Refinement

Refinement on *F*
$R = 0.0249$
$wR = 0.0246$
$S = 0.333$
1062 reflections
112 parameters
Only coordinates of H atoms refined
$w = 1/\sigma^2(F)$
$(\Delta/\sigma)_{max} = 0.005$
$\Delta\rho_{max} = 0.575$ e Å^{-3}
$\Delta\rho_{min} = -0.245$ e Å^{-3}
Extinction correction: Stout & Jensen (1968)
Extinction coefficient: 2.7496×10^{-6}
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$B_{eq} = (4/3)\Sigma_i\Sigma_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	B_{eq}
S	0.27908 (7)	1/2−x	0.61369 (9)	3.187 (5)
O	0.2124 (1)	1/2−x	0.4577 (3)	5.82 (3)
C(1)	0.2467 (2)	1/2−x	0.8895 (5)	4.45 (3)
C(2)	0.4266 (2)	0.2439 (2)	0.5827 (3)	4.48 (4)
Cl(1)	0	0	0	3.709 (9)
Cl(2)	0	1/2	0.9136 (1)	3.67 (1)
O(10)	0.0999 (1)	0.0129 (2)	0.1289 (3)	8.55 (4)
O(20)	0.0534 (3)	1/2−x	1.0922 (9)	10.38 (9)
O(21)	0.0403 (4)	1/2−x	0.712 (1)	11.7 (1)
O(22)	−0.0188 (3)	0.3794 (2)	0.9165 (6)	7.63 (9)

Table 2. *Selected geometric parameters* (Å, °)

Cl(1)—O(10)	1.402 (2)	S—O	1.439 (2)
Cl(2)—O(20)	1.385 (5)	S—C(1)	1.739 (3)
O(20)···O(21)	2.292 (8)	S—C(2)	1.742 (2)
O(20)···O(22)	2.314 (4)	O—C(1)	2.653 (3)
Cl(2)—O(21)	1.379 (5)	O—C(2)	2.646 (2)
Cl(2)—O(22)	1.417 (3)	C(1)···C(2)	2.786 (3)
O(21)···O(22)	2.249 (4)		
O(10)—Cl(1)—O(10)	113.0 (2)	O(21)—Cl(2)—O(22)	107.1 (2)
O(10)—Cl(1)—O(10)	107.7 (1)	O—S—C(1)	112.82 (9)
O(20)—Cl(2)—O(21)	112.1 (2)	O—S—C(2)	112.13 (9)
O(20)—Cl(2)—O(22)	111.3 (2)	C(1)—S—C(2)	106.34 (9)

Systematic absences, $0k0$ ($k = 2n$) and $h00$ ($h = 2n$), indicated space group $P\bar{4}2_1m$ (No. 113) or $P42_12$ (No. 90). Intensity data were corrected for decay and Lorentz–polarization effects. Direct methods (*MULTAN77*; Main, Lessinger, Woolfson, Germain & Declercq, 1977) were used for structure determination in $P\bar{4}2_1m$. H atoms were located by difference Fourier synthesis. Anisotropic full-matrix least-squares refinement was performed for non-H atoms, isotropic for H atoms. *SDP* (Enraf–Nonius, 1977) was used for all calculations on a VAX 730 computer.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: DU1067). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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2,4,6-Triphenylcyanobenzene and 2,4,6-Triphenylnitrobenzene

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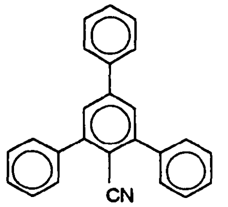
Abstract

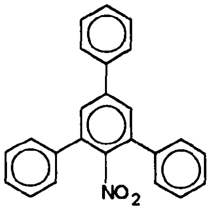
The structures of the title compounds, the cyano derivative $C_{25}H_{17}N$ (TPCB; 2,4,6-triphenylbenzonitrile) and the nitro derivative $C_{24}H_{17}NO_2$ (TPNB), have been determined. In the two symmetry independent molecules of TPNB the nitro group is twisted by almost the same amount, 64 and 65°.

