estimated for the degree of disorder from the total number of observed reflections (Hosemann & Bagchi, 1962) agree with those derived from the integral widths after correcting for the small crystallite sizes.

Discussion

In view of the absence of a unique solution within the statistical approach, it is preferable to obtain a first approximation to the electron density profile by using the X-ray data uncorrected for the diffuse scattering and then to refine the approximate profile using the model calculations presented above.

The paracrystal approach is particularly useful for removing the diffuse scattering which would otherwise lead to artificial details in the reconstructed electron density profile (Baianu, 1978).

To account for membrane asymmetry (Moody, 1975) additional terms have to be included in (2)–(5). In this case, however, the refinement procedure proposed above cannot be applied unless the asymmetric membrane lamellae are stacked back-to-back as in myelin (to form centrosymmetric units), or an alternative method of phase determination is found.

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Crystallographic Pedigree of Organic Compounds

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A scheme of systematization of organic crystals is proposed on the basis of morphotropism. The organic crystal structures are classified into two main families, $Fm3m$ and $Pbca$, whose prototypes are provided by methane and benzene respectively. The system of organic crystals is made up from these prototypes by chemical substitutions frequently accompanied by descent in symmetry of the crystal structures by way of the isotranslational subgroups. The $Pbca$ family is predominant in organic molecular crystals. Polymorphism suggests the pedigree relation for descent or ascent in symmetry. The concept of an extended isomorphism is proposed to describe the crystallographic pedigree of organic compounds.

Introduction

Every chemical individual has its own characteristic crystalline form or sometimes forms (polymorphs). To discover the systematic relation between the chemical composition and the crystal structure is a fundamental task in organic crystal chemistry. Previous investigations in this field have dealt almost exclusively with inorganic crystals. This is because organic crystals are not uniformly distributed over all the space groups, but rather are concentrated into a small number of groups. This fact has been attributed by Nowacki (1943) to a zigzag chain structure of dipoles for which the appropriate symmetry element is either a twofold screw axis or a glide plane. Kitaigorodsky (1961) has demonstrated on the grounds of his close-packing

theory that organic molecules may attain closest packing in the special space groups.

It is instructive in the systematization of organic crystallography to consider the relation between chemical composition and crystal structure from the viewpoint of morphotropism. The present paper proposes the crystallographic pedigree of organic compounds on the basis of morphotropism and shows that the space group *Pbca* is a main prototype of organic crystal structures.

Morphotropism in organic crystals

Morphotropism has been defined as the process that, when by chemical substitution the limit of homogeneous deformation in the crystal structure is surpassed, a new atomic arrangement in space takes place. According to this definition polymorphism is an equivalence of morphotropism brought about not by chemical substitution but by physical conditions so that the substance is no longer isomorphous with itself. For applying this notion to organic crystals we shall extend the category of chemical substitution so as to include the group and homologous substitutions; then the terms isomorphism and polymorphism for atomic substitution will be replaced by the terms homomorphism and heteromorphism respectively.

As a first step towards a systematization of organic crystals methane and benzene are considered as the prototypes of the aliphatic and aromatic compounds respectively. The whole system of organic compounds can be made up from the prototypes by means of atomic, group and homologous substitutions, which are not necessarily realized by actual chemical reactions. By this chemical substitution the molecule changes its size and shape and then the symmetry is generally lowered by a new anisotropy caused by the substituents. The lowering of the symmetry results in the alteration of the mutual arrangement of neighboring molecules in the crystal structure. The distance between the nearest neighboring lattice sites increases, and about each lattice site a cavity grows by the influence of the molecular shape at the neighboring sites. The angular location of the pits and valleys of the cavity is determined by the symmetry elements of the lattice, while the direction of knobs and ridges of the molecule is determined by the symmetry of the

molecule. So far as the molecule fits into the cavity with its knobs and ridges fitting into the pits and valleys of the cavity, the space group and the number of molecules in the unit cell, Z, remain the same. This indicates that the general arrangement of the molecules conforms to the same symmetry operations. However, the values of the cell dimensions, the dihedral angles and spacings between nearest-neighbor molecules, and the other geometrical quantities vary homogeneously by successive substitutions. Sometimes the variation of the geometrical quantities may be drastic, in particular for polar-group substitution owing to such an occurrence as hydrogen bonding, indicating that besides the packing requirement the intermolecular forces play an important role in the alignment of molecules. However, it is to be remembered that even if the hydrogen bond changes greatly the orientation of the molecules, the general arrangement in the structures of the same space group and Z conforms to the same symmetry principle as that without the hydrogen bond. The molecular orientations have to be among those for which the effective symmetry of the molecule is aligned with the symmetry elements of the lattice.

