maintaining covalent bond distances from the zinc atom. These approaches are aided by in-plane distortions about the same bonds C(5)–C(6) and C(10)–C(11) which make the mean value of the four internal angles of the type N(1) C(5)C(6) 9° smaller than the mean of the four external angles of the type C(4)C(5)C(6). Some distortion of this type is to be expected on account of the non-equivalence of the N–C and C–C bonds within the rings, and has been observed in the dipyridyl molecule (Merritt & Schroeder, 1956). Even with the distortions described, if N(1) and N(3) are to approach the zinc atom to within bonding distances, then N(2) must approach even closer. Hence the shortening of Zn–N(2), although statistically only possibly significant, is probably real.

Although 2,2′,2″-terpyridyl might exist as a *trans* form in isolation it is unlikely that it would coordinate as such because of the strong repulsions which would exist between the coordinated metal atom and the non-bonding C–H groups in the 2-positions. On the assumption then that it is functioning in the *cis* form, 2,2′,2″-terpyridyl will coordinate as a tridentate ligand, or not at all. The preference shown by zinc for tetrahedral coordination must therefore be sacrificed in the present situation and the coordination mode must rather be based on the arrangement of the three nitrogen atoms in the approximately planar ligand. The stoichiometry of the compound then favours 5-coordination with a trigonal bipyramidal arrangement a natural consequence.

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## Diamagnetic anisotropies of naphthalene tetrachloride and 1,3,5-triphenylbenzene molecules.

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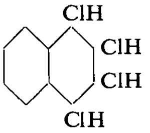
**Naphthalene tetrachloride,** $C_{10}H_8Cl_4$



The crystal structure has been determined and refined by Lasheen (1952, 1956).

$$a=7{\cdot}925,\ b=10{\cdot}25,\ c=14{\cdot}25\ \text{Å},$$
$$\beta=112{\cdot}6°;\ Z=4;\ I2/c.$$

The unsubstituted ring and the two neighbouring carbon atoms in the molecule are found to be closely planar.

Lasheen (1952) measured the crystal diamagnetic anisotropies and Lasheen & Heddewi (1966) the mean molecular susceptibility (all in $10^{-6}$ e.m.u./g) $\chi_1-\chi_2=56{\cdot}2$, $\chi_1-\chi_3=2{\cdot}6$, $\chi_3-\chi_2=53{\cdot}6$, $\bar{\chi}_M=-164{\cdot}55$ where $\chi_3$ is along [010] and $\psi$ (angle $\chi_1$: [001], positive in obtuse $\beta$)$=0{\cdot}5°$.

Hence $\chi_1=-144{\cdot}95$, $\chi_2=-201{\cdot}15$, $\chi_3=-147{\cdot}55$.

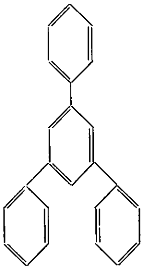
Lonsdale & Krishnan (1936) showed how to calculate molecular susceptibilities from crystal susceptibilities, given the molecular direction cosines, which in this case are:

| | | $a'$ | $b$ | $c$ |
|---|---|---|---|---|
| (length) | $L$ | 0 | 1 | 0 |
| (breadth) | $M$ | −0·1154 | 0 | 0·9933 |
| (normal) | $N$ | 0·9934 | 0·0026 | 0·1149 |

$a'$ is perpendicular to $c$ in (010). Hence the values given in Table 1.

Table 1 shows that the molecular anisotropy of naphthalene tetrachloride has almost the same value as that of a benzene ring with two hydrogen atoms substituted. Thus the cyclohexane ring has no or very small magnetic anisotropy and hence does not contribute to that of the whole molecule.

1.3.5-**Triphenylbenzene,** $C_{24}H_{18}$



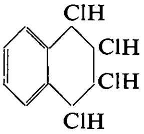
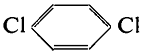
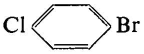
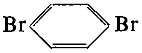
The crystal structure was determined by Farag (1954), who gave: $a=7{\cdot}47$, $b=19{\cdot}66$, $c=11{\cdot}19$ Å; $Z=4$; $Pna2_1$. The molecules, which form an approximately layer arrangement, are not planar, the substituted phenyl groups being twisted about the formal single bonds by (+34°, −27°, +24°)±2° respectively, out of the plane of the central ring. The benzene rings are planar to within ±0·08 Å.

