Instrumental	And S	ize	Broader	ning								
Type Of Rad:												
Radiation	х-ка lamb	y da1	lambo	da2 rat	io							
Wavelength	1.5	406	0.000	0.0	000							
instrumental Aberrations	aberra	tions	2	zero	sycos	3 3	sysin					
Aberrations			(0.000	0.000	00	0.00					
Aberrations instr. broad Pseudo-Voigt	dening		u	V		W		Х	Ι)g	D]	L
Pseudo-Voigt		0.032	948 -	-0.003558	0.	.22740	0.0	00000	479	.26	459.	.87 Trim
		1	.00	0.00		0.0	U	0.00	1	.00	1.	.00
Structural												
! a Cell 3.	100000	b	100000	C 4 COO		gamı	ma n no					
Cell 3	21.00	٥.	21.00	c 4.608 1	.00	12	0.00					
Laue symmeti	Э											
Symm -3M number of la	+											
Nlayers 4	rier cyp	63										
layer width												
Lwidth Inf:	inite											
Layer 1												
Layer symmet												
LSYM Centi				7.7	7		Biso	000				
Atom name Atom Ni2+		0.6	7000	У 0.33000	0.00	0000	1.06197	0.50	000			
			0.00	0.00	(0.00	0.00	0	.00			
Atom name	number	υ s	3000	У 0 67000	Z 0 22	2265	Biso 0 75961	0cc	200			
Atom O2-	2	0.3	0.00	0.00	71	L.00	0.00	0	.00			
Layer 2 = 1												
Layer 3 = 1												
Layer 4 Layer symmet	2017											
Layer symmet Lsym Centi		ric										
Atom name	number	х		У	Z		Biso	0cc				
Atom Ni2+	3	0.0	0000	0.0000	0.00	1000	1.06197	0.500	100			
			0.00	0.0000	0.00	0.00	0.00	n 0	.00			
		X			Z		Biso	0cc				
Stacking stacking type Recursive number of la	4 De	x 0.3		У 0.67000	z 0.22	2265	Biso	0cc 1.000	000			
Stacking stacking type Recursive	4 De	x 0.3	3000	У 0.67000	z 0.22	2265	Biso 0.75961	0cc 1.000	000			
Stacking Stacking type Recursive number of 18 40.0	4 De	x 0.3	3000	У 0.67000	z 0.22	2265	Biso 0.75961	0cc 1.000	000			
Stacking stacking type Recursive Inumber of 1a 40.0	4 De ayers	x 0.3	3000	У 0.67000	z 0.22	2265	Biso 0.75961	0cc 1.000	000			
Stacking stacking type Recursive number of 12 40.0 1.0 Transitions layer 1 to 0.808196	4 pe ayers layer 5 0.000	x 0.3	3000 0.00	y 0.67000 0.00	z 0.22 71	2265	Biso 0.75961	0cc 1.000	000			
Atom 02- Stacking stacking typ Recursive number of 1a 40.0 1.0 Transitions clayer 1 to ct 0.808196 -92.00000	layer 5 0.000 0.000	x 0.3	3000 0.00 0.00000 0.00000	y 0.67000 0.00	2 0.22 7J	2265	Biso 0.75961 0.00	Occ 1.000	000			
Atom O2- Stacking stacking typ Recursive number of 1a 40.0 1.0 Transitions layer 1 to t 0.808196 -92.000000	layer 5 0.000 0.000	x 0.3	3000 0.00 0.00000 0.00000	y 0.67000 0.00	2 0.22 7J	2265	Biso 0.75961 0.00	Occ 1.000	000			
1.0 Transitions layer 1 to to 0.808196 -92.000000 FW 0.00 0.00 layer 1 to	layer 5 0.000 0 0 0 0 0 0 0 0 0 1 ayer	x 0.3	0.00000 0.00000 0.00000 0.00000	y 0.67000 0.000 0.000 0.000 0.000 0.000	2 0.222 73	2265	Biso 0.75961 0.00	Occ 1.000	000			
Atom 02- Stacking stacking tym Recursive number of 1a 40.0 1.0 Transitions layer 1 to tt 0.808194 -92.000000 w 0.00 0.00 layer 1 to LT 0.095902	layer 5 0.000 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	1 000 000 .00 .00 2	0.00000 0.00000 0.00000 0.00000	y 0.67000 0.00 0.00 0.00 0.00 0.00 0.00 0	2 0.222 71 0000 0000 0000 0.00	2265	Biso 0.75961 0.00	Occ 1.000	000			
