tropic thermal parameters while the other atoms were refined anisotropically by block-diagonal least-squares calculations using counting-statistics weights. The scattering factors from Cromer & Waber (1974) were used. The final residuals are $R_F = 6.6\%$ and $wR_F = 4.4\%$. The atomic positional parameters are listed in Table 1.* All the calculations were performed using the NRC system of programs for the PDP8-E computer (Larson & Gabe, 1978).

Discussion. The molecule (Fig. 1) extends along z while the two parts of the dimer are related by the twofold axis parallel to y and passing through the middle of the N=N bond at $x = z = \frac{1}{4}$. The interatomic distances and angles except those involving H atoms are shown in Fig. 2. The high thermal motion observed at the C(81) and C(82) positions probably indicates some degree of disorder at these positions. Consequently the H atoms bonded to C(8), C(81) and C(82) are not considered to be located with certainty. Their refined positions are

nevertheless given in Table 1. The average C—H distance is 1.05 Å.

The 76.2° angle between the planes of the benzene rings is such that little interference occurs between the isopropyl groups on C(2) and C(6) and their equivalents on the symmetry-related part of the dimer. Consequently, contrary to what is observed in the hexa-*tert*-butyl derivative, the C(1) and N atoms lie approximately in the plane defined by the C(2), C(3), C(4), C(5) and C(6) atoms.

The torsion angle between the N—C(1) and N'—C(1') bonds is 174.3°. A comparative study of the geometry of hindered azobenzenes will be reported separately.

References

CROMER, D. T. & WABER, J. T. (1974). *International Tables for X-ray Crystallography*, Vol. IV, p. 99. Birmingham: Kynoch Press.
GERMAIN, G., MAIN, P. & WOOLFSON, M. M. (1971). *Acta Cryst.* A27, 368–376.
GRANT, D. F. & GABE, E. J. (1978). *J. Appl. Cryst.* 11, 114–120.
LARSON, A. C. & GABE, E. J. (1978). *Computing in Crystallography*, edited by H. SCHENK, R. OLTHOF-HAZEKAMP, H. VAN KONINGSVELD & G. C. BASSI, p. 81. Delft Univ. Press.
LE PAGE, Y., GABE, E. J., WANG, Y., BARCLAY, L. R. C. & HOLM, H. L. (1980). *Acta Cryst.* B36, 2846–2848.

2,2',4,4',6,6'-Hexamethylazobenzene*†

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Abstract. $C_{18}H_{22}N_2$, monoclinic, $P2_1/c$, $a = 4.870$ (2), $b = 10.017$ (2), $c = 16.431$ (4) Å, $\beta = 108.05$ (2)° at room temperature, giving $Z = 2$ and $D_c = 1.16$ Mg m^{-3}. The molecule is planar, utilizes a symmetry center and is relatively undistorted. The final R_F value is 3.8% for 708 observed data.

Introduction. The structures of a series of hindered azobenzenes have been determined (Le Page, Gabe, Barclay & Dust, 1981). The diffraction intensities of a crystal, 0.3 × 0.3 × 0.3 mm, of the title compound were measured with graphite-monochromatized Cu $K\alpha$ radiation using profile analysis (Grant & Gabe, 1978) with the $\theta/2\theta$ scan technique. Three unique sets of 776 reflections for $2\theta \leq 100°$ were collected and averaged to give 708 with significant and 68 with insignificant

Table 1. *Atomic parameters x,y,z and B_{iso}*

E.s.d.'s refer to the last digit printed. B_{iso} is the arithmetic mean of the principal axes of the thermal ellipsoid.

