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The Crystal Structures of Two Pyrazolinone Azomethine Dyes

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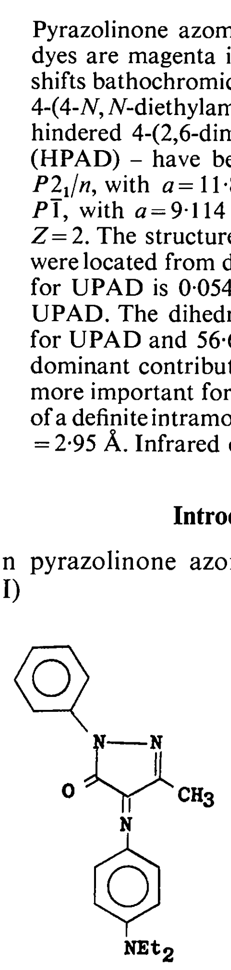
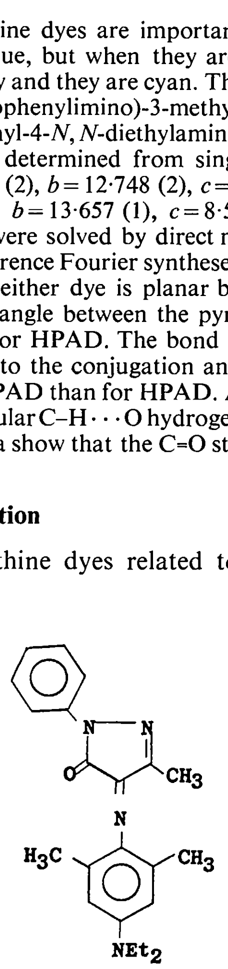
Pyrazolinone azomethine dyes are important as image formers in color photography. Usually these dyes are magenta in hue, but when they are overcrowded by suitable substituents, their absorption shifts bathochromically and they are cyan. The structures of two of these dyes – the relatively uncrowded 4-(4-*N*,*N*-diethylaminophenylimino)-3-methyl-1-phenyl-2-pyrazolin-5-one (UPAD) and the highly hindered 4-(2,6-dimethyl-4-*N*,*N*-diethylaminophenylimino)-3-methyl-1-phenyl-2-pyrazolin-5-one (HPAD) – have been determined from single-crystal X-ray diffraction data. UPAD is monoclinic, $P2_1/n$, with a = 11·840 (2), b = 12·748 (2), c = 11·982 (2) Å, β = 93·02 (1)° and Z = 4; HPAD is triclinic, $P\bar{1}$, with a = 9·114 (1), b = 13·657 (1), c = 8·502 (1) Å, α = 103·19 (1), β = 102·92 (1), γ = 91·63 (1)°, and Z = 2. The structures were solved by direct methods and refined by least squares. The hydrogen atoms were located from difference Fourier syntheses and were refined. The final R value for HPAD is 0·042 and for UPAD is 0·054. Neither dye is planar but HPAD deviates considerably more from planarity than UPAD. The dihedral angle between the pyrazolinone ring and the p-phenylenediamine ring is 13·9° for UPAD and 56·6° for HPAD. The bond lengths show that the unexcited canonical structure is the dominant contributor to the conjugation and that the quinoid form of the p-phenylenediamine part is more important for UPAD than for HPAD. A striking feature of the structure of UPAD is the presence of a definite intramolecular C–H···O hydrogen bond. The atomic separations are O···H = 2·03 Å, O···C = 2·95 Å. Infrared data show that the C=O stretch frequency is 24 cm^{-1} less for UPAD than for HPAD.

Introduction

Certain pyrazolinone azomethine dyes related to (I) and (II)



(I) UPAD



(II) HPAD

are important as image formers in color photography (Weissberger, 1966). These dyes are formed during color development by oxidative condensation of pyrazolinones and p-phenylenediamines, where silver ion is the oxidizing agent. Usually these dyes are magenta in hue and exhibit two maxima in their visible absorption spectra, a low intensity y band near 440 nm and a high intensity x band near 500 nm (Brown, Graham, Vittum & Weissberger, 1951; Smith, 1964). Fig. 1 shows the spectra of the unhindered dye (I) (UPAD) and of the hindered dye (II) (HPAD) measured in CCl_4 with a Carey 14 spectrophotometer (Figueras, 1967). For UPAD, ε_{max}, the molar extinction coefficient, is $3{\cdot}30 \times 10^4 M^{-1}.cm^{-1}$ at λ_{max} = 495 nm and for HPAD, ε_{max} = $1{\cdot}28 \times 10^4 M^{-1}.cm^{-1}$ at λ_{max} = 632 nm.

Knott & Pauwels (1968) have discussed this unusual bathochromic shift arising from nonplanarity of an asymmetric conjugated system. Normally one would expect the change of structure from the presumed planarity of UPAD to the presumed nonplanarity of HPAD to occur through twisting of the bonds about the azomethine nitrogen, especially the N-phenyl bond. Such twisting should decrease the extent of conjugation thus increasing the energetic asymmetry of the dye, and cause the absorption maximum to shift to shorter wavelengths. Knott & Pauwels suggested that if the twisting about the N-pyrazolinyl bond were great enough, the bond orders of both bridge bonds would become equal, resulting in an isoenergetic system. It is known that any loss of coplanarity of the end nuclei in isoenergetic dyes such as the symmetrical cyanine dyes results in bathochromic shifts and decreased extinction (Dewar, 1958; Brooker, White, Sprague, Dent & Van Zandt, 1947). In addition, unpublished Hückel molecular orbital calculations of Figueras (1967) of our laboratories have indicated that an appreciable twist about the N-pyrazolinyl bond is necessary to explain the observed spectra.

To obtain detailed information about the actual molecular conformations of these dyes, we have determined the crystal structures of UPAD and HPAD by X-ray diffraction. The chemical name for UPAD is 4-(4-*N*,*N*-diethylaminophenylimino)-3-methyl-1-phenyl-2-pyrazolin-5-one; for HPAD it is 4-(2,6-dimethyl-4-*N*,*N*-diethylaminophenylimino)-3-methyl-1-phenyl-2-pyrazolin-5-one.

Crystal data

	UPAD	HPAD
Formula	$C_{20}H_{22}N_4O$	$C_{22}H_{26}N_4O$
Molecular weight	334·42	362·48
Color	green	reddish-brown
Habit	thick tabular (10$\bar{1}$)	chunky
Crystal system	monoclinic	triclinic
Wavelength (Cu $K\alpha_1$)	1·5405 Å	1·5405 Å
Unit cell: a	11·840 (2) Å	9·114 (1) Å
b	12·748 (2)	13·657 (1)
c	11·982 (2)	8·502 (1)
α		103·19 (1)°
β	93·02 (1)°	102·92 (1)
γ		91·63 (1)
V	1805·8 (5) Å^3	1000·8 (2) Å^3
Z	4	2
D_{obs} (flotation)	1·21 g.cm^{-3}	1·19 g.cm^{-3}
D_{calc}	1·230 g.cm^{-3}	1·203 g.cm^{-3}
μ (Cu $K\alpha$)	6·2 cm^{-1}	6·0 cm^{-1}
F(000)	712	388
Absent spectra	$h0l$, $h+l$ odd $0k0$, k odd	none
Space group	$P2_1/n(C_{2h}^5)$	$P\bar{1}(C_i)$
General position	$\pm(x,y,z;\frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}+z)$	$\pm(x,y,z)$

Experimental

Single crystals of both dyes were supplied by J. Figueras. Space group extinctions and preliminary lattice dimensions were obtained from precession photographs The unit cell reported above for HPAD is the reduced crystallographic cell (Lawton & Jacobson, 1965). Small chunky crystals of UPAD (0·41 × 0·38 × 0·23 mm) and HPAD (0·23 × 0·25 × 0·18 mm), fastened to thin glass rods with Canada balsam, were chosen for intensity data collection on an automatic Picker four-circle goniostat. To minimize the effect of multiple reflections (Zachariasen, 1965), the crystals were oriented so no symmetry axis lay along the spindle of the goniometer head. Narrow source, open-counter ω scans (Furnas, 1957) through several reflections showed the mosaicity of both crystals to be approximately 0·20°. Twenty-six reflections for UPAD and thirty-four reflections for HPAD, all at moderately high Bragg angles (Cu $K\alpha_1$ radiation), were accurately centered through very narrow vertical and horizontal slits at a take-off angle of 0·5°. These observations were used as input to the computer program *PICK*2 (Ibers, 1966), which refined the cell and orientation parameters by the method of least squares and generated the cards to control the automated goniostat.

