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Part I
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MODEL COMPOUND STUDIES OF RIGID ROD AROMATIC HETEROCYCLIC POLYMER SYSTEMS, PART I: THE CRYSTAL AND MOLECULAR STRUCTURES OF 2,6-DIPHENYLBENZO (1,2-D:4,5-D') BISTHIAZOLE & 2,6-DIPHENYLBENZO (1,2-D:5,4-D') BISOXAZOLE

Polymer Branch
Nonmetallic Materials Division

February 1980

TECHNICAL REPORT AFML-TR-79-4184, Part I

Final Report for Period April 1977 to April 1978

AIR FORCE MATERIALS LABORATORY
AIR FORCE WRIGHT AERONAUTICAL LABORATORIES
AIR FORCE SYSTEMS COMMAND
WRIGHT-PATTERSON AIR FORCE BASE, OHIO 45433

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E. E. Arnold
Project Scientist

R. L. Van Deusen, Chief
Polymer Branch
Nonmetallic Materials Division

FOR THE COMMANDER

F. D. CHERRY, Chief
Nonmetallic Materials Division

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X-ray Crystal Structure	Benzobisoxazole	Rigid Rod Polymer
Polybisbenzoxazoles	Benzobisthiazole	Fully Extended Polymer
Polybisbenzthiazoles	Molecular Packing	
Model Compounds	Aromatic Heterocyclic Polymers	

20. ABSTRACT *(Continue on reverse side if necessary and identify by block number)*

The x-ray crystal structures of two monomeric model compounds for polybisbenzoxazole (PBO) and polybisbenzthiazole (PBT) are presented. The PBO model compound molecules stack along the b crystallographic axis in two vertical columns of differing orientation and are inclined to b by an angle of 36°. The repeat distance along b is 5.94A and the perpendicular distance between adjacent molecules in a particular stack is 3.4A. The PBT model compound molecules stack most efficiently along its b crystallographic axis with an inclination angle

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of 36.8°. Adjacent molecules along c exhibit a crossing pattern with a dihedral angle of 73.6°. The relationship between the model compound structures and the gross packing features of polymer chains in PBO and PBT are discussed.

FOREWORD

This report was prepared by the Polymer Branch, Nonmetallic Materials Division. The work was initiated under Project No. 2303, "Research to Define the Structure Property Relationships," Task No. 2303Q3 Work Unit Directive 2303Q307, "Structural Resins." It was administered under the direction of the Air Force Materials Laboratory, Air Force Wright Aeronautical Laboratories, Air Force Systems Command, Wright-Patterson Air Force Base, Ohio, with Dr. F. E. Arnold as the AFML Project Scientist. Co-authors were Dr. D. R. Wiff and Dr. A. V. Fratini, University of Dayton Research Institute, and Captain M. W. Wellman and Mr. W. W. Adams, Air Force Materials Laboratory (AFML/MBP).

This report covers research conducted from April 1977 to April 1978.

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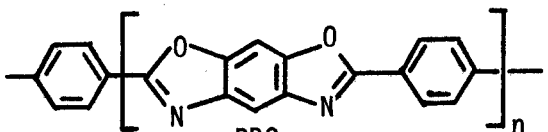
BACKGROUND

The Materials Laboratory at Wright-Patterson Air Force Base is presently investigating the applicability of ordered polymer systems as self-reinforced polymer composites. The preparation of high strength materials consisting of rod-like polymers, such as Kevlar, requires a high degree of orientation of the rods. Of the numerous rod-like polymer systems that have been studied to date, the paraconfigured aromatic heterocyclic class of polymers, such as the polybenzoxazoles (PBO) and the polybenzthiazoles (PBT), are especially promising, since precipitated films and fibers of these materials exhibit high tensile strengths and good thermal oxidative stabilities. These systems are also excellent alternatives to the more widely known aromatic polyamides.

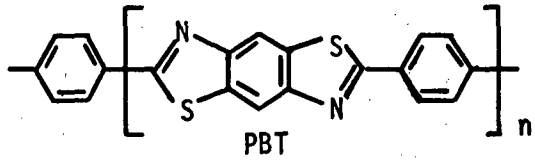
G. Berry of Carnegie-Mellon University has shown that 8.25% PBO in methane sulfonic acid forms an ordered solution under certain conditions (Reference 1). At 50°C the solution is optically isotropic, but develops an ordered phase which is characterized by the onset of birefringence as the temperature is decreased. The rheological behavior of the ordered phase implies that it is a nematic liquid crystal and is more susceptible to orientation under shear flow than the isotropic phase of randomly oriented rods. The molecular order present in fibers and precipitated films of PBO is believed to exist to some degree in solution just prior to fiber formation and film precipitation.

Diffraction patterns of films of PBO exhibited strong Bragg reflections at 3.4 and 5.9Å. These spacings have been interpreted by Berry in terms of a structure in which the polymer chains position themselves in a pleated array that is analogous to the "herring-bone" packing in quaterphenyl. The interpretation relied heavily on the apparent structure of one monomeric model compound possessing the PBO repeat unit.



PBO

To achieve a better understanding of precipitated film formation, film and fiber morphology, and microstructure in the polybenzoxazoles and polybenzthiazoles, a systematic study of the x-ray structures of a variety of possible model compounds has been initiated. These compounds embrace the different chemical environments for the repeat units of those PBO and PBT polymers which have already been synthesized.



PBT

The work described herein is the detailed structural analysis of two monomeric compounds which may function as model compounds for PBO and PBT.

