108.8 (1)°]. The bond length P(1)—O(1) = 1.482 (3) Å [1.487 (2) Å], and the P—C bond lengths are P(1)—C(11) = 1.799 (3), P(1)—C(21) = 1.798 (3) and P(1)—C(31) = 1.799 (4) Å [1.796 (2), 1.797 (3), 1.806 (3) Å].

Both the O atom [O(1*s*), which lies on a twofold axis] and the H atom [H(1*s*)] of the solvent water molecule were found and their positions were refined. The distances O(1*s*)—H(1*s*) and O(1*s*)—H(1*sa*) are each 0.846 (50) Å. In the hydrogen bond O(1)···O(1*s*) = 2.810 (4) [2.856 (3)], O(1)···H(1*s*) = 2.05 (6) Å and P(1)—O(1)···H(1*s*) = 145.3 (1.5)°. The position and bond lengths involving the H atoms of the solvent molecule were not reported in the previous structural study of P=O(phenyl)$_3\cdot\frac{1}{2}H_2O$.

Other related structures include $(o\text{-}CH_3C_6H_4)_3PO$ (Cameron & Dahlen, 1975) and $(m\text{-}CH_3C_6H_4)_3PO\cdot H_2NSO_2(p\text{-}CH_3C_6H_4)$ (Ferguson, Lough & Glidewell, 1989).

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Low-Temperature Structures of *cis*-4-*tert*-Butylcyclohexyl *p*-Nitrobenzoate (1) and *trans*-4-*tert*-Butylcyclohexyl *p*-Nitrobenzoate (2)

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Abstract. *cis*- and *trans*-4-*tert*-Butylcyclohexyl *p*-nitrobenzoate, $C_{17}H_{23}NO_4$, $M_r = 305.4$. (1) *cis* isomer, triclinic, $P\bar{1}$, $a = 6.3555$ (7), $b = 11.615$ (4), $c = 12.365$ (4) Å, $\alpha = 111.44$ (3), $\beta = 100.06$ (2), $\gamma = 96.38$ (2)°, $V = 821.16$ Å^3, $Z = 2$, $D_x = 1.23$ Mg m^{-3}, λ(Cu $K\alpha$) = 1.5418 Å, $\mu = 0.66$ mm^{-1}, $F(000) = 328$, $T = 130$ (2) K, $R = 0.033$ for 2237 unique observed reflections. (2) *trans* isomer, triclinic, $P\bar{1}$, $a = 5.9963$ (7), $b = 15.511$ (4), $c = 17.244$ (4) Å, $\alpha = 83.15$ (2), $\beta = 89.73$ (1), $\gamma = 87.94$ (2)°, $V = 1591.4$ Å^3, $Z = 4$, $D_x = 1.27$ Mg m^{-3}, λ(Cu $K\alpha$) = 1.5418 Å, $\mu = 0.64$ mm^{-1}, $F(000) = 656$, $T = 130$ (2) K, $R = 0.032$ for 4504 unique observed reflections. Structure (2) consists of two independent molecules in the asymmetric unit, which have essentially identical conformations. In both structures the ester function adopts the preferred *Z* configuration. The axial C—OPNB (PNB = *p*-nitrobenzoate) bond length in (1) is 1.473 (2) Å, which is slightly longer than the two equatorial C—OPNB bond lengths observed in (2) [C(1)—O(1) and C(1′)—O(1′) for the two molecules are 1.463 (2) and 1.468 (2) Å, respectively].

Experimental. A Philips PW1100/20 diffractometer with graphite monochromator was used for data collection. Crystal temperatures were maintained at 130 (2) K with a Leybold–Heraeus nitrogen cooling device. Lattice parameters were determined from least-squares analysis of the setting angles of 25 reflections with $50 < 2\theta < 60°$. Three check reflections measured every 120 min during data collection for (1) and (2) showed no significant decrease in intensity. Structure solution was by direct methods (*SHELXS*86, Sheldrick, 1985), ΔF synthesis and full-matrix least-squares refinement. Non-H atoms were refined with anisotropic displacement factors. H atoms were refined with isotropic thermal parameters. Weighting scheme $w = [\sigma^2(F) + (0.0005)F^2]^{-1}$.