When the limit of homogeneous deformation is surpassed by further substitution, the descent in symmetry of the crystal structure occurs through the subgroups by stepwise removal of certain symmetry elements characteristic of the chemical substitution. The order of the subgroup should be a factor of the order of the original group. Thus, for favourable orientation the effective point symmetry of the molecule would be a sub-point group of the space group at the lattice sites. In such a manner the pedigree relation occurs in organic crystals.

In considering the pedigree it should be noted that the resemblance and parallelism of the cell dimensions are necessary but not always sufficient conditions for a criterion of isostructure. For example, we have recently compared the crystal structures of isatin and isatoic anhydride and their isomers (Kashino, Nakashima & Haisa, 1978). The crystal data are shown in Table 1.

In this series, phthalimide is clearly heteromorphous with the other three homomorphs, because its cell dimensions are different from those of the other three. In fact the crystals of phthalimide (Matzat, 1972) do not comprise the sheet structure found in the other three. Despite the difference in the number of atoms in the rings, the sheet structure of isatin is closely similar

Table 1. *Crystal data of isatin, isatoic anhydride and their isomers*

	Space group	Z	a (Å)	b (Å)	c (Å)	β (°)
Isatin	$P2_1/a$	4	7·17	14·46	6·19	94·8
Isatoic anhydride	$P2_1/a$	4	7·18	14·35	6·73	91·9
Phthalimide	$P2_1/n$	4	22·83	7·651	3·810	91·36
O,N-Carbonylsalicylamide	$P2_1/a$	4	8·41	15·87	5·27	90·5

to that of isatoic anhydride. In this sense isatin is literally homomorphous with isatoic anhydride. On the other hand, the crystals of *O,N*-carbonylsalicylamide are alike in cell dimensions but are different in the details of the sheet structure from those of isatoic anhydride. Thus, *O,N*-carbonylsalicylamide is homomorphous but not isostructural with isatoic anhydride and isatin.

The *Fm3m* family

A prototype of aliphatic compounds, methane crystallizes in the space group *Fm3m* with $Z = 4$ (Müller & Schallmach, 1939). Organic molecules with cubic (tetrahedral or octahedral) symmetry crystallize frequently in the degenerate space groups which have symmetry axes of order higher than three.

On the basis of thermodynamics and crystallography Nitta (1959) has shown that the predominant structures of the face- and body-centered cubic crystals result from orientational and rotational disorder. This suggests that the highly symmetrical molecules should act like spheres, as observed in inorganic crystals. Therefore, the pedigree of the *Fm3m* family would resemble that in inorganic crystallography. We shall not mention further particulars in the present paper, and shall confine our attention to molecular crystals of simple organic compounds for the sake of brevity.

The *Pbca* family

According to recent statistics by Belsky & Zorkii (1977) the most common space groups of organic molecular crystals in decreasing order of abundance (Fig. 1) are $P2_1/c$, $P2_12_12_1$, $P\bar{1}$, $P2_1$, $C2/c$, *Pbca*, $Pna2_1$, *Pnma*, *Pbcn* and the others, in accordance with the prediction by Kitaigorodsky (1961). It is of particular interest to note that the first four of the groups are isotranslational (*zellengleich*, or *z*-) subgroups of the sixth, *Pbca* (*Internationale Tabellen zur Bestimmung von Kristallstrukturen*, 1935). A number of organic crystals belong to this group and the following may be considered to be representative.

(i) *For aliphatics*: methylamine, pentaerythritol tetraformate, oxalic acid (α form), hexamethylenediamine, succinimide.

(ii) *For alicyclics*: *o*-cyclohexanediol (α form).

