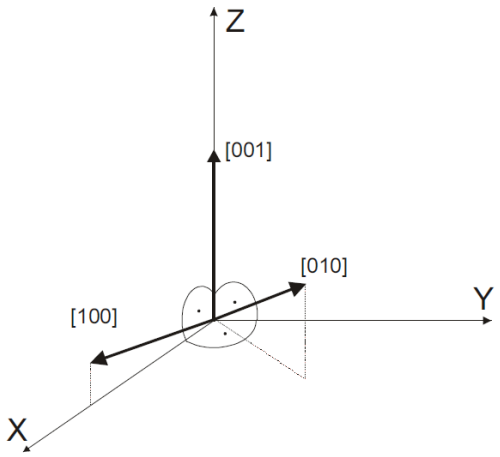
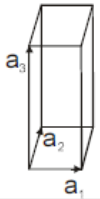
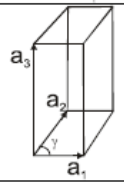
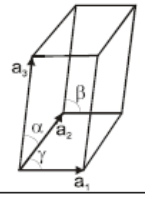
LaboTexのZ軸定義



Orthorhombic	D_2	D_{2h},D_2	a < b < c	90° 90° 90°	
	C_2	C_{2v}			
Monoclinic	C_2	C_{2h},C_2	a < b c	90° 90° γ < 90°	
	C_1	C_1			
Triclinic	C_1	C_1	a < b < c	α β γ < 90°	

Poly(phenylene sulfide)

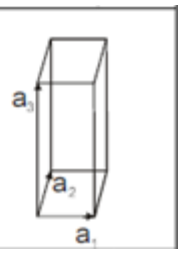
ポリプロピレン

PET

Poly(phenylene sulfide)

No: 00-040-1536 ↓
Name: Poly(phenylene sulfide)↓
Chemical Formula: (C6 H4 S2)n↓
Formula: C6 H4 S2↓
Z value: --↓
Space Group: (0)↓
Cell: 8.6700 5.6100 10.2600 90.000 90.000 90.000↓
Volume: 499.033↓
Crystal System: Orthorhombic↓
Quality: B↓
RIR(I/Ic): ---↓
Subfile: Organic, Polymer↓
---------- Experiment↓
Radiation: lambda: ↓
Reference: Schoch, K., Bartko, J. Polymer28(1987)556.↓
---------- Physical↓
---------- Comment↓
---------- d-I list (2theta are calculated with ↓
2theta range: 18.91 - 51.91↓

2theta	d	I	(hkl)↓
18.91	4.690	25.0	(1,1,0)↓
20.59	4.310	100.0	(2,0,0)↓
25.58	3.480	16.0	(1,1,2)↓
27.42	3.250	19.0	(2,1,1)↓
31.94	2.800	8.0	(0,2,0)↓
33.15	2.700	3.0	(0,2,1)↓
36.04	2.490	7.0	(3,1,1)↓
39.86	2.260	6.0	(1,1,4)↓
45.55	1.990	5.0	(4,1,1)↓
51.91	1.760	2.0	(2,1,5)↓

a < b < c	90° 90° 90°	

Orthorhombic
8.67 (1.0)
5.61 (0.6471)
10.26 (1.1834)
90.0
90.0
90.0
1.54056
10

1	1	0	25.0	18.825
2	0	0	100.0	20.47
1	1	2	16.0	25.655
2	1	1	19.0	27.393
0	2	0	8.0	31.878
0	2	1	3.0	33.08
3	1	1	7.0	36.007
1	1	4	6.0	39.991
4	1	1	5.0	45.698
2	1	5	2.0	51.879

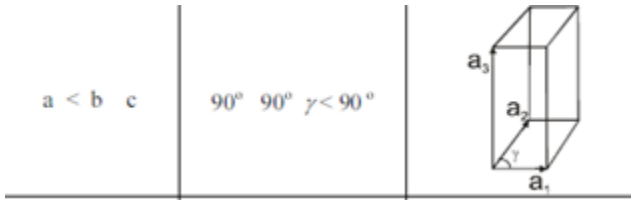
Orthorhombic
5.61 (1.0)
8.67 (1.5455)
10.26 (1.8289)
90.0
90.0
90.0
1.54056
10