Comment

In a continuation of our studies of sterically affected chemical species (Krygowski, Anulewicz, Daniluk & Drapala, 1990; Wozniak, Krygowski, Kariuki, Jones & Grech, 1990) we have investigated 2,4,6-triphenylcyanobenzene (TPCB) and 2,4,6-triphenylnitrobenzene (TPNB). These two derivatives of 1,3,5-triphenylbenzene (Farag, 1954; Shekata, 1959; Lin & Williams, 1975) are convenient examples to use for studying weak steric interactions between a central ring and a phenyl ring at the 4 position, and slightly stronger interactions between a central ring and phenyl substituents at positions 2 and 6 when additional interactions with the substituent at position 1 also take place.



TPCB



TPNB

Estimation of the aromaticity index HOMA (Krygowski, 1993; Krygowski & Kruszewski, 1972; Gdaniec, Turowska-Tyrk & Krygowski, 1989) for these geometries revealed that the rings in the three title molecules (two independent TPNB molecules) have HOMA < 0.943, indicating only a slight loss of aromatic character. Endocyclic bond angles do not differ significantly between respective positions. In all three molecules only the exocyclic angles C21—C2—C1 and C21—C2—C3 differ significantly. The values of Δ [φ(C21—C2—C1) − φ(C21—C2—C3), and similarly for other positions] are 4.2 and 3.0 for TPCB and 2.2, 2.7, 4.1 and 5.1 for TCNB. These values indicate relatively strong overcrowding in this region which can be attributed to the presence of NO_2 or CN substituents.

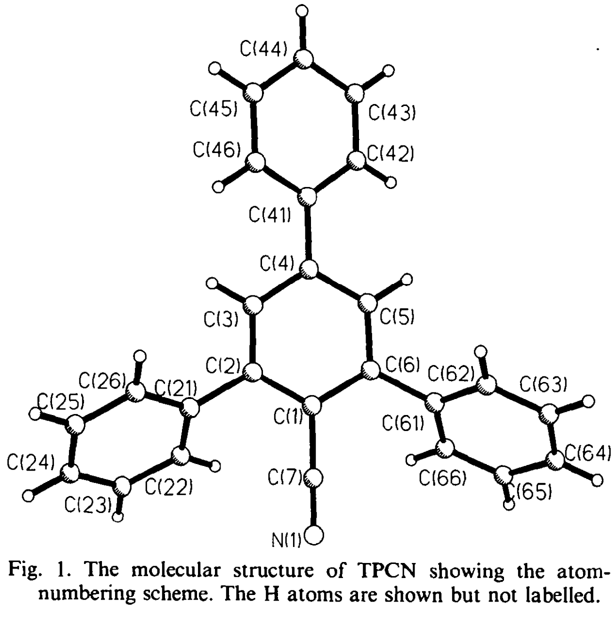


Fig. 1. The molecular structure of TPCN showing the atom-numbering scheme. The H atoms are shown but not labelled.

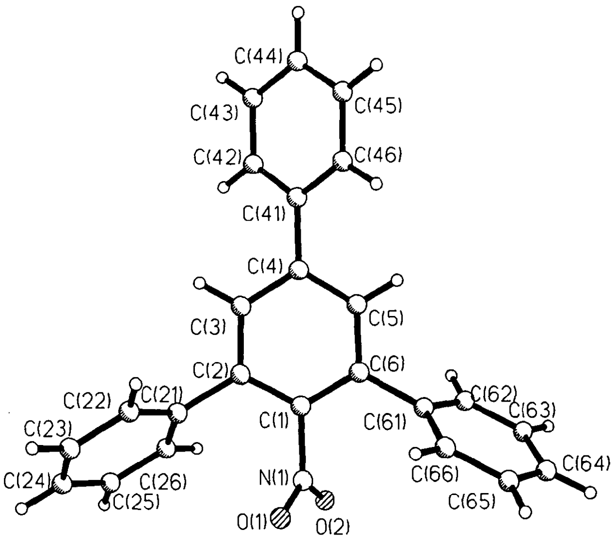


Fig. 2. The molecular structure of TPNB showing the atom-numbering scheme. The symmetry independent molecules (1) and (2) are distinguished in Table 2 by addition of 1 and 2, respectively, to the atomic labelling.