(iii) *For aromatics*: benzene, acetanilide, *p*-diiodobenzene, *p*-nitrotoluene, *p*-dimethoxybenzene, dimethyl terephthalate, *o*-aminophenol, *o*-aminobenzoic acid, dibenzoylmethane, ethylene dibenzoate, *p*-nitrobiphenyl, *s*-trinitrobenzene, 2,6-dimethylnaphthalene, α-naphthylamine, *N*-2-naphthylacetamide, 2,5,7,8-tetranitronaphthalene, triketoindane, 9-fluorenone, dibenz[*a,h*]anthracene.

(iv) *For heterocyclics*: 2-aminopyridine, thiophthene, tetramethylpyrazine, 2,5-distyrylpyrazine, 5-ethyl-5-phenylbarbituric acid monohydrate (form XIII), 1,2,4-triazole.

There is a natural reason why benzene and many other simpler molecules crystallize in this space group: it is because the *Pbca* group comprises as many as possible twofold screw axes and glide planes in all three dimensions, which are considered to be the most appropriate elements for the low-symmetry molecules. The reason for this is as follows: if a molecule deviates from its position parallel to an adjacent molecule, owing to low symmetry and intermolecular forces, a third molecule can ultimately obtain a parallel translation with the first molecule. This arrangement can be continued indefinitely only by a twofold screw axis or a glide plane. In this sense *Pbca* is the highest symmetrical group of non-degenerate primitive groups. A primitive lattice should be most suitable for anisotropic objects. Thus, *Pbca* is eligible for the prototype of organic molecular crystals.

For illustration we shall start with a consideration of the relation between homologous substitution and morphotropism of aromatic compounds.

In the benzene crystals belonging to *Pbca* with $Z = 4$ (Cox, Cruickshank & Smith, 1958), the molecules lie at the corners and face centers of the unit cell and make a dihedral angle of 85.0° with each other. The crystal structures of linear polyphenyls and linear and nonlinear condensed aromatics are compared in Table 2.

Some interesting aspects of morphotropism may be suggested from these examples. At first, increasing the number of benzene rings by homologous substitution decreases the dihedral angle and when the limit of homogeneous decrease is surpassed the descent in symmetry of the crystal structures by way of the *z*-subgroups results. The limits occur between benzene and the others, between anthracene and tetracene and also between perylene and coronene. The limit in the polyphenyls is remarkably extended far from the expectation from the degree of similarity of molecules by Kitaigorodsky (1961). This extension of homomorphism is of particular interest in connection with the scope of morphotropism in organic crystals. Interesting examples of homomorphism are provided also by the series benzoic acid–2-naphthoic acid (Sim, Robertson & Goodwin, 1955; Trotter, 1960) and acetanilide–*N*-2-naphthylacetamide (Brown & Corbridge, 1954; Haisa *et al.*, unpublished data).

Secondly, the mode of descent in symmetry by way of *z*-subgroups, *Pbca*–$P2_1/c$–$P\bar{1}$ seems to be a main line of heteromorphism of organic crystals. An excellent example is provided by the polymorphs of 5-ethyl-5-phenylbarbituric acid monohydrate (phenobarbitone) (Williams, 1973) as shown in Table 3.

Among these forms a variety of intermolecular hydrogen-bonding schemes are found and the density

(D_x) parallels with the symmetry. In such a manner the occurrence of polymorphs gives a clue in the search for the mode of descent in the symmetry of the crystal structures.

Further examples of atomic, group and homologous substitutions are illustrated for p-dihalobenzenes, p-disubstituted benzenes and aliphatic dicarboxylic acids in Tables 4, 5 and 6 respectively. The space groups given on the same line in the tables indicate the occurrence of polymorphism.

In Table 5 it should be noted that the type of molecular overlapping is oblique for the first two and is parallel for the others, indicating that the former undergoes a different descent from the latter (Haisa & Kashino, 1977). 4-Formylbenzoic acid is associated with this series by means of disordering (Haisa, Kashino, Ikejiri, Ohno & Teranishi, 1976).

The *Pbca*-related families

The interrelation between *Pbca* and the other related families can be derived by successive substitutions. For illustration, the pedigree of p-substituted acetanilides is shown in Table 7.

