Chapter III

EXPERIMENTAL

3.1 The Powder Photographs

In order to take the powder photograph, Stemonone crystal was carefully ground to fine powders. By using Guinier-Hägg type focusing powder camera, and monochromatized CrKα radiation (λ = 2.28962 Å), the x-ray powder photograph was obtained at 22°C. To eliminate error due to film shrinkage, a complete scale was printed on the film before processing, and cobolt phosphide (CoP_3) was used as an internal standard substance[6], which from the graph of Fig. 14 gives diffraction ares of Stemonone at accurately known angles.

The x- ray powder diffraction pattern for cobolt phosphide (CoP_3) is given in Table 1. The indices of the diffraction lines of Stemonone were obtained by using the Ito method, and preliminary cell parameters obtained from rotation and Weissenberg photographs. Powder diffraction data for Stemonone with indices calculated using a desk calculator are shown in Table 2. The following cell parameters were obtained:

$a^* = 0.2983 \pm .0011$ rlu., $a = 9.782 \pm .002$ Å ;

$b^* = 0.2198 \pm .0011$ rlu., $b = 12.903 \pm .002$ Å ;

$c^* = 0.2926 \pm .0011$ rlu., $c = 8.210 \pm .002$ Å ,

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[6] S. Rundquist, and N.O. Ersson, Arkiv För Kemi, 30(1968), p.103.

$\alpha^* = 79.030 \pm .005^\circ$, $\alpha = 92.950 \pm .004^\circ$,

$\beta^* = 72.650 \pm .005^\circ$, $\beta = 103.883 \pm .003^\circ$,

$\gamma^* = 53.920 \pm .005^\circ$, $\gamma = 124.700 \pm .003^\circ$,

$V^* = 0.01478\ (\mathrm{r.l.u.})^3$, $V = 812.1\ \text{Å}^3$,

$a : b : c = 1 : 1.32 : 0.84$.

Table I

X-Ray Powder-Diffraction Data for CoP_3

I	$s-s_o$	hkl	Θ	$\frac{\Theta}{s-s_o}$
m	42.40	110	12.1255	0.28598
s	60.39			
m	74.65	211	21.3359	0.28581
s	86.85	220	24.8422	0.28604
vs	98.00	310	28.0154	0.28587
s	108.28	222	30.9667	0.28599
s	118.12	321	33.7636	0.28584
m	127.48	400	36.4514	0.28593
m	136.64	330	39.0635	0.28587
vs	145.64	420	41.6263	0.28582
s	154.46	332	44.1622	0.28591

The crystal system of CoP_3 is cubic, the cell dimension is $a = 7.70735 \pm 0.00005$ Å. The angles, Θ, are known.

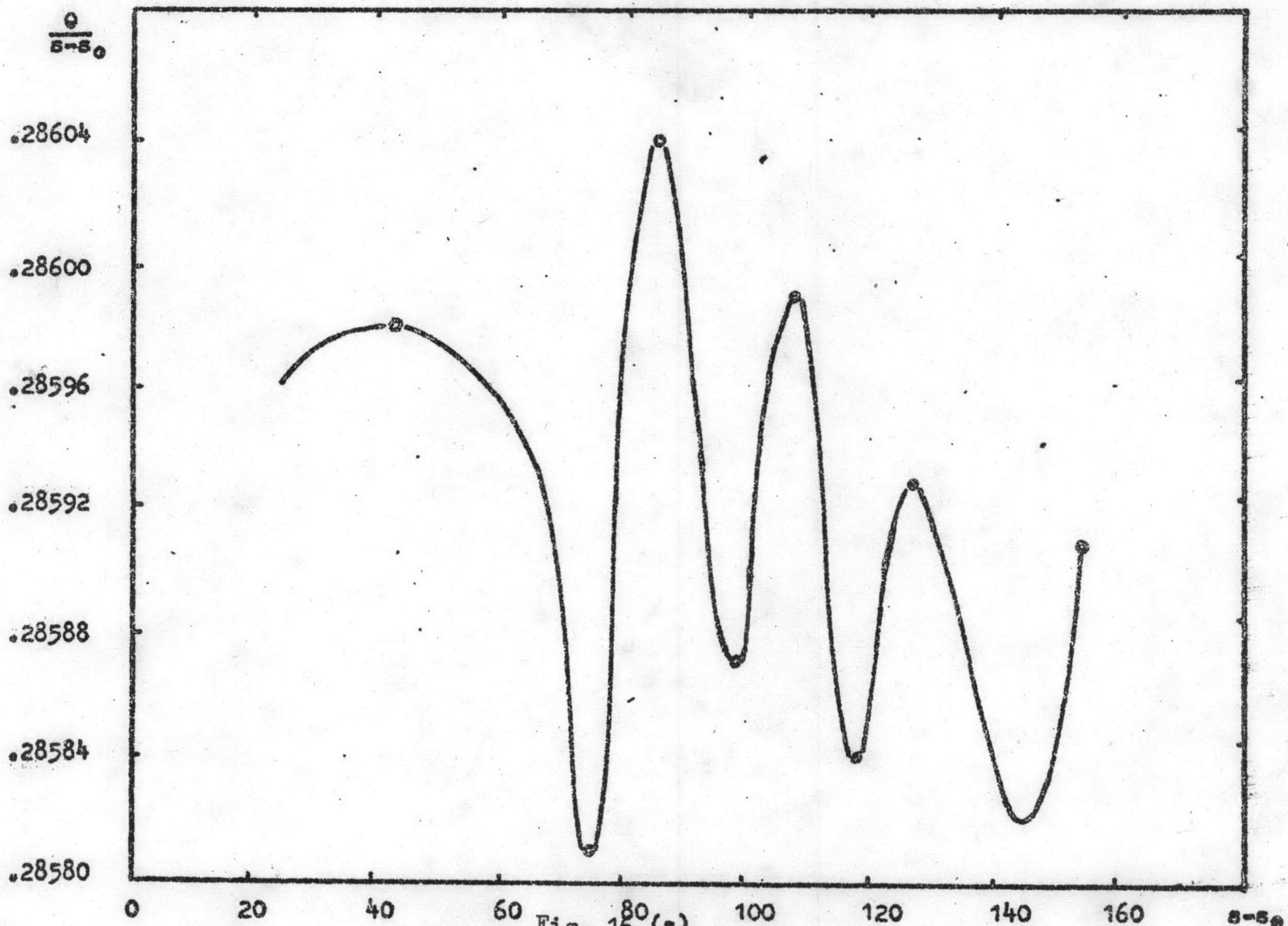


Fig. 16 (a)

Graph of $s-s_o$ VS $\frac{\theta}{s-s_o}$ for Stemonone crystal+C_oP_3 obtained by (a) a desk calculator (b) an I B M 1800 Computer.