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Table 1. *Non-*H *atomic coordinates and equivalent isotropic thermal parameters* (Å^2) *for cis-4-tert-butylcyclohexyl p-nitrobenzoate* (1)

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

	x	y	z	U_{eq}
O(1)	0.2919 (1)	0.82548 (8)	0.15174 (8)	0.0217 (4)
O(2)	0.5075 (2)	0.68832 (9)	0.07984 (9)	0.0295 (4)
O(3)	−0.2131 (2)	0.23793 (9)	0.14469 (9)	0.0302 (4)
O(4)	−0.3800 (2)	0.3832 (1)	0.2368 (1)	0.0415 (5)
N(1)	−0.2355 (2)	0.3479 (1)	0.1857 (1)	0.0250 (5)
C(1)	0.4328 (2)	0.9271 (1)	0.1391 (1)	0.0217 (5)
C(2)	0.2866 (2)	1.0156 (1)	0.1197 (1)	0.0235 (5)
C(3)	0.2019 (2)	1.0836 (1)	0.2304 (1)	0.0217 (5)
C(4)	0.3898 (2)	1.1547 (1)	0.3411 (1)	0.0207 (5)
C(5)	0.5243 (2)	1.0595 (1)	0.3609 (1)	0.0229 (5)
C(6)	0.6125 (2)	0.9917 (1)	0.2518 (1)	0.0239 (5)
C(7)	0.3183 (2)	1.2374 (1)	0.4538 (1)	0.0252 (5)
C(8)	0.1807 (3)	1.3276 (2)	0.4246 (2)	0.0399 (7)
C(9)	0.1844 (3)	1.1581 (2)	0.5019 (2)	0.0336 (6)
C(10)	0.5217 (3)	0.3173 (2)	0.5508 (2)	0.0445 (7)
C(11)	0.3504 (2)	0.7134 (1)	0.1207 (1)	0.0205 (5)
C(12)	0.1973 (2)	0.6200 (1)	0.1411 (1)	0.0194 (5)
C(13)	0.0164 (2)	0.6529 (1)	0.1867 (1)	0.0219 (5)
C(14)	−0.1239 (2)	0.5641 (1)	0.2028 (1)	0.0232 (5)
C(15)	−0.0807 (2)	0.4436 (1)	0.1725 (1)	0.0212 (5)
C(16)	0.0974 (2)	0.4082 (1)	0.1276 (1)	0.0230 (5)
C(17)	0.2371 (2)	0.4984 (1)	0.1122 (1)	0.0219 (5)