Experimental

TPCB

Crystal data

$C_{25}H_{17}N$
$M_r = 331.4$
Monoclinic
$P2_1/c$
$a = 4.096$ (2) Å
$b = 11.558$ (5) Å
$c = 37.250$ (15) Å
$\beta = 99.15$ (3)°
$V = 1741.1$ Å^3
$Z = 4$
$D_x = 1.264$ Mg m^{-3}

Cu $K\alpha$ radiation
$\lambda = 1.54178$ Å
Cell parameters from 25 reflections
$\theta = 13$–27°
$\mu = 0.524$ mm^{-1}
$T = 298$ K
Plate
0.30 × 0.25 × 0.1 mm
Pale yellow

Data collection

KM-4 Kuma Diffraction diffractometer
$\omega/2\theta$ scans
Absorption correction: none
2674 measured reflections
2491 independent reflections
2099 observed reflections [$F_o \geq 3\sigma(F_o)$]

$R_{\text{int}} = 0.0285$
$\theta_{\text{max}} = 60°$
$h = -4 \rightarrow 4$
$k = 0 \rightarrow 12$
$l = 0 \rightarrow 37$
3 standard reflections monitored every 100 reflections
intensity variation: 4.8%

Refinement

Refinement on F
$R = 0.0579$
$wR = 0.0577$
$S = 3.488$
2099 reflections
252 parameters
H atoms refined isotropically
$w = 1/[\sigma^2(F) + 0.0001F^2]$

$(\Delta/\sigma)_{\text{max}} = 0.22$
$\Delta\rho_{\text{max}} = 0.28$ e Å^{-3}
$\Delta\rho_{\text{min}} = -0.35$ e Å^{-3}
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

TPNB

Crystal data

$C_{24}H_{17}NO_2$
$M_r = 351.4$
Monoclinic
$P2_1/a$
$a = 10.011\ (5)$ Å
$b = 13.163\ (5)$ Å
$c = 28.896\ (8)$ Å
$\beta = 98.12\ (3)°$
$V = 3769.7$ Å^3
$Z = 8$
$D_x = 1.238$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 7.5–15°$
$\mu = 0.073$ mm^{-1}
$T = 298$ K
Plate
0.35 × 0.30 × 0.20 mm
Yellow

Data collection

Siemens $P3$ diffractometer
ω–2θ scans
Absorption correction: none
4022 measured reflections
3529 independent reflections
2723 observed reflections $[F_o \geq 3\sigma(F_o)]$
$R_{int} = 0.0184$

$\theta_{max} = 25°$
$h = -9 \rightarrow 9$
$k = 0 \rightarrow 12$
$l = 0 \rightarrow 27$
3 standard reflections monitored every 100 reflections intensity variation: 4.6%

Refinement

Refinement on F
$R = 0.0724$
$wR = 0.0566$
$S = 2.53$
2723 reflections
522 parameters
H atoms refined isotropically
$w = 2.1729/[\sigma^2(F) + 0.0001F^2]$