In this series *Pbca* is interrelated with $Pna2_1$ by way of $P2_1/c$. $Pna2_1$ is not a z-subgroup of *Pbca* but of *Pnma*. However, $P2_1/c$ is a common z-subgroup of *Pbca* and *Pnma*. Thus, the *Pbca* family is interrelated

Table 2. *Crystal features of linear polyphenyls, and linear and non-linear condensed aromatics*

	Space group	Z	Dihedral angle (°)	Intermolecular spacing (Å)
Linear polyphenyl				
Biphenyl	$P2_1/a$	2	69·1	
Terphenyl	$P2_1/a$	2	67·9	
Quaterphenyl	$P2_1/a$	2	64·1	
Linear condensed aromatics				
Naphthalene	$P2_1/a$	2	52·5	
Anthracene	$P2_1/a$	2	49·6	
Tetracene	$P\bar{1}$	2	50·9	
Pentacene	$P\bar{1}$	2	52·7	
Non-linear condensed aromatics				
Pyrene	$P2_1/a$	4	0	3·53
Perylene	$P2_1/a$	4	0	3·46
Coronene	$P2_1/a$	2	0	3·46
Ovalene	$P2_1/a$	2	0	3·45

Table 3. *Polymorphs of 5-ethyl-5-phenylbarbituric acid monohydrate*

Form	XIII	V	III	I	II
Space group	*Pbca*	$P2_1/c$	$P2_1/c$	$P2_1/n$	$P\bar{1}$
Z	8	8	4	12	6
Density (g cm^{-3})	1·384	1·362	1·360	1·352	1·354

Table 4. *Atomic substitution in p-dihalobenzenes, X—Ph—Y*

X	Y			
I	I	*Pbca*, $Z = 4$		
Br	Br	$P2_1/a$, $Z = 2$		
Br	Cl	$P2_1/a$, $Z = 2$		
Cl	Cl	$P2_1/a$, $Z = 2$	$P2_1/c$, $Z = 2$	$P\bar{1}$, $Z = 2$

with the *Pnma* family by way of their common z-subgroup.

Again, it is to be emphasized that p-amino- and p-hydroxyacetanilides belong to the same space group and Z as acetanilide. This indicates that the benzene rings of the former two acetanilides are arranged in the unit cells by the same symmetry operations as that of acetanilide, although the orientations of the rings in the crystals are altered by different hydrogen-bonding schemes (Haisa, Kashino, Matsuzaki, Kawai & Kunitomi, 1977).

Another example is provided by the series of o-nitrophenols, as shown in Table 8. In this series $P2_1na$ is not a z-subgroup but an isoclass (*klassengleich*, or k-) subgroup of $P2_1ca$ (Boyle & Lawrenson, 1972). It may be relevant to consider that $P2_12_12_1$ and $P2_1/c$ are z-subgroups of both *Pnma* and *Pbca* and that $P2_1na$ and $P2_1ca$ are z-subgroups of *Pnma* and *Pbca* respectively. Thus, the *Pnma* family is interrelated with the *Pbca* family.

In a similar manner the *Pbcn* and *Pbcm* families are also interrelated with the *Pbca* family. The representatives of these *Pbca*-related families are as follows.

Pnma: thiourea, chloroform, hexachloroethane, N-methylacetamide, aniline-m-sulfonic acid, 3,5-dibromo-p-aminobenzoic acid, p-toluidine, carbazole, fluorene, 4-nitropyridine N-oxide, 2-methyl-5-aminotetrazole.

Pbcn: pentane, tetraacetylethane, nitrosobenzene, benzalazine, *cis*-azobenzene, *trans*-1,4-diphenyl-butenyne, 3,3'-dibromobenzophenone, 2,2'-dichloro-benzidine, bis(7-methoxycoumarin), difluorenylidene (α form).

Pbcm: n-tricosane, 2,6-dinitrophenol, o-aminobenzoic acid (form II), m-azotoluene, o-nitro-diphenylamine, o-benztoluidine, 1,3,5,7-tetranitronaphthalene.

By the way, *Cmcm* is a z-supergroup of *Pnma* but not of *Pbca*. The *Cmcm* family has z-subgroups $C2/c$ and $C2/m$, and considerable numbers of organic crystals belong to $C2/c$. The molecular crystals belonging to the *Cmcm* group amount merely to methanol (β form), dimethyl sulfone and *trans*-bis(nitrosomethane).

In any event, it is evident that the *Pbca* family contains broad and widespread lines of descent in symmetry, and the related families hence comprise more than 80% of all the organic crystals.