SECTION II

EXPERIMENTAL

1. BENZOBISOXAZOLE

Crystalline material of the benzobisoxazole was furnished by Dr. Guy Berry of Carnegie-Mellon University. Optical examination under crossed polars as well as diffraction photographs taken on a Buerger precession camera showed the material to be polycrystalline and therefore not suitable for single crystal analysis. Precession photographs were characterized by rather broad and diffuse alignment streaks and diffraction spots. A request was then made to Dr. Berry for an additional sample of the model compound for use in the growth of fresh crystals by a sublimation technique. Approximately 50 mg of the material, consisting mostly of colorless flakes, were placed in a microsublimator (Kontes Glass vacuum sublimator, model K-306500) and heated by means of an oil bath and under reduced pressure to a final temperature of 180°C. A slow and uniform sublimation rate was maintained by gradually raising the temperature over a period of about three days. The crystals grew as tiny platelets — a feature not considered desirable for a good 'data' crystal — but continued examination under crossed polars finally yielded a needle-like crystal of dimensions 0.1 x 0.3 x 1.0 mm. Subsequent Weissenberg and precession photographs revealed the crystal to be orthorhombic with the following systematic absences: $h + k = 2n + 1$ for hkl, $l = 2n + 1$ for h0l, and $h = 2n + 1$ for hk0. These absences are consistent with two space groups, one of which is centric C_{mca}, No. 64, D_{2h}^{18}, and the other acentric A_{c2a} (a nonstandard setting of the standard space group A_{ba2}, No. 41, C_{2v}^{17}).

The crystal was then mounted on a Picker FACS-1 computer controlled diffractometer with $\underline{b}$ coincident with ϕ. A detailed account of the experimental apparatus is given in Reference 2. Unit cell dimensions were calculated by least squares refinement of the angular settings of 13 Friedel pairs ($28° < 2\theta < 41°$) using Nb-filtered MoK_α radiation. A total of 5422 reflections were measured using the θ-2θ scan mode, amounting to four equivalent octants (hkl, $\bar{h}$kl, h$\bar{k}$l, and $\bar{h}\bar{k}$l) of the sphere of reflection. Intensities were recorded with a scan speed of 1°/min for reflections

with $2\theta<55°$ and a 0.5°/min scan speed for $55°<2\theta<60°$. Background count times were approximately one-half peak scan times. Due to a breakdown in the air conditioning system, the prevailing temperature was as high as 28°C for the first three octants, finally stabilizing at 20°C for the final octant. Three standard reflections (115, 006, 202) were recorded every 75 reflections with no observable decrease in intensity during the three weeks of continuous data collection. Absorption corrections were estimated to be less than 1% and were not applied. The observed reflections were corrected for Lorentz and polarization effects and variances $\sigma(F)$ assigned on the basis of counting statistics using the method of Miller, Lenhert, and Joesten (Reference 3). The pertinent crystal data are summarized in Table 1.

2. BENZOBISTHIAZOLE

Single crystals of the benzobisthiazole were grown by vacuum sublimation using material supplied to us by Dr. Jim Wolfe of SRI International. Approximately 4 mg of the model compound were placed in a sample chamber (7 mm glass tubing, 58 cm long) which was then inserted into a thermal gradient sublimer (Scientific Instrument Accessories, Austin, Tx,78746 Model 240). The tube was evacuated and then heated to 205°C which was maintained for a period of 24 hours. The best crystals grew with material that had been previously sublimed. Crystals grew as needles elongated along the b axis and extinguished light along the needle axis when examined under a polarizing microscope. Although many of the crystals were twinned or polycrystalline, a single crystal of volume 0.0553 mm^3 was selected for a complete x-ray structural analysis. Weissenberg and precession photographs indicated that the crystal was monoclinic, space group $P2_1/c$, No. 14, C_{2h}^5.

The experimental configuration for the benzobisthiazole was similar to that used for the benzobisoxazole. Unit cell dimensions were computed from 15 Friedel pairs ($34° < 2\theta < 49°$). Intensities were measured with a scan speed of 1°/min for reflections with $2\theta < 50°$ and 0.5°/min for reflections having $50° < 2\theta < 65°$. Three standard reflections (104, 025, $\bar{1}12$) were measured periodically with no observable variation in intensity.

A total of 7653 diffraction intensities were recorded, yielding 2868 reflections after averaging equivalent reflections. Absorption corrections were applied using the Oak Ridge absorption program ORABS (Reference 4). The transmission factors ranged from 0.886 to 0.959 with an average of 0.937. The prevailing temperature was maintained at 21°C.

TABLE 1

PERTINENT CRYSTAL DATA FOR THE BENZOBISOXAZOLE AND THE BENZOBISTHIAZOLE

	BENZOBISOXAZOLE	BENZOBISTHIAZOLE
Formula	$C_{20}H_{12}N_2O_2$	$C_{20}H_{12}S_2N_2$
Formula Weight	312	344.5
a (Å)	11.370(7)	11.041(3)
b	5.940(3)	6.633(2)
c	22.275(14)	11.720(3)
β	——	112.36(5)°
Volume	1504.4 Å^3	793.8Å^3
space group	orthorhombic, C_{mca}	Monoclinic, $P2_1/c$
No. of molecules in cell (Z)	4	2
μ(MoKα)	0.99cm^{-1}	3.32 cm^{-1}
D_{meas}	1.39gcm^{-3}(flotation in acetone-chloroform mixture)	1.42gcm^{-3} (aqueous CsCl)
D_{calc}	1.38gcm^{-3}	1.44gcm^{-3}
$2\theta_{max}$	60°	65°
Total reflections measured	5422	7653
Independent reflections	1152	2868
weighting scheme	$1/\sigma^2(F)$	$1/\sigma^2(F)$
R, Rw	0.073, 0.077	0.051, 0.054

SECTION III

PHASE DETERMINATION AND REFINEMENT

1. BENZOBISOXAZOLE

The centric space group C_{mca} was initially chosen based on the averages and distributions of the normalized structure factor magnitudes. The 16-fold multiplicity of the general positions requires the model compound to possess 2/m symmetry or be disordered. 2/m molecular symmetry was not considered a realistic possibility, thus the structure analysis continued with the knowledge that the crystal was probably disordered.