1	1	0	25.0	18.825
0	2	0	100.0	20.47
1	1	2	16.0	25.655
1	2	1	19.0	27.393
2	0	0	8.0	31.878
2	0	1	3.0	33.08
1	3	1	7.0	36.007
1	1	4	6.0	39.991
1	4	1	5.0	45.698
1	2	5	2.0	51.879

α-Polypropylene

Name: α-Polypropylene↓
Chemical Formula: (C3 H6)n↓
Formula: C3 H6↓
Z value: 12↓
Space Group: P21/c(14)↓
Cell: 6.6300 20.7800 6.5000 90.000 99.500 90.000↓
Volume: 883.233↓
Crystal System: Monoclinic↓
Quality: C↓
RIR(I/Ic): 1.06↓
Subfile: Organic, Polymer↓
---------- Experiment↓
Radiation: CuKa1 lambda: 1.54060↓
Reference: Kaduk, J., Amoco Corporation, Naperville, I
ion(1998).↓
---------- Physical↓
Dcalc: 0.949↓
---------- Comment↓
General Comments: Hydrogen atoms included in calculate
2.5 for C and 5.0 for H. Symmetric Cauchy ↓
profile function with resolution FWHM=0.08° at 2θ=30
Single Crystal.↓
---------- d-I list (2theta are calculated with
2theta range: 8.50 - 76.00↓

2theta	d	I	(hkl)
8.50	10.390	2.6	(0,2,0)↓
13.53	6.539	1.2	(1,0,0)↓
14.19	6.238	100.0	(1,1,0)↓
17.05	5.195	54.0	(0,4,0)↓
18.65	4.755	71.4	(1,3,0)↓
19.66	4.513	2.3	(-1,2,1)↓
21.36	4.156	36.9	(1,1,1)↓
21.88	4.059	70.4	(-1,3,1)↓
22.63	3.927	1.8	(1,2,1)↓

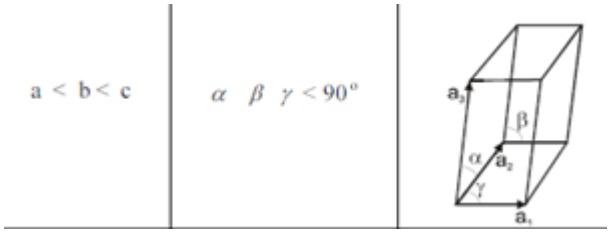


Monoclinic					Monoclinic				
6.63	(1.0)				6.5	(1.0)			
20.78	(3.1342)				6.63	(1.02)			
6.5	(0.9804)				20.78	(3.1969)			
90.0					90.0				
99.5					90.0				
90.0					80.5				
1.54056					1.54056				
145					145				
0	2	0	2.6	8.503	0	0	2	2.6	8.503
1	0	0	1.2	13.53	0	-1	0	1.2	13.53
1	1	0	100.0	14.187	0	-1	1	100.0	14.187
0	4	0	54.0	17.054	0	0	4	54.0	17.054
1	3	0	71.4	18.645	0	-1	3	71.4	18.645
-1	2	1	2.3	19.656	1	1	2	2.3	19.656
1	1	1	36.9	21.364	1	-1	1	36.9	21.364
-1	3	1	70.4	21.877	1	1	3	70.4	21.877
1	2	1	1.8	22.626	1	-1	2	1.8	22.626