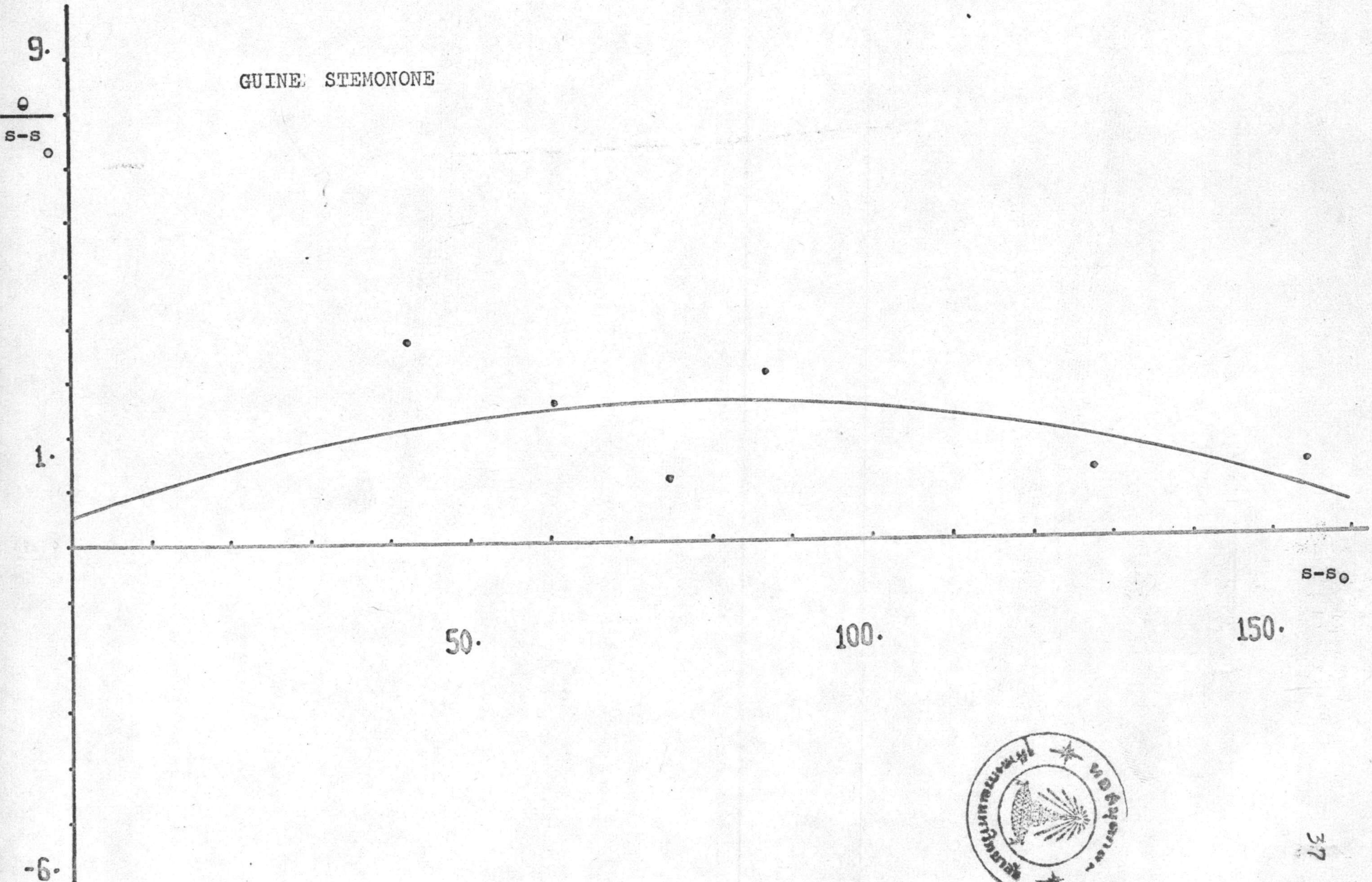
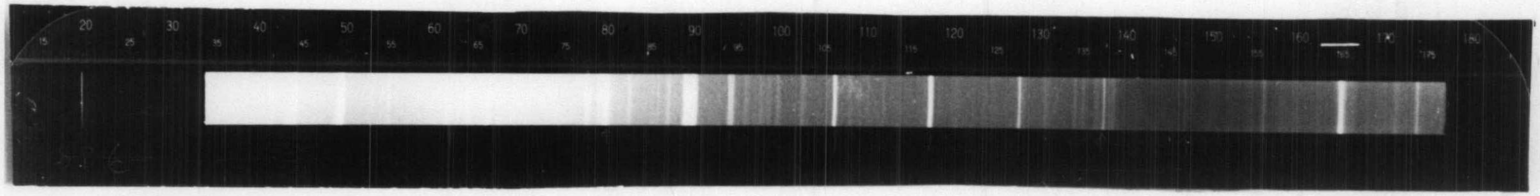
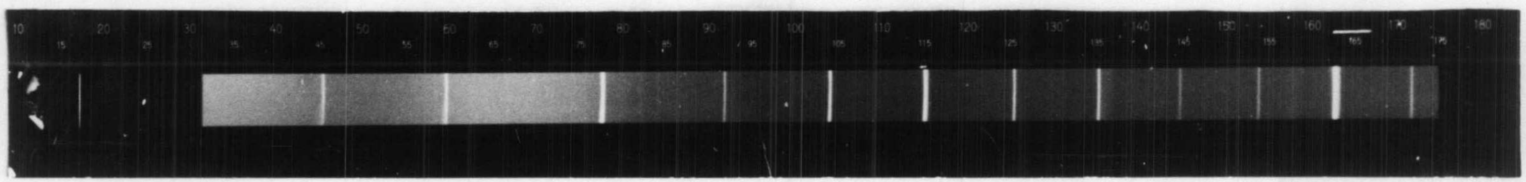


Fig. 16 (b)



(a)



(b)

Fig.17 Powder photographs for (a) Stemonone crystal + CoP_3, (b) CoP_3 CrK radiation

Table 2

X-ray Powder-diffraction data for Stemonone (unrefined)

h	k	l	I	θ	$Sin^2θ_{obs}$	$Sin^2θ_{cal}$	$sin^2θ_{obs}-Sin^2θ_{cal}$
0	1	0	m	6.31067	.01208	.01208	.00000
$\bar{1}$	1	0	s	7.04002	.01502	.01501	.00001
1	0	0	s	8.57890	.02225	.02225	.00000
0	$\bar{1}$	1	w	9.52278	.02737	.02737	.00000
$\bar{1}$	1	1	vw	9.89178	.02951	.02951	.00000
$\bar{1}$	0	1	w	10.10058	.03076	.03062	.00014
$\bar{1}$	2	0	vw	10.32082	.03210	.03197	.00013
1	$\bar{1}$	1	m	12.01116	.04331	.04334	-.00003
0	2	0	m	12.70892	.04840	.04832	.00008
1	1	0	m	13.39804	.05369	.05362	.00007
1	0	1	w	13.77260	.05668	.05667	.00001
$\bar{2}$	2	0	w	14.21290	.06028	.06008	.00020
$\bar{1}$	0	2	m	16.63967	.08200	.08181	.00019
0	2	1				.08195	.00005
0	$\bar{1}$	2	w	17.01400	.08562	.08547	.00015
0	0	2				.08562	.00000
$\bar{1}$	1	2	w	17.13687	.08682	.08679	.00003
1	$\bar{3}$	1	vvw	17.40261	.08945	.08916	.00029
2	$\bar{2}$	1	w	18.02255	.09573	.09537	.00036
$\bar{2}$	3	1				.09559	.00014
2	$\bar{1}$	1	vvw	18.81087	.10397	.10384	.00013
$\bar{1}$	$\bar{2}$	1	w	18.97931	.10577	.10532	.00045
1	2	0	m	19.30757	.10933	.10916	.00017
0	1	2				.10992	.00057
0	3	$\bar{1}$	vvw	19.52446	.11170	.11179	-.00009
$\bar{1}$	2	2	vs	19.89801	.11584	.11596	-.00012
$\bar{2}$	2	2	vvs	20.09464	.11804	.11805	-.00001
3	$\bar{2}$	0	m	21.4186	.13336	.13278	.00058
1	0	2				.13393	-.00057
$\bar{1}$	4	0	w	21.8565	.13860	.13830	.00030

Table 2 cont.

h	k	l	I	Θ	$Sin^2\Theta_{obs}$	$Sin^2\Theta_{cal}$	$Sin^2\Theta_{obs}-Sin^2\Theta_{cal}$
1	2	$\bar{2}$	w	22.37410	.14490	.14426	.00064
1	$\bar{3}$	2	vvw	22.65702	.14839	.14808	.00031
0	3	1				.14846	-.00007
$\bar{2}$	3	2	m	22.95296	.15208	.15210	-.00002
0	2	2	vw	23.46834	.15860	.15838	.00022
$\bar{3}$	4	0	w	23.79106	.16273	.16175	.00082
$\bar{1}$	4	1	vw	24.47913	.17169	.17112	.00057
3	$\bar{3}$	1	vw	24.94243	.17783	.17743	.00040
3	0	$\bar{1}$	vw	25.37006	.18358	.18257	.00101
2	$\bar{3}$	2				.18282	.00076
$\bar{1}$	1	3	vvw	25.6265	.18705	.18691	.00014
0	$\bar{1}$	3				.18638	.00067
$\bar{2}$	$\bar{2}$	1	vw	26.46531	.19861	.19763	.00098
3	$\bar{4}$	1				.19794	.00067
$\bar{2}$	0	3	vw	26.80866	.20341	.20342	.00001
3	$\bar{4}$	2	w	31.83451	.27822	.27679	.00143
2	$\bar{6}$	0	vvw	32.7822	.29316	.29222	.00094
1	4	0				.29269	.00047
1	$\bar{4}$	3	w	33.04986	.29743	.29667	.00076
2	$\bar{3}$	3				.29771	-.00028
2	3	0	vvw	34.07534	.31392	.31352	.00040
1	$\bar{6}$	1	vvw	35.74273	.34123	.33902	.00212
$\bar{1}$	6	0				.34126	-.00003
1	$\bar{5}$	3	w	37.32984	.36773	.36774	.00001

The refinement of the unit cell dimension was carried out by the least-squares method. Eighteen reflections were chosen and performed on the NEAC 2200 computer at the unit of Computer Science, Chulalongkorn University. The data after refinement was shown in Table 3. The refined cell dimensions are

$a^* = .2988 \pm .0011$ rlu., $a = 9.746 \pm .002$ Å ,

$b^* = .2200 \pm .0011$ rlu., $b = 12.866 \pm .002$ Å ,

$c^* = .2925 \pm .0011$ rlu., $c = 8.198 \pm .002$ Å ,

$\alpha^* = 79.206 \pm .005^\circ$, $\alpha = 90.956 \pm .004^\circ$,

$\beta^* = 72.754 \pm .005^\circ$, $\beta = 1103.566 \pm .003^\circ$,

$\gamma^* = 53.9\ 88 \pm .005^\circ$, $\gamma = 124.580 \pm .003^\circ$,

$V^* = .01485$ (r.l.u.)^3, $V = 808.2$.