|	x	y	z	B_{iso} (Å²)
N	0·0033 (4)	0·48984 (18)	0·46379 (9)	4·94 (8)
C(1)	0·1882 (4)	0·38338 (19)	0·45303 (12)	4·02 (9)
C(2)	0·1717 (4)	0·36410 (20)	0·36685 (12)	4·37 (9)
C(3)	0·3429 (4)	0·26660 (20)	0·34675 (12)	4·80 (10)
C(4)	0·5283 (4)	0·18765 (20)	0·40850 (13)	4·78 (10)
C(5)	0·5404 (4)	0·20722 (20)	0·49338 (13)	4·73 (10)
C(6)	0·3739 (4)	0·30327 (19)	0·51738 (12)	4·29 (9)
C(7)	−0·0315 (5)	0·44416 (23)	0·29567 (12)	5·95 (11)
C(8)	0·7135 (5)	0·08242 (23)	0·38466 (15)	6·52 (12)
C(9)	0·4009 (5)	0·31353 (23)	0·61111 (12)	5·94 (12)
H(31)	0·330 (3)	0·2548 (15)	0·2809 (9)	5·8 (4)
H(51)	0·689 (3)	0·1443 (17)	0·5410 (10)	6·5 (5)
H(71)	−0·001 (4)	0·4174 (19)	0·2374 (12)	9·3 (6)
H(72)	0·013 (5)	0·5458 (20)	0·3067 (12)	11·2 (7)
H(73)	−0·227 (4)	0·4402 (19)	0·2949 (11)	9·5 (6)
H(81)	0·734 (6)	0·001 (3)	0·4143 (15)	15·0 (9)
H(82)	0·907 (6)	0·095 (3)	0·4074 (16)	16·4 (9)
H(83)	0·684 (6)	0·085 (3)	0·3231 (16)	15·4 (9)
H(91)	0·553 (4)	0·2456 (18)	0·6447 (10)	8·2 (5)
H(92)	0·461 (4)	0·4083 (18)	0·6353 (11)	7·8 (5)
H(93)	0·217 (4)	0·2992 (18)	0·6235 (11)	9·0 (6)
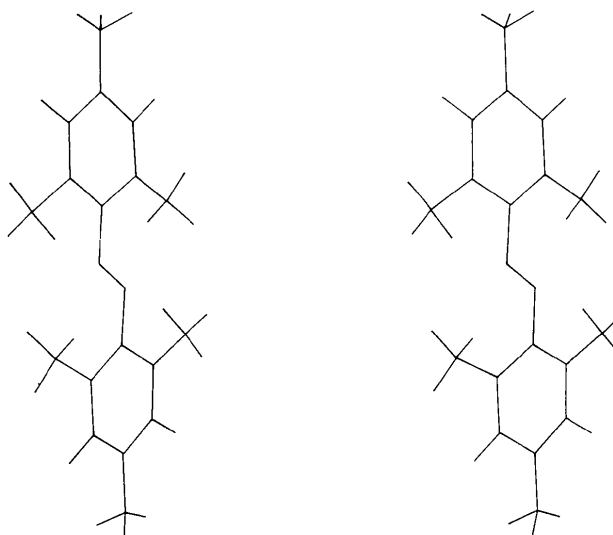
Fig. 1. Stereoscopic view of the skeleton of the molecule.

net counts at the $2\sigma(I)$ level. Only 5 out of the 63 measurements of the systematic absences satisfied the observation criterion. The intensity agreement of the equivalent measurements with the mean was 4·8%. No absorption correction was applied ($\mu = 0.529$ mm^{-1}). The structure was solved by a routine application of *MULTAN* (Germain, Main & Woolfson, 1971) to the 128 largest E values. The resulting map revealed all the non-hydrogen atoms. Successive isotropic and anisotropic refinement reduced R_F to 10·4% at which point all H atoms were located from a difference map. The final refinement cycle gave $R_F = 3.8\%$ and $wR_F = 3.2\%$. Counting-statistics weights were used throughout. The atomic positional parameters are listed in Table 1.* The calculations were performed using the NRC system of programs (Larson & Gabe, 1978).

Discussion. The molecule (Fig. 1) is planar and a symmetry center relates its two chemically equivalent parts. The distances and angles (Fig. 2) show that the molecule is relatively undistorted. The only remarkable distortions are the C(6)—C(1)—N and C(2)—C(1)—N angles, respectively 127·5 and 112·5°. The center of symmetry requires the benzene rings to be parallel and the C(1)—N—N'—C(1') torsion angle to be 180°.

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* The tables of anisotropic thermal parameters and the final observed and calculated structure factors have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 35857 (7 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.
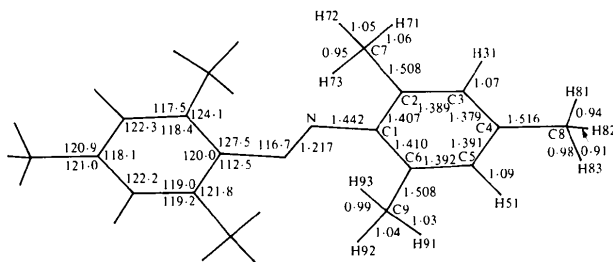

Fig. 2. Distances (Å) and angles (°) for the non-hydrogen atoms. The e.s.d.'s are 0·003 Å on all the distances and 0·2° on all the angles shown. The C—H bond lengths range from 0·91 (3) to 1·05 (2) Å. The molecule utilizes a symmetry center in the middle of the N—N' bond,

A comparative study of the geometry of the hindered azobenzenes will be reported separately.

References

GERMAIN, G., MAIN, P. & WOOLFSON, M. M. (1971). *Acta Cryst.* A27, 368–376.

GRANT, D. F. & GABE, E. J. (1978). *J. Appl. Cryst.* 11, 114–120.

LARSON, A. C. & GABE, E. J. (1978). *Computing in Crystallography*, edited by H. SCHENK, R. OLTHOF-HAZEKAMP, H. VAN KONINGSVELD & G. C. BASSI, p. 81. Delft Univ. Press.

LE PAGE, Y., GABE, E. J., BARCLAY, L. R. C. & DUST, J. M. (1981). *Acta Cryst.* B37, 976–978.