Table 2. *Non-*H *atomic coordinates and equivalent isotropic thermal parameters* (Å^2) *for trans-4-tert-butylcyclohexyl p-nitrobenzoate* (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}
Molecule *A*				
O(1)	0.3528 (2)	0.32298 (6)	0.37789 (5)	0.0223 (5)
O(2)	0.0692 (2)	0.38145 (6)	0.44266 (6)	0.0257 (6)
O(3)	0.6691 (2)	0.75577 (6)	0.42433 (6)	0.0316 (6)
O(4)	0.9262 (2)	0.69736 (7)	0.35637 (6)	0.0324 (6)
N(1)	0.7463 (2)	0.69582 (7)	0.39084 (6)	0.0234 (7)
C(1)	0.2590 (2)	0.23664 (8)	0.39074 (8)	0.0200 (7)
C(2)	0.4574 (2)	0.17312 (9)	0.39353 (8)	0.0233 (8)
C(3)	0.3805 (2)	0.07955 (9)	0.40144 (8)	0.232 (8)
C(4)	0.2228 (2)	0.06411 (8)	0.33486 (7)	0.0198 (7)
C(5)	0.0248 (2)	0.12988 (8)	0.33354 (8)	0.0223 (8)
C(6)	0.0997 (2)	0.22410 (9)	0.32550 (8)	0.0229 (8)
C(7)	0.1546 (2)	−0.03204 (8)	0.33690 (8)	0.0231 (8)
C(8)	0.0397 (3)	−0.0653 (1)	0.41329 (9)	0.0338 (9)
C(9)	−0.0028 (3)	−0.0416 (1)	0.2688 (1)	0.034 (1)
C(10)	0.3622 (3)	−0.0900 (1)	0.3263 (1)	0.039 (1)
C(11)	0.2468 (2)	0.38761 (8)	0.40931 (7)	0.0186 (7)
C(12)	0.3766 (2)	0.46882 (8)	0.3997 (7)	0.0179 (7)
C(13)	0.5850 (2)	0.47194 (9)	0.36322 (7)	0.0205 (7)
C(14)	0.7054 (2)	0.54666 (9)	0.35938 (7)	0.0217 (7)
C(15)	0.6150 (2)	0.61700 (8)	0.39286 (7)	0.0196 (7)
C(16)	0.4073 (2)	0.61626 (9)	0.42820 (7)	0.0208 (7)
C(17)	0.2883 (2)	0.54100 (8)	0.43130 (7)	0.0194 (7)
Molecule *B*				
O(1′)	0.0554 (1)	0.37914 (6)	0.12708 (5)	0.0209 (5)
O(2′)	−0.2791 (2)	0.39450 (6)	0.18505 (6)	0.0301 (6)
O(3′)	−0.1721 (2)	−0.03739 (7)	0.06634 (7)	0.0429 (7)
O(4′)	−0.5191 (2)	−0.01298 (8)	0.09477 (8)	0.0514 (8)
N(1′)	−0.3243 (2)	0.00877 (8)	0.08755 (7)	0.0330 (8)
C(1′)	0.0914 (2)	0.47205 (8)	0.12823 (7)	0.0195 (7)
C(2′)	0.2529 (2)	0.49814 (8)	0.06274 (8)	0.0214 (7)
C(3′)	0.2880 (2)	0.59560 (8)	0.05778 (7)	0.0211 (7)
C(4′)	0.3809 (2)	0.62064 (8)	0.13486 (7)	0.0184 (7)
C(5′)	0.2234 (2)	0.58847 (8)	0.20201 (7)	0.0201 (7)
C(6′)	0.1834 (2)	0.49071 (8)	0.20588 (7)	0.0198 (7)
C(7′)	0.4338 (2)	0.71850 (8)	0.13085 (7)	0.0209 (7)
C(8′)	0.5866 (3)	0.7439 (1)	0.06087 (8)	0.0292 (9)
C(9′)	0.5602 (3)	0.73430 (9)	0.20465 (8)	0.0268 (8)
C(10′)	0.2222 (3)	0.77766 (9)	0.12380 (9)	0.0291 (9)
C(11′)	−0.1430 (2)	0.35124 (8)	0.15359 (7)	0.0206 (7)
C(12′)	−0.1794 (2)	0.26009 (8)	0.13769 (7)	0.0192 (7)
C(13′)	−0.0214 (2)	0.21178 (9)	0.10046 (8)	0.0225 (8)
C(14′)	−0.0656 (2)	0.12854 (9)	0.08454 (8)	0.0251 (8)
C(15′)	−0.2722 (2)	0.09661 (8)	0.10564 (7)	0.0235 (8)
C(16′)	−0.4331 (2)	0.14293 (9)	0.14254 (8)	0.0252 (8)
C(17′)	−0.3855 (2)	0.22540 (9)	0.15895 (8)	0.0237 (8)

Table 3. *Interatomic distances* (Å) *and angles* (°) *for cis-4-tert-butylcyclohexyl p-nitrobenzoate* (1) *and trans-4-tert-butylcyclohexyl p-nitrobenzoate* (2)

For compound (2) molecule *B*, atom labels should carry a prime.