The structure was solved by the direct phasing method of Karle and Karle (Reference 5), employing Stewart's XRAY 72 system of programs (Reference 6). NORMSF, SINGEN and PHASE subprograms were used to assign the phases of 90 reflections with $|E| > 1.5$, followed by computation of an E-map to locate atomic positions. Hydrogens were found in a difference Fourier map.

Atomic coordinates and anisotropic thermal parameters (isotropic for H atoms) were refined by the full-matrix least squares method using the complete data set of 959 reflections. Atomic scattering factors for carbon, nitrogen, and oxygen were taken from Cromer and Mann (Reference 7) and those for hydrogen were from Stewart, Davidson, and Simpson (Reference 8). A disordered model was incorporated into the final cycles of refinement by inserting a hypothetical atom at the position of the heteroatom (nitrogen or oxygen). The atomic scattering factor for the hypothetical atom was computed by simply averaging the values for nitrogen and oxygen assuming 50% occupancy for each atom. The last cycle gave a mean shift/error value for all atoms of 0.019, and a maximum value of 0.081 for the non-hydrogen atoms. The final residuals (R, Rw) are 0.073 and 0.077. Weights were assigned as $1/\sigma^2(F)$.

An attempt at refinement in the acentric space group Ac2a did not prove successful. Although there was little change in R, the distances and angles in the phenyl substituents were obviously incorrect. In the absence of any disorder, one might expect the centric and the acentric refinements to eventually converge to the same final structure. This did not prove to be the case. The final parameters are listed in Table 2.

2. BENZOBISTHIAZOLE

The phase determination for the benzobisthiazole followed essentially the same procedure used for the benzobisoxazole. XRAY 72 determined the phases of 395 reflections with $E_{min} > 1.4$. An E-map clearly revealed the positions of all the nonhydrogen atoms.

Atomic parameters were refined using 2536 reflections whose $F_{obs} > 1.5\sigma(F_{obs})$. The atomic scattering factor for sulfur is that of Cromer and Mann (Reference 7). 471 reflections had F_{obs} less than $1.5\sigma(F)$ and were excluded except for 138 reflections whose F_{calc} exceeded the threshold. The final residuals, R and R_w, are 0.051 and 0.054, respectively. The mean shift/error value for all atoms is 0.02. The final parameters are presented in Table 3.

TABLE 2

ATOMIC AND TEMPERATURE PARAMETERS FOR THE BENZOBISOXAZOLE**

	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(1)	0.1275(5)	0.5000(0)	0.0000(0)	4.5(3)	6.5(4)	7.1(4)	0	0	-.7(3)
C(2)	0.0621(3)	0.3428(7)	-.0302(2)	4.7(2)	5.2(2)	5.7(2)	0.1(2)	0.1(2)	0.3(2)
C(3)	0.0000(0)	0.0661(11)	-.0843(3)	5.9(3)	5.9(4)	5.1(3)	0	0	0.4(3)
C(4)	0.0000(0)	-.1312(11)	-.1231(3)	7.3(4)	5.3(3)	4.8(3)	0	0	0.6(3)
C(5)	0.1039(6)	-.2273(12)	-.1424(3)	10.1(5)	9.6(5)	6.9(3)	3.0(4)	-.4(3)	-.9(3)
C(6)	0.1024(9)	-.4099(13)	-.1795(3)	20.5(11)	9.9(5)	7.5(4)	7.7(6)	-.9(5)	-1.4(4)
C(7)	0.0000(0)	-.5004(19)	-.1988(5)	37.2(27)	6.2(6)	5.3(5)	0	0	-.4(4)
O,N*	0.0984(3)	0.1617(6)	-.0651(1)	5.2(2)	6.7(2)	7.1(2)	0.4(2)	-.3(2)	-.3(2)
H(1)	0.208(5)	0.500(0)	0.000(0)						
H(5)	0.160(5)	-.177(10)	-.128(2)						
H(6)	0.156(5)	-.489(10)	-.176(2)						
H(7)	0.000(0)	-.629(13)	-.215(3)						

*These atoms were given occupancies of 0.5.

**Parameters are in the form $\exp[-2\pi^2\{U_{11}h^2a^{*2} + \ldots 2U_{12}hka^*b^* + \ldots\}]$.

U_{ij} are times 100.

Hydrogen atoms were given an isotropic thermal parameter U = 0.08.