$(\Delta/\sigma)_{max} = 0.3$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.31$ e Å^{-3}
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
TPCB				
C1	0.1834 (7)	0.2142 (2)	0.3887 (1)	0.034 (1)
C2	0.1561 (7)	0.2915 (2)	0.4173 (1)	0.035 (1)
C3	0.0184 (7)	0.3995 (2)	0.4088 (1)	0.037 (1)
C4	−0.0941 (7)	0.4344 (2)	0.3730 (1)	0.035 (1)
C5	−0.0700 (7)	0.3541 (2)	0.3454 (1)	0.036 (1)
C6	0.0627 (7)	0.2447 (2)	0.3524 (1)	0.034 (1)
C7	0.3610 (8)	0.1071 (2)	0.3963 (1)	0.041 (1)
N1	0.5106 (7)	0.0243 (2)	0.4025 (1)	0.059 (1)
C21	0.2789 (7)	0.2624 (2)	0.4561 (1)	0.035 (1)
C22	0.1992 (8)	0.1579 (2)	0.4712 (1)	0.044 (1)
C23	0.3114 (8)	0.1346 (3)	0.5077 (1)	0.052 (1)
C24	0.5034 (9)	0.2136 (3)	0.5291 (1)	0.057 (1)
C25	0.5840 (9)	0.3174 (3)	0.5144 (1)	0.058 (1)
C26	0.4700 (8)	0.3418 (2)	0.4780 (1)	0.046 (1)
C41	−0.2249 (7)	0.5523 (2)	0.3648 (1)	0.035 (1)
C42	−0.4566 (7)	0.5753 (2)	0.3339 (1)	0.040 (1)
C43	−0.5703 (7)	0.6870 (2)	0.3262 (1)	0.046 (1)
C44	−0.4585 (8)	0.7773 (2)	0.3492 (1)	0.046 (1)
C45	−0.2296 (8)	0.7560 (2)	0.3798 (1)	0.047 (1)
C46	−0.1146 (7)	0.6446 (2)	0.3873 (1)	0.043 (1)
C61	0.0795 (7)	0.1648 (2)	0.3213 (1)	0.037 (1)
C62	0.2013 (7)	0.2059 (2)	0.2906 (1)	0.046 (1)
C63	0.2077 (8)	0.1334 (3)	0.2610 (1)	0.059 (1)
C64	0.0993 (9)	0.0205 (3)	0.2620 (1)	0.062 (1)
C65	−0.0226 (8)	−0.0203 (2)	0.2920 (1)	0.054 (1)
C66	−0.0270 (7)	0.0516 (2)	0.3219 (1)	0.044 (1)
TPNB molecule (1)				
N11	0.6313 (5)	−0.2021 (4)	0.3228 (2)	0.058 (2)
O11	0.6781 (4)	−0.1643 (3)	0.2900 (2)	0.080 (1)
O21	0.5394 (4)	−0.1661 (3)	0.3406 (1)	0.092 (1)
C11	0.6909 (5)	−0.2987 (4)	0.3420 (2)	0.044 (2)
C21	0.6773 (5)	−0.3851 (4)	0.3137 (2)	0.045 (2)
C31	0.7343 (5)	−0.4739 (4)	0.3331 (2)	0.050 (2)
C41	0.8002 (5)	−0.4780 (4)	0.3787 (2)	0.044 (2)
C51	0.8106 (5)	−0.3895 (4)	0.4054 (2)	0.047 (2)
C61	0.7570 (5)	−0.2990 (4)	0.3874 (2)	0.044 (2)
C211	0.6072 (6)	−0.3821 (4)	0.2645 (2)	0.047 (2)
C221	0.6770 (6)	−0.4047 (4)	0.2280 (2)	0.065 (2)
C231	0.6116 (8)	−0.4017 (4)	0.1826 (2)	0.078 (2)
C241	0.4777 (8)	−0.3774 (4)	0.1736 (2)	0.069 (2)
