FOR
MINOR RESEARCH PROJECT IN PHYSICS
[F. No. PSW-134/13-14(ERO) dated: 18-03-2014]
UNIVERSITY GRANTS COMMISSION,
NEW DELHI-11002**



BY

ARPITA DAS

**DEPARTMENT OF PHYSICS
MUGBERIA GANGADHAR MAHAVIDYALAYA
BHUPATINAGAR, PURBA MEDINIPUR
WEST BENGAL - 721425, INDIA**

CONTENTS

Preface	i
Publication list	ii
Chapter-1: Single crystal structure determination by X-ray diffraction	1-16
1.1. Fourier synthesis of the electron density	2
1.2. One-dimensional Synthesis	3
1.3. Phase Problem in Crystallography	5
1.4. Structure determination from single crystal X-ray data	7
1.4.1. Collection of X-ray intensity data	7
1.4.2. Space group determination	7
1.4.3. Crystal structure solution	8
1.4.4. Structure refinement	13
References	15
Chapter-2: Molecular recognition and crystal engineering	17-36
2.1. Molecular Recognition	18
2.2. Self-assembly	19
2.3. Crystal engineering	20
2.3.1. Supramolecular synthon	21
2.3.2. Non-covalent interactions	21
2.3.2.1. Hydrogen Bonding interactions	22
2.3.2.2. Interactions involving π -cloud of aromatic rings	23
2.3.2.3. Metal-Metal Interactions	29
References	31
Chapter-3: Supramolecular self-assembly and Hirshfeld surface analysis of 4,4'-Oxybis(benzoic acid)	37-51
3.1. Introduction	38
3.2. Experimental	39
3.2.1. Synthesis	39
3.2.2. Crystallographic analysis	40
3.2.2. Hirshfeld surface analysis	41
3.3. Result and discussions	42
3.3.1. Structural description	42
3.3.2. Hirshfeld surface	45
3.4. Conclusions	48
References	49
Reprints of the Published paper	52
Summary and Future plan	61