Table 3 Data after refinement

h	k	l	$\sin^2\theta_{obs}$	$\sin^2\theta_{cal}$	$\sin^2\theta_{obs} - \sin^2\theta_{cal}$
0	1	0	.012080	.012104	-.000024
$\bar{1}$	1	0	.015020	.015093	-.000073
1	0	0	.022250	.022316	-.000066
0	$\bar{1}$	1	.027370	.027463	-.000093
$\bar{1}$	1	1	.029510	.029551	-.000041
$\bar{1}$	0	1	.030756	.030747	.000009
1	$\bar{2}$	0	.032098	.032079	.000019
1	$\bar{1}$	1	.043310	.043406	-.000096
0	2	0	.048399	.048415	-.000016
1	1	0	.053690	.053745	-.000055
1	0	1	.056676	.056655	.000021
$\bar{2}$	2	0	.060280	.060374	-.000094
$\bar{1}$	1	2	.086819	.086780	.000039
1	2	$\bar{1}$	.105773	.105762	.000011
$\bar{1}$	2	2	.115840	.115818	.000022
$\bar{1}$	4	0	.138595	.138671	-.000076
1	2	$\bar{2}$	.144901	.144912	-.000011
$\bar{3}$	4	0	.162731	.162590	.000142

With the same powder diffraction photographs of Stemonone (Fig. 19), the positions of diffraction lines were measured by Miss S. Pramatus at the Institute of Chemistry, University of Uppsala, Sweden. The calculation of observed $\sin^2\theta$ for each reflections was determined by her by compputing program GUINE with an IBM 1800 Computer, the powder data were shown in Table 3. Twenty seven reflections with unambiguity of indices were chosen for least-squares refinement with computing program CELCIUS using a CDC 3600 Computer. The data after last refinement was shown in Table 4. The final cell parameters are

a = 12.864 (2)* Å ,	α = 103.564 (8)° ,
b = 9.748 (2) Å ,	β = 90.955 (5)° ,
c = 8.192 (2) Å ,	γ = 124.605 (22)° ,
V = 807.4 (Å)³ .	

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* Numbers in parenthesis here and throughout this paper are the estimated standard deviations in the least significant digits.

Table 4

Stemonone Powder Data

h	k	l	I	θ	$\sin^2\theta_{obs}$	$\sin^2\theta_{cal}$	$\sin^2\theta_{obs}-\sin^2\theta_{cal}$
1	0	0	m	6.313	.01209	.01212	-.00003
1	$\bar{1}$	0	vvs	7.037	.01501	.01509	-.00008
0	1	0	vvs	8.567	.02219	.02232	-.00013
$\bar{1}$	0	1	w	9.534	.02743	.02750	-.00007
1	$\bar{1}$	1	vvw	9.903	.02958	.02957	.00001
0	$\bar{1}$	1	w	10.109	.03081	.03077	.00004
2	$\bar{1}$	0	vvw	10.318	.03208	.03210	-.00002
$\bar{1}$	1	1	s	12.015	.04333	.04343	-.00010
2	0	0	s	12.713	.04843	.04848	-.00005
1	1	0	s	13.405	.05375	.05379	-.00004
0	1	1	w	13.765	.05662	.05670	-.00008
2	$\bar{2}$	0	vvw	14.215	.06030	.06035	-.00005
2	0	1	s	16.646	.08206	{.08197	.00009
0	$\bar{1}$	2				.08205	.00001
0	0	2	vw	17.026	.08574	{.08566	.00008
$\bar{1}$	0	2				.08571	.00003
1	$\bar{1}$	2	w	17.138	.08683	.08689	.00006
$\bar{3}$	1	1	vw	17.413	.08955	.08962	.00007
$\bar{2}$	2	1	**bm	18.027	.09577	{.09562	.00015
3	$\bar{2}$	1				.09584	-.00007
$\bar{1}$	2	1	vvw	18.823	.10410	.10400	.00010
$\bar{2}$	$\bar{1}$	1	m	18.989	.10587	.10588	-.00001
2	1	0	bm	19.326	.10952	{.10950	.00002
1	0	2				.10986	-.00034
$\bar{3}$	2	1	vvw	19.489	.11131	.11149	-.00018
$\bar{3}$	0	1	vvw	19.578	.11228	.11239	-.00011

** b = broad

Table 4 cont.

h k l	I	θ	$\sin^2\theta_{obs}$	$\sin^2\theta_{cal}$	$\sin^2\theta_{obs}-\sin^2\theta_{cal}$
2 $\bar{1}$ 2	vvs	19.915	.11603	.11597	.00006
2 $\bar{2}$ 2	vvs	20.147	.11863	.11829	.00034
2 $\bar{3}$ 0	vbm	21.431	.13351	.13324	.00027
4 $\bar{1}$ 0	vw	21.874	.13881	.13884	.00003
$\bar{2}$ $\bar{1}$ 2	vvw	22.389	.14508	.14508	.00000
3 0 1	vvw	22.672	.14858	.14861	-.00003
$\bar{3}$ 1 2				.14872	-.00014
3 $\bar{2}$ 2	m	22.958	.15215	.15226	-.00011
4 $\bar{3}$ 0	w	23.779	.16258	.16257	.00001
2 $\bar{3}$ 2	vvw	23.856	.16358	.16524	-.00166
$\bar{2}$ 2 2	vvw	24.631	.17371	.17373	-.00002
0 $\bar{3}$ 1	bw	25.355	.18338	.18338	.00000
$\bar{3}$ 2 2				.18356	-.00018
$\bar{1}$ 0 3	w	25.604	.18675	.18675	.00000
1 $\bar{1}$ 3				.18704	.000029
$\bar{4}$ 0 1	vvw	25.921	.19109	.19119	-.00010
$\bar{2}$ $\bar{2}$ 1	w	26.465	.19860	.19856	.00004
$\bar{4}$ 3 1				.19874	-.00014
$\bar{4}$ 2 2	vw	27.809	.21764	.21762	.00002
$\bar{4}$ 3 2	vw	31.815	.27792	.27774	.00018
$\bar{4}$ $\bar{1}$ 1				.27795	-.00003
$\bar{6}$ 2 0	vvw	32.799	.29343	.29339	.000004
4 1 0				.29365	-.00022
$\bar{4}$ 1 3	w	33.067	.29771	.29803	-.00032
$\bar{4}$ 0 3	bm	34.108	.31445	.31422	.00023
3 2 0				.31446	-.00001
$\bar{6}$ 1 1	w	35.698	.34049	.34070	-.00041

Table 5

The data after last refinement

h	k	l	$\sin^2\theta_{obs}$	$\sin^2\theta_{cal}$	$(\sin^2\theta_{obs}-\sin^2\theta_{cal})$
1	0	0	0.012092	0.012115	.00023
1	$\bar{1}$	0	0.015010	0.015086	-.000076
0	1	0	0.022195	0.022319	-.000124
$\bar{1}$	0	1	0.027439	0.027498	-.000059
1	$\bar{1}$	1	0.029582	0.029573	.000009
0	$\bar{1}$	1	0.030813	0.030773	.000040
2	$\bar{1}$	0	0.032085	0.032083	.000002
$\bar{1}$	1	1	0.043335	0.043433	-.000098
2	0	0	0.048431	0.048460	-.000029
1	1	0	0.053750	0.053783	-.000033
0	1	1	0.056622	0.056700	-.000078
$\bar{2}$	2	0	0.060300	.0.60345	-.000045
1	$\bar{1}$	2	0.086836	0.086893	-.000057
$\bar{3}$	1	1	0.089554	0.089589	-.000035
$\bar{1}$	2	1	0.104101	0.104007	.000094
$\bar{2}$	$\bar{1}$	1	0.105876	0.105862	.000014
$\bar{3}$	2	1	0.111312	0.111467	-.000155
$\bar{3}$	0	1	0.112287	0.112351	-.000064
2	$\bar{1}$	2	0.116033	0.115957	.000076
4	$\bar{1}$	0	0.138817	0.138766	.000051
$\bar{2}$	$\bar{1}$	2	0.145088	0.145081	.000007
3	$\bar{2}$	2	0.152154	0.152238	-.000084
$\bar{4}$	3	0	0.162587	0.162536	.000051
$\bar{2}$	2	2	0.173711	0.173733	-.000022
$\bar{4}$	0	1	0.191093	0.191122	-.000029
$\bar{4}$	2	2	0.217648	0.217585	.000063
$\bar{6}$	1	1	0.340493	0.340549	-.000056

3.2 The Rotation and Weissenberg Photographs

Two suitable well-formed single crystals were selected and mounted separately perpendicular and parallel to the c axis (needle axis) on the goniometer heads. Following the methods described in a previous thesis (Chaipayungpun, 1970), the x-ray data were obtained from rotation and Weissenberg photographs with CuKα radiation along b and c rotation axes, as shown in Table 6-9.