Intensity data were collected with Ni-filtered Cu radiation at a take-off angle of 2·5°. A scintillation detector was used and the pulse-height analyzer was set for an approximately 90% window. All unique reflections for $2\theta < 130°$ were measured by the θ–2θ scan technique (Furnas, 1957) at a 2θ scan rate of 1·0°.min^{-1} The scan range varied from 0·9° at low 2θ to 2·7° at high 2θ. Stationary-crystal stationary-counter background counts were taken for 40 sec at each end of the scan. For count rates above 13,000 cps, brass attenuators were automatically inserted in the diffracted beam by the Picker system. To check electronic and crystal stability during the period of data collection, the intensities of standard reflections (452 for UPAD, 422 for HPAD) were measured every 50th reflection. No systematic variation was observed for these standard intensities

The background for a reflection was approximated by a straight line between the two measured background points. The intensities were corrected for background and for Lorentz and polarization effects and were reduced to structure amplitudes, $|F_o|$. Absorption corrections were not applied because of the low absorption coefficients and the small size and regularity of the crystals. We estimate the maximum error in F_o caused by absorption to be 3% for UPAD and 1% for HPAD. Standard deviations $\sigma(I)$ were based on counting statistics and were corrected to $\sigma(F)$. Those intensities less than $2\sigma(I)$ were considered unobserved and were set equal to $2\sigma(I)$ and corrected to structure amplitudes, F_{lim}. For UPAD the unobserved reflections numbered 626 out of a total of 3077 measured intensities, and for HPAD 577 out of 3400 were unobserved.

Determination and refinement of the structures

The observed structure factors of the dyes were converted to normalized structure factor magnitudes, $|E_H|$ (Hauptman & Karle, 1953); their statistical averages indicated the centrosymmetric space groups in both cases. Both structures were solved by the direct phasing of the structure amplitudes. Three-dimensional E maps based on these phases yielded the positions of most of

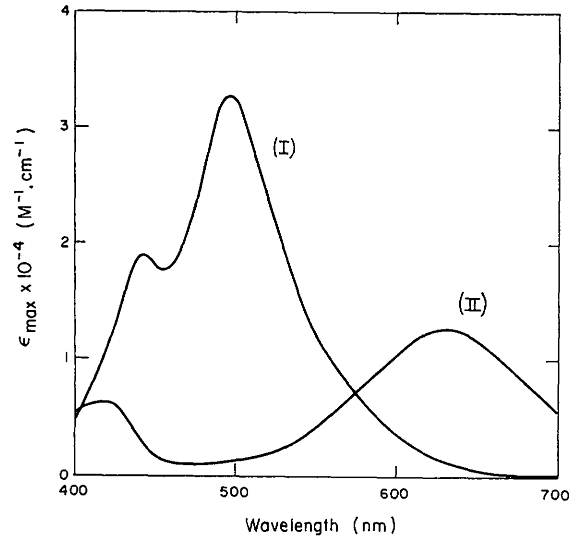


Fig. 1. Visible absorption spectra in CCl_4 solution of dyes (I) and (II).

the heavy atoms. Refinement was by the method of least squares. The initial cycles were computed by the full-matrix program *ORFLS* (Busing, Martin & Levy, 1962) but a block-diagonal least-squares program (Trotter, 1965), which utilized a 3 × 3 block for coordinates and was diagonal in temperature factors, was used for most of the refinement. This program minimized $\sum w(F_o^*-F_c)^2$, where

$$F_o^*=K\left(1+g\frac{(1+\cos^4 2\theta)}{(1+\cos^2 2\theta)\sin 2\theta}F_c^2\right)^{1/2}F_o=KGF_o\,,$$

in which K is the scale factor, g is the extinction parameter (Zachariasen, 1963; Larson, 1967) and F_c is the usual calculated structure factor. The weights were defined as

$$w=[\{qK\sigma(F_o)\}^2+(rF_o^*)^2+s(F_o^*-KF_o)^2]^{-1},$$

where q, r, and s were chosen by inspection to make the averages of $\sum w(F_o^*-F_c)^2$ constant for groups of increasing F_o's (Cruickshank, 1965). In addition to the observed reflections, unobserved reflections were included in the refinement and the agreement indices if $|F_c|>F_{\text{lim}}^*$. The usual agreement index was defined as $R_1=\sum|F_o^*-F_c|/\sum|F_o^*|$ and the weighted agreement index as $R_2=(\sum w(F_o^*-F_c)^2/\sum wF_o^{*2})^{1/2}$. The atomic scattering factors were obtained from *International Tables for X-ray Crystallography* (1962). All computations were performed on an IBM 360/65 computer.

UPAD

Of the 335 reflections with $|E|>1{\cdot}6$, 330 were phased by the multiple solution computer program of Long (1965) (modified by Tsai, 1968) based on the reiterative application of Sayre's (1952) equation. An E map calculated from the most consistent set of phases yielded all of the heavy atoms except the two methyl carbons of the ethyl groups. Two cycles of full-matrix least-squares refinement with individual isotropic temperature factors, $g=s=0$, $q=1$, and $r=0{\cdot}04$ were followed by the calculation of a difference electron density map, in which the remaining carbon atoms were found. Two further cycles of refinement reduced R_1 to 0·18. Three cycles of block-diagonal least squares with anisotropic thermal parameters decreased R_1 to 0·13. The largest structure factors were obviously affected by extinction, so several refinement cycles in which only g varied were computed. Additional cycles of anisotropic refinement with $g=5{\cdot}6\times10^{-6}$, $q=1$, $r=0{\cdot}04$, and $s=0{\cdot}01$ yielded $R_1=0{\cdot}11$.

All 22 hydrogen atoms were located from a difference Fourier synthesis although some difficulty was experienced in finding the hydrogen atoms of the C(20) methyl group. The hydrogen atoms were assigned isotropic temperature factors of 4·0 Å^2 and several cycles of refinement of the heavy atoms ($g=5{\cdot}6\times10^{-6}$, $q=1$, $r=0{\cdot}04$, $s=0{\cdot}03$) reduced R_1 to 0·077. Extinction effects needed further correction and g was redetermined from the 105 strongest reflections, except for 103, which was by far the most intense reflection. The value, $2{\cdot}03\times10^{-5}$ determined for g, caused the correction for 103 ($G=2{\cdot}66$) to exceed greatly the applicable range of the correction (Zachariasen, 1963), so this reflection was omitted from the remainder of the refinement and from the R indices.

Least-squares refinement continued with $q=1{\cdot}8$, $r=0{\cdot}04$, $s=0$, $g=2{\cdot}03\times10^{-5}$, and the parameters of all atoms being allowed to vary. Refinement appeared to be complete when R_1 was 0·054 and R_2 was 0·073; this point was eventually adopted as the end of the refinement. A three-dimensional difference electron density map, calculated to verify the correctness of the structure, was essentially featureless, with residual electron densities which ranged from $-0{\cdot}12$ to $+0{\cdot}18$ e.Å^{-3} *except* for negative areas to $-0{\cdot}15$ e.Å^{-3} around the C(20) position and a well-formed hydrogen-like peak (0·52 e.Å^{-3}). This 'atom' with coordinates $x=0{\cdot}949$, $y=0{\cdot}769$ and $z=-0{\cdot}075$ was 1·42 Å from N(4), 1·23 Å from C(19), and 1·18 Å from C(20) and made no particular chemical sense, especially since it would result in a tetrahedral nitrogen rather than the expected planar nitrogen. Attempts to eliminate the peak by redetermining hydrogen positions and by refinement of occupancy parameters for the diethylamino heavy atoms did not succeed but did indicate that C(20) might have a reduced occupancy (0·92), in agreement with the difference map. The extra atom, C(21), was then assigned carbon scattering factors, an occupancy factor of 0·10 and an isotropic temperature factor of 9·1 Å^2. Six cycles of least squares in which all parameters except g and the occupancy factors were varied reduced R_1 to 0·049 and R_2 to 0·065, a highly significant improvement in agreement according to the Hamilton (1965) R-ratio test. The C(21) temperature factor decreased to 4·9 Å^2 and it would appear possible that there might be electron density at C(21). However, we believe it is more likely that there is systematic error in the intensity data and in the proposed model owing to partial decomposition of the molecule during data collection. It was known (Rossiter, 1969) that in ultraviolet light UPAD decomposes at the diethylamino group to form a variety of products, with eventual total dealkylation and formation of an unsubstituted amino group. A portion of the original sample of UPAD was exposed for seven days to X-rays from a copper target tube. Thin-layer chromatography revealed small amounts of four unidentified dyes in the irradiated sample which were not present in the original sample and showed that some decomposition of the crystal had undoubtedly occurred during data collection. We were unable to propose a chemically satisfactory model with an atom at C(21) so the refinement was considered final at the convergence of the original model. A similar experience with an extra hydrogen-like peak was reported recently by Hanson & Huml (1969).