The crystal diamagnetic anisotropies and susceptibilities were measured by Krishnan & Banerjee (1934) and later confirmed by Lonsdale (1937). The crystal susceptibilities are:

$$\chi_a=-313,\ \chi_b=-155,\ \chi_c=-140$$

(all in $10^{-6}$ e.m.u./g.).

Table 1. *Molecular susceptibilities of naphthalene tetrachloride compared with those of some p-substituted benzene molecules* (*Lasheen*, 1964) *all in* $10^{-6}$ *e.m.u./g.*

| Name and formula ($L \leftrightarrow$ and $M \updownarrow$ in each case) | | $K_L$ | $K_M$ | $K_N$ | $\Delta K$ |
|---|---|---|---|---|---|
| Naphthalene tetrachloride |  | −147·5 | −145·0 | −201·2 | 54·9 |
| *p*-Dichlorobenzene |  | −78·8 | −50·3 | −120·2 | 55·9 |
| *p*-Bromochlorobenzene |  | −87·6 | −59·9 | −129·0 | 55·2 |
| *p*-Dibromobenzene |  | −97·1 | −70·5 | −136·7 | 52·9 |

The direction cosines calculated from the atomic coordinates given by Farag (1954) are:

Central ring

| | *a* | *b* | *c* |
|---|---|---|---|
| *L* | 0·1730 | −0·0055 | −0·9847 |
| *M* | 0·1000 | −0·9949 | 0·0231 |
| *N* | 0·9789 | 0·1025 | 0·1768 |

First phenyl ring

| | *a* | *b* | *c* |
|---|---|---|---|
| *L* | 0·1374 | 0 | −0·9837 |
| *M* | 0·5218 | 0·8498 | 0·0729 |
| *N* | 0·8416 | −0·5269 | 0·1179 |

Second phenyl ring

| | *a* | *b* | *c* |
|---|---|---|---|
| *L* | 0·2085 | −0·0072 | 0·9780 |
| *M* | 0·3073 | 0·9498 | −0·0585 |
| *N* | 0·9311 | −0·3128 | −0·1875 |

Third phenyl ring

| | *a* | *b* | *c* |
|---|---|---|---|
| *L* | 0·1651 | 0·0754 | 0·9834 |
| *M* | 0·2994 | −0·9538 | 0·0229 |
| *N* | 0·9400 | 0·2908 | −0·1786 |

Thus the mean molecular susceptibilities and anisotropy for one benzene ring are:

$$K_L = -33{\cdot}7,\ K_M = -32{\cdot}5,\ K_N = -85{\cdot}9,$$
$$\Delta K = 52{\cdot}8 \text{ (all in } 10^{-6} \text{ e.m.u./g.).}$$

Comparing the value of the molecular anisotropy with that of the benzene molecule $\Delta K = 59{\cdot}7$ given by Hoarau, Joussot-Dubien, Lemanceau, Lumbroso & Pacault (1956), it is evident that the replacement of one hydrogen atom by a phenyl ring decreases the molecular anisotropy. Considering three replacements in the central benzene ring and one in each phenyl ring, it follows that the decrease in anisotropy due to each substitution is equal to 4·6. This gives the molecular anisotropy of the central ring as $\Delta K = 45{\cdot}9$ and that of any of the three phenyl rings as $\Delta K = 55{\cdot}1$.

It should be noted that the 1,3,5-triphenylbenzene molecule is non-planar and thus some approximation is involved with the consequence that the conclusions drawn are less rigorous.

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## A table of the real part of the dispersion correction for X-ray scattering.

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In a previous paper, one of us (Caticha-Ellis, 1962), described a method using the real part of the dispersion correction $\Delta f'$ in the X-ray atomic scattering factor for the solution of centrosymmetric crystal structures.

Until now, values of $\Delta f'$ have been available only for a few wavelengths. The table published by Dauben & Templeton (1955) includes the real and imaginary parts of the dispersion corrections for elements with $Z \geq 20$ for the wavelengths: Cr $K\alpha$, Cu $K\alpha$ and Mo $K\alpha$. A second table calculated by Templeton (1962), includes the effect of the diffraction angle $\theta$, for the same three wavelengths, for elements with $Z \geq 5$. Cooper (1963) performed similar cal-