TABLE 3

ATOMIC AND TEMPERATURE PARAMETERS FOR THE BENZOBISTHIAZOLE**

	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(1)	0.49420(13)	0.02454(24)	0.11905(13)	4.46(9)	3.77(9)	2.73(7)	0.78(8)	1.88(7)	0.23(7)
C(2)	0.43260(13)	0.15676(22)	0.02413(12)	3.73(8)	3.05(8)	3.09(7)	0.62(7)	1.70(6)	0.20(7)
C(3)	0.43775(13)	0.13501(23)	-.09461(12)	3.57(8)	3.02(8)	2.86(7)	0.20(7)	1.48(6)	0.30(7)
C(4)	0.31570(13)	0.40881(22)	-.13120(12)	3.50(8)	3.20(9)	3.37(8)	0.09(7)	1.51(1)	0.21(7)
C(5)	0.23489(14)	0.57883(23)	-.19894(14)	3.61(8)	3.37(9)	4.22(9)	0.46(7)	1.99(7)	0.80(7)
C(6)	0.21428(16)	0.74636(27)	-.13836(16)	4.96(11)	3.85(11)	5.23(10)	0.65(9)	2.05(9)	0.35(9)
C(7)	0.13492(18)	0.90239(29)	-.20417(21)	6.56(12)	3.81(12)	8.14(16)	1.32(10)	4.01(12)	0.70(11)
C(8)	0.07531(19)	0.89067(33)	-.33010(21)	6.52(13)	5.85(15)	7.46(15)	2.98(11)	3.42(12)	3.31(12)
C(9)	0.09560(18)	0.72482(33)	-.39139(18)	6.95(13)	6.98(15)	5.36(11)	2.89(12)	2.55(11)	2.37(12)
C(10)	0.17570(17)	0.57003(28)	-.32706(15)	5.69(11)	4.88(12)	4.47(11)	1.65(9)	2.24(9)	1.05(9)
S	0.34010(4)	0.36837(6)	0.02428(3)	4.87(2)	3.71(2)	3.41(2)	1.25(2)	2.00(2)	0.30(2)
N	0.36994(11)	0.28036(19)	-.17986(10)	3.93(7)	3.63(8)	3.19(6)	0.63(6)	1.70(6)	0.60(6)
H(1)	0.4888(11)	0.0400(19)	0.1969(11)	2.9(3)					
H(6)	0.2541(13)	0.7521(23)	-.0533(13)	4.3(4)					
H(7)	0.1244(14)	1.0178(27)	-.1605(14)	5.9(4)					
H(8)	0.0187(16)	0.9927(28)	-.3732(15)	6.9(4)					
H(9)	0.0533(15)	0.7156(27)	-.4821(16)	8.1(5)					
H(10)	0.1902(15)	0.4468(24)	-.3707(14)	6.3(4)					

**Parameters are in the form $\exp[-2\pi^2\{U_{11}h^2a^{*2} + \ldots 2U_{12}hka^*b^* + \ldots\}]$.

U_{ij} are times 100.

Hydrogen atoms were given an isotropic thermal parameter U = 0.08.

SECTION IV

DISCUSSION OF RESULTS

1. BENZOBISOXAZOLE

The pertinent bond distances and angles for the benzobisoxazole are shown in Figure 1. Estimated standard deviations for bonds involving non-hydrogen atoms range from 0.002 to 0.005Å, while those involving hydrogens average 0.03Å. Space group symmetry requires the molecule to be planar and oriented with its 2-fold axis coincident with a. As mentioned previously, the crystal is disordered, thereby generating a pseudo-mirror plane which is perpendicular to the molecular plane. The average C-C distance in the terminal phenyl rings is 1.379Å, while the internal angles of the terminal phenyl rings average 119.8°. The disorder in the crystal precludes a complete and unambiguous structural characterization of the benzobisoxazole moiety at this time.

The c-glide plane perpendicular to b causes the molecules to stack along b in two vertical columns of different orientation (Figures 2, 3, and 4). The molecular planes are inclined at an angle of 36° to the b-axis. The repeat distance along the stacking direction is the same as the b-axis length, 5.94Å. The perpendicular distance between adjacent molecules in a stack is 3.48Å. These spacings correspond directly with the 5.9 and 3.4Å Bragg spacings observed in the oriented films of PBO (Reference 1).

Dr. Deane K. Smith of Pennsylvania State University has written a FORTRAN program for calculating x-ray powder patterns from atomic positions (Reference 9). Figure 5 presents the diffractometer tracing which results when the atomic parameters in Table 2 are read into the program. The first five peaks at 11.14, 5.69, 3.83, 3.40, and 3.03Å are in good agreement with values reported by Berry for the five strongest reflections from Debye-Scherrer photographs of the benzobisoxazole. Other features of the structure which are noteworthy are: (1) The molecular plane does not correspond to the 115 reflection, even though the Bragg spacing is 3.4Å. Molecular planes are restricted to the 0kl type; (2) A separation as short as 3.0Å between molecular planes, as is assumed in Figure 25 of