PET

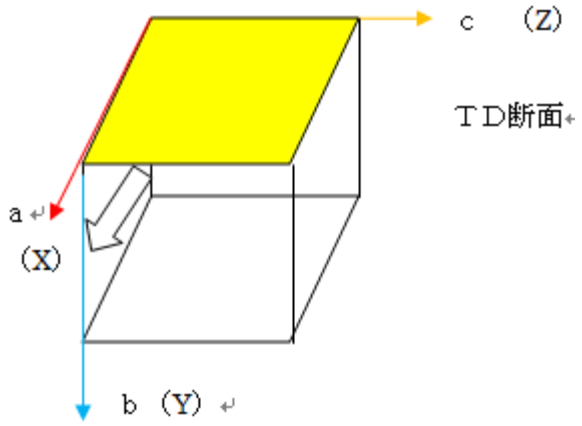
Name: PET, PETE↓
Chemical Formula: (C10 H8 O4)n↓
Formula: C10 H8 O4↓
Z value: 1↓
Space Group: P-1(2)↓
Cell: 4.5370 5.9220 10.7710 99.920 118.620 111.370↓
Volume: 214.225↓
Crystal System: Triclinic↓
Quality: C↓
RIR(I/Ic): 1.15↓
Subfile: Organic, Polymer↓
---------- Experiment↓
Radiation: CuKa1 lambda: 1.54060↓
Reference: Kaduk, J., Amoco Corporation, Naperville, I
unication(1997).↓
CAS: 25038-59-9↓
---------- Physical↓
Dcalc: 1.490↓
---------- Comment↓
Additional Patterns: See PDF 02-072-2446, 00-058-1447
omments: Pattern calculated using the results ↓
of a Rietveld refinement of a highly crystalline PET c
profiles. Instrument resolution function yields ↓
FWHM of 0.08° at 2θ=35° . Unit Cell Data Source: Rie
sis.↓
---------- d-I list (2theta are calculated with
2theta range: 16.31 - 89.80↓

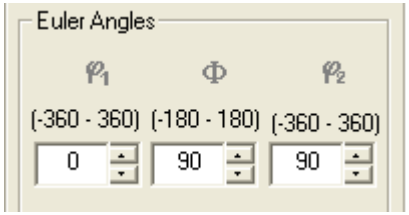
2theta	d	I	(hkl)↓
16.31	5.432	30.6	(0,-1,1)↓
17.75	4.994	37.0	(0,1,0)↓
21.46	4.137	21.8	(-1,1,1)↓
22.72	3.910	61.7	(-1,1,0)↓
24.12	3.687	13.1	(0,1,1)↓
24.97	3.564	13.5	(-1,1,2)↓
26.11	3.410	100.0	(1,0,0)↓

