

# Table of Contents

<b>Acknowledgements</b>	iii
<b>Abstract</b>	v
<b>Zusammenfassung</b>	vii
<b>Table of contents</b>	ix
<b>Chapter 1: Introduction</b>	
1.1 Motivation of the thesis	1
1.2 Complexity of crystals	3
1.3 Probes for local crystallography	5
1.3.1 Monte Carlo (MC) simulation technique	6
1.3.2 Atomic Pair Distribution Function (PDF) technique	8
1.4 The structure of the thesis	11
1.5 Bibliography	12
<b>Chapter 2: Mathematical and symmetry aspects of crystals</b>	
2.1 Disorder in crystals	15
2.1.1 Different types of disorder present in crystals	21
2.1.1.1 Static disorder	21
2.1.1.1.1 Substitutional disorder	21
2.1.1.1.2 Displacement disorder	27
2.1.1.1.2.1 Stacking faults	32
2.1.1.2 Dynamic disorder	34
2.1.1.3 Magnetic disorder	35
2.2 Polytypism in layered structures	36
2.2.1 Order-Disorder (OD) theory of polytypes	37
2.2.2 Stacking ambiguities in close-packed structures and NFZ relationship	40
2.2.3 MDO polytypes	42
2.2.4 The groupoid symbol	44
2.2.5 Diffraction features of OD structures	45
2.2.6 Categories of OD structures	48
2.2.6.1 OD structures of equivalent layers	48
2.3 Bibliography	50

<b>Chapter 3: Diffraction pattern of a crystal of the <math>\beta</math>-phase of Pigment Red 170</b>	
3.1	Pigment Red 170 53
3.1.1	Crystallization of the $\beta$ -phase of Pigment Red 170 55
3.1.2	X-ray data collection 55
3.2	Diffraction pattern 56
3.2.1	Coarse features 56
3.2.2	Fine features 57
3.3	Bibliography 60
<b>Chapter 4: The average structure of <math>\beta</math>-Pigment Red 170</b>	
4.1	Introduction to the average structure of $\beta$ -Pigment Red 170 61
4.1.1	Indexing and unit cell determination 61
4.1.2	Extraction of the Bragg intensities 63
4.1.3	Space group determination 64
4.1.4	Attempts at structure solution and refinement 65
4.2	Description of the average structure 68
4.2.1	Model 1 69
4.2.2	Model 2 70
4.2.3	Similarities and differences between model 1 and model 2 72
	4.2.3.1 Similarities and differences in direct space, OD analysis 72
	4.2.3.2 Similarities and differences in reciprocal space 76
4.3	Subgroup analysis 79
4.4	Summary and Conclusions 80
4.5	Bibliography 82
<b>Chapter 5: Beyond the average structure of <math>\beta</math>-P.R.170</b>	
5.1	Introduction to the local structure of $\beta$ -P.R.170 85
5.2	Experimental data for the local structure modeling 86
5.2.1	Measurement of diffuse scattering 86
5.2.2	Preparation of diffuse data for modeling 91
5.3	Construction of the model crystal 94
5.3.1	Disentanglement of the average structure and defining chemical units 94
5.3.2	Model crystal building and energy minimization 97
5.4	Intensity calculation and qualitative analysis of models 105
5.5	Summary and conclusions 116

5.6	Bibliography	117
	<b>Chapter 6: Conclusions and Outlook</b>	<b>119</b>
	<b>Appendix: Crystallographic Information Files (CIF)</b>	<b>123</b>
	for the average structure models 1 and 2 (only in electronic version).	
	They are also available from the International Union of Crystallography	
	electronic archives <i>via</i> <a href="http://journals.iucr.org">journals.iucr.org</a> (search keyword: og5065).	