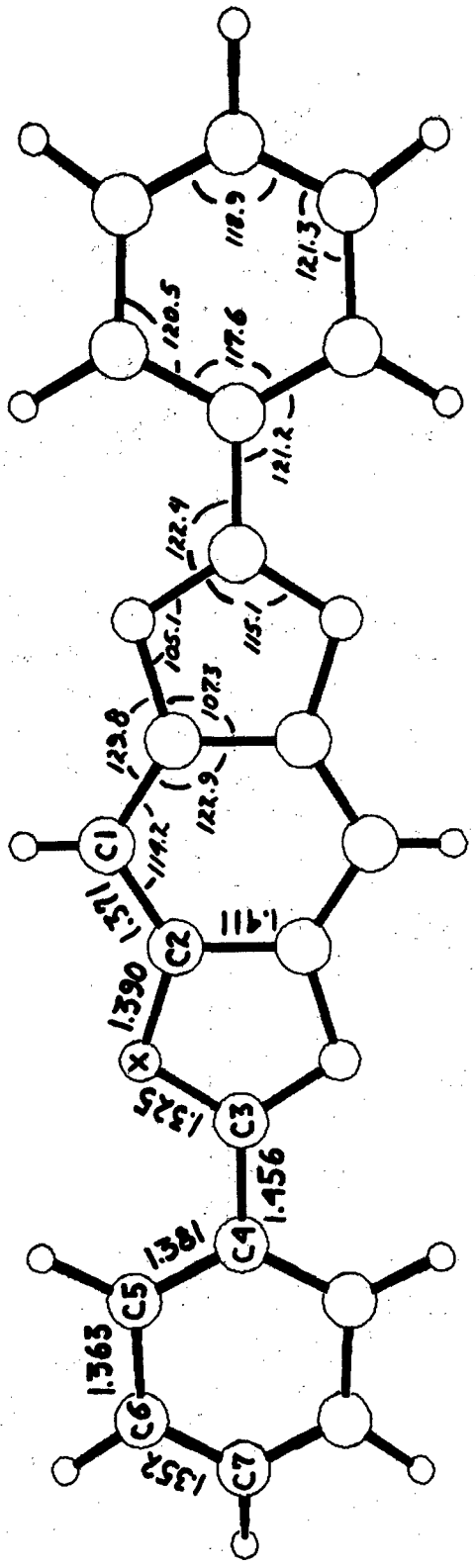


Figure 1. Bond Distances (Å) and Angles (°) of the Benzobisoxazole. (Carbon-hydrogen parameters have been omitted for clarity. The disordered heteroatom is denoted with the letter x)

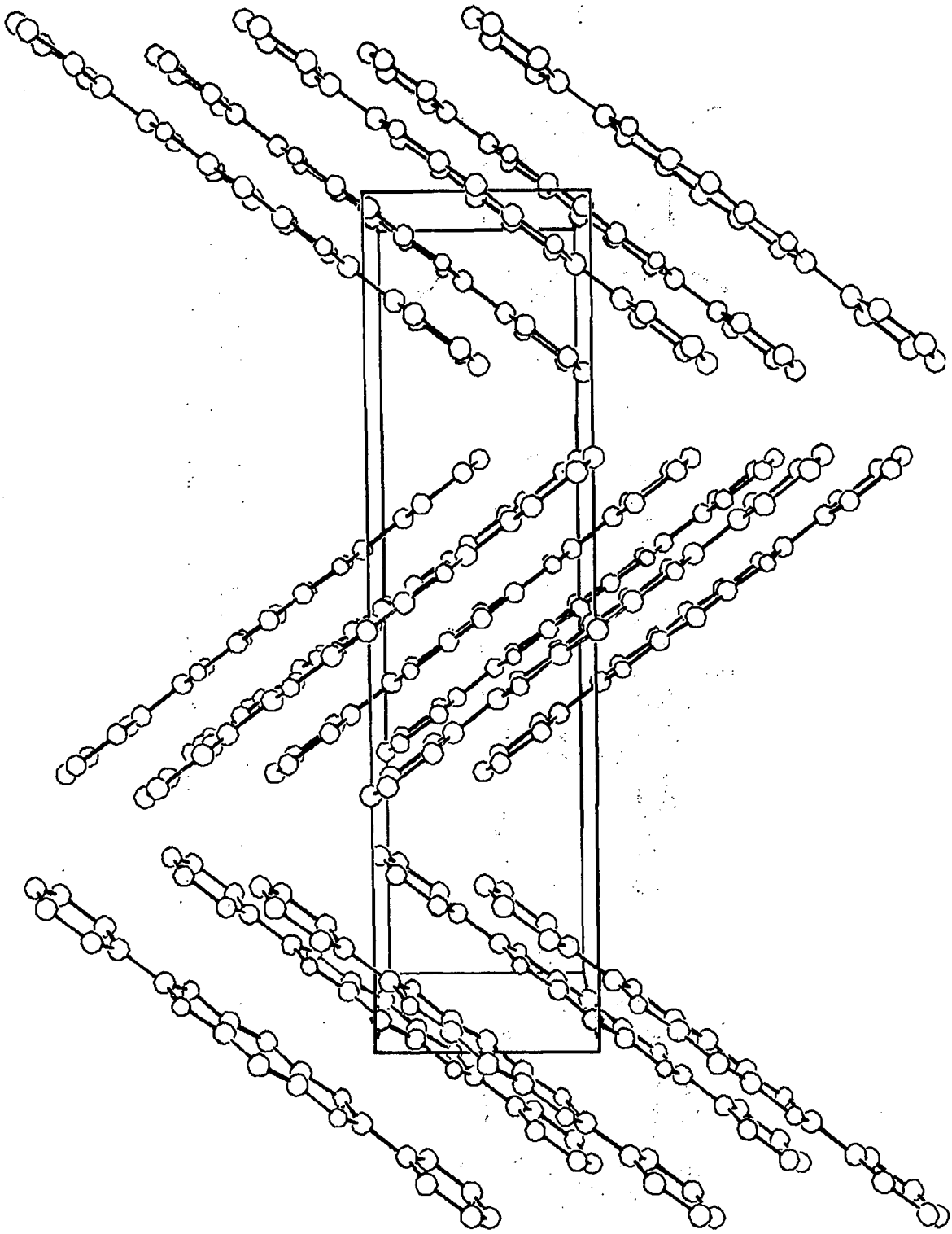


Figure 2. A Negative a-Axis View of the Molecular Stacking in the Benzobisoxazole Unit Cell. (The b-axis is vertical and the c-axis is horizontal)