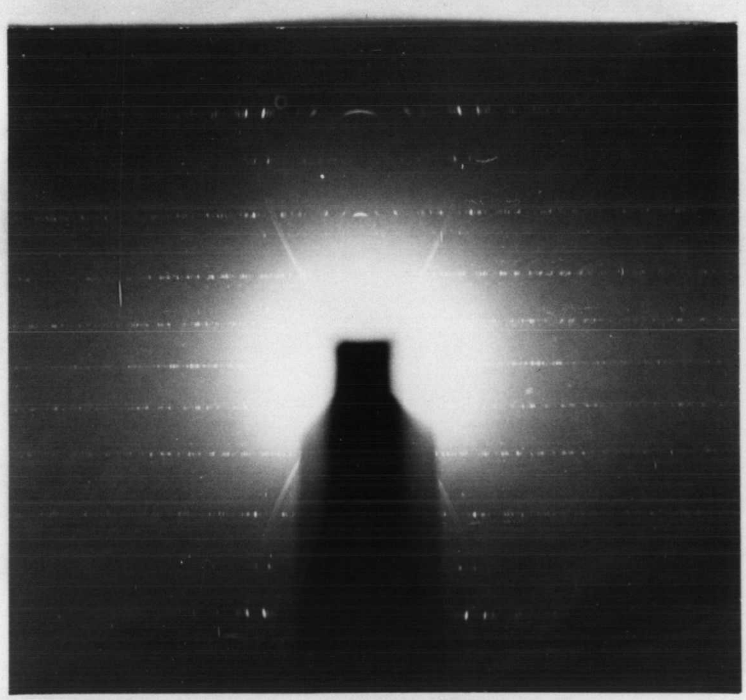
Table 6

Determination of cell parameter, b, from [010] rotation Photograph

layer (n)	2 y (mm)	y (mm)	tan ν =tan $\frac{y}{r}$	ν	sin ν = ζ	$\frac{b}{n}=\frac{\lambda}{\zeta}$	b A°
Cu Kα radiation, $\lambda_{K\alpha}$ = 1.5418 Å							
1	6.95	3.475	0.1213	6°57'	.1210	12.743	12.743
2	14.30	7.150	0.2496	14° 3'	.2427	6.353	12.706
3	22.40	11.200	0.3909	21°21'	.3641	4.234	12.702
4	31.70	15.850	0.5532	28°57'	.4841	3.185	12.740
Cu Kβ radiation, $\lambda_{K\beta}$ = 1.3922 Å							
1	6.20	3.100	0.1082	6°10'	.1076	12.939	12.939
2	12.90	6.450	0.2251	12°41'	.2195	6.342	12.684
3	19.60	9.800	0.3420	18°53'	.3235	4.304	12.912
4	28.60	14.300	0.4991	26°31'	.4466	3.117	12.468
							av. 12.73

r = radius of the camera = 28.65 mm.

(a)



(b)

Fig. 18 Rotation photographs (a) about [010] rotation axis (b) [001] rotation axis

Table 7

Determination of cell parameter, C, from [001] rotation photograph

layer	2y mm	y mm	tan ν	ν	ζ	c/n	c A°
Cu Kα radiation, $\lambda_{K\alpha}$ = 1.5418 Å							
1	10.975	5.488	0.1915	10°50'	0.1878	8.210	8.210
2	23.20	11.600	0.4049	22° 3'	0.3753	4.108	8.216
3	39.40	19.700	0.6876	34°30'45"	0.5666	2.721	8.163
Cu Kβ radiation, $\lambda_{K\beta}$ = 1.3922 Å							
1	9.75	4.875	0.1702	9°40'	0.1679	8.292	8.292
2	20.67	10.340	0.3609	19°51'	0.3395	4.101	8.202
3	34.10	17.050	0.5951	30°45'	0.5113	2.723	8.188
							av. 8.21

Table 8

Determination of the inclination angle μ, and layer line screen setting, S, from rotation photographs

layer	ζ	ζ/2 = sin μ	μ	tan μ	S = r tan μ r = 24.238 mm.
[010] ratation axis					
1	0.1210	0.0605	3°28'	0.0606	1.47
2	0.2427	0.1214	6°58'30"	0.1224	2.97
3	0.3641	0.1820	10°29'20"	0.1851	4.49
4	0.4841	0.2420	14°20"	0.2494	6.04
[001] rotation axis					
1	0.1878	0.0939	5°23'20"	0.0945	2.29
2	0.3753	0.1876	10°48'40"	0.1910	4.63
3	0.5666	0.2833	16°27'40"	0.2954	7.16