Table 5. *Group substitution in p-disubstituted benzenes, X—Ph—Y*

1,4-Dimethoxybenzene	$Pbca, Z = 4$			
1,4-Diethoxybenzene		$P2_1, Z = 2$		
Dimethyl terephthalate	$Pbca, Z = 4$			
Diethyl terephthalate		$P2_1/n, Z = 2$		
4-Formylbenzoic acid		$P2_1/a, Z = 4$	$P\bar{1}, Z = 1$	
Terephthalic acid			$P\bar{1}, Z = 1$ $P\bar{1}, Z = 1$	
Terephthalimide			$P\bar{1}, Z = 1$	

Table 6. *Homologous substitution in aliphatic dicarboxylic acids*

Oxalic acid	$Pbca, Z = 4$ (α-form)	$P2_1/c, Z = 2$ (β form)	
Succinic acid		$P2_1/a, Z = 2$ (β form)	$P\bar{1}, Z = 2$ (α form)
Adipic acid		$P2_1/a, Z = 2$	
Suberic acid		$P2_1/a, Z = 2$	
Sebacic acid		$P2_1/c, Z = 2$	

Table 7. *The pedigree of p-substituted (p-X) acetanilides*

X			
H	$Pbca, Z = 8$		
OMe	$Pbca, Z = 8$		
NH$_2$	$Pbca, Z = 8$		
OH	$Pbca, Z = 8$		$P2_1/a, Z = 4$
Me		$Pna2_1, Z = 4$	$P2_1/c, Z = 4$
Cl		$Pna2_1, Z = 4$	
Br		$Pna2_1, Z = 4$	

The pedigree diagram

Examination of polymorphism among orthorhombic, monoclinic and triclinic crystals suggests the crystallographic pedigree of organic compounds as illustrated in Fig. 1, where only the most common groups are given for the sake of clarity with Schönflies and Hermann–Mauguin symbols and the relative abundance in parentheses, ( ) indicating less than 1%. Every symmetry-descending route shown by a solid line represents the group-theoretical transition from a space group into one of its maximal z-subgroups. A broken line connects the space groups between which actual polymorphs have been reported. As can be seen from the diagram the z-subgroup relation of the structures results in a hierarchical arrangement resembling a family tree.

The routes of the polymorphic transition can be classified into three types: homo-, hetero- and hypo- or hypersymmetric ones.

1. *Homosymmetric route.* The transition occurs sometimes within the same or equivalent space groups to the original one. For example, p-nitrophenol crystallizes in $P2_1/a$, $Z = 4$ (α form) from diethyl ether solution and in $P2_1/n$, $Z = 4$ (β form) from hot toluene

solution (Coppens & Schmidt, 1965). Both structures consist of chains of glide-related molecules linked by hydrogen bonds. The only difference is observed in the
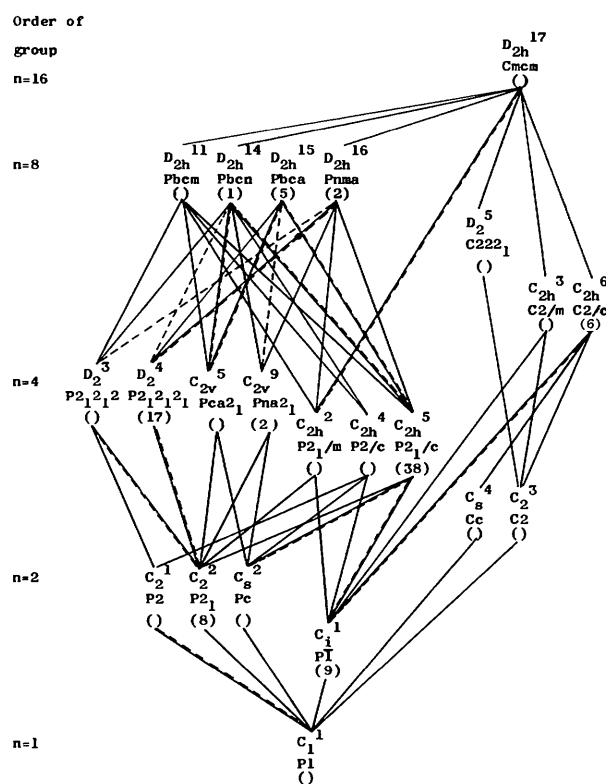

Fig. 1. The crystallographic pedigree of organic compounds. The most common space groups are arranged in decreasing order of the groups. Schönflies and Hermann–Mauguin symbols are accompanied by the relative abundances in parentheses, ( ) indicating less than 1%. A solid line connects the z-super-sub-groups and a broken line the groups between which polymorphs occur.