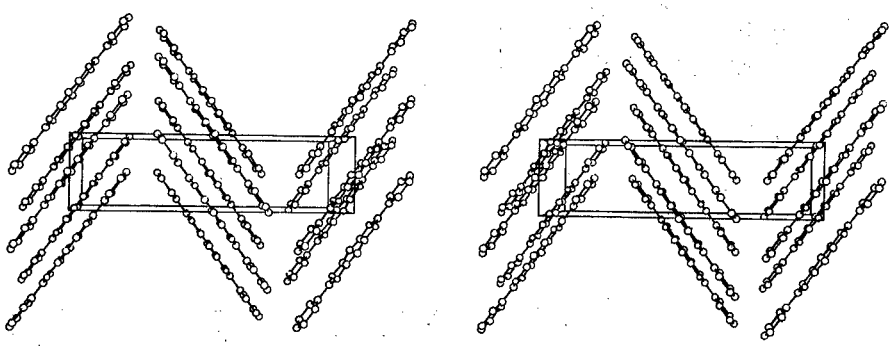


Figure 3. Stereoscopic View Down the Negative a-Axis of the Packing in the unit cell of the Benzobisoxazole. (The b-axis is vertical and the c-axis is horizontal. Only two adjacent layers of molecules are drawn for clarity)

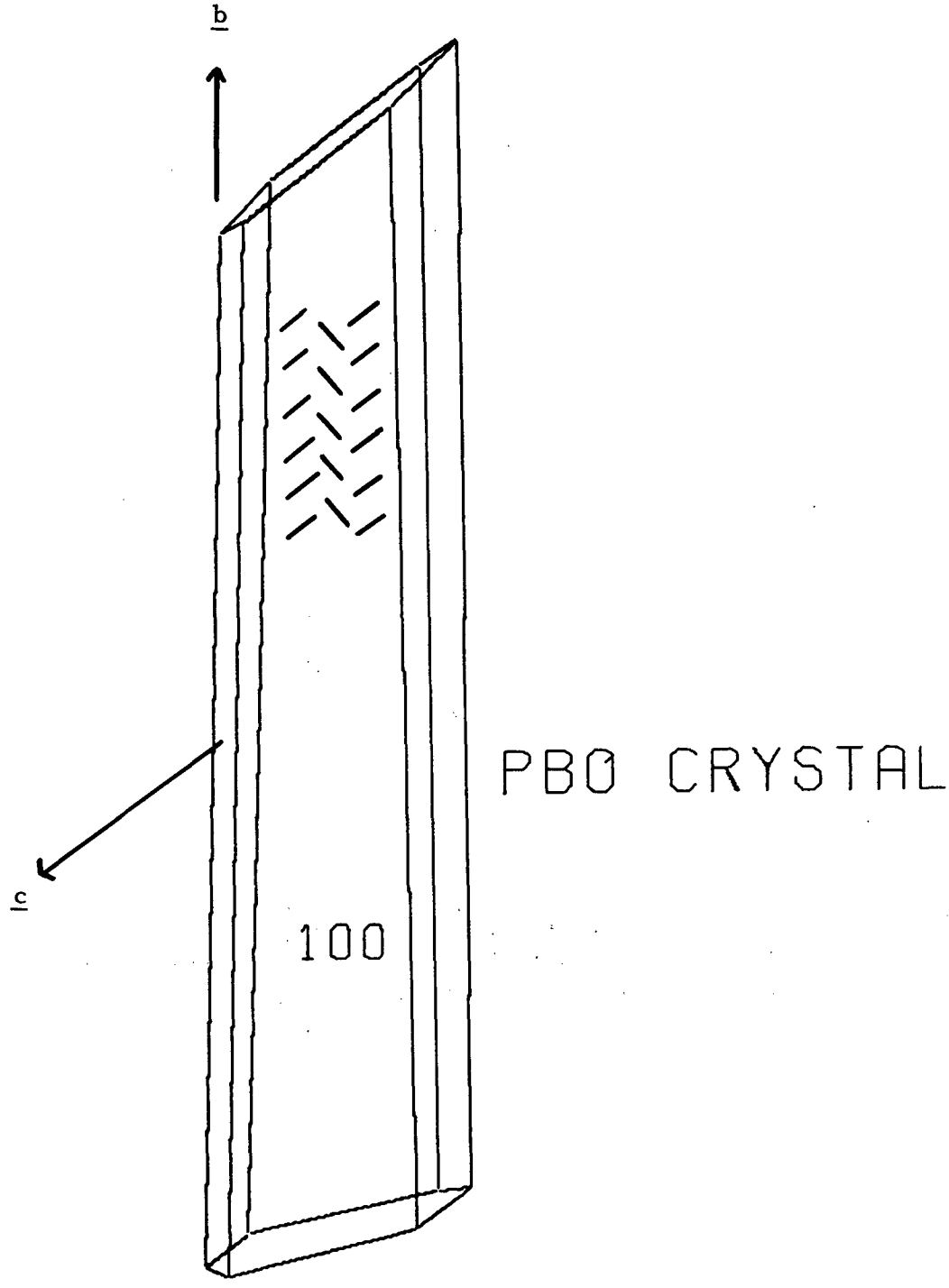


Figure 4. A sketch of the Benzobisoxazole Data Crystal Depicting the Orientation of the Crystallographic Axes, the Prominent (100) Face and the Molecular Stacking Along b