Table 9

Cell parameters determined

from Weissenberg photographs

a) [010] rotational axis

$a^* = 0.200 \pm .002$ rlu., $a = 9.929 \pm .003$ Å ,

$b^* = 0.151 \pm .002$ rlu., $b = 12.730 \pm .003$ Å ,

$c^* = 0.197 \pm .002$ rlu., $c = 8.221 \pm .003$ Å ,

$\alpha^* = 79.62 \pm .10^\circ$, $\alpha = 92.800 \pm .004^\circ$,

$\beta^* = 72.40 \pm .10^\circ$, $\beta = 104.583 \pm .004^\circ$,

$\gamma^* = 53.35 \pm .10^\circ$, $\gamma = 125.450 \pm .004^\circ$,

$V^* = 0.004544$ (r.l.u.)^3, $V = 806.5$ Å^3 ,

$a : b : c = 1 : 1.28 : 0.83$

b) [001] rotational axis

$a^* = 0.200 \pm .002$ rlu., $a = 9.885 \pm .003$ Å ,

$b^* = 0.151 \pm .002$ rlu., $b = 12.764 \pm .003$ Å ,

$c^* = 0.197 \pm .002$ rlu., $c = 8.210 \pm .003$ Å ,

$\alpha^* = 79.63 \pm .10^\circ$, $\alpha = 90.000 \pm .004^\circ$,

$\beta^* = 72.30 \pm .10^\circ$, $\beta = 104.045 \pm .004^\circ$,

$\gamma^* = 53.50 \pm .10^\circ$, $\gamma = 125.050 \pm .004^\circ$,

$V^* = 0.004534$ (r.l.u.)^3, $V = 808.4$ Å^3 ,

$a : b : c = 1 : 1.29 : 0.83$

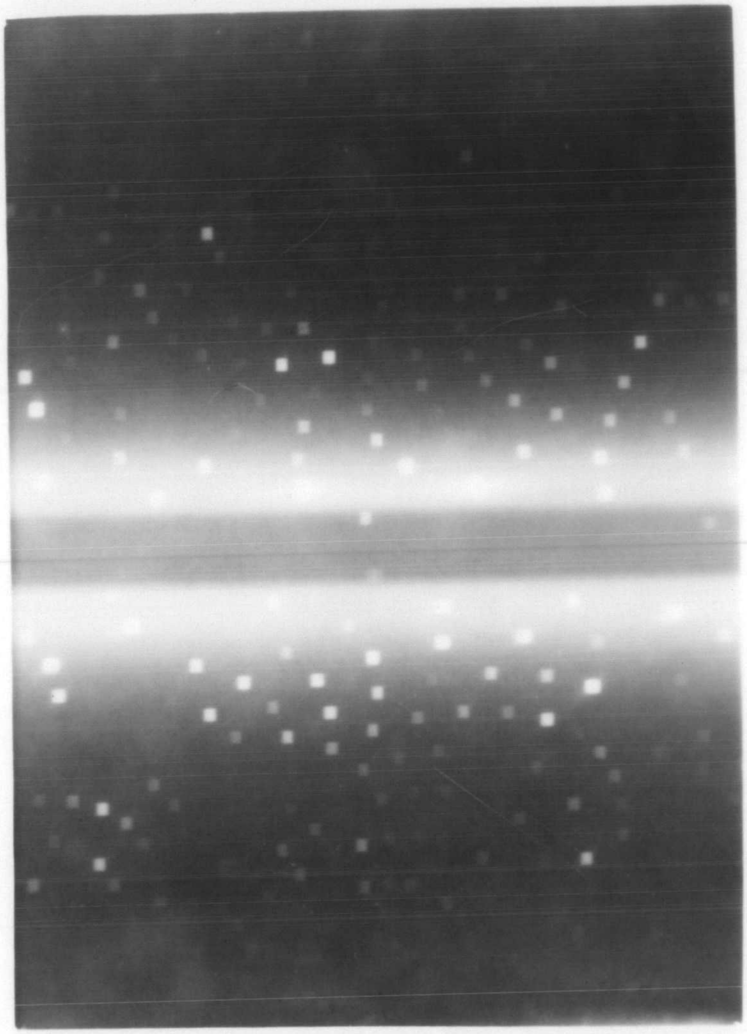


Fig. 19 Integrated Weissenberg photograph

[001] 2-nd layer

3.3 The Structure Factor

In order to collect the intensity data, Integrating Weissenberg photographs, multiple-film technique, were taken along the C rotation axis. The Integrated photograph of the 2nd layer, [001] rotational axis is shown in Fig. 19. A pack of 3 photographic films was used for each x-ray photograph instead of the customary single film. The intensities of the strong reflections are estimated by examining the film of the pack farthest from the crystal, and the weak reflections are estimated from the films nearest the crystal.

The relative intensities, I_{rel}, obtained from the number of oscillations (n), of each spectra determined from the graph are shown in Table 10, column 2. The values of $\sin^2\theta$, 1/LP, and the structure factors of each spectra are listed in column 3, 4 and 5 of the same table. The reciprocal lattice net of the 0-th layer and the 2nd layer, [001] rotation axis are shown in the Appendix.

Table 10

The Structure Factors (observed)

h	k	l	I_{rel}	$\sin^2\theta$	1/LP	F
0	2	0	609.9	.021965	.153149	9.664643
0	3	0	5.8	.049421	.239222	1.177915
0	4	0	63.3	.087859	.337125	4.619521
0	5	0	40.0	.137280	.450961	4.247169
1	0	0	1370.2	.010120	.102132	11.829650
1	1	0	1035.7	.024375	.161912	12.949600
1	2	0	524.9	.049613	.239755	11.218150
1	3	0	68.8	.085834	.332262	4.781170
1	4	0	629.6	.133037	.441446	16.671350
1	5	0	5.0	.191222	.569380	1.687275
1	7	0	8.3	.340541	.860284	2.672143
1	8	0	2.5	.431673	.972459	1.559213
2	0	0	95.1	.040478	.213676	4.507832
2	1	0	235.8	.063498	.276775	8.078577
2	2	0	23.8	.097501	.359994	2.927089
2	3	0	675.2	.142486	.462590	17.673160
2	4	0	84.4	.198454	.584923	7.026197
2	6	0	6.6	.343336	.864749	2.389004
2	8	0	4.2	.532148	.993823	2.043050
2	9	0	10.8	.643028	.885737	3.092887
3	0	0	11.6	.091076	.344803	1.999928
3	1	0	82.8	.122860	.418470	5.886366
3	2	0	42.4	.165628	.513739	4.667173
3	3	0	5.8	.219377	.629393	1.910622
3	5	0	10.0	.359824	.889950	2.983203
3	7	0	5.3	.544200	.988362	2.288737
3	8	0	3.3	.652862	.870735	1.695117
3	9	0	1.0	.772506	.646418	.804001
4	2	0	18.2	.253993	.700913	3.571639
4	6	0	1.7	.569945	.971164	1.284903
4	8	0	5.0	.793815	.601448	1.734138
5	0	0	19.7	.252988	.698880	3.710514
5	1	0	11.6	.302302	.794327	3.035488
5	3	0	10.0	.433877	.974180	3.121185
6	0	0	96.5	.364303	.896441	9.300888
6	1	0	10.8	.422381	.964631	3.227694
6	2	0	22.6	.491442	.999562	4.752904
7	0	0	56.6	.495856	.999898	7.522911
1	-1	0	101.7	.006846	.083595	2.915747
1	-2	0	69.6	.014555	.123301	2.929461
1	-3	0	11.6	.033247	.1[illegible]	1.490811
1	-4	0	288.2	.062921	.275283	8.907098
1	-6	0	10.3	.155216	.490829	2.248452
1	-7	0	1.0	.217837	.626147	.791294
1	-8	0	9.2	.291441	.774158	2.668754
1	-9	0	14.7	.376027	.912666	3.662811
1	-10	0	34.4	.471595	.995173	5.850979
1	-11	0	6.6	.578146	.964161	2.522590
2	-1	0	88.6	.028440	.175950	3.948312
2	-2	0	287.5	.027385	.172385	7.039924

h	k	l	I_{rel}	$Sin^2 \theta$	1/LP	F
2	-3	0	363.4	.037312	.204194	8.614169
2	-4	0	32.9	.058221	.263003	2.941561
2	-5	0	9.2	.090113	.342510	1.775130
2	-6	0	123.1	.132987	.441334	7.370763
2	-7	0	1.0	.186844	.559930	.748285
2	-8	0	15.8	.251683	.696236	3.316704
2	-10	0	10.8	.414308	.957092	3.215056
2	-11	0	6.6	.512095	.999123	2.567919
2	-12	0	1.0	.620863	.916776	.957484
3	-1	0	16.7	.070273	.294027	2.215909
3	-2	0	675.2	.060453	.268867	13.473630
3	-3	0	21.7	.061616	.271898	2.429029
3	-4	0	465.9	.073760	.307748	11.876450
3	-7	0	208.4	.176090	.536598	10.574820
3	-8	0	2.5	.232164	.656148	1.280769
3	-9	0	10.8	.299221	.788663	2.918485
3	-10	0	7.5	.377260	.914306	2.618643
3	-11	0	2.5	.466282	.993207	1.575759
3	-12	0	38.8	.566286	.974054	6.147625
3	-13	0	1.7	.677273	.830628	1.188304
4	-1	0	4.2	.132345	.439891	1.359242
4	-2	0	3.3	.113761	.397715	1.145626
4	-3	0	363.3	.106159	.380193	11.752610
4	-4	0	10.0	.109539	.388007	1.969788
4	-5	0	106.7	.123902	.420832	6.700950
4	-6	0	97.7	.149247	.477620	6.831068
4	-7	0	5.0	.185574	.557185	1.669108
4	-8	0	20.8	.232884	.657644	3.698513
4	-11	0	2.5	.440709	.979176	1.564589
4	-13	0	2.5	.634171	.898618	1.498848
5	-1	0	15.2	.214656	.619429	3.068439
5	-2	0	17.5	.187307	.560932	3.133097
5	-3	0	288.7	.170941	.525367	12.315570
5	-4	0	80.6	.165556	.513582	6.433868
5	-5	0	38.7	.171155	.525834	4.511074
5	-6	0	1.0	.187735	.561856	.749571
5	-8	0	30.4	.253844	.700610	4.615034
5	-9	0	3.3	.303372	.796283	1.621028
6	-1	0	2.5	.317206	.821042	1.432691
6	-2	0	5.8	.281093	.754452	2.091845
6	-4	0	66.9	.241813	.676089	6.725351
6	-5	0	1.0	.238647	.669571	.818273
6	-6	0	5.8	.246463	.685614	1.994131
6	-8	0	9.2	.295042	.780907	2.680362
6	-9	0	12.5	.335805	.852599	3.264579
7	-2	0	29.0	.395117	.936543	5.211500
7	-4	0	19.8	.338308	.856679	4.118524
7	-5	0	5.8	.326378	.836866	2.203139
7	-9	0	22.6	.388478	.928612	4.581115
8	-2	0	2.5	.529381	.994838	1.577052