Table 8. *The pedigree of o-nitrophenols*

4-	6-				
Nitro	nitro	$P2_1ca, Z = 8$			
Nitro			$P2_12_12_1, Z = 4$		
	Nitro	$P2_1na, Z = 8$			
Nitro	chloro		$P2_12_12_1, Z = 4$		
Nitro	bromo			$P2_1/c, Z = 4$	
Chloro				$P2_1/a, Z = 4$	
Chloro	nitro				$P2_1, Z = 2$

triene, 1,8-diphenyl-1,3,5,7-octatetraene, 1,10-diphenyl-1,3,5,7,9-decapentaene, 1,5-naphthyridine dihydrate.

$P2_12_12_1–P2_1$: ($Z = 4$–4) oestrone, cholestane-3,5,6-triol, 9-phenyl-9-arsafluorene; ($Z = 4$–2) methyl β-L-arabinoside; ($Z = 8$–2) β-phenylglyceric acid.

$Bmab–P2_1/n$: ($Z = 4$–2) 1,3-diiodoethane, trans-1,3-diiodoethylene.

$Pcab–Pc2_1n$: ($Z = 8$–8) o-aminobenzoic acid.

$Pcab–P2_1$: ($Z = 4$–2) 1,2,5,6-dibenzanthracene.

$Pcan–P2_12_12_1$: ($Z = 12$–4) difluorenylidene.

inclination of O···C vectors to the benzene rings. Such a transition does not change the general structure, coordination and intermolecular linkage, but the details of the structure, such as orientation angle, intermolecular dihedral angle, and so on, vary.

2. *Heterosymmetric route.* Polymorphic transition occurs occasionally between groups in which a certain symmetry element is converted into another of the same order. For example, N-methylacetamide crystallizes in $Pnma$, $Z = 4$ at low temperature and in $Pnmm$, $Z = 2$ at high temperature (Katz & Post, 1960). $Pnma$ is a k-subgroup of $Pnmm$, with the ratio of the volume of the unit cell in the subgroup symmetry to that in the supergroup, $z = 2, 4, 8, 16$ or 32 (Boyle & Lawrenson, 1972). There is a phase transition near 10°C, above which the dimension of the a axis is halved since the a-glide plane degenerates into a mirror plane cutting the a axis in half. In this case the orientational disorder causes the transition. It may be considered that the transition occurs by way of the common z-subgroup $P2_1/m$, which is kept during the transition.

3. *Hypo- or hypersymmetric route.* This route is most common and illustrated explicitly in the diagram. The descent routes fall into three types in terms of the z-subgroup relation.

3.1. Polymorphs occur predominantly between space groups directly related by a z-subgroup relation. Some examples for this route are mentioned above, and further examples are as follows.

$P2_1/c–P\bar{1}$: ($Z = 4$–2) m-nitro-trans-cinnamic acid, m-chloro-trans-cinnamic acid, o-methoxy-cis-cinnamic acid, hexadecanamide; ($Z = 8$–4) 5-nitrobarbituric acid; ($Z = 6$–1) fumaric acid; ($Z = 2$–1) quinhydrone.

$Pbca–P2_1/c$: ($Z = 8$–4) sulfanilamide; ($Z = 4$–2) 1,4-diphenyl-1,3-butadiene, 1,6-diphenyl-1,3,5-hexa-

$Pnma–P2_12_12_1$: ($Z = 4$–4) D-mannitol.

$Pbcn–Pbc2_1$: ($Z = 8$–4) chalcone.

$Pbnb–P2_122_1$: ($Z = 4$–2) aniline hydrobromide.

$Pbnb–P2_1/a$: ($Z = 4$–4) aniline hydrobromide.

$Pmmn–P2_1/a$: ($Z = 8$–2) anthraquinone.

$Cmcm–P2_1/m$: ($Z = 4$–2) methanol.