The final agreement indices for 2450 observed reflections (103 omitted) plus 104 unobserved reflections with $|F_c|>F_{\text{lim}}^*$ are, as noted above, $R_1=0{\cdot}054$ and $R_2=0{\cdot}073$. Of these 104 unobserved reflections, none have $|F_c| > 1{\cdot}9\ F^*_{\text{lim}}$. The standard deviation of an observation of unit weight is 1·30. On the last cycle of refinement, only six of the 313 atomic parameters shifted more than 0·2 σ and the maximum shift was 0·36σ. The final positional and thermal parameters with standard deviations estimated from the least-squares process are given in Tables 1 and 2. Since there is residual systematic error in the structure, the reported standard deviations are probably low. Expressed in Å, the average e.s.d.'s are 0·0017 for oxygen and nitrogen (range: 0·0014 to 0·0019), 0·0023 for carbon (range: 0·0019 to 0·0031), and 0·026 for hydrogen (range: 0·017 to 0·044). Two other parameters determined were the scale factor, $K=0{\cdot}1792$, and the extinction coefficient, $g=2{\cdot}03\times 10^{-5}$. The final values of the observed and calculated structure factors are compared in Table 3. Their agreement leaves no doubt as to the essential correctness of the proposed structure.

Table 2. *Final atomic parameters for the hydrogen atoms of UPAD*

Estimated standard deviations are given in parentheses.

	x	y	z	B
H(1)	0.6452(23)	0.1836(24)	0.0858(20)	7.7(7)
H(2)	0.5967(24)	0.1144(22)	0.1716(21)	7.9(7)
H(3)	0.6969(28)	0.1948(28)	0.1925(25)	11.6(10)
H(4)	0.2817(17)	0.2163(16)	0.3147(15)	4.2(5)
H(5)	0.0970(21)	0.2274(20)	0.3833(20)	6.6(6)
H(6)	−0.0063(21)	0.3858(19)	0.3581(20)	6.3(6)
H(7)	0.0738(20)	0.5294(19)	0.2759(19)	5.9(6)
H(8)	0.2569(18)	0.5155(17)	0.1999(16)	4.7(5)
H(9)	0.7464(32)	1.0065(29)	0.0389(27)	12.1(11)
H(10)	0.8571(30)	0.9729(27)	0.0953(28)	11.0(10)
H(11)	0.7359(24)	0.9093(22)	0.1206(22)	7.8(7)
H(12)	0.7270(18)	0.8528(19)	−0.0691(16)	5.1(5)
H(13)	0.8540(19)	0.9184(19)	−0.0903(18)	5.6(6)
H(14)	1.0360(17)	0.7458(17)	0.0706(16)	4.4(5)
H(15)	1.0231(20)	0.8802(19)	0.0199(19)	6.4(6)
H(16)	1.0054(30)	0.8434(28)	−0.1553(27)	11.3(10)
H(17)	1.0034(39)	0.6986(34)	−0.1207(34)	15.3(13)
H(18)	1.1336(31)	0.7850(29)	−0.0784(27)	13.0(12)
H(19)	0.6589(16)	0.7561(15)	0.0426(15)	3.4(4)
H(20)	0.9598(16)	0.6012(15)	0.0404(14)	3.4(4)
H(21)	0.8611(18)	0.4441(17)	0.0827(17)	4.6(5)
H(22)	0.5668(17)	0.5986(17)	0.1033(16)	4.5(5)

HPAD

Of the 361 reflections with $|E| > 1{\cdot}6$, 329 were phased by hand by the symbolic addition procedure for centrosymmetric crystals (Karle & Karle, 1966). The three most likely sets of phases were used to calculate E maps of which one showed all 27 heavy atoms. Three cycles of full-matrix least-squares refinement with individual isotropic temperature factors and four cycles of block-diagonal least squares with anisotropic temperature factors ($q=1$, $r=0{\cdot}03$, $s=g=0$) reduced R_1 to 0·12. Extinction effects were apparent, so two refinement cycles in which only K and g varied were computed. A three-dimensional difference electron density map revealed all 26 hydrogen atoms. Isotropic temperature factors (4·0 Å^2) were assigned to the hydrogen atoms and all parameters were refined for several cycles to $R_1=0{\cdot}046$. The sixty largest F's were used to refine g only ($q=2$, $r=0{\cdot}03$, $s=0$), after which several cycles in which all parameters except g varied ($q=2$, $r=0{\cdot}03$, $s=0{\cdot}04$) completed the refinement.

For the last refinement cycle, five of the 347 atomic parameters shifted more than 0·2σ and the maximum shift was 0·34σ. The final agreement indices for the 2823 observed reflections plus the 82 unobserved reflections with $|F_c| > F^*_{\text{lim}}$ are $R_1=0{\cdot}042$ and $R_2=0{\cdot}051$. The standard deviation of an observation of unit weight is 1·09. Of the 82 unobserved reflections with $|F_c| > F^*_{\text{lim}}$, none had $|F_c| > 1{\cdot}7F^*_{\text{lim}}$. A final three-dimensional difference electron density map was featureless, with resid-

Table 1. *Final atomic parameters for the non-hydrogen atoms of UPAD*

Estimated standard deviations are given in parentheses.
The anisotropic thermal parameters are in the form $\exp\left[-0{\cdot}25(h^2a^{*2}B_{11}+\cdots 2klb^*c^*B_{23})\right]$.