h	k	l	I_{rel}	$\sin^2 \theta$	1/LP	F
8	-9	0	3.3	.461390	.991105	1.808492
8	-11	0	7.4	.540806	.990071	2.706755
8	-12	0	22.0	.596987	.945435	4.560653
9	-5	0	10.0	.562557	.976852	3.125463
9	-6	0	13.7	.544079	.988425	3.679866
9	-10	0	19.1	.579993	.962485	4.287593
10	-8	0	11.6	.662226	.855813	3.150782
10	-9	0	9.2	.667931	.846433	2.790552
10	-10	0	5.0	.684618	.817836	2.022171
0	2	1	18.0	.037124	.177724	1.788582
0	3	1	31.0	.067309	.267048	2.877233
0	4	1	2.5	.108476	.369505	.961125
0	5	1	36.7	.160626	.488719	4.235086
1	0	1	439.2	.025692	.134879	7.696666
1	1	1	5.8	.042677	.195986	1.066170
1	2	1	14.0	.070644	.275881	1.965283
1	3	1	94.3	.109594	.372145	5.923953
1	4	1	47.8	.159526	.486266	4.821153
1	5	1	10.8	.220440	.618831	2.585221
1	6	1	2.4	.292337	.764018	1.354120
1	7	1	5.0	.375216	.900774	2.122232
2	0	1	1.0	.061922	.252474	.502467
2	3	1	28.8	.172117	.514196	3.848224
2	4	1	36.5	.230814	.640702	4.835869
2	5	1	1.0	.300493	.779281	.882769
2	6	1	5.8	.381154	.908669	2.295709
3	0	1	5.0	.118391	.392760	1.401355
3	1	1	15.8	.152905	.471468	2.729321
3	2	1	86.4	.198401	.571629	7.027712
3	4	1	25.1	.322341	.818499	4.532584
3	5	1	5.0	.400785	.932525	2.159310
4	0	1	7.6	.195100	.564479	2.071241
4	1	1	1.0	.238378	.656490	.810241
4	2	1	2.5	.292639	.764589	1.382559
4	3	1	103.2	.357882	.876059	9.508377
5	0	1	13.0	.292047	.763470	3.150413
5	1	1	7.2	.344090	.854744	2.480757
5	2	1	43.2	.407115	.939443	6.370553
5	3	1	14.7	.481123	.988653	3.812242
6	0	1	79.3	.409233	.941671	8.641439
6	1	1	8.0	.470040	.985232	2.807464
6	2	1	2.5	.541830	.981461	1.566413
7	0	1	9.7	.546658	.979026	3.081648
7	1	1	5.8	.616230	.916099	2.305075
8	0	1	2.5	.704323	.777167	1.393885
1	-1	1	753.2	.019690	.107259	8.988168
1	-2	1	36.9	.024670	.130525	2.194624
1	-3	1	164.9	.040633	.189403	5.588606
1	-4	1	46.8	.067578	.267764	3.539966
1	-5	1	18.2	.105505	.362460	2.568418

h	k	l	I_{rel}	$Sin^2 \theta$	1/LP	F
1	-6	1	24.1	.154415	.474849	3.382877
1	-8	1	2.5	.285182	.750381	1.369653
1	-9	1	2.5	.367039	.889416	1.491153
1	-10	1	76.2	.459878	.980829	8.645183
1	-11	1	2.5	.563700	.968326	1.555896
2	-1	1	373.0	.047155	.209930	8.848944
2	-2	1	164.0	.043371	.198189	5.701134
2	-3	1	125.6	.050569	.220180	5.258766
2	-4	1	52.1	.068749	.270880	3.756703
2	-5	1	18.5	.097912	.344274	2.523701
2	-6	1	445.4	.138058	.437963	13.966690
2	-7	1	14.3	.189185	.551625	2.808599
2	-8	1	46.7	.251295	.683104	5.648094
2	-9	1	3.3	.324388	.822036	1.647033
2	-10	1	51.9	.408463	.940865	6.987910
2	-11	1	3.3	.503520	.991107	1.808494
3	-1	1	26.1	.094860	.336880	2.965224
3	-2	1	7.0	.082311	.305862	1.463227
3	-3	1	24.0	.080745	.301910	2.691807
3	-4	1	78.1	.090160	.325387	5.041105
3	-5	1	5.8	.110559	.374420	1.473647
3	-6	1	122.2	.141939	.446768	7.388844
3	-7	1	113.2	.184303	.540967	7.825439
3	-8	1	1.7	.237648	.654973	1.055202
3	-9	1	5.8	.301976	.782022	2.129724
3	-10	1	1.7	.377287	.903562	1.239376
3	-11	1	2.5	.463579	.982573	1.567300
3	-12	1	2.5	.560855	.970337	1.557511
4	-1	1	27.5	.162804	.493564	3.684156
4	-2	1	76.9	.141490	.445751	5.854760
4	-3	1	39.8	.131159	.422226	4.099341
4	-4	1	2.5	.131810	.423717	1.029219
4	-5	1	3.3	.143464	.450172	1.218838
4	-6	1	11.5	.166060	.500795	2.399821
4	-7	1	2.5	.199659	.574347	1.198276
4	-8	1	5.0	.244240	.668625	1.828421
4	-9	1	5.0	.299803	.778003	1.972311
4	-10	1	1.7	.366349	.888433	1.228957
4	-12	1	12.7	.532388	.985444	3.537672
4	-13	1	2.5	.631881	.895514	1.496256
5	-1	1	5.0	.250986	.682473	1.847259
5	-2	1	7.5	.220908	.619823	2.156078
5	-3	1	110.3	.201813	.578996	7.991445
5	-5	1	78.3	.196569	.567663	6.666933
5	-6	1	1.7	.210420	.597488	1.007833
5	-7	1	7.6	.235254	.649988	2.222589
5	-8	1	20.1	.271071	.722867	3.811773
5	-13	1	9.6	.614889	.917764	2.968254
6	-1	1	4.2	.359408	.878330	1.920673
6	-4	1	16.4	.275827	.732227	3.465331

h	k	l	I_{rel}	$Sin^2\theta$	1/LP	F
6	-5	1	3.3	.269932	.720613	1.542083
6	-8	1	7.6	.318141	.811162	2.482908
6	-13	1	23.4	.618137	.913705	4.623925
7	-2	1	3.3	.440462	.969127	1.788327
7	-4	1	15.3	.378195	.904773	3.720619
7	-6	1	2.5	.359857	.878995	1.482392
7	-7	1	2.5	.367162	.889592	1.491301
7	-9	1	104.9	.414719	.947230	9.968167
7	-10	1	42.4	.454972	.978277	6.440414
7	-11	1	16.1	.506206	.990998	3.994378
8	-5	1	2.5	.477376	.987658	1.571351
8	-6	1	4.2	.464934	.983170	2.032071
8	-7	1	1.7	.463475	.982526	1.292398
8	-8	1	3.3	.472998	.986287	1.804091
8	-9	1	4.2	.493503	.990751	2.039890
8	-10	1	84.5	.524991	.987836	9.136306
8	-13	1	3.3	.685348	.811263	1.636205
9	-4	1	2.5	.643646	.878716	1.482156
9	-5	1	2.5	.611457	.921952	1.518183
9	-6	1	23.5	.590250	.945379	4.713427
9	-7	1	2.5	.580026	.955089	1.545225
9	-8	1	4.2	.580785	.954406	2.002125
9	-11	1	3.3	.648954	.870789	1.695170
9	-12	1	3.3	.693642	.796587	1.621338
10	-7	1	3.3	.716817	.753777	1.577169
10	-11	1	2.5	.750686	.687342	1.310859
0	-2	1	89.9	.026208	.137033	3.509874
0	-3	1	98.3	.050935	.221262	4.663697
0	-4	1	110.9	.086645	.316697	5.926354
0	-5	1	21.7	.133[illegible]37	.427206	3.044729
0	-7	1	12.7	.259668	.700095	2.981813
0	-8	1	4.2	.339307	.847038	1.886148
0	-9	1	13.9	.429928	.961021	3.654885
0	-10	1	20.4	.531532	.985753	4.484344
0	-11	1	4.2	.644119	.878018	1.920332
-1	-1	1	96.4	.025476	.133967	3.593661
-1	-2	1	288.0	.047985	.212449	7.822098
-1	-3	1	396.0	.081477	.303760	10.967620
-1	-4	1	347.1	.125951	.410264	11.933240
-1	-5	1	4.4	.181407	.534629	1.533742
-1	-6	1	3.3	.247846	.676044	1.493634
-1	-7	1	4.4	.325267	.823549	1.903578
-1	-8	1	16.6	.413671	.946191	3.963176
-2	0	1	177.2	.038436	.1[illegible]2152	5.681315
-2	-1	1	78.1	.058727	.243625	4.362006
-2	-2	1	166.2	.090001	.324996	7.349438
-2	-3	1	6.8	.132257	.424739	1.699478
-2	-4	1	98.8	.185496	.543576	7.328387
-2	-5	1	3.3	.249717	.679878	1.497863
-2	-6	1	20.5	.324920	.822952	4.107372