Atom 02- Stacking stacking typ Recursive number of 1a 40.0 1.0 Transitions layer 1 to to 0.00 0.00 0.00 0.00 0.00 0.00 0.0	layer 5 0.000 0 0.000 0 0 0 0 0 0 0 0 0 0 0 0	1 000 000 .00 .00 2 000 .00	0.00000 0.00000 0.00000 0.00000 0.00000 0.000000	y 0.67000 0.00 0.00 0.00 0.00 0.00 0.00 0	2 0.222 71 0000 0000 0000 0.00	0.i 0.i	Biso 0.75961 0.00	Oce 1.000 0	000			
Atom O2- Stacking stacking tym Recursive number of 1: 40.0 1.0 Transitions layer 1 to .t 0.808194 -92.000000 W 0.00 layer 1 to .T 0.095902 91.000000 W 0.00	layer 5 0.000 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	1 000 000 .00 .00 2 000 .00 .00	0.00000 0.00000 0.00000 0.00000 0.00000 0.000000	y 0.67000 0.00 0.00 0.00 0.00 0.00 0.00 0	2 0.22 71	0.i 0.i	Biso 0.75961 0.00	Oce 1.000 0	000			
Stacking	layer 5 0.000 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	1 0000 0000 0000 0000 2 0000 0000 0000	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	Y 0.67000 0.	z 0.22 71	0.i 0.i	Biso 0.75961 0.00	Oce 1.000 0	000			
Atom 02- Stacking stacking tym Recursive number of 1a 40.0 1.0 Transitions layer 1 to bt 0.80819a -92.000000 FW 0.00 0.00 clayer 1 to 0.7 0.000000	layer 5 0.000 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	y 0.67000 0.00 0.00 0.00 0.00 0.00 0.00 0	2 0.22 71	0.i 0.i	Biso 0.75961 0.00	Oce 1.000 0	000			
Stacking	layer 5 0.000 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	1 0000 0000 .000 .000 .000 .000 .000 .0	3000 0.00 0.00 0.00 0.00 0.00 0.00 0.00	Y 0.67000 0.	2 0.22 71	0.i 0.i	Diso 0.75961 0.00	0.00 0.00 0.00 0.00	000			
Atom 02- Stacking Stacking typ Recursive Lumber of 1a 40.0 1.0 Transitions Layer 1 to 0.00 0.00 Layer 1 to 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.	layer 5 0.000 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	1 000 000 000 .00 .00 2 000 .00 .00 .00	3000 0.00 0.00 0.00 0.0 0.0 0.0 0.0 0.0	Y 0.67000 0.	2 0.22 71 0.000 0.000 0.000 0.000 0.000 0.000 0.000	0.i 0.i	Diso 0.75961 0.00	0.00 0.00 0.00 0.00	000			
Atom 02- Stacking stacking tym Recursive number of 1: 40.0 1.0 Transitions layer 1 to 1.0 0.00000000000000000000000000000000	layer 5 0.000 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	1 0000 0000 .000 .000 .000 .000 .000 .0	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000	Y 0.67000 0.	2 0.222 773 773 773 773 773 773 773 773 773	0.i 0.i	Diso 0.75961 0.00	0.00 0.00 0.00 0.00	000			
Atom 02- Stacking stacking tym Recursive number of 1a 40.0 1.0 Transitions layer 1 to be 0.808194 -92.000000 0.000 0.000000 0.000000 0.000000	layer 5 0.000 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	1 0000 0000 .000 .000 .000 .000 .000 .0	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	y 0.67000 0.000	2 0.22 73	0 0 0	Diso 0.75961 0.00	0.00 0.00 0.00 0.00	000			
Atom 02- Stacking stacking tym Recursive number of 1a 40.0 1.0 Transitions layer 1 to be 0.808194 -92.000000 0.000 0.000000 0.000000 0.000000	layer 5 0.000 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	1 0000 0000 .000 .000 .000 .000 .000 .0	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	y 0.67000 0.000	2 0.22 73	0 0 0	Biso 0.75961 0.00	0.00 0.00 0.00 0.00	000			