	x	y	z	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
O	0.44449(13)	0.52869(11)	0.19018(15)	6.97(7)	4.11(6)	11.87(10)	0.12(6)	2.36(7)	−1.24(7)
N(1)	0.39440(13)	0.35571(12)	0.21245(13)	5.81(7)	4.03(6)	6.30(7)	0.24(6)	0.41(7)	−0.39(6)
N(2)	0.44356(15)	0.25576(13)	0.20329(14)	6.80(8)	4.19(6)	6.18(8)	0.35(6)	0.71(7)	−0.11(6)
N(3)	0.66929(15)	0.40874(13)	0.12281(14)	6.61(8)	4.56(7)	5.43(7)	0.54(7)	1.06(6)	0.16(6)
N(4)	0.87079(15)	0.78560(13)	0.00873(16)	5.96(8)	5.00(6)	8.39(10)	0.85(7)	1.20(8)	1.45(7)
C(1)	0.62346(21)	0.18114(18)	0.15363(20)	8.48(12)	4.60(9)	8.46(12)	1.33(9)	2.86(10)	0.80(9)
C(2)	0.54447(18)	0.26996(15)	0.17039(16)	6.69(10)	4.39(8)	5.13(9)	0.49(8)	0.83(8)	−0.00(7)
C(3)	0.57074(17)	0.37951(15)	0.15364(16)	6.23(9)	4.24(8)	5.15(8)	0.40(7)	0.55(7)	−0.19(7)
C(4)	0.46527(18)	0.43523(15)	0.18430(17)	5.99(10)	4.01(8)	6.62(10)	0.02(7)	0.34(8)	−0.78(7)
C(5)	0.28412(17)	0.36328(15)	0.25175(17)	5.47(9)	4.83(8)	5.81(9)	−0.40(7)	−0.15(8)	−1.06(7)
C(6)	0.23810(19)	0.27829(17)	0.30526(19)	6.28(10)	5.09(9)	7.63(11)	−0.82(8)	0.19(9)	−0.84(9)
C(7)	0.13104(20)	0.28676(20)	0.34597(23)	6.45(11)	6.60(12)	9.89(15)	−1.46(10)	1.15(11)	−1.14(11)
C(8)	0.07069(21)	0.37786(22)	0.33354(24)	5.83(11)	8.07(14)	11.12(15)	−1.07(11)	1.15(11)	−2.29(13)
C(9)	0.11646(21)	0.46176(21)	0.27956(25)	6.10(11)	6.55(12)	11.10(16)	0.26(10)	0.15(12)	−1.51(12)
C(10)	0.22214(18)	0.45500(17)	0.23777(22)	5.63(10)	5.40(10)	8.70(13)	0.21(9)	0.17(10)	−0.56(10)
C(11)	0.71037(18)	0.50632(15)	0.09805(17)	6.22(9)	4.31(8)	5.18(8)	0.65(7)	0.77(7)	0.08(7)
C(12)	0.64987(18)	0.60048(16)	0.08391(18)	5.47(9)	5.03(9)	6.69(10)	0.53(8)	0.29(8)	0.38(8)
C(13)	0.70223(18)	0.69057(16)	0.05300(18)	5.81(9)	4.57(8)	6.97(10)	1.07(8)	0.27(8)	0.62(8)
C(14)	0.81984(17)	0.69517(15)	0.03787(17)	5.78(9)	4.64(8)	5.85(9)	0.66(8)	0.74(8)	0.42(7)
C(15)	0.88092(18)	0.60067(17)	0.05426(19)	5.99(10)	5.23(9)	7.77(11)	1.27(8)	1.81(8)	1.19(9)
C(16)	0.82667(19)	0.51069(16)	0.08118(18)	6.77(10)	4.62(8)	7.13(10)	1.43(8)	1.95(8)	0.84(8)
C(17)	0.76424(26)	0.95080(23)	0.06711(26)	9.86(17)	6.81(14)	11.26(18)	1.43(12)	0.89(15)	−1.36(13)
C(18)	0.80554(20)	0.87872(17)	−0.02829(20)	7.44(12)	4.92(9)	8.02(12)	0.87(9)	0.56(10)	0.98(9)
C(19)	0.99728(21)	0.79744(19)	0.01243(22)	7.31(12)	6.34(12)	8.17(13)	−0.18(10)	0.34(11)	1.24(10)
C(20)	1.04368(24)	0.77729(24)	−0.09798(25)	9.03(16)	8.57(16)	9.84(16)	0.92(14)	1.61(14)	1.37(13)

Table 3. *Observed and calculated structure factors for UPAD*

The column headings are k, l, $10F_o$*, and $10|F_c|$.
* denotes unobserved reflections.
\+ denotes observed reflection omitted from least squares.