h	k	l	I_{rel}	$Sin^2\Theta$	1/LP	F
-2	-7	1	2.5	.411106	.943602	1.535905
-2	-8	1	3.3	.508274	.990857	1.808266
-3	0	1	35.2	.083162	.308002	3.292666
-3	-1	1	181.0	.112218	.378324	8.275058
-3	-3	1	73.9	.203277	.582151	6.559035
-3	-7	1	1.7	.517184	.989660	1.297082
-4	0	1	49.4	.148127	.460736	4.770779
-4	-2	1	27.0	.234750	.648936	4.185840
-4	-3	1	5.7	.294536	.768164	2.092494
-4	-4	1	3.8	.365303	.886935	1.835852
-4	-5	1	2.5	.447053	.973577	1.560109
-4	-6	1	3.3	.539786	.982411	1.800543
-5	0	1	17.8	.233331	.645972	3.390914
-5	-1	1	22.5	.279916	.740206	4.081007
-5	-2	1	10.1	.337484	.844059	2.919759
-5	-5	1	7.6	.576080	.958548	2.699067
-6	0	1	22.6	.338774	.846170	4.373034
-6	-1	1	99.5	.394124	.924829	9.592730
-6	-2	1	4.2	.460456	.981112	2.029943
-6	-3	1	1.7	.537770	.983299	1.292906
-6	-4	1	5.8	.626067	.903404	2.289048
-6	-6	1	2.5	.835608	.508319	1.127295
-7	0	1	32.2	.464456	.982962	5.625955
-7	-1	1	2.5	.528571	.986758	1.570635
-7	-3	1	1.7	.689746	.803528	1.168758
-7	-4	1	8.3	.786807	.612859	2.255377
-7	-5	1	2.5	.894851	.375982	.969513
-8	-3	1	5.8	.861961	.450334	1.616147
-9	0	1	6.6	.776538	.634337	2.046124
-9	-1	1	2.5	.858181	.458723	1.070890
-1	3	1	92.2	.045263	.204113	4.338111
-2	1	1	37.9	.029127	.148746	2.374333
-2	2	1	35.8	.030801	.155144	2.356726
-2	3	1	359.7	.043457	.198459	8.449010
-2	4	1	153.0	.067095	.266476	6.385204
3	1	1	54.7	.152905	.471468	5.078315
-3	2	1	80.0	.057998	.241580	4.396180
-3	3	1	32.8	.061889	.252382	2.877176
-3	4	1	106.4	.076763	.291767	5.571715
-4	1	1	9.3	.121289	.399490	1.927500
-4	2	1	2.5	.105434	.362291	.951697
-4	3	1	14.7	.100560	.350649	2.270360
-4	4	1	2.5	.106670	.365226	.955545
-5	1	1	13.0	.197729	.570174	2.722547
-5	3	1	97.7	.159471	.486144	6.891755
-5	4	1	6.6	.156816	.480219	1.780292
-5	6	1	1.0	.184452	.541295	.735727
-5	7	1	4.2	.214744	.606724	1.596320
-6	3	1	2.5	.238620	.656993	1.281593
-6	4	1	22.8	.227201	.633112	3.799335

h	k	l	I_{rel}	$Sin^2\theta$	1/LP	F
-6	5	1	57.4	.226763	.632191	6.023932
-6	6	1	5.0	.237308	.654266	1.808681
-6	7	1	5.0	.258836	.698416	1.868710
-6	8	1	6.6	.291346	.762143	2.242797
-7	1	1	28.7	.411325	.943825	5.204592
-7	2	1	12.4	.369176	.892438	3.326592
-7	4	1	1.7	.317825	.810606	1.173895
-7	5	1	11.5	.308623	.794171	3.022080
-7	6	1	7.6	.310403	.797387	2.461734
-7	7	1	9.6	.323166	.819927	2.805583
-7	8	1	5.8	.346911	.859216	2.232365
-8	1	1	5.0	.548482	.978038	2.211377
-8	2	1	75.7	.497568	.991040	8.661507
-8	4	1	2.5	.428688	.959988	1.549183
-9	1	1	5.0	.705877	.774294	1.967605
-9	6	1	5.0	.517310	.989637	2.224451
-9	8	1	4.2	.518760	.989350	2.038447
-9	10	1	1.0	.564140	.968006	.983873
-10	6	1	1.0	.651122	.867491	.931392
-10	7	1	1.0	.637591	.887496	.942070
-10	8	1	2.5	.635043	.891108	1.492571
-11	6	1	5.8	.805173	.573962	1.824548
-11	8	1	5.6	.771565	.644658	1.900021
-11	9	1	6.1	.771234	.645341	1.984081
0	1	2	251.6	.049754	.129119	5.699685
0	2	2	137.6	.071685	.211797	5.398446
0	3	2	5.2	.104599	.306360	1.262168
0	4	2	10.8	.148496	.415422	2.118148
0	5	2	146.4	.203374	.541200	8.901216
0	6	2	42.2	.269236	.681613	5.363213
0	11	2	5.8	.763278	.649992	1.941636
1	0	2	891.7	.060667	.173980	12.455420
1	1	2	51.1	.080381	.238749	3.492856
1	4	2	6.4	.205416	.545730	1.868869
1	5	2	10.8	.269060	.681256	2.712483
1	6	2	5.8	.343686	.819570	2.180252
1	10	2	5.8	.752013	.672334	1.974723
2	0	2	8.8	.102769	.301515	1.628904
2	1	2	11.8	.131247	.373863	2.100375
2	3	2	5.8	.221151	.580290	1.834579
2	4	2	5.8	.282576	.708324	2.026888
2	9	2	5.0	.754440	.667551	1.826951
3	1	2	13.3	.202352	.538928	2.677264
3	2	2	6.6	.250577	.643151	2.060289
3	9	2	2.5	.895661	.368472	.959781
4	0	2	32.7	.247689	.637093	4.564311
4	1	2	18.7	.293697	.730018	3.694771
4	2	2	11.0	.350686	.830867	3.023166
4	3	2	7.0	.418658	.919738	2.537353
4	4	2	7.5	.497613	.963774	2.688549

h	k	l	I_{rel}	$Sin^2\theta$	1/LP	F
4	7	2	7.5	.800371	.574314	2.075417
5	0	2	20.0	.350508	.830583	4.075740
5	2	2	72.8	.471034	.956896	8.346375
5	4	2	1.0	.635490	.871427	.933502
6	0	2	5.8	.473566	.957909	2.357089
3	-1	2	802.7	.138849	.392339	17.746270
4	-1	2	6.6	.212664	.561727	1.925459
4	-2	2	140.9	.188622	.508170	8.461749
5	-2	2	13.6	.273912	.691056	3.065673
6	-2	2	10.0	.379440	.873380	2.955299
7	-2	2	5.0	.505208	.964204	2.195681
7	-3	2	14.7	.465854	.954593	3.745999
7	-6	2	1.7	.413688	.914683	1.246980
8	-4	2	5.8	.565961	.943369	2.339132
8	-6	2	10.8	.524636	.962195	3.223615
8	-7	2	2.5	.520448	.963005	1.551615
8	-8	2	9.2	.527242	.961587	2.974323
9	-7	2	2.5	.642871	.861253	1.467355
-1	0	2	22.5	.037181	.044977	1.005971
-1	1	2	48.2	.039366	.067023	1.797358
-1	2	2	1527.6	.052533	.141616	14.708230
-1	3	2	48.2	.076682	.227523	3.311588
-1	4	2	49.1	.111814	.325152	3.995615
-1	5	2	5.0	.157928	.437657	1.479284
-1	6	2	171.6	.215025	.566908	9.863135
-2	0	2	34.3	.055796	.155233	2.307483
-2	1	2	271.5	.049216	.126586	5.862419
-2	2	2	1652.7	.053619	.146261	15.547500
-2	3	2	602.8	.069004	.203043	11.063180
-2	4	2	70.0	.095371	.281562	4.439516
-2	5	2	12.7	.132721	.377466	2.189479
-2	6	2	4.2	.181053	.491017	1.436060
-2	7	2	7.0	.240368	.621623	2.085990
-2	8	2	5.0	.310665	.761990	1.951909
-3	1	2	37.6	.079306	.235521	2.975830
-3	2	2	126.6	.074944	.222133	5.303022
-3	3	2	81.6	.081565	.242276	4.446317
-3	4	2	7.2	.099167	.291880	1.449666
-3	5	2	4.2	.127753	.365273	1.238606
-3	6	2	17.5	.167320	.459512	2.835746
-3	7	2	10.8	.217870	.573136	2.487943
-3	10	2	1.7	.435415	.934895	1.260682
-3	12	2	11.4	.635357	.871606	3.152190
-4	2	2	21.9	.116509	.337150	2.717274
-4	3	2	55.9	.114365	.331691	4.305987
-4	4	2	43.4	.123203	.353988	3.919573
-4	5	2	41.5	.143023	.402373	4.086377
-4	6	2	31.6	.173826	.474501	3.872239
-4	7	2	6.8	.215612	.568195	1.965635

