frequency range. The same method yielded the temperature coefficients of all wave velocities in a temperature range from -20 to 20°C. From these coefficients the thermoelastic constants $T_{ij} = d \log c_{ij}/\mathrm{d}T$ were derived. The values of thermal expansion necessary for correction of the thickness and density change of the crystals in that temperature interval were obtained with an optical dilatometer. The problem of sign ambiguity which occurs in evaluating the elastic constants c_{12}, c_{13}, and c_{23} was solved by some static measurements of Young's modulus and Poisson's ratio in some directions also employing the stability criteria which forbid negative values for s_{ii} and K.

All values are tabulated in Table 1. The probable errors are within the following limits:

c_{11}, c_{22}, c_{33}: 0·3%; other c_{ij}: 2%.
T_{11}, T_{22}, T_{33}: 3%; other T_{ij} except T_{55}: 10%
For T_{55} the error limit may be larger.

Table 1. *Elastic constants* c_{ij}, *thermoelastic constants* T_{ij} *and coefficients of thermal expansion* α_i *of* 1,3,5-*triphenylbenzene*

In brackets the values of Suresh Chandra & Hemkar (1973). Units: c_{ij} in 10^{11} erg cm^{-3}, T_{ij} in 10^{-3}/°C, α_i in 10^{-6}/°C. c_{ij} for 20°C; T_{ij} and α_i for 0°C.

c_{11}	c_{22}	c_{33}	c_{12}	c_{13}	c_{23}
0·720	1·353	1·433	0·430	0·421	0·468
(0·031)	(0·136)	(0·233)	(−0·178)	(0·092)	(0·080)
c_{44}	c_{55}	c_{66}	α_1	α_2	α_3
0·632	0·097	0·185	125	5	5
(0·502)	(0·034)	(0·369)			
T_{11}	T_{22}	T_{33}	T_{12}	T_{13}	T_{23}
−1·371	−1·504	−1·403	−1·37	−1·33	−2·65
T_{44}	T_{55}	T_{66}			
−1·08	−0·09	−0·75			

The large discrepancy between the older values published by Suresh Chandra & Hemka (see Table 1) and the values of this paper indicates that only some rough idea of the elastic anisotropy and the order of magnitude of the constants can be derived from thermal diffuse scattering of X-rays. In other cases the discrepancies were not of this magnitude. At the moment one cannot decide whether the experimental procedure of the authors was inadequate or whether the first-order approximation of X-ray scattering by phonons is insufficient. In molecular crystals, such as TPHB, a certain contribution to the background from thermal diffuse scattering by low-frequency internal molecular vibrations and librational movements should be expected. Still other perturbations may originate from stronger deviations of the ideal undisturbed lattice structure.

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Conditions for the diffraction enhancement of symmetry of types 1 and 2.

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A re-examination of the conditions for the diffraction enhancement of symmetry for the structures of types 1 and 2 [Iwasaki H. (1972). *Acta Cryst.* A**28**, 253–260] has brought out the existence of some additional solutions. The conditions for these types of structures have been systematically tabulated.

Diffraction enhancement of symmetry, which means the appearance of a higher Laue symmetry than normally expected, has been studied by several authors (Sadanaga & Takeda, 1968; Iwasaki, 1971, 1972; Marumo & Saito, 1972: Ohsumi, Okamura & Sadanaga, 1972). In particular, Iwasaki (1972) has classified the structures into four types, and systematically investigated, using a general expression for the square of the structure amplitude, the necessary conditions of enhancement for each type of structure. By a re-examination of these conditions, we have come across some additional solutions of the equation (12) as given by Iwasaki (1972) for the case of the Laue symmetry $2/m$, mmm, $4/m$ and $4/mmm$ of the structures of types 1 and 2, which are composed of substructures with the same space group.

For instance, the enhancement condition for monoclinic Laue symmetry $2/m$, unique axis c [equation (18) in Iwasaki (1972)], is given by

$$\cos 2\pi(hu_{pq} + kv_{pq} + lw_{pq}) = \cos 2\pi(hu_{pq} + kv_{pq} - lw_{pq}) \quad (1)$$

for any combination of p and q, where u_{pq}, v_{pq} and w_{pq} are the three components of the difference vector from the origin of the pth substructure to that of the qth substructure, and hkl are the indices of a reflexion. By taking the origin of the crystal coincident with that of an arbitrarily chosen substructure, the solution of equation (1) can be written in the form