***** H= 0 *****			
0	2	197	211
0	4	24	24
0	6	80	86
0	8	137	148
0	10	14	20
0	12	18	19
0	14	13	13
1	1	528	526
1	2	144	147
1	3	497	511
1	4	588	619
1	5	145	170
1	6	182	191
1	7	177	183
1	8	99	99
1	9	15	11
1	10	15	1
1	11	15	20
1	12	13*	1
1	13	12*	7
1	14	11*	6
2	0	357	387
2	1	946	875
2	2	273	296
2	3	781	809
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4	-8	19	23
4	9	20	19
4	-9	12*	2
4	-10	11*	9
5	0	68	71
5	1	160	158
5	-1	117	125
5	2	172	173
5	-2	150	154
5	3	30	29
5	-3	150	147
5	4	85	85
5	-4	139	138
5	5	47	49
5	-5	14*	13
5	6	13*	5
5	-6	71	70
5	7	21	22
5	-7	13*	16
5	8	12*	10
5	-8	37	38
5	9	11*	1
5	-9	12*	13
5	-10	11*	1
6	0	14*	9
6	1	87	89
6	-1	101	105
6	2	76	81
6	-2	147	143
6	3	13*	15
6	-3	128	130
6	4	53	47
6	-4	145	137
6	5	34	33
6	-5	76	74
6	6	34	33
6	-6	46	42
6	7	29	25
6	-7	20	21
6	8	17	13
6	-8	12*	3
6	-9	14	11
7	0	97	95
7	1	47	49
7	-1	45	41
7	2	62	58
7	-2	130	131
7	3	13*	6
7	-3	26	21
7	4	24	18
7	-4	31	31
7	5	78	75
7	-5	63	64
7	6	43	42
7	-6	28	21
7	7	12*	9
7	-7	35	37
7	8	11*	1
7	-8	12*	5
8	0	34	40
8	1	30	35
8	-1	18	16
8	2	13*	1
8	-2	54	49
8	3	32	31
8	-3	35	30
8	4	59	57
8	-4	23	29
8	5	41	40
8	-5	12*	2
8	6	12*	0
8	-6	33	33
8	7	27	31
8	-7	19	21
8	-8	13	15
9	0	13*	4
9	1	25	24
9	-1	16	13
9	2	14	9
9	-2	12*	11
9	3	16	16
9	-3	18	18
9	4	44	45
9	-4	12*	10
9	5	12*	8
9	-5	12*	10
9	6	12*	17
9	-6	12*	8
9	-7	17	18
10	0	12*	8
10	1	16	19
10	-1	12*	7
10	2	19	12
10	-2	12*	16
10	3	12*	6
10	-3	22	18
10	4	13	12
10	-4	26	21
10	-5	15	7
11	0	14	9
11	1	11*	9
11	-1	12*	9
11	2	12	11
11	-2	36	35
11	-3	19	18
***** H=10 *****			
0	0	30	28
0	2	101	98
0	-2	37	47
0	4	64	57
0	-4	96	105
0	6	35	39
0	-6	54	55
0	8	40	37
0	-8	15	22
0	-10	49	42
1	0	13*	4
1	1	18	21
1	-1	40	40
1	2	14*	15
1	-2	47	39
1	3	17	20
1	-3	28	28
1	4	13*	0
1	-4	47	38
1	5	64	63
1	-5	32	38
1	6	13*	14
1	-6	40	41
1	7	13*	9
1	-7	29	30
1	8	21	23
1	-8	12*	10
1	9	11*	14
1	-9	13*	17
1	-10	11*	4
2	0	23	24
2	1	18	24
2	-1	70	74
2	2	42	39
2	-2	27	29
2	3	15	8
2	-3	89	96
2	4	27	24
2	-4	17	15
2	5	13*	10
2	-5	42	42
2	6	14	17
2	-6	27	23
2	7	55	51
2	-7	13*	14
2	8	12*	14
2	-8	33	32
2	9	12	13
2	-9	12*	13
2	-10	11*	4
3	0	96	95
3	1	97	95
3	-1	74	77
3	2	84	82
3	-2	13*	2
3	3	45	43
3	-3	23	19
3	4	42	47
3	-4	35	47
3	5	33	40
3	-5	44	43
3	6	36	33
3	-6	115	115
3	7	74	68
3	-7	12*	0
3	8	19	13
3	-8	12*	8
3	-9	12*	1
4	0	88	53
4	1	68	67
4	-1	13*	6
4	2	13*	11
4	-2	127	127
4	3	60	63
4	-3	26	25
4	4	70	74
4	-4	13*	16
4	5	45	48
4	-5	30	27
4	6	27	33
4	-6	28	29
4	7	21	21
4	-7	12*	6
4	8	19	17
4	-8	14	13
4	-9	11*	7
5	0	81	80
5	1	57	54
5	-1	174	173
5	2	66	71
5	-2	26	32
5	3	35	31
5	-3	76	73
5	4	80	79
5	-4	31	30
5	5	50	49
5	-5	37	32
5	6	26	22
5	-6	16	16
5	7	26	28
5	-7	12*	9
5	8	26	26
5	-8	11*	2
5	-9	11*	8
6	0	130	127
6	1	105	103
6	-1	51	74
6	2	72	71
6	-2	71	66
6	3	14*	7
6	-3	30	26
6	4	23	26
6	-4	21	21
6	5	28	32
6	-5	40	33
6	6	12*	1
6	-6	20	17
6	7	11*	4
6	-7	12*	8
6	-8	12*	9
7	0	33	32
7	1	42	43
7	-1	35	32
7	2	44	49
7	-2	42	42
7	3	41	44
7	-3	13*	13
7	4	42	44
7	-4	40	44
7	5	28	18
7	-5	12*	5
7	6	12*	12
7	-6	22	22
7	-7	31	32
8	0	27	23
8	1	74	75
8	-1	53	55
8	2	22	23
8	-2	15	14
8	3	39	40
8	-3	48	40
8	4	14	11
8	-4	15	13
8	5	12*	8
8	-5	18	15
8	-6	18	12
9	0	19	18
9	1	12*	3
9	-1	14	9
9	2	20	18
9	-2	19	19
9	3	30	27
9	-3	12*	1
9	4	11*	11
9	-4	12*	7
9	-5	21	15
10	0	12*	8
10	1	11*	4
10	-1	15	14
10	2	25	25
10	-2	32	25
10	-3	11*	4
***** H=11 *****			
0	1	14	16
0	-1	66	77
0	3	13*	0
0	-3	84	90
0	5	29	24
0	-5	49	43
0	7	21	20
0	-7	54	56
0	-9	18	16
1	0	20	21
1	1	37	42
1	-1	59	56
1	2	21	20
1	-2	36	40
1	3	28	23
1	-3	36	30
1	4	13*	9
1	-4	43	44
1	5	21	20
1	-5	36	34
1	6	12*	6
1	-6	34	36
1	7	12*	6
1	-7	19	13
1	8	16	15
1	-8	22	23
1	-9	11*	5
2	0	69	70
2	1	49	39
2	-1	34	28
2	2	73	72
2	-2	26	25
2	3	33	34
2	-3	13*	11
2	4	13*	7
2	-4	13*	18
2	5	37	32
2	-5	27	23
2	6	12*	7
2	-6	13*	2
2	7	19	18
2	-7	12*	9
2	-8	11*	2
2	-9	16	18
3	0	24	23
3	1	13*	7
3	-1	48	58
3	2	35	35
3	-2	45	45
3	3	28	29
3	-3	75	69
3	4	69	70
3	-4	32	28
3	5	26	28
3	-5	12*	2
3	6	12*	5
3	-6	29	23
3	7	16	26
3	-7	13	6
3	-8	12*	13
4	0	14*	17
4	1	80	53
4	-1	33	32
4	2	53	47
4	-2	15	11
4	3	62	57
4	-3	62	61
4	4	19	17
4	-4	13*	3
4	5	21	19
4	-5	26	26
4	6	31	29
4	-6	12*	0
4	7	14	17
4	-7	12*	4
4	-8	16	14
5	0	37	32
5	1	31	35
5	-1	13*	5
5	2	84	88
5	-2	13*	10
5	3	13*	8
5	-3	12*	1
5	4	19	11
5	-4	22	24
5	5	21	26
5	-5	12*	1
5	6	17	10
5	-6	16	17
5	-7	13	14
6	0	12	5
6	1	20	19
6	-1	24	22
6	2	13*	18
6	-2	37	32
6	3	61	65
6	-3	15	12
6	4	33	34
6	-4	19	21
6	5	34	33
6	-5	13	11
6	-6	16	14
6	-7	14	16
7	0	12*	8
7	1	27	30
7	-1	21	22
7	2	12*	14
7	-2	23	23
7	3	45	42
7	-3	12*	4
7	4	12*	0
7	-4	25	25
7	5	21	25
7	-5	32	30
7	-6	14	15
8	0	36	33
8	1	16	13
8	-1	12*	5
8	2	58	57
8	-2	12*	10
8	3	12*	12
8	-3	16	16
8	-4	11*	9
9	0	19	18
9	1	11*	8
9	-1	11*	7
9	-2	17	10
***** H=12 *****			
0	0	86	91
0	2	37	35
0	-2	17	15
0	4	13*	14
0	-4	54	63
0	6	21	16
0	-6	12*	6
1	0	13*	10
1	1	33	36
1	-1	28	32
1	2	19	21
1	-2	51	44
1	3	24	22
1	-3	22	22
1	4	32	32
1	-4	12*	17
1	5	12*	4
1	-5	33	31
1	6	26	28
1	-6	17	17
1	-7	12*	9
2	0	13	7
2	1	13	3
2	-1	13*	13
2	2	31	32
2	-2	12*	2
2	3	49	52
2	-3	30	27
2	4	29	28
2	-4	26	18
2	5	45	40
2	-5	13*	13
2	6	12*	16
2	-6	12*	11
2	-7	15	16
3	0	12*	5
3	1	41	40
3	-1	31	25
3	2	56	53
3	-2	12*	7
3	3	12*	7
3	-3	20	15
3	4	13	9
3	-4	12*	3
3	5	14	15
3	-5	12	12
3	-6	20	20
3	-7	11*	6
4	0	42	37
4	1	12*	10
4	-1	14	9
4	2	13*	12
4	-2	39	39
4	3	16	15
4	-3	12*	4
4	4	47	51
4	-4	19	10
4	5	32	34
4	-5	25	22
4	-6	11*	5
5	0	12	9
5	1	12*	13
5	-1	20	17
5	2	17	12
5	-2	15	4
5	3	13	0
5	-3	20	22
5	4	11*	3
5	-4	21	20
5	-5	11*	8
5	-6	11*	5
6	0	12*	5
6	1	20	15
6	2	11*	9
6	-2	12*	4
6	3	11	0
6	-3	19	17
6	-4	26	25
6	-5	11*	2
7	0	27	21
7	1	11*	7
7	2	11*	5
7	-2	12*	6
7	-3	11*	10
***** H=13 *****			
0	1	12*	3
0	-1	44	49
0	3	36	38
0	-3	12*	0
0	-5	31	24
1	0	12*	2
1	1	27	18
1	-1	18	29
1	2	15	20
1	-2	15	18
1	3	22	21
1	-3	12*	18
1	4	13	10
1	-4	11*	11
1	-5	11*	4
2	0	14	13
2	1	12*	6
2	-1	12*	12
2	2	15	16
2	-2	12*	1
2	3	15	16
2	-3	12*	2
2	4	17	15
2	-4	12*	11
2	-5	13	11
3	0	11*	1
3	1	12*	1
3	-1	12*	7
3	2	12*	16
3	-2	12*	9
3	3	11*	6
3	-3	27	19
3	-4	11*	7
4	0	11*	10
4	1	34	32
4	-1	26	21
4	2	11*	7
4	-2	21	24
4	-3	11*	1
4	-4	11*	12
5	0	23	22
5	1	11*	3
5	-1	17	17
5	-2	11*	0

Table 4. *Final atomic parameters for the non-hydrogen atoms of HPAD*

Estimated standard deviations are given in parentheses.
The anisotropic thermal parameters are in the form $\exp[-0.25(h^2a^{*2}B_{11}+\cdots 2klb^*c^*B_{23})]$.