		(2)	
	(1)	Molecule *A*	Molecule *B*
O(1)—C(1)	1.473 (2)	1.463 (2)	1.468 (2)
O(1)—C(11)	1.332 (2)	1.335 (2)	1.340 (2)
O(2)—C(11)	1.213 (2)	1.209 (2)	1.205 (2)
O(3)—N(1)	1.225 (2)	1.228 (2)	1.221 (2)
O(4)—N(1)	1.228 (2)	1.229 (2)	1.229 (2)
N(1)—C(15)	1.475 (2)	1.475 (2)	1.478 (2)
C(1)—C(2)	1.514 (2)	1.514 (2)	1.512 (2)
C(1)—C(6)	1.516 (2)	1.514 (2)	1.514 (2)
C(2)—C(3)	1.532 (2)	1.529 (2)	1.526 (2)
C(3)—C(4)	1.538 (2)	1.537 (2)	1.541 (2)
C(4)—C(5)	1.533 (2)	1.536 (2)	1.539 (2)
C(4)—C(7)	1.553 (2)	1.557 (2)	1.555 (2)
C(5)—C(6)	1.529 (2)	1.535 (2)	1.537 (2)
C(7)—C(8)	1.537 (3)	1.527 (2)	1.534 (2)
C(7)—C(9)	1.526 (3)	1.534 (2)	1.533 (2)
C(7)—C(10)	1.532 (2)	1.532 (2)	1.535 (2)
C(11)—C(12)	1.496 (2)	1.496 (2)	1.496 (2)
C(12)—C(13)	1.397 (2)	1.396 (2)	1.389 (2)
C(12)—C(17)	1.388 (2)	1.389 (2)	1.396 (2)
C(13)—C(14)	1.381 (2)	1.382 (2)	1.387 (2)
C(14)—C(15)	1.383 (2)	1.386 (2)	1.382 (2)
C(15)—C(16)	1.384 (2)	1.384 (2)	1.380 (2)
C(16)—C(17)	1.386 (2)	1.385 (2)	1.383 (2)
C(1)—O(1)—C(11)	117.4 (1)	118.0 (1)	115.9 (1)
O(3)—N(1)—O(4)	123.8 (1)	124.1 (1)	124.2 (1)
O(3)—N(1)—C(15)	118.2 (1)	117.6 (1)	118.2 (1)
O(4)—N(1)—C(15)	118.0 (1)	118.3 (1)	117.6 (1)
O(1)—C(1)—C(2)	105.9 (1)	105.5 (1)	106.5 (1)
O(1)—C(1)—C(6)	108.8 (1)	110.5 (1)	111.82 (9)
C(2)—C(1)—C(6)	112.0 (1)	111.7 (1)	110.8 (1)
C(1)—C(2)—C(3)	112.4 (1)	110.7 (1)	109.2 (1)
C(2)—C(3)—C(4)	111.4 (1)	111.9 (1)	111.5 (1)
C(3)—C(4)—C(5)	108.2 (1)	108.5 (1)	108.9 (1)
C(3)—C(4)—C(7)	114.5 (1)	113.7 (1)	113.3 (1)
C(5)—C(4)—C(7)	114.0 (1)	114.2 (1)	114.1 (1)
C(4)—C(5)—C(6)	111.7 (1)	112.3 (1)	112.4 (1)
C(1)—C(6)—C(5)	112.1 (1)	110.3 (1)	108.9 (1)
C(4)—C(7)—C(8)	110.1 (1)	112.3 (1)	109.7 (1)
C(4)—C(7)—C(9)	112.1 (1)	110.3 (1)	109.6 (1)
C(4)—C(7)—C(10)	108.9 (1)	109.6 (1)	112.4 (1)
C(8)—C(7)—C(9)	108.3 (1)	108.7 (1)	107.3 (1)
C(8)—C(7)—C(10)	107.9 (1)	108.9 (1)	109.2 (1)
C(9)—C(7)—C(10)	109.4 (1)	106.8 (1)	108.6 (1)
O(1)—C(11)—O(2)	124.7 (1)	124.5 (1)	124.5 (1)
O(1)—C(11)—C(12)	111.9 (1)	111.8 (1)	111.9 (1)
O(2)—C(11)—C(12)	123.4 (1)	123.7 (1)	123.6 (1)
C(11)—C(12)—C(13)	121.2 (1)	121.6 (1)	122.6 (1)
C(11)—C(12)—C(17)	118.4 (1)	118.1 (1)	117.2 (1)
C(13)—C(12)—C(17)	120.3 (1)	120.2 (1)	120.2 (1)
C(12)—C(13)—C(14)	119.9 (1)	119.9 (1)	120.5 (1)
C(13)—C(14)—C(15)	118.4 (1)	118.5 (1)	117.7 (1)
N(1)—C(15)—C(14)	118.2 (1)	118.5 (1)	118.5 (1)
N(1)—C(15)—C(16)	118.8 (1)	118.7 (1)	118.3 (1)
C(14)—C(15)—C(16)	123.0 (1)	122.8 (1)	123.2 (1)
C(15)—C(16)—C(17)	117.9 (1)	118.0 (1)	118.4 (1)
C(12)—C(17)—C(16)	120.4 (1)	120.5 (1)	119.9 (1)