$$(u_p, v_p) = (0,0) \quad \text{or} \quad (0,\tfrac{1}{2}) \quad \text{or} \quad (\tfrac{1}{2},0) \quad \text{or} \quad (\tfrac{1}{2},\tfrac{1}{2})$$

and

$$w_p \neq 0 \tag{2}$$

or

$$w_p = 0 \text{ or } \tfrac{1}{2},\ u_p \text{ and } v_p \text{ arbitrary,} \tag{3}$$

for any p, where u_p, v_p, w_p are the coordinates of the origin of the pth substructure. Therefore, if the substructures belong to the point group m and their relative locations satisfy one of the four sets of possible combinations of the relation (2), the diffraction symmetry of the entire structure becomes $2/m$, even though the structure has a true point-group symmetry 1 as a whole. Similarly, if the local point-group symmetry is 2 and the substructures are shifted perpendicular to the unique axis to the heights 0 or $\frac{1}{2}$, the point group of the crystal will be 1 and the diffraction symmetry becomes a higher one, $2/m$. The solutions with the value $\frac{1}{2}$ for u_p, v_p and w_p had not been given in the previous report by Iwasaki (1972). In the case of other enhancement (mmm, $4/m$ and $4/mmm$) also, the solutions with the value of $\frac{1}{2}$ should be added to those given before.

Table 1. *The necessary conditions for the diffraction enhancement in the case of types* 1 *and* 2

For simplicity, u_p, v_p and w_p are designated as u, v, w respectively.

Diffraction symmetry	Crystal symmetry (point group)		Enhancement condition	Symmetry of substructures
$2/m$ *c* axis unique	1		$00w$, $0\frac{1}{2}w$, $\frac{1}{2}0w$, $\frac{1}{2}\frac{1}{2}w$	m
			$uv0$, $uv\frac{1}{2}$	2
mmm	2	*a* axis unique	$u00$, $u0\frac{1}{2}$, $u\frac{1}{2}0$, $u\frac{1}{2}\frac{1}{2}$	
		b axis unique	$0v0$, $0v\frac{1}{2}$, $\frac{1}{2}v0$, $\frac{1}{2}v\frac{1}{2}$	222
		c axis unique	$00w$, $0\frac{1}{2}w$, $\frac{1}{2}0w$, $\frac{1}{2}\frac{1}{2}w$	
	m	*a* axis unique	$0v0$, $0v\frac{1}{2}$, $\frac{1}{2}v0$, $\frac{1}{2}v\frac{1}{2}$	$mm2$
			$00w$, $0\frac{1}{2}w$, $\frac{1}{2}0w$, $\frac{1}{2}\frac{1}{2}w$	$m2m$
		b axis unique	$u00$, $u0\frac{1}{2}$, $u\frac{1}{2}0$, $u\frac{1}{2}\frac{1}{2}$	$mm2$
			$00w$, $0\frac{1}{2}w$, $\frac{1}{2}0w$, $\frac{1}{2}\frac{1}{2}w$	$2mm$
		c axis unique	$u00$, $u0\frac{1}{2}$, $u\frac{1}{2}0$, $u\frac{1}{2}\frac{1}{2}$	$m2m$
			$0v0$, $0v\frac{1}{2}$, $\frac{1}{2}v0$, $\frac{1}{2}v\frac{1}{2}$	$2mm$
$4/m$	2		$00w$, $\frac{1}{2}\frac{1}{2}w$	$\bar{4}$
$4/mmm$	$mm2$		$00w$, $\frac{1}{2}\frac{1}{2}w$	$\bar{4}m2$, $\bar{4}2m$
	4		$00w$, $\frac{1}{2}\frac{1}{2}w$	422
$\bar{3}1m$	3		$00w$	312
$\bar{3}m1$	3		$00w$	321
$6/m$	3		$00w$	$\bar{6}$
$6/mmm$	$31m$		$00w$	$\bar{6}2m$
	$3m1$		$00w$	$\bar{6}m2$
	6		$00w$	622

Including these solutions, the enhancement conditions for types 1 and 2 are summarized in Table 1. It must be noticed that, in addition to those given in Table 1, another condition [equation (44) in Iwasaki (1972)] is also necessary for type 2. In all cases, the symmetry of the entire structure satisfying these conditions is lower than that of the substructures. However, if the local symmetry elements in any two arbitrarily chosen substructures, instead of substructures themselves, are combined to form a new set of symmetry elements, the corresponding space group will be isogonal with the point group identical with that of the substructures. When this relation exists between the symmetry of the substructures and their relative locations, the composite structure of types 1 or 2 shows the diffraction enhancement of symmetry.

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