	x	y	z	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
O	0.13895(13)	0.81885(8)	0.24004(14)	5.41(5)	4.36(5)	4.98(5)	0.66(4)	-0.52(4)	-0.41(4)
N(1)	0.20806(13)	0.97428(9)	0.42754(14)	4.48(5)	3.61(5)	3.60(5)	0.45(4)	0.66(4)	0.33(4)
N(2)	0.31568(14)	1.01441(9)	0.57852(14)	4.92(5)	3.59(5)	3.69(5)	-0.08(4)	0.86(4)	0.33(4)
N(3)	0.39885(13)	0.76278(9)	0.50472(14)	3.98(5)	3.58(5)	4.13(5)	0.07(4)	0.80(4)	0.59(4)
N(4)	0.22988(16)	0.39441(9)	0.03687(16)	5.92(7)	3.17(5)	5.08(6)	-0.38(5)	0.59(5)	0.50(4)
C(1)	0.51470(20)	0.95642(12)	0.76915(20)	5.83(8)	4.32(6)	4.10(6)	-0.06(6)	0.10(6)	0.67(5)
C(2)	0.39384(16)	0.94178(10)	0.61481(17)	4.39(6)	3.43(6)	3.58(5)	-0.10(5)	1.05(5)	0.61(4)
C(3)	0.34858(16)	0.84827(10)	0.48820(17)	3.96(5)	3.39(5)	3.67(5)	0.14(5)	0.96(4)	0.56(4)
C(4)	0.22037(17)	0.87348(11)	0.36426(18)	4.31(6)	3.45(6)	3.81(6)	0.22(5)	0.88(5)	0.25(5)
C(5)	0.10119(17)	1.03790(11)	0.36665(17)	4.64(6)	4.03(6)	3.99(5)	0.88(5)	1.71(5)	1.08(4)
C(6)	0.10233(23)	1.13583(13)	0.45731(22)	8.15(10)	4.57(7)	4.67(7)	1.95(7)	1.04(7)	0.42(6)
C(7)	-0.00374(25)	1.19743(14)	0.39754(25)	9.52(11)	5.20(8)	6.16(9)	3.17(8)	1.85(8)	0.78(7)
C(8)	-0.10727(21)	1.16458(14)	0.25053(22)	6.57(8)	6.72(8)	6.02(8)	2.82(7)	2.31(7)	2.41(6)
C(9)	-0.10862(20)	1.06809(14)	0.16265(23)	5.22(8)	6.56(8)	6.07(8)	1.47(7)	0.95(7)	1.66(7)
C(10)	-0.00572(20)	1.00411(13)	0.21928(22)	5.20(7)	4.91(7)	5.21(7)	1.00(6)	0.62(6)	0.85(6)
C(11)	0.36315(15)	0.67275(10)	0.38118(17)	3.49(5)	3.16(5)	4.09(6)	0.23(4)	0.57(5)	0.67(4)
C(12)	0.36987(15)	0.66205(10)	0.21405(18)	3.80(6)	3.16(5)	4.25(6)	0.31(5)	0.85(5)	0.86(4)
C(13)	0.33192(17)	0.56869(10)	0.10465(18)	4.36(6)	3.44(6)	4.09(6)	0.30(5)	0.92(5)	0.80(4)
C(14)	0.28190(16)	0.48349(10)	0.15174(19)	3.92(6)	3.14(5)	4.80(6)	0.32(5)	0.51(5)	0.72(5)
C(15)	0.29082(17)	0.49433(10)	0.32229(18)	4.43(6)	3.34(5)	5.04(6)	0.20(5)	0.97(5)	1.44(4)
C(16)	0.33359(16)	0.58559(11)	0.43620(18)	3.84(6)	3.73(6)	4.25(6)	0.47(5)	0.75(5)	1.16(4)
C(17)	0.07504(22)	0.43132(15)	-0.21836(25)	5.90(9)	5.83(8)	6.32(9)	0.19(8)	0.09(8)	1.05(7)
C(18)	0.21533(20)	0.38602(12)	-0.14012(21)	5.63(8)	3.81(6)	5.26(8)	0.31(6)	0.78(6)	0.06(6)
C(19)	0.14818(19)	0.31270(12)	0.07884(23)	5.13(8)	3.69(6)	6.68(9)	-0.56(6)	0.53(7)	0.85(6)
C(20)	0.24720(23)	0.23064(13)	0.11374(27)	6.40(9)	4.48(7)	9.95(11	0.23(7)	1.59(9)	2.81(7)
C(21)	0.42726(19)	0.74698(11)	0.15127(19)	5.85(7)	3.61(6)	4.89(6)	-0.13(6)	1.78(5)	0.94(5)
C(22)	0.33894(20)	0.59290(12)	0.61623(20)	6.28(8)	4.95(7)	4.64(6)	0.40(7)	1.41(6)	1.67(5)

ual electron densities between -0.15 and $+0.18$ e.Å^{-3} and verified the structure. The final positional and thermal parameters, with standard deviations estimated from the least-squares process, are given in Tables 4 and 5. The average standard deviations of the positional parameters, expressed in Å, are 0·0012 for nitrogen and oxygen (range: 0·0011 to 0·0015), 0·0017 for carbon (range: 0·0014 to 0·0023), and 0·019 for hydrogen (range: 0·015 to 0·023). Two other parameters that were refined are the scale factor, $K=0.1647$, and the extinc-

Table 5. *Final atomic parameters for the hydrogen atoms of HPAD*

Estimated standard deviations are given in parentheses.

	x	y	z	B
H(1)	0.6078(22)	0.9329(15)	0.7406(23)	5.6(5)
H(2)	0.5169(21)	1.0276(14)	0.8392(22)	5.2(5)
H(3)	0.4943(20)	0.9087(14)	0.8325(20)	4.3(4)
H(4)	0.1833(20)	1.1604(14)	0.5640(21)	4.6(4)
H(5)	0.0020(22)	1.2655(15)	0.4583(24)	5.9(5)
H(6)	-0.1816(20)	1.2174(13)	0.2090(21)	4.3(4)
H(7)	-0.1855(22)	1.0405(15)	0.0548(24)	6.2(5)
H(8)	-0.0084(21)	0.9350(14)	0.1569(22)	5.0(5)
H(9)	0.0733(22)	0.4260(15)	-0.3393(23)	5.6(5)
H(10)	-0.0198(24)	0.3919(16)	-0.2103(24)	6.3(5)
H(11)	0.0773(21)	0.5063(14)	-0.1572(22)	5.0(5)
H(12)	0.3067(17)	0.4203(11)	-0.1592(18)	2.8(3)
H(13)	0.2102(19)	0.3110(12)	-0.1893(20)	3.5(4)
H(14)	0.1009(18)	0.3413(12)	0.1848(19)	3.8(4)
H(15)	0.0590(19)	0.2847(12)	-0.0193(19)	3.1(4)
H(16)	0.2749(24)	0.1985(17)	0.0067(26)	7.3(6)
H(17)	0.3318(24)	0.2575(16)	0.2206(26)	7.0(6)
H(18)	0.1849(21)	0.1738(14)	0.1330(22)	4.8(5)
H(19)	0.3387(16)	0.5639(11)	-0.0104(17)	2.3(3)
H(20)	0.2682(16)	0.4362(11)	0.3655(18)	2.5(3)
H(21)	0.4206(23)	0.6441(15)	0.6949(25)	6.0(5)
H(22)	0.3542(22)	0.5257(15)	0.6464(23)	5.8(5)
H(23)	0.2439(23)	0.6150(15)	0.6486(24)	6.2(5)
H(24)	0.4786(18)	0.7183(12)	0.0617(20)	3.8(4)
H(25)	0.4958(18)	0.7995(12)	0.2417(19)	3.4(4)
H(26)	0.3442(18)	0.7802(12)	0.0985(19)	3.4(4)

tion coefficient, $g = 3{\cdot}89 \times 10^{-5}$. The final values of the observed and calculated structure factors are compared in Table 6. The largest structure factors are somewhat overcorrected for extinction effects.

Description and discussion of the structures

Stereoscopic views (Johnson, 1965) of the molecules are given in Figs. 2 and 3. Intramolecular distances and angles, uncorrected for thermal motion, are shown in Figs. 4 and 5. The cell parameter errors and the coordinate standard deviations obtained from the least-squares refinement were used to calculate the estimated standard deviations tabulated in Table 7 for the distances and angles.

In both molecules the *p*-phenylenediamine ring is *syn* to the carbonyl group, in agreement with the predictions of Brown *et al.* (1951) and Smith (1964) and the nuclear magnetic resonance results of Pauwels (1967). Neither molecule is planar but the intramolecular overcrowding due to the added methyl groups has caused HPAD to deviate considerably more from planarity than the comparatively uncrowded UPAD. The molecules can be divided into five relatively planar regions shown in Fig. 6. The equations of these planes and the deviations of various atoms from them are given in Tables 8 and 9. All of these regions are reasonably planar except for *D* and *E* of HPAD, which depart systematically from planarity. In plane *E* (HPAD), N(4) is 0·12 Å out of the plane of its neighbors. Plane *D* (HPAD) can be divided into two planes, *F* and *G*, as though the *p*-phenylenediamine phenyl were creased at C(11) and C(14). The substituent atoms N(3), C(1), C(5), and O of plane *B* of both molecules are systematically on one side of the plane.

