

# CONTENTS

## PART I

### CHAPTER I. SOME FUNDAMENTAL IDEAS

1.1. What are direct methods ?	1
1.2. The unitary structure factor	2
1.3. The derivation of unitary structure factors	6
1.4. The normalized structure factor	13

### CHAPTER II. INEQUALITY RELATIONSHIPS

2.1. Harker-Kasper inequalities	15
2.2. Inequalities for structures with symmetry element $\bar{1}$	17
2.3. Structure invariants	21
2.4. An application of Harker-Kasper inequalities	25
2.5. Inequality relationships for other symmetry elements	35
2.6. The scope and limitations of inequality relationships	41

### CHAPTER III. SIGN RELATIONSHIPS

3.1. Sayre's equation	43
3.2. The basic sign relationship	48
3.3. Other sign relationships for $P\bar{1}$	52
3.4. Sign relationships in conjunction with inequalities	55

### CHAPTER IV. THE APPLICATION OF SIGN RELATIONSHIPS TO STRUCTURE DETERMINATION

4.1. The general problem	63
4.2. The hit-or-miss method	64
4.3. The coincidence method	65
4.4. The method of structure invariants	73
4.5. The use of relationships between sign relationships	80
4.6. The scope and limitation of the hand application of sign relationships	84

## PART II

### CHAPTER V. COMPUTER METHODS OF APPLYING SIGN RELATIONSHIPS

5.1. The Hauptman and Karle procedure	88
5.2. The Cochran and Douglas method	94
5.3. The Vand and Pepinsky method	101
5.4. An extension of the method of structure invariants	106

CHAPTER VI. ADDITIONAL CRITERIA FOR SIGN DETERMINATION	
6.1. The necessity for additional criteria	107
6.2. The upper and lower bound criterion	107
6.3. The zero-check	108
6.4. The $Z$ -test	112
CHAPTER VII. THE PAST, THE PRESENT, AND THE FUTURE	
7.1. What has been achieved by direct methods ?	122
7.2. What can be done now ?	123
7.3. What does the future hold ?	128
APPENDIXES I TO V	130
SOLUTIONS TO EXAMPLES	137
REFERENCES	140
INDEX	143