For *cis*-4-*tert*-butylcyclohexyl *p*-nitrobenzoate (1), a colourless crystal, 0.13 × 0.14 × 0.25 mm, was used for data collection with θ–2θ, scans of width $(1.1 + 0.142\tan\theta)^\circ$ in θ and rate 4° $\min^{-1}$ in θ with 7 s backgrounds on each side of every scan, to $2\theta_{\max} = 128^\circ$ with $0 \le h \le 8$, $-13 \le k \le 13$, $-14 \le l \le 14$. 2860 reflections were measured, of which 2535 were unique ($R_{\rm int} = 0.007$), and 2237 with $I > 3\sigma(I)$ were regarded as observed. Data were corrected for absorption (maximum/minimum transmission 0.94/0.87). Refinement on F of 292 parameters converged to $R = 0.033$, $wR = 0.049$, $S = 1.66$. Data were corrected for extinction with isotropic extinction parameter 0.24 (2). Maximum $\Delta/\sigma = 0.09$. Maximum and minimum heights in the final $\Delta\rho$ map were 0.2 and -0.2 e Å^{-3}.

For *trans*-4-*tert*-butylcyclohexyl *p*-nitrobenzoate (2), a colourless crystal, 0.50 × 0.07 × 0.25 mm, was used for data collection with θ–2θ scans of width $(1.0 + 0.142\tan\theta)^\circ$ in θ and rate 4° min^{-1} in θ with 5 s backgrounds on each side of every scan, to $2\theta_{\max} = 128^\circ$ with $0 \le h \le 7$, $-18 \le k \le 18$, $-20 \le l \le 20$. 5268 reflections were measured, of which 5149 unique ($R_{\rm int} = 0.006$), and 4504 with $I > 3\sigma(I)$ were regarded as observed. Data were corrected for absorption (maximum/minimum transmission 0.95/0.83). Refinement on F of 582 parameters converged to $R = 0.032$, $wR = 0.048$, $S = 1.70$. Data were corrected for extinction with isotropic extinction parameter 0.29 (3). Maximum $\Delta/\sigma = 0.005$. Maximum and minimum heights in the final $\Delta\rho$ map were 0.2 and -0.3 e Å^{-3}.