Atom 02- Stacking stacking tym Recursive number of 1a 40.0 1.0 Transitions layer 1 to be 0.808194 -92.000000 0.000 0.000000 0.000000 0.000000	layer 5 0.000 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	1 0000 0000 .000 .000 .000 .000 .000 .0	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	Y 0.67000 0.	2 0.22 73	0 0 0	Biso 0.75961 0.00	0.00 0.00 0.00 0.00	000			
Atom O2- Stacking stacking tym Recursive number of 1a 40.0 1.0 Transitions layer 1 to 0.808194 -92.000000 0.00 W 0.00 0.00 W 0.00 0.00 Layer 1 to 0.00000 0.00 Layer 1 to 0.00000 0.00000 0.000000 0.000000 0.000000	layer 5 0.000 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	1 0000 0000 .000 .000 .000 .000 .000 .0	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	y 0.67000 0.000	2 0.22 73	0 0 0	Biso 0.75961 0.00	0.00 0.00 0.00 0.00	000			
Atom 02- Stacking Stacking Stacking Recursive Rumber of 1a 40.0 1.0 Transitions Rayer 1 to 0.0 0.00 0.00 0.00 0.00 0.00 0.00 0.0	layer 5 0.000 0.000 0 0 0 0 0 0 0 0 0 0 0 0 0	x 0.3 1 0000 0000 .000 .000 2 0000 .000 .000	3000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000	Y 0.67000 0.	2 0.22773	0 0 0	Biso 0.75961 0.00	0.00 0.00 0.00 0.00	000			
Atom 02- Stacking Stacking Stacking typ Recursive Lumber of 1a 40.0 1.0 Transitions Llayer 1 to 0.0 0.00 0.00 0.00 0.00 0.00 0.00 0.0	layer 5 0.000 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	x 0.3 1 0000 .000 .000 .000 .000 .000 .00	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000	Y 0.67000 0.	2 0.22 73	0 0 0	Biso 0.75961 0.00	0.00 0.00 0.00 0.00	000			
Atom 02- Stacking stacking tymecursive number of lade 40.0 1.0 Transitions 1 to 0.808194 -92.000000	layer 5 0.000 0.000 0 0 0 0 0 0 0 0 0 0 0 0 0	x 0.3 1 0000 0000 .000 .000 2 0000 .000 .000	3000 0.0000 0.000	Y 0.67000 0.	2 0.22773	0 0 0	Biso 0.75961 0.00	0.00 0.00 0.00 0.00 0.00	000			
Atom 02- Stacking stacking tymecursive number of lade 40.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0	layer 5 0.000 0 0.000 0 0 0 0 0 0 0 0 0 0 0 0	x 0.33 1 0000 .000 .000 .000 .000 .000 .000 .	3000 0.0000 0.000	Y 0.67000 0.	2 0.227777777777777777777777777777777777	0 0 0	Biso 0.75961 0.00	0.00 0.00 0.00 0.00 0.00	000			
Atom 02- Stacking stacking tymecursive number of lade 40.0 1.0 Transitions 1 to to to 88819492.000000 1 to 1.0 Layer 1 to 0.005950 1 to 0.00000 1 to 0.000000 1 to 0.0000000 1 to 0.0000000 1 to 0.00000000 1 to 0.00000000 1 to 0.00000000 1 to 0.0000000000000000000000000000000000	layer 5 0.000 0.00	x 0.3 1 0000 0000 .000 .000 2 0000 .000 .000	3000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.0000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.00000000	Y 0.67000 0.	2 0.22773	0 0 0	Biso 0.75961 0.00	0.00 0.00 0.00 0.00 0.00	000			