$I2mm–I\bar{2}$: ($Z = 12$–12) 2-chloro-5-methylbenzo-quinone-4-oxime.

$C2/c–P\bar{1}$: ($Z = 8$–2) o-ethoxy-trans-cinnamic acid.

$P2/n–P\bar{1}$: ($Z = 4$–2) 5-formylvanillic acid.

$P2–P\bar{1}$: ($Z = 8$–4) 2,2'-dihydroxy-5,5'-dimethyldiphenylmethane.

3.2. There is an alternative route via the common z-supergroup shown in parentheses in the following examples.

$P2_12_12_1–(Pbca)–P2_1/c$: ($Z = 4$–4) acridine, 3,4-benzopyrene, monobromodurene, N-picryl-p-iodoaniline; ($Z = 4$–8) acridine.

$Pna2_1–(Pmna)–P2_1/c$: ($Z = 4$–4) p-methylacetanilide, 3-chloro-4-nitrophenol.

$Pbc2_1–(Pbca)–P2_1/c$: ($Z = 4$–4) glycylglycine.

$Pmn2_1–(Pmna)–P2_1/c$: ($Z = 2$–2) 1,4-dithiane 1,4-dioxide.

It could be a powerful tool in the elucidation of the very complex mechanism of polymorphic transition of organic crystals, which is yet to be solved, to investigate the physical significance of the promotion to the common supergroup. It may be presumable that the supergroup plays the role of the excited state in a chemical reaction.

3.3. Finally, we shall call attention to the fact that there are a few routes other than 3.1 and 3.2, as follows.

$Pmna–P2_12_12$: ($Z = 4$–4) D-mannitol.

$P2_12_12_1–I2/a$: ($Z = 4$–8) 1,8-dinitronaphthalene.

$P2_12_12_1–B2$: ($Z = 4$–4) 5'-bromo-5-deoxythymidine.

$P2_1nb–Aa$: ($Z = 4$–4) thiodipropionic acid.

$F222–P2_1/m$: ($Z = 16$–4) 1,2; 7,8-dibenzocarbazole.

$Fdd2–P2_1/n$: ($Z = 8$–2) cyclotetramethylenetetranitramine.

Conclusion

Organic crystals are classified on the basis of morphotropism into two main families, $Fm3m$ and $Pbca$,

whose prototypes are provided by methane and benzene respectively. The *Pbca* family is predominant. The isotranslational subgroup relation serves as the route of descent or ascent in symmetry of the crystal structures by chemical (atomic, group and homologous) substitutions, and constitutes the pedigree of organic crystals. Elucidation of the physical significance of the descent and ascent in symmetry will give a powerful clue to the better understanding of the mechanism of polymorphic transition and the systematization of organic molecular crystals.

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Debye–Waller Factors of CuBr by Powder Neutron Diffraction at 295 K

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Zinc blende structures are of interest because of their semiconducting properties. Lattice dynamical properties of copper halides which belong to this class of structures have recently been studied. A powder neutron diffraction study of the Debye–Waller factors of the cubic (zinc blende) γ phase of CuBr is reported here. The diffraction pattern was obtained on the high-resolution diffractometer PANDA installed at the PLUTO reactor, Harwell. A neutron wavelength of 1·524 Å was used in the experiment. The B factors determined were $B_{Cu} = 2·85 \pm 0·33$ and $B_{Br} = 2·71 \pm 0·33$ Å^2. A mean value $\bar{B} = \sum m_i B_i / \sum m_i = 2·77$ Å^2, $i = $ Cu, Br, gives the corresponding Debye temperature of 131 ± 8 K.

Introduction

Crystals of zinc blende structure have been the subject of investigations in recent years. One of the reasons for the interest is their semiconducting properties. Copper halides CuI, CuCl and CuBr belong to the above class

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of structures. Investigations on the crystal structure and the temperature-dependent phase transitions have been made on CuI (Miyake, Hoshino & Takenada, 1952) and on CuBr (Hoshino, 1952). Recent studies of the anharmonicity of atomic vibrations of these substances have been made by the method of neutron diffraction on single-crystal samples (Sakata, Hoshino & Harada, 1974; Hoshino, Fuji, Harada & Axe, 1975). Results of these experiments similar to that for fluorite