C251	0.4077 (7)	−0.3554 (4)	0.2096 (2)	0.072 (2)
C261	0.4724 (7)	−0.3579 (4)	0.2555 (2)	0.070 (2)
C411	0.8614 (6)	−0.5743 (4)	0.3980 (2)	0.046 (2)
C421	0.7982 (6)	−0.6670 (4)	0.3889 (2)	0.054 (2)
C431	0.8562 (7)	−0.7562 (5)	0.4074 (2)	0.066 (2)
C441	0.9774 (7)	−0.7530 (5)	0.4363 (2)	0.070 (2)
C451	1.0411 (7)	−0.6618 (5)	0.4457 (2)	0.070 (2)
C461	0.9852 (6)	−0.5726 (4)	0.4267 (2)	0.053 (2)
C611	0.7802 (6)	−0.2039 (4)	0.4157 (2)	0.052 (2)
C621	0.7228 (6)	−0.1904 (5)	0.4561 (2)	0.061 (2)
C631	0.7509 (7)	−0.1033 (6)	0.4826 (2)	0.078 (2)
C641	0.8373 (7)	−0.0309 (5)	0.4694 (3)	0.080 (2)
C651	0.8945 (7)	−0.0434 (5)	0.4293 (3)	0.088 (2)
C661	0.8664 (7)	−0.1310 (5)	0.4026 (2)	0.075 (2)
TPNB molecule (2)				
N12	0.4371 (5)	0.2410 (3)	0.0623 (2)	0.047 (1)
O12	0.5538 (4)	0.2114 (3)	0.0659 (1)	0.072 (1)
O22	0.3684 (4)	0.2620 (3)	0.0255 (1)	0.062 (1)
C12	0.3753 (5)	0.2533 (4)	0.1055 (1)	0.037 (2)
C22	0.3569 (5)	0.1686 (4)	0.1325 (2)	0.040 (2)
C32	0.2945 (5)	0.1844 (4)	0.1720 (2)	0.045 (2)
C42	0.2542 (5)	0.2810 (4)	0.1846 (2)	0.043 (2)
C52	0.2783 (5)	0.3635 (4)	0.1567 (2)	0.041 (2)
C62	0.3393 (5)	0.3518 (4)	0.1166 (2)	0.038 (1)
C212	0.3928 (5)	0.0622 (4)	0.1205 (2)	0.042 (2)
C222	0.4567 (5)	0.0010 (4)	0.1561 (2)	0.050 (2)
C232	0.4871 (6)	−0.1002 (4)	0.1471 (2)	0.064 (2)
C242	0.4510 (6)	−0.1388 (4)	0.1024 (3)	0.071 (2)
C252	0.3858 (6)	−0.0784 (5)	0.0670 (2)	0.067 (2)
C262	0.3571 (5)	0.0218 (4)	0.0763 (2)	0.050 (2)
C412	0.1856 (5)	0.2951 (4)	0.2263 (2)	0.045 (2)
C422	0.1024 (5)	0.2197 (5)	0.2407 (2)	0.057 (2)
C432	0.0376 (6)	0.2337 (6)	0.2798 (2)	0.072 (2)
C432	0.0565 (7)	0.3225 (6)	0.3049 (2)	0.084 (2)
C452	0.1388 (7)	0.3987 (5)	0.2918 (2)	0.083 (2)
C462	0.2032 (6)	0.3840 (4)	0.2525 (2)	0.064 (2)
C612	0.3584 (6)	0.4425 (3)	0.0875 (2)	0.035 (1)
C622	0.4834 (5)	0.4690 (4)	0.0758 (2)	0.042 (2)
C632	0.4975 (6)	0.5581 (4)	0.0502 (2)	0.049 (2)
C642	0.3868 (7)	0.6184 (4)	0.0368 (2)	0.050 (2)
C652	0.2624 (6)	0.5922 (4)	0.0486 (2)	0.049 (2)
C662	0.2474 (6)	0.5040 (4)	0.0740 (2)	0.047 (2)

