Abstract. C_{28}H_{26}N_{2}, monoclinic, P2_1, \( a = 9.94 \) (2), \( b = 14.58 \) (2), \( c = 7.91 \) (2) Å, \( \beta = 106.5 \) (2)°, \( V = 1099.86 \) Å\(^3\), \( Z = 2\); \( D_m = 1.177\), \( D_x = 1.179\) g cm\(^{-3}\); \( F(000) = 416\). Full-matrix least-squares refinement gave \( R = 0.084\) and \( R_w = 0.072\) for 375 parameters and 1928 significant reflexions. The molecule exhibits a cis configuration and the phenyl groups are twisted out of the plane of the ethylene group to avoid steric hindrance. The N atoms have a planar configuration.

Discussion. The molecule with the numbering of atoms is shown in Fig. 1. The configuration around the double bond is cis and a pseudo twofold axis is present. The final coordinates, interatomic distances and bond angles are listed in Tables 1, 2, and 3, respectively. The ethylenic bond, C(1)—C(2) (1.356 Å), agrees well with the corresponding bond, \( \alpha—\beta \) (1.35 Å), refined was continued using full-matrix least squares (LINUS, Coppens & Hamilton, 1970) minimizing the quantity \( r = \sum w(|F_o| - |F_c|)^2 / \sum w|F_o|^2 \) where \( w = |\sigma(F_o^2) + 1.02F_o^2|^{1/2} - |F_o|^2 \).

The scattering factors used for C and N were those of Cromer & Mann (1968) and of Stewart, Davidson & Simpson (1965) for H. Final refinement of the coordinates, overall scale factor, thermal parameters (anisotropic for C and N, isotropic for H) gave an \( R \) value of 0.084 (\( wR = 0.070\)) for 56 atoms, 1928 reflexions \( |\sum 2\sigma(I)| \) and 375 parameters refined in batches of 210.* Illustrations were drawn by ORTEP (Johnson, 1965) while interatomic distances, angles, least-squares planes and dihedral angles were calculated with ORFFE (Busing, Martin & Levy, 1964).

* Lists of structure factors, thermal parameters, hydrogen atom coordinates and C—H distances have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 33721 (12 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.
in 2,6-dibromo-a-cyanostilbene (d'Enghien & Van Meersse, 1962), where the stilbene group is in a cis configuration, and with Pariser-Parr-Pople calculations. It is slightly longer than the corresponding bonds in 2,6-dibromo-(t-cyanostilbene (d'Enghien & Van Meerssche, 1962), where the stilbene group is in a cis configuration, and with Pariser-Parr-Pople calculations. It is slightly longer than the corresponding bonds in 1,2-diphenylcyclopentene (Bernstein, 1975b; Finder, Newton & Allinger, 1974), 1.334 Å in a,β-bis-(phenylazo)stilbene (Chesick, 1973), and 1.339 Å in a cis-stilbene derivative, 1,2-diphenylcyclopentene (Bern-
energetically favourable, compared to the common pyramidal configuration (sp\(^3\) hybridization), because of the interaction of the N lone pair with the \(\pi\)-electron system of the phenyl ring. Extensive discussions about the influence of the N lone pair on the geometry of N-containing molecules are given by Genson & Christoffersen (1972). The angle between the phenyl ring and the plane of coordination around N is 15 and 35°, whereas the torsion angles C(36)—N(1)—C(1)—C(2) and C(46)—N(2)—C(2)—C(1) are 52 and 46°, respectively, so that interaction between the lone pairs and the ethylenic bond is less likely.

The molecule is considerably twisted around both the double bond (17.5°) and the two C—C single bonds (44.3 and 41.7°) in order to avoid steric hindrance between the two phenyl groups in cis positions. Similar angles were found in the cis-stilbene derivative 1,2-diphenylcyclopentene (Bernstein, 1975a).

The packing of molecules in the unit cell is shown in Fig. 2. No intermolecular contacts shorter than normal van der Waals distances were found.

References