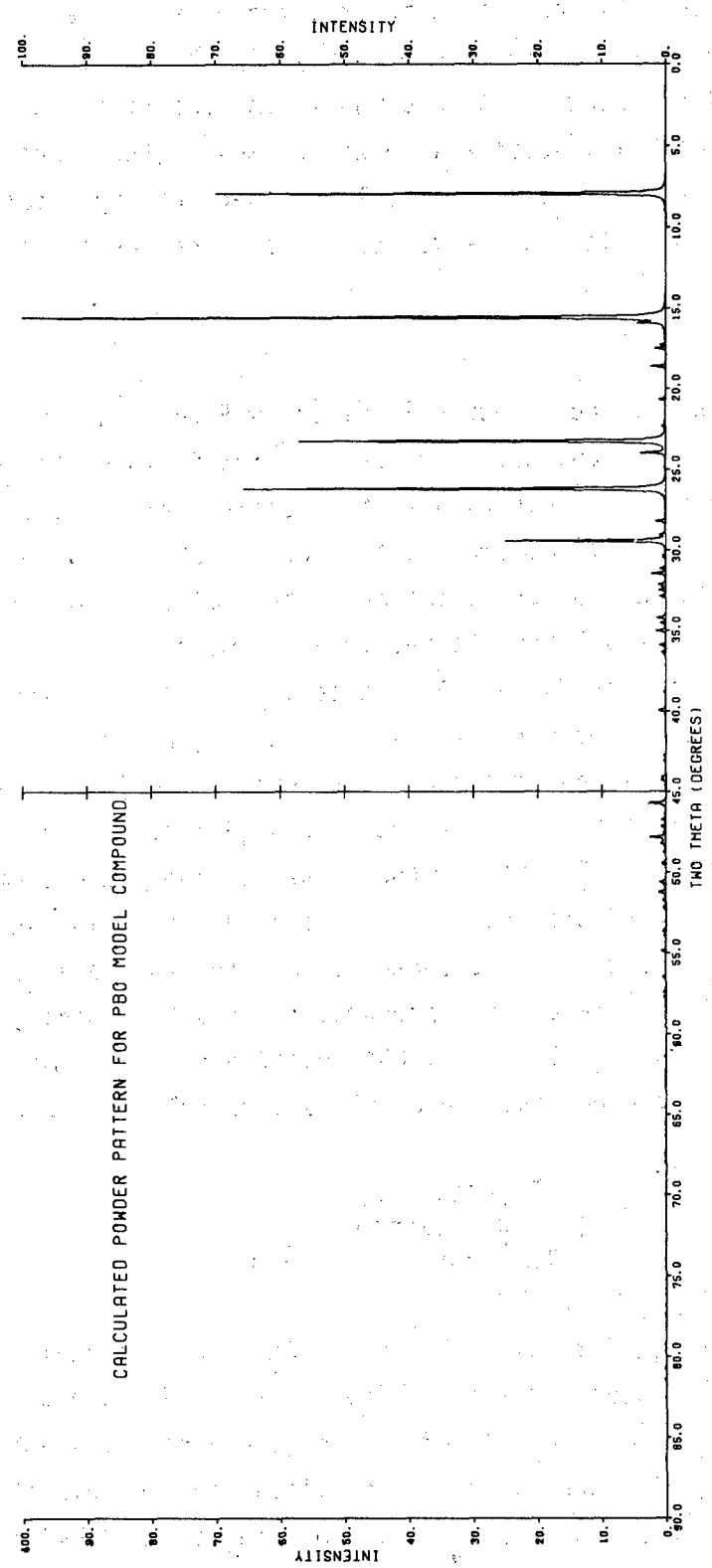
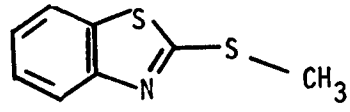


Figure 5. Calculated Powder Pattern of the Model Compound (Benzobisoxazole) Computed from the Atomic Parameters Listed in Table 2

Reference 1, is unreasonable on account of severe intermolecular repulsions between π-electrons; and (3) There is a major difference in the molecular packing of the benzobisoxazole proposed by Berry and that which is presented herein. Molecules of the benzobisoxazole model compound tilt out of the ac plane as a result of rotation about a line which lies in the plane and is perpendicular to the backbone of the molecule, rather than by rotation about a line which is parallel to the molecular backbone, as proposed by Berry (Reference 1).

2. BENZOBISTHIAZOLE

A perspective view of the molecule is given in Figure 6, along with selected bond distances and angles. The centrosymmetric molecule is not entirely planar as in the benzobisoxazole, but consists of two planar segments — the benzobisthiazole framework and the phenyl substituent — which are twisted relative to each other, creating a dihedral angle of 23.2°. The twist angles of ring systems bonded to the thiazole moiety are usually less than 20° [e.g., 10° in thiabendazole (Reference 10) and 19° in 2-amino-4-phenylthiazole hydrobromide monohydrate (Reference 11)] except in cases where steric interference is an important consideration (e.g., 36° in [2-phenyl-4-(p-chlorophenyl)-5-thiazolyl]-acetic acid (Reference 12)). The two S-C distances, 1.736 and 1.758Å, in the thiazole ring would seem to indicate minimal double bond character for these bonds, assuming shortening due to hybridization is taken into account. In 2-methyl-aminobenzothiazole, a molecule where the C-S distances are presumed to be single bonds, the corresponding distances are 1.739 and 1.763Å (Reference 13). A molecule which closely resembles the present structure is 2-methylthiobenzothiazole (Reference 14).



The corresponding S-C distances are 1.73 and 1.78Å. The internal valency angles about the S and N atom, 88.9 and 110.8°, are in good agreement with literature values [e.g., 89.3 and 111.8° in bis (benzothiazole-2-thiolato) bis(pyridine) cobalt (Reference 15); 90.1 and 111.4° in the thiazole-substituted acetic acid; and 89.3 and 109.9° in 2-amino-4,5-dihydro-7,8-dimethoxynaphtho (1,2-d)thiazole] (Reference 16).