Atom 02- Stacking stacking tym Recursive number of 1a 40.0 1.0 Transitions layer 1 to 0.0000000000000000000000000000000000	layer 0.000 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	x 0.3 1 0000 0000 .000 .000 .000 .000 .000 4 0000 .000 .	3000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.0000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.000000 0.00000000	Y 0.67000 0.	2 0.22 73 73 73 73 73 73 73 73 73 73 73 73 73	000 000	Biso 0.75961 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00	000			
Atom 02- Stacking stacking tym Recursive number of 1a 40.0 1.0 Transitions layer 1 to 0.0000000000000000000000000000000000	layer 0.000 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	x 0.3 1 0000 0000 .000 .000 .000 .000 .000 4 0000 .000 .	3000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.0000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.000000 0.00000000	Y 0.67000 0.	2 0.227 773	000 000 000.	Biso 0.75961 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00	000			
Atom 02- Stacking stacking stacking typ Recursive number of 1a 40.0 1.0 Transitions layer 1 to 0.80819 -92.000000 0.000000 0.000000 0.000000 0.000000	layer 0.000 0.000 0 0.	x 0.33 1 0000 .000 .000 .000 .000 .000 .000 .	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000	Y 0.67000 0.	2 0.22 73 3 0000 0000 0000 0000 0000 0000 00	000 000 000.	Biso 0.75961 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00	000			
Atom 02- Stacking stacking stacking rym Recursive number of 1a 40.0 1.0 Transitions layer 1 to to to 0.00 0.00 0.00 0.00 0.00 0.00	layer 5 0.000 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	x 0.3 1 1 0000 000000 3 0000 000000 1 1 0000 0000	0.000000 0.000000 0.000000 0.000000 0.000000	Y 0.67000 0.	2 0.227 773 0000 0000 0000 0000 0000 0000 00	000 000 000.	Biso 0.75961 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00	000			
Atom 02- Stacking stacking stacking typ Recursive number of 1a 40.0 1.0 Transitions layer 1 to 0.808194 -92.000000 0.000000000 0.0000000000000000	layer 5 0.000 0 0.000 0 0 0 0 0 0 0 0 0 0 0 0	x 0.3 1 0000 0000 .000 .000 .000 .000 .000 .	3000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.0000000 0.000000 0.0000000 0.00000000	Y 0.67000 0.	2 0.227 773 8 10000 10000 1.00	0 0 0 0	Biso 0.75961 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00	000			
Atom 02- Stacking Stacking Stacking Recursive Lumber of 1a 40.0 1.0 Transitions Clayer 1 to Ct 0.808194 -92.000000 FW 0.00 Clayer 1 to CT 0.000000 FW 0.00 Clayer 2 to CT 0.000000 FW 0.00 CD 0.00	layer 5 0.000 0 0.000 0 0 0 0 0 0 0 0 0 0 0 0	x 0.3 1 1 0000 0000 000 000 000 000 000 000	3000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.0000000 0.000000 0.0000000 0.00000000	Y 0.67000 0.	2 0.227 773 8 10000 10000 1.00	0000 0000	Biso 0.75961 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00	000			
Atom 02- Stacking stacking tym Recursive number of 1a 40.0 1.0 1.0 Transitions 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0	layer 5 0.000 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	x 0.3 1 0000 .000 .000 .000 .000 .000 .000 .	0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000	Y 0.67000 0.	2 0.22 73 73 73 73 73 73 73 73 73 73 73 73 73	0000 0000	Biso 0.75961 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	000			