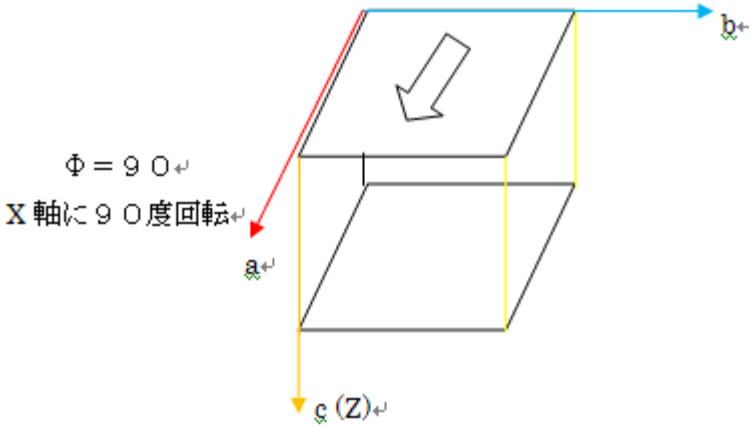


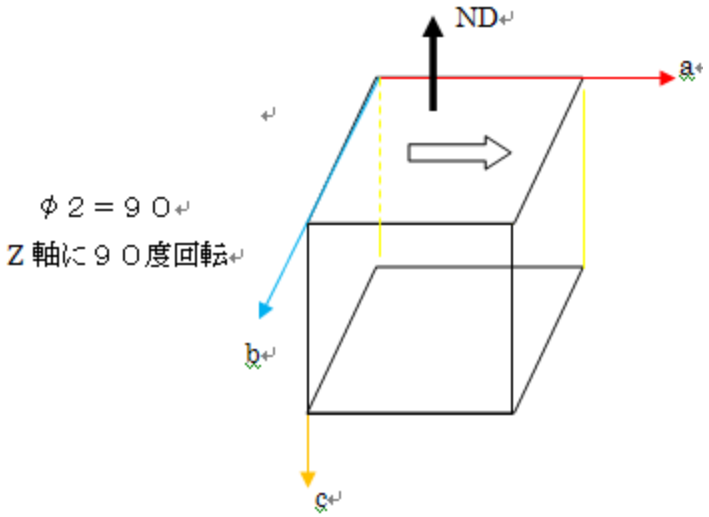
Triclinic					Triclinic				
4.537	(1.0)				4.537	(1.0)			
5.922	(1.3053)				5.922	(1.3053)			
10.771	(2.374)				10.771	(2.374)			
99.92					99.92				
118.62					61.38				
111.37					68.63				
1.54056					1.54056				
142					142				
0	-1	1	30.6	16.305	0	-1	1	30.6	16.305
0	1	0	37.0	17.746	0	1	0	37.0	17.746
-1	1	1	21.8	21.463	1	1	1	21.8	21.463
-1	1	0	61.7	22.724	1	1	0	61.7	22.724
0	1	1	13.1	24.122	0	1	1	13.1	24.122
-1	1	2	13.5	24.966	1	1	2	13.5	24.966
1	0	0	100.0	26.114	-1	0	0	100.0	26.114
1	-1	1	25.2	28.149	-1	-1	1	25.2	28.149
0	-1	3	2.2	28.673	0	-1	3	2.2	28.673
0	0	3	3.9	31.317	0	0	3	3.9	31.317
-1	-1	3	2.8	32.081	1	-1	3	2.8	32.081
0	-2	1	3.7	32.798	0	-2	1	3.7	32.798

TD->ND軸変換

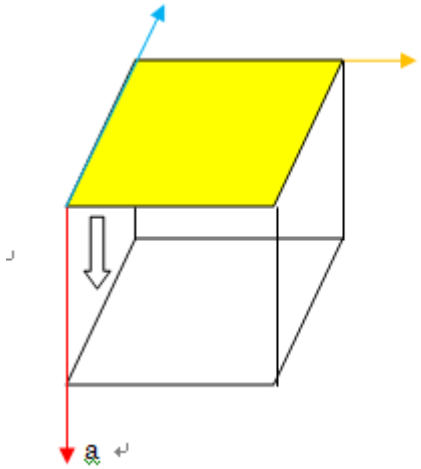

c (Z)
ＴＤ断面
a
(X)
b (Y)


Euler Angles
φ1
Φ
φ2
(-360 - 360)
(-180 - 180)
(-360 - 360)
0
90
90

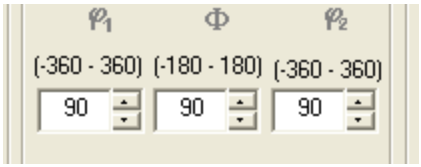

Φ＝９０
Ｘ軸に９０度回転
b
a
c (Z)


ND
a
φ２＝９０
Ｚ軸に９０度回転
b
c

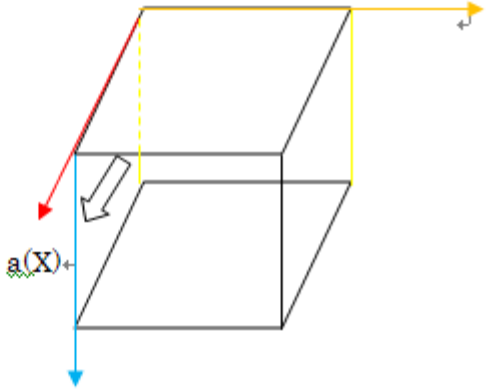
RD->ND軸変換



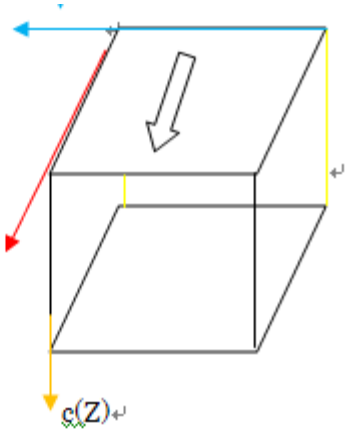
RD断面



φ１＝９０
Ｚ軸に９０度回転



Φ＝９０
Ｘ軸に９０度回転



φ２＝９０
Ｚ軸に９０度回転