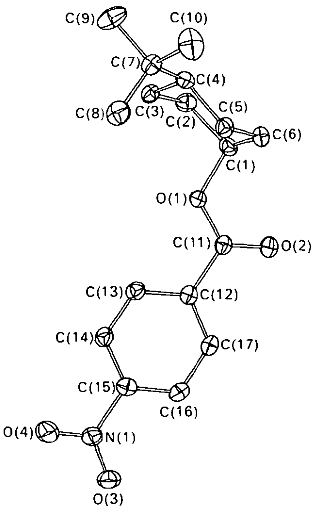


Fig. 1. Thermal-ellipsoid diagram of (1) showing labelling of non-H atoms. Ellipsoids show 50% probability levels.

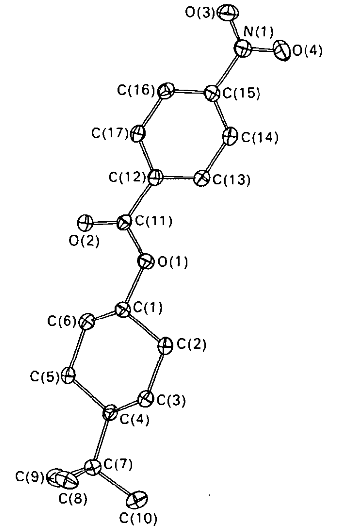
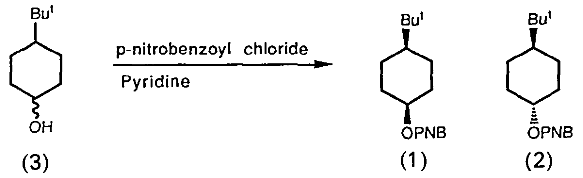


Fig. 2. Thermal ellipsoid plot for (2) molecule *A* showing labelling of non-H atoms. Ellipsoids show 50% probability levels.

Atomic scattering factors for neutral atoms and real and imaginary dispersion terms were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV). Data reduction was carried out as described elsewhere (Robertson & Whimp, 1975) and refinement computations were performed with *Xtal*2.6 (Hall & Stewart, 1989). Final parameters for non-H atoms for (1) and (2) are given in Tables 1 and 2, respectively. Interactomic distances and angles are given in Table 3.* Perspective views of (1) and the independent molecules *A* and *B* of (2) with labelling are presented in Figs. 1, 2 and 3, respectively.

Related literature. As part of our studies on the factors affecting C—O bond lengths (White & Robertson 1992), we required the C—O bond



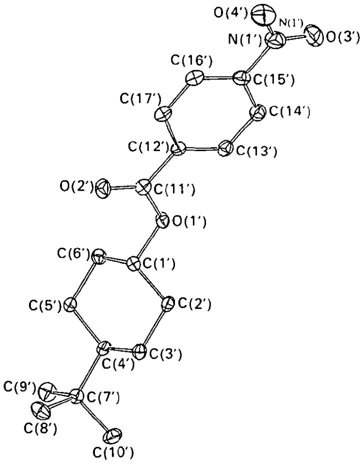


Fig. 3. Thermal ellipsoid plot for (2) molecule *B* showing labelling of non-H atoms. Ellipsoids show 50% probability levels.

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* Lists of H-atom coordinates, anisotropic thermal parameters, additional bond distances, angles and dihedral angles, and structure factor amplitudes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55483 (64 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: HL1002]

lengths for both axial and equatorial cyclohexyl *p*-nitrobenzoates at low temperature for comparison purposes. Thus *cis* (1) and *trans* (2) 4-*tert*-butylcyclohexyl *p*-nitrobenzoate were prepared by treatment of a *ca* 1:1 mixture of *cis* and *trans* 4-*tert*-butylcyclohexanol (3) (as supplied by Aldrich) with *p*-nitrobenzoyl chloride in the presence of pyridine. The resulting mixture of isomers was separated by chromatography on silica gel. Crystals of (1) and (2) suitable for X-ray analysis were grown from pentane.