Atom 02- Stacking St	layer 0.000 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	x 0.3 1 0000 0000 .000 .000 2 0000 .000 .000 4 0000 .000 1 0000 .000 .000 2 0000 .000 .000 .000 .000	3000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.0000000 0.000000 0.00000000	Y 0.67000 0.	2 0.22 713 0000 0000 0000 0000 0000 0000 0000	0000 0000	Biso 0.75961 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	000			
Atom 02- Stacking stacking stacking typ Recursive number of 1a 40.0 1.0 Transitions layer 1 to t 0.808194 -92.000000 W 0.00 layer 1 to T 0.095902 91.000000 W 0.00 layer 1 to T 0.095902 91.000000 W 0.00 layer 1 to T 0.095902 91.000000 W 0.00 layer 2 to T 0.000000	layer 5 0.000 0 0.000 0 0 0 0 0 0 0 0 0 0 0 0	x 0.33 1 1 0000 000000 2 0000 0.0000 3 0000 0.0000 3 0000 0.000	0.00000 0.000000 0.000000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.0000	Y 0.67000	2 0.22771	0000	Diso 0.75961 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	000			

!la	yer 3 to	laver 1					
LT	0.132589	0.333000	0.666700	1.000000			
-	111.000000	0.000000	0.000000	0.000000			
FW	0.00	0.00	0.00	0.00	0.00	0.00	
11a	0.00 ver 3 to	layer 2	0.00	0.00	0.00	0.00	
LT	0.000000	0.000000	0.000000	0.000000			
	0.000000	0.000000	0.000000	0.000000			
FW	0.00	0.00	0.00	0.00	0.00	0.00	
	0.00	0.00 layer 3	0.00	0.00	0.00	0.00	
		l 0.000000	0 000000	1 000000			
		0.000000					
FW	0.00	0.00	0.00	0.00	0.00		
	0.00	0.00	0.00	0.00	0.00	0.00	
!la	yer 3 to	layer 4	0 000000	1 000000			
шт	0.000000	0.000000	0.000000	0.000000			
FW	0.00	0.000000 0.000000 0.000000 0.00	0.00	0.00	0.00	0.00	
	0.00	0.00	0.00	0.00	0.00	0.00	
	4 +	1 1					
T.T	yer 4 to 0.108204	0.000000	0.000000	1.000000			
	-41.000000	0.000000	0.000000	0.000000			
FW	0.00	0.000000	0.00	0.00	0.00	0.00	
	0.00	0.00 layer 2	0.00	0.00	0.00	0.00	
1.17	yer 4 to n nnnnn	1ayer 2	0 000000	1 000000			
111		0.000000					
FW		0.00					
	0.00	0.00	0.00	0.00	0.00	0.00	
!la	yer 4 to	layer 3	0 000000	0 000000			
LT	0.000000	0.000000	0.000000	0.000000			
FW	0.00	0.00	0.00	0.00	0.00	0.00	
	0.00	0.000000	0.00	0.00	0.00	0.00	
!la	yer 4 to	layer 4					
LT		0.000000					
FW	0.00	0.000000	0.000000	0.000000	0 00	0 00	
2	0.00	0.00	0.00	0.00	0.00	0.00	
	lculation						
Lm	iq rrmav	3.0					
Ma	orrmax exfun 2	2400					
I C) I U .	100000E-04					
Np	rint	0					
17.4	perimental						
	lename		Scale	factor	code		
	LE cer+si	imul.dat		0.812	1.00		
	cluded_Reg						
	0.0000						
	.35.0000 1 ORMAT fre						
	near inter						
Во	rinter	Sim.Bgr					
		Number of o	coefficient	S			
		2 coefficients					
:PC		0.20000					
	1.0	1.0					
	mber of pa	attern backo	rounds				
Bg	rnum 1		T. 1	0 1		,	
!Pa	ittern file irnatt	cerus	rilename	Scale 0 02	ractor	code 1.00 cer	neita
ьú		Cerus		0.02	5555	1.00 CEI	. u u ± t E

Scale factor code 0.026000 1.00 cerusite.hkl