The dihedral angles between the planes are compared in Table 10 for the two molecules. These angles represent mostly twists about bonds but do include some bending as well. UPAD and HPAD have similar intramolecular steric requirements at the ends of the molecules. The difference in the dihedral angles between the 1-phenyl group and the pyrazolinone ring, the *A*–*B* angles, is probably determined by the molecular packing. On the other hand, the similarity of the *D*–*E* angles (11·9 and 11·6°) probably arises from a balance between the relatively high C(14)–N(4) bond order and the intramolecular steric interaction of H(19) and H(20) with the ethyl groups. The conformation of the central portion of the molecules is determined by the substituent on C(12). When this is methyl, as in HPAD, severe overcrowding results and the dihedral angle between

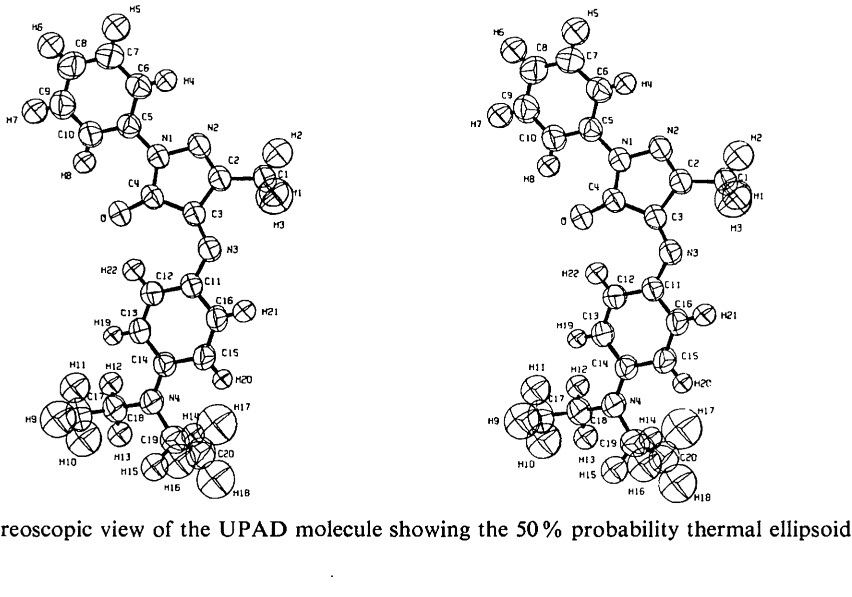

Fig. 2. Stereoscopic view of the UPAD molecule showing the 50% probability thermal ellipsoids.

Table 6. *Observed and calculated structure factors for HPAD*

The column headings are k, l, $10F_o$*, and $10|F_c|$.
* denotes unobserved reflections.

***** H= 0 *****

k	l	$10F_o$	$10\lvert F_c\rvert$
1	0	180	192
2	0	327	353
3	0	74	76
4	0	133	129
5	0	452	435
6	0	103	103
7	0	86	86
8	0	9*	6
9	0	56	51
10	0	11	4
11	0	182	179
12	0	90	87
13	0	20	20
14	0	30	28
15	0	10*	9
0	1	361	370
1	1	440	464
1	-1	748	689
2	1	505	527
2	-1	203	220
3	1	33	32
3	-1	167	177
4	1	193	200
4	-1	161	176
5	1	287	282
5	-1	114	110
6	1	252	252
6	-1	54	54
7	1	153	149
7	-1	53	55
8	1	46	44
8	-1	76	73
9	1	66	64
9	-1	9*	0
10	1	183	122
10	-1	26	29
11	1	16	20
11	-1	123	124
12	1	91	93
12	-1	115	115
13	1	54	57
13	-1	11*	13
14	1	12	10
14	-1	31	30
15	1	20	21
15	-1	10*	7
0	2	84	58
1	2	41	41
1	-2	73	70
2	2	251	254
2	-2	31	31
3	2	101	110
3	-2	10	13
4	2	234	234
4	-2	165	163
5	2	151	140
5	-2	34	31
6	2	73	66
6	-2	285	282
7	2	47	44
7	-2	240	238
8	2	127	126
8	-2	56	39
9	2	12	7
9	-2	87	88
10	2	61	62
10	-2	91	94
11	2	120	127
11	-2	16	15
12	2	10*	4
12	-2	75	72
13	2	16	9
13	-2	126	125
14	2	18	17
14	-2	36	33
15	-2	34	33
16	-2	9	9
0	3	323	333
1	3	238	229
1	-3	61	63
2	3	125	121
2	-3	106	105
3	3	140	142
3	-3	42	42
4	3	9*	8
4	-3	226	234
5	3	14	13
5	-3	137	139
6	3	10*	12
6	-3	101	103
7	3	24	22
7	-3	40	40
8	3	25	27
8	-3	190	182
9	3	65	60
9	-3	162	164
10	3	122	128
10	-3	30	32
11	3	10*	4
11	-3	30	28
12	3	10*	0
12	-3	133	128
13	3	16	16
13	-3	81	79
14	-3	52	51
15	-3	16	17
16	-3	9*	6
0	4	145	140
1	4	20	20
1	-4	219	210
2	4	20	23
2	-4	418	406
3	4	165	157
3	-4	86	84
4	4	55	55
4	-4	53	54
5	4	69	65
5	-4	89	89
6	4	11	8
6	-4	203	197
7	4	11*	14
7	-4	115	111
8	4	65	62
8	-4	97	92
9	4	14	15
9	-4	10*	6
10	4	60	61
10	-4	28	26
11	4	24	23
11	-4	90	92
12	4	13	7
12	-4	40	38
13	-4	115	117
14	-4	32	31
15	-4	9*	3
0	5	199	194
1	5	78	76
1	-5	169	163
2	5	173	166
2	-5	143	139
3	5	191	193
3	-5	146	148
4	5	23	26
4	-5	9*	5
5	5	149	154
5	-5	11	9
6	5	95	93
6	-5	25	22
7	5	106	105
7	-5	112	110
8	5	38	41
8	-5	64	66
9	5	10*	11
9	-5	32	31
10	5	13	4
10	-5	41	39
11	5	9*	5
11	-5	10*	4
12	-5	35	33
13	-5	78	76
14	-5	13	13
15	-5	9*	4
0	6	67	66
1	6	78	76
1	-6	83	81
2	6	10*	7
2	-6	75	75
3	6	158	156
3	-6	16	17
4	6	15	2
4	-6	10*	8
5	6	186	185
5	-6	10*	9
6	6	141	141
6	-6	68	71
7	6	33	33
7	-6	109	107
8	6	10*	4
8	-6	244	249
9	6	16	12
9	-6	70	71
10	-6	50	48
11	-6	11	1
12	-6	10*	3
13	-6	27	24
14	-6	14	16
0	7	47	48
1	7	33	33
1	-7	11*	10
2	7	70	72
2	-7	16	18
3	7	10*	7
3	-7	23	15
4	7	59	57
4	-7	26	20
5	7	52	51
5	-7	14	8
6	7	12	10
6	-7	73	72
7	7	10*	5
7	-7	16	11
8	7	46	42
8	-7	11*	3
9	-7	32	30
10	-7	50	51
11	-7	49	51
12	-7	16	17
13	-7	9*	10
0	8	68	68
1	8	11*	5
1	-8	38	39
2	8	26	24
2	-8	55	58
3	8	57	58
3	-8	10*	7
4	8	18	19
4	-8	72	75
5	8	23	24
5	-8	10*	7
6	-8	34	34
7	-8	12	10
8	-8	48	48
9	-8	61	60
10	-8	69	69
11	-8	45	43
12	-8	14	15
0	9	10*	2
1	9	9*	3
1	-9	15	12
2	9	37	36
2	-9	25	28
3	-9	43	44
4	-9	21	19
5	-9	60	61
6	-9	55	54
7	-9	55	53
8	-9	27	30
9	-9	38	39