Table 2. *Selected geometric parameters* (Å, °)

	TPCB	TPNB	
		Molecule (1)	Molecule (2)
C1—C7	1.441 (4)		
C7—N1	1.140 (4)		
C1—N1		1.479 (7)	1.478 (7)
N1—O1		1.221 (8)	1.222 (6)
N1—O2		1.212 (8)	1.214 (6)
C1—C2	1.408 (5)	1.396 (8)	1.388 (7)
C1—C6	1.409 (5)	1.383 (8)	1.395 (7)
C2—C3	1.386 (3)	1.384 (7)	1.392 (8)
C2—C21	1.491 (5)	1.495 (8)	1.499 (8)
C3—C4	1.399 (5)	1.389 (8)	1.398 (8)
C4—C5	1.400 (5)	1.393 (8)	1.394 (8)
C4—C41	1.478 (3)	1.482 (7)	1.480 (8)
C5—C6	1.385 (3)	1.378 (7)	1.392 (8)
C6—C61	1.492 (5)	1.495 (8)	1.488 (7)

C2—C1—C7	119.7 (3)		
C6—C1—C7	119.5 (3)		
C1—C7—N1	177.8 (3)		
N1—C1—C2		118.7 (5)	119.4 (4)
N1—C1—C6		118.2 (5)	116.6 (4)
O1—N1—C1		117.6 (5)	118.2 (4)
O2—N1—C1		117.9 (5)	117.5 (4)
O1—N1—O2		124.6 (5)	124.3 (5)
C2—C1—C6	120.6 (3)	123.2 (5)	123.9 (5)
C1—C2—C3	118.5 (3)	116.8 (5)	116.8 (5)
C1—C2—C21	122.3 (3)	122.0 (5)	124.4 (5)
C3—C2—C21	119.1 (3)	121.3 (5)	118.7 (5)
C2—C3—C4	122.5 (3)	122.0 (5)	121.9 (5)
C3—C4—C5	117.2 (3)	118.8 (5)	118.6 (5)
C3—C4—C41	121.1 (3)	120.4 (5)	120.7 (5)
C5—C4—C41	121.7 (3)	120.8 (5)	120.7 (5)
C4—C5—C6	122.6 (3)	121.3 (5)	121.8 (5)
C1—C6—C5	118.5 (3)	118.0 (5)	116.9 (5)
C1—C6—C61	122.6 (3)	122.2 (5)	123.9 (5)
C5—C6—C61	119.0 (3)	119.7 (5)	119.2 (5)
C1—C2—C21—C22	−49.1 (4)	117.7 (6)	137.0 (6)
C1—C2—C21—C26	132.5 (3)	−63.1 (8)	−47.1 (8)
C3—C2—C21—C22	132.8 (3)	−61.1 (8)	−46.5 (7)
C3—C2—C21—C26	−45.6 (3)	118.2 (6)	129.4 (6)
C3—C4—C41—C42	−152.7 (3)	−40.4 (8)	−31.5 (8)
C3—C4—C41—C46	28.9 (4)	140.5 (6)	148.0 (5)
C5—C4—C41—C42	28.9 (3)	141.3 (6)	147.6 (6)
C5—C4—C41—C46	−149.6 (3)	−37.8 (8)	−32.9 (8)
C1—C6—C61—C62	−131.6 (3)	116.6 (6)	−56.3 (8)
C1—C6—C61—C66	49.3 (4)	−67.1 (8)	126.9 (6)
C5—C6—C61—C62	46.9 (3)	−68.0 (8)	125.8 (6)
C5—C6—C61—C66	−132.1 (3)	108.3 (7)	−51.0 (7)

For both compounds, the data were corrected for Lorentz and polarization effects but not for absorption. The structures were solved by direct methods. Full-matrix least-squares refinement minimizing $\Sigma w(|F_o|-|F_c|)^2$ was employed. Non-H atoms were refined anisotropically and all H atoms were placed in calculated positions and refined with isotropic displacement parameters. Calculations were carried out using the *SHELX*76 and *SHELXS*86 programs (Sheldrick, 1976, 1990). The final geometry calculations were performed with the *CSU* program (Vickovic, 1988).

We thank Professor T. M. Krygowski for helpful discussions.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: KA1051). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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5,6-Dihydro-5,6-diphenyl-1,3-dithiolo[4,5-*b*]-[1,4]dithiine-2-thione (DHPT-DTT), $C_{17}H_{12}S_5$

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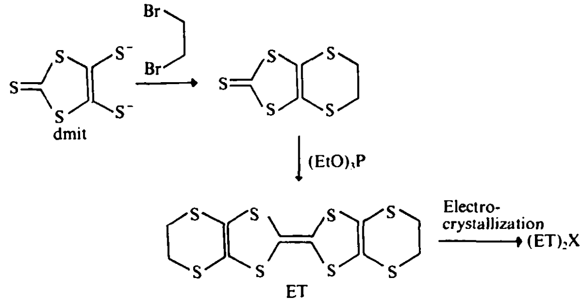
Abstract

The DHPT-DTT molecule contains a conjugated 4,5-dimercapto-1,3-dithiole-2-thione plane and two phenyl planes, all of which are approximately perpendicular to one another. The crystal packing is stabilized by an S···S interaction between pairs of neighbouring molecules, which may account for the rather high thermal stability of the crystal.

Comment

The ring closure of 4,5-dimercapto-1,3-dithiole-2-thione (dmit) with a dihalohydrocarbon to produce a suitable π-donor precursor is the first step of a three-stage procedure for the preparation of dmit-based organic electric conductors, such as the well known $(ET)_2X$ type of charge-transfer salts, where X^- is a charge-compensating monovalent anion (Williams *et al.*, 1987; Bryce, 1991).



During attempts to prepare new organic superconductors, many smaller precursors of dmit-based π donors have been synthesized, some of which rep-