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Structure of 4′-Dimethylamino-4-methyl-4-azastilbenium *p*-Toluenesulfonate Hydrate

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Abstract. 4′-Dimethylamino-*N*-methyl-4-stilbazolium tosylate hydrate, $C_{16}H_{19}N_2^+.C_7H_7O_3S^-.H_2O$, M_r = 428.5, triclinic, $P\bar{1}$, a = 8.006 (2), b = 9.548 (2), c = 14.647 (12) Å, α = 80.34 (2), β = 80.30 (2), γ = 77.98 (2)°, V = 1069.2 Å^3, Z = 2, D_x = 1.330 g cm^{-3}, λ(Mo $K\alpha$) = 0.71069 Å, μ = 1.75 cm^{-1}, $F(000)$ = 456, T = 213 K, R = 0.0649 for 3754 unique reflections with $I > 2\sigma(I)$. The 4-methyl-4′-dimethylamino-4-azastilbenium molecules pack head to tail within a sheet and are aligned in the opposite direction in the neighboring sheets. The phenyl rings in the *p*-toluenesulfonate groups lie at an angle of 72° relative to the aromatic rings in the azastilbenium groups. The axes for both molecules lie along the *a* axis. The rings for the azastilbenium group lie in the *ab* plane and the phenyl ring of the *p*-tolunesulfonate group lies in the *ac* plane.

Experimental. Compound obtained by reaction of one equivalent of γ-picoline and one equivalent of methyl *p*-toluenesulfonate heated at reflux for 1 h in 1 l of ethanol. Treatment with 1.1 equivalents of *N*,*N*-dimethylaminobenzaldehyde and 0.2 equivalents of piperidine yielded dark green crystals of the desired product. Large platelets of the reported crystals were grown by slow evaporation at 300 K from a saturated solution of 4-methyl-4′-dimethylamino-4-azastilbenium *p*-toluenesulfonate and 95% methanol/water solution. The crystal was sealed in a glass capillary for low-temperature data collection. Siemens *R*3*m*/*V* upgrade of Nicolet *P*3*F* automated diffractometer, 2θ–θ scan with variable scan speeds. Structure solved by direct methods and refined on *F* using the *SHELXTL-Plus* (MicroVAX II) program package (Sheldrick, 1988). H atoms were placed in idealized positions and constrained to have C—H = 0.96 Å and isotropic thermal parameters, U = 0.08 Å^2. All non-H atoms treated as anisotropic. No absorption correction was applied. Details of the data collection are in Table 1.* Scattering factors from *International Tables for X-ray Crystallography*

Table 1. *Experimental details*

Crystal habit and size (mm)	Plate 0.40 × 0.24 × 0.04
Number of reflections, 2θ range (°) for lattice parameters	29, 13.3–36.6
Range of h,k,l	−1 to 10, −12 to 12, −18 to 19
Max. $\sin\theta/\lambda$ (Å^{-1})	0.650
Check reflections	$1\bar{1}\bar{3}$, 104, $31\bar{3}$
% variation	5, 5, 3
Reflections collected	4932
Unique observed reflections	3754
$R_{\rm int}$	0.014
Observed criterion	$I > 2\sigma(I)$
Number of parameters	272
R	0.065
wR	0.070
S	1.34
Secondary-extinction parameter (χ) $F^* = F[1 + 0.002\chi F^2/\sin(2\theta)]^{-1/4}$	0.0007 (4)
Weighting factor (g), $w^{-1} = \sigma^2(F) + gF^2$	0.0011
Fourier difference peaks, max., min. (e Å^{-3})	0.47, −0.43
Max. Δ/σ	0.002

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* Lists of structure factors, anisotropic thermal parameters, bond lengths and angles and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55456 (23 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: CR0417]

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