h	k	l	I_{rel}	$\sin^2\theta$	1/LP	F
-4	8	2	9.2	.268380	.679876	2.500971
-4	9	2	5.2	.332130	.800189	2.039848
-4	13	2	5.0	.696956	.775233	1.968798
-5	4	2	52.1	.167477	.459875	4.894840
-5	5	2	2.5	.178533	.485274	1.101445
-5	6	2	40.2	.200572	.534966	4.637416
-5	7	2	10.1	.233593	.607167	2.476365
-5	9	2	11.6	.332582	.800963	3.048142
-5	12	2	5.0	.563434	.945070	2.173787
-6	4	2	2.5	.231991	.603730	1.228545
-6	5	2	96.0	.234282	.608644	7.643937
-6	8	2	11.5	.307051	.755304	2.947200
-6	10	2	5.8	.410476	.911284	2.299009
-6	11	2	1.0	.478662	.959720	.979653
-7	4	2	13.8	.316743	.773077	3.266260
-7	5	2	6.4	.310270	.761263	2.207279
-7	7	2	29.8	.330271	.796990	4.873426
-7	9	2	2.0	.394202	.892520	1.336053
-8	6	2	2.0	.402242	.902107	1.343210
-8	7	2	6.0	.408969	.909654	2.336220
-8	8	2	5.0	.426679	.927361	2.153324
-8	10	2	5.0	.495046	.963473	2.194848
-9	10	2	4.2	.567689	.942166	1.989245
-9	11	2	1.0	.609581	.903560	.950558
0	1	3	2.6	.100988	.169499	.663850
0	2	3	19.4	.125649	.257207	2.233789
0	3	3	6.4	.161292	.358878	1.515525
0	4	3	1.0	.207917	.475419	.689506
0	5	3	5.2	.265525	.605868	1.774967
1	0	3	7.6	.115044	.222442	1.300215
1	1	3	31.3	.137487	.292960	3.028143
1	2	3	3.0	.170912	.383999	1.073310
1	3	3	5.0	.215320	.492925	1.569911
1	4	3	6.4	.270710	.616949	1.987076
1	5	3	4.2	.337082	.747010	1.771282
1	6	3	11.8	.414437	.860418	3.186364
2	0	3	71.0	.163018	.363437	5.079762
2	1	3	7.0	.194225	.442409	1.759789
2	3	3	1.7	.289586	.656277	1.056252
2	4	3	5.8	.353741	.775492	2.120813
2	5	3	12.1	.428278	.875571	3.254903
2	6	3	1.0	.514997	.918254	.958256
3	0	3	6.0	.231230	.529796	1.782912
3	4	3	9.0	.457011	.898761	2.844089
3	5	3	22.9	.540913	.914293	4.575730
4	0	3	1.7	.319681	.715285	1.102717
4	1	3	3.3	.368417	.798892	1.623681
4	2	3	5.0	.428136	.874845	2.091464
4	3	3	12.9	.498837	.916760	3.438924
4	4	3	17.1	.580521	.893630	3.909100

h	k	l	I_{rel}	$Sin^2\theta$	1/LP	F
5	2	3	30.4	.554355	.909212	5.257379
6	2	3	1.0	.700814	.742475	.861670
3	-1	3	47.4	.202241	.461837	4.678788
4	-1	3	8.4	.281927	.640518	2.319558
4	-2	3	2.5	.255156	.583367	1.207648
5	-1	3	1.7	.381853	.818800	1.179813
5	-2	3	1.0	.346317	.763040	.873522
5	-3	3	9.5	.321763	.719181	2.613851
6	-2	3	1.7	.457717	.899231	1.236402
7	-2	3	8.7	.589357	.886743	2.777520
7	-3	3	2.5	.547274	.912142	1.510084
7	-4	3	30.8	.516174	.918244	5.318073
7	-6	3	5.0	.486921	.913698	2.137402
8	-5	3	5.1	.621641	.855132	2.088342
-1	1	3	484.3	.084729	.081225	6.271939
-1	2	3	90.9	.100625	.167967	3.907458
-1	3	3	7.2	.127503	.262988	1.376048
-1	4	3	1.7	.165364	.369596	.792662
-1	5	3	45.1	.214207	.490308	4.702434
-1	6	3	5.0	.274033	.623990	1.766337
-1	7	3	1.7	.344841	.760518	1.137048
-1	8	3	16.8	.426631	.873353	3.830447
-1	12	3	2.5	.863618	.427767	1.034125
-2	0	3	167.3	.092559	.130421	4.671121
-2	1	3	52.4	.088708	.108776	2.387439
-2	2	3	3.5	.095839	.146653	.716440
-2	3	3	7.5	.113953	.218666	1.280622
-2	4	3	49.8	.143050	.308960	3.922527
-2	5	3	5.2	.183128	.414991	1.468996
-2	6	3	5.2	.234189	.536545	1.670338
-2	7	3	6.8	.296233	.669721	2.134034
-2	8	3	19.4	.369259	.800182	3.939991
-2	9	3	1.0	.453267	.896175	.946665
-2	12	3	5.8	.771187	.614765	1.888289
-3	1	3	57.4	.112926	.215071	3.513558
-3	2	3	59.6	.111293	.209268	3.531625
-3	3	3	48.2	.120643	.241191	3.409601
-3	4	3	143.2	.140974	.303042	6.587531
-3	5	3	7.9	.172288	.387537	1.749726
-3	6	3	19.7	.214585	.491198	3.110722
-3	7	3	6.6	.267864	.610881	2.007937
-3	8	3	2.5	.332125	.738169	1.358462
-3	9	3	5.8	.407369	.852240	2.223283
-3	12	3	1.7	.698995	.745503	1.125768
-3	13	3	1.7	.818169	.521690	.941739
-4	13	3	23.4	.757452	.641016	3.872953
-4	2	3	23.2	.146986	.320036	2.724853
-4	3	3	44.9	.147571	.321665	3.800361
-4	4	3	5.8	.159138	.353154	1.431184
-4	5.	3	3.0	.181688	.411383	1.110922

h	k	l	I_{rel}	$Sin^2\theta$	1/LP	F
-4	6	3	9.2	.215220	.492690	2.129025
-4	7	3	2.5	.259734	.593357	1.217945
-4	8	3	2.5	.315231	.706874	1.329355
-4	9	3	4.0	.381710	.818596	1.809525
-4	10	3	3.9	.459172	.900182	1.873688
-4	12	3	1.7	.647043	.823825	1.183428
-4	13	3	7.5	.757452	.641016	2.192628
-4	14	3	32.2	.878843	.395384	3.568103
-5	2	3	4.2	.202918	.463465	1.395189
-5	3	3	6.0	.194738	.443662	1.631555
-5	4	3	2.5	.197541	.450483	1.061228
-5	6	3	4.4	.236093	.540868	1.542666
-5	7	3	2.5	.271843	.619356	1.244343
-5	8	3	1.7	.318576	.713207	1.101113
-5	9	3	1.7	.376290	.810740	1.173991
-5	10	3	12.3	.444988	.889904	3.308445
-5	12	3	2.5	.615329	.862069	1.468050
-6	3	3	2.5	.262145	.598582	1.223296
-6	4	3	1.0	.256183	.585615	.765255
-6	5	3	23.1	.261203	.596544	3.712162
-6	6	3	7.9	.277206	.630668	2.232100
-6	7	3	5.0	.304192	.685523	1.851381
-6	9	3	3.3	.391110	.831616	1.656603
-6	10	3	25.9	.451042	.894564	4.813438
-6	11	3	28.8	.521957	.917956	5.141703
-6	12	3	1.0	.603855	.873759	.934751
-7	4	3	1.0	.335064	.743429	.862223
-7	5	3	7.5	.331320	.736717	2.350611
-7	6	3	1.0	.338558	.749611	.865800
-7	7	3	2.5	.356779	.780471	1.396845
-7	8	3	5.8	.385982	.824610	2.186946
-7	9	3	2.5	.426168	.872890	1.477235
-7	11	3	2.5	.539486	.914713	1.512210
-8	4	3	2.5	.434184	.880597	1.483742
-8	6	3	12.7	.420149	.866665	3.317625
-8	8	3	2.5	.450044	.893824	1.494844
-9	6	3	1.0	.521979	.917954	.958099
-9	7	3	1.0	.522670	.917894	.958068
-9	8	3	4.2	.534345	.916031	1.961460
-9	10	3	10.8	.590640	.885676	3.092782
-10	9	3	15.9	.652776	.816059	3.602128