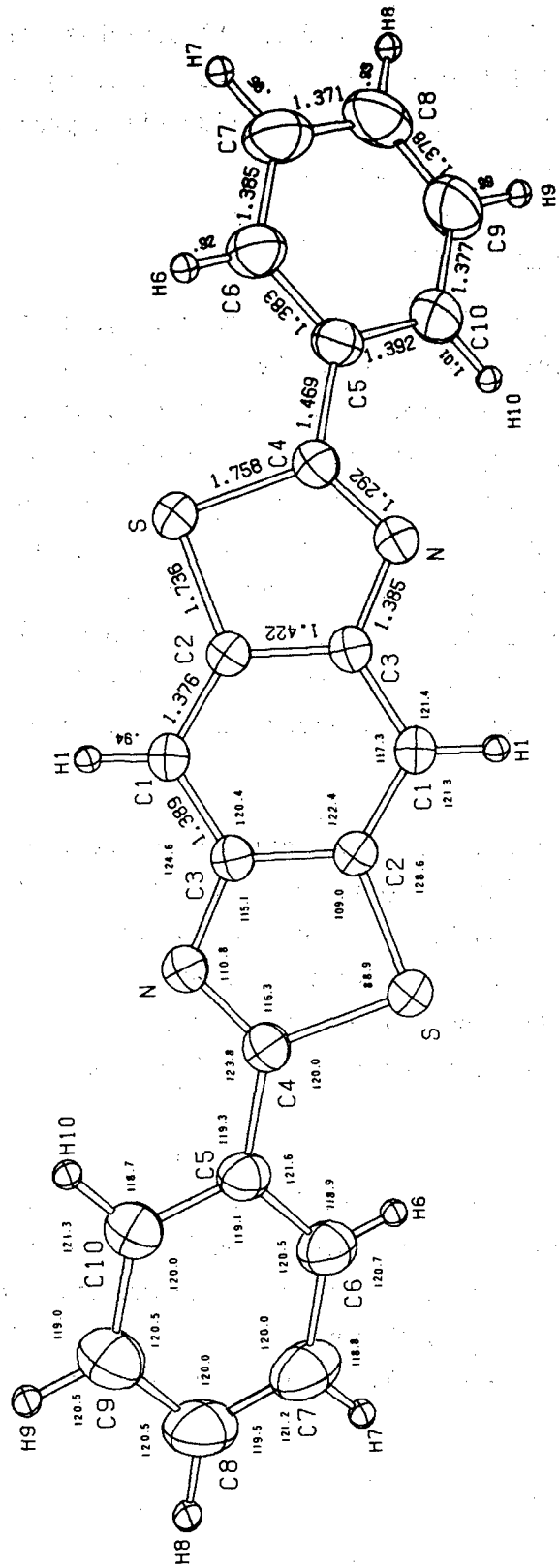


Figure 6. Selected Bond Distances (Å) and Angles (°) for the Benzobisthiazole

A stereoscopic view of the packing is shown in Figure 7. The packing is similar in many respects to that found in the benzobisoxazole. The molecules stacked most efficiently along the b-axis, being inclined to b by 36.8°, as in the benzobisoxazole. The c-glide plane produces the criss-cross pattern depicted in Figure 7.

3. RELATIONSHIP TO POLYMER SYSTEMS

The molecular packing in the two model compounds just discussed is not easily adapted to the packing of polymer chains in PBO and PBT. A more plausible model for packing in fibers and stretched films would involve chains of molecules extending in the direction of elongation, with the ring systems comprising the repeat units in a parallel or nonparallel arrangement. Tadorkoro has been successful in combining fiber diffraction data together with accurate molecular parameters toward the solution of the structures of several aromatic polyamides (Reference 17). It would seem that this type of an approach is now possible for PBO and PBT, since good quality diffraction patterns for fibers and films of PBO have been achieved.

It is also interesting to note that neither the benzobisoxazole nor the benzobisthiazole exhibits intermolecular interactions stronger than the Van der Waals type. Thus hydrogen bonding, which is believed to be an important interchain interaction in the aromatic polyamides, is absent in PBO and PBT. The rather low heat of sublimation for the benzobisoxazole reflects the absence of significant intermolecular interactions in these systems (Reference 1).

Lastly, the phenomenon of polymorphism has recently been observed for monomeric aromatic amides (References 18 and 19). We find two different modes of packing, depending on the crystal growth medium. The question naturally arises whether the model compounds selected for PBO and PBT exhibit similar behavior. Hopefully, this will become the topic of future study.

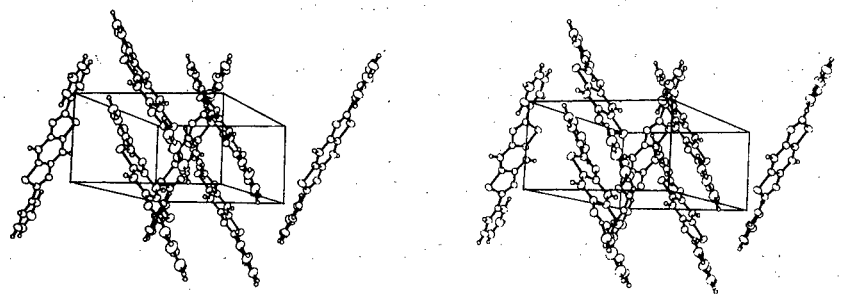


Figure 7. A Stereoscopic View Down the c-Axis of the Unit Cell of the Benzobisthiazole. (The a-Axis is horizontal and the b-axis is vertical)

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