***** H= 1 *****

k	l	$10F_o$	$10\lvert F_c\rvert$
0	0	37	40
1	0	601	581
-1	0	10	6
2	0	309	326
-2	0	239	250
3	0	89	92
-3	0	295	309
4	0	172	171
-4	0	81	84
5	0	43	61
-5	0	173	186
6	0	163	167
-6	0	199	197
7	0	162	163
-7	0	14	13
8	0	24	24
-8	0	108	107
9	0	59	61
-9	0	16	26
10	0	156	158
-10	0	29	31
11	0	77	76
-11	0	231	231
12	0	11*	3
-12	0	122	124
13	0	10*	5
-13	0	16	15
14	0	26	26
-14	0	40	38
15	0	9*	2
-15	0	9*	3
0	1	247	262
0	-1	678	634
1	1	588	606
1	-1	498	502
-1	1	658	679
-1	-1	54	58
2	1	336	345
2	-1	177	156
-2	1	75	75
-2	-1	290	302
3	1	361	370
3	-1	323	337
-3	1	213	227
-3	-1	294	312
4	1	173	163
4	-1	299	304
-4	1	163	162
-4	-1	35	34
5	1	233	237
5	-1	187	194
-5	1	8*	2
-5	-1	85	85
6	1	226	225
6	-1	40	37
-6	1	126	130
-6	-1	236	238
7	1	88	93
7	-1	43	41
-7	1	41	39
-7	-1	169	166
8	1	47	44
8	-1	90	87
-8	1	30	27
-8	-1	89	90
9	1	57	58
9	-1	72	72
-9	1	44	43
-9	-1	10*	1
10	1	47	46
10	-1	28	27
-10	1	97	94
-10	-1	10*	7
11	1	11*	6
11	-1	172	168
-11	1	39	37
-11	-1	28	28
12	1	104	103
12	-1	204	201
-12	1	77	76
-12	-1	29	27
13	1	33	37
13	-1	17	16
-13	1	193	194
-13	-1	12	11
14	1	10	12
14	-1	10*	2
-14	1	16	17
-14	-1	26	22
15	-1	9*	7
-15	1	14	16
-15	-1	27	28
0	2	243	252
0	-2	144	155
1	2	35	37
1	-2	285	293
-1	2	284	297
-1	-2	85	89
2	2	94	97
2	-2	293	308
-2	2	117	119
-2	-2	13	3
3	2	169	164
3	-2	231	234
-3	2	126	131
-3	-2	67	70
4	2	234	244
4	-2	209	217
-4	2	91	87
-4	-2	50	50
5	2	140	145
5	-2	216	226
-5	2	440	442
-5	-2	382	383
6	2	46	45
6	-2	147	151
-6	2	97	98
-6	-2	27	27
7	2	26	25
7	-2	222	223
-7	2	114	122
-7	-2	9*	0
8	2	47	49
8	-2	28	22
-8	2	25	30
-8	-2	19	16
9	2	11*	11
9	-2	60	57
-9	2	91	90
-9	-2	33	31
10	2	26	30
10	-2	12	11
-10	2	92	89
-10	-2	28	23
11	2	34	32
11	-2	98	96
-11	2	107	106
-11	-2	50	53
12	2	73	73
12	-2	45	45
-12	2	115	117
-12	-2	16	18
13	2	53	56
13	-2	14	17
-13	2	69	70
-13	-2	10*	7
14	2	10*	11
14	-2	10	8
-14	2	28	30
-14	-2	12	16
15	-2	34	33
-15	2	16	17
-16	2	13	12
0	3	157	158
0	-3	276	279
1	3	97	103
1	-3	84	90
-1	3	322	325
-1	-3	217	218
2	3	156	161
2	-3	263	263
-2	3	100	106
-2	-3	142	149
3	3	8*	10
3	-3	25	24
-3	3	23	25
-3	-3	127	130
4	3	167	165
4	-3	22	20
-4	3	84	83
-4	-3	100	106
5	3	34	36
5	-3	35	33
-5	3	204	203
-5	-3	31	25
6	3	42	44
6	-3	188	186
-6	3	105	101
-6	-3	28	34
7	3	140	143
7	-3	172	170
-7	3	29	24
-7	-3	30	29
8	3	30	30
8	-3	39	42
-8	3	149	141
-8	-3	33	32
9	3	11*	1
9	-3	42	41
-9	3	93	89
-9	-3	77	75
10	3	51	59
10	-3	26	21
-10	3	18	14
-10	-3	87	88
11	3	81	80
11	-3	47	48
-11	3	34	31
-11	-3	126	132
12	3	10*	12
12	-3	10*	0
-12	3	49	47
-12	-3	10*	14
13	3	25	23
13	-3	25	27
-13	3	10*	2
-13	-3	10*	2
14	-3	59	60
-14	3	16	13
15	-3	74	71
-15	3	9*	3
0	4	9*	11
0	-4	130	129
1	4	74	71
1	-4	142	136
-1	4	136	138
-1	-4	124	127
2	4	75	79
2	-4	146	140
-2	4	136	135
-2	-4	31	37
3	4	183	179
3	-4	161	155
-3	4	133	129
-3	-4	111	109
4	4	92	91
4	-4	86	93
-4	4	39	37
-4	-4	47	48
5	4	61	61
5	-4	46	48
-5	4	110	115
-5	-4	22	21
6	4	75	75
6	-4	37	44
-6	4	12	9
-6	-4	73	79
7	4	92	90
7	-4	193	197
-7	4	44	42
-7	-4	22	27
8	4	45	48
8	-4	9*	6
-8	4	35	34
-8	-4	10*	4
9	4	59	62
9	-4	20	21
-9	4	72	72
-9	-4	20	26
10	4	55	55
10	-4	49	47
-10	4	16	15
-10	-4	107	113
11	4	38	37
11	-4	51	56
-11	4	55	53
-11	-4	10*	4
12	4	32	33
12	-4	34	32
-12	4	74	73
-12	-4	38	40
13	-4	52	51
-13	4	71	71
14	-4	85	88
-14	4	25	26
15	-4	12	13
-15	4	10	9
0	5	10*	7
0	-5	122	121
1	5	78	76
1	-5	53	46
-1	5	16	18
-1	-5	35	34
2	5	10*	1
2	-5	89	85
-2	5	10	8
-2	-5	10*	4
3	5	145	145
3	-5	37	36
-3	5	166	162
-3	-5	83	80
4	5	225	224
4	-5	58	57
-4	5	69	69
-4	-5	91	91
5	5	11*	1
5	-5	56	55
-5	5	107	107
-5	-5	259	263
6	5	79	80
6	-5	139	138
-6	5	32	32
-6	-5	13	15
7	5	59	61
7	-5	35	38
-7	5	54	52
-7	-5	39	35
8	5	40	37
8	-5	54	57
-8	5	126	127
-8	-5	10*	1
9	5	42	38
9	-5	79	80
-9	5	82	80
-9	-5	16	16
10	5	11	11
10	-5	42	47
-10	5	31	31
-10	-5	12	14
11	-5	50	50
-11	5	33	34
-11	-5	9*	1
12	-5	70	72
-12	5	12	9
13	-5	44	47
-13	5	36	35
14	-5	33	36
-14	5	72	72
15	-5	14	15
-15	5	14	15
0	6	38	37
0	-6	59	53
1	6	11*	3
1	-6	10*	6
-1	6	23	20
-1	-6	35	37
2	6	196	194
2	-6	75	77
-2	6	67	64
-2	-6	41	38
3	6	11*	9
3	-6	39	36
-3	6	21	20
-3	-6	240	242
4	6	30	31
4	-6	17	13
-4	6	24	24
-4	-6	154	157
5	6	13	10
5	-6	83	86
-5	6	48	47
-5	-6	22	20
6	6	88	92
6	-6	10	12
-6	6	39	38
-6	-6	10*	5
7	6	29	33
7	-6	34	37
-7	6	94	94
-7	-6	18	19
8	6	9*	8
8	-6	103	106
-8	6	71	71
-8	-6	43	40
9	6	9	5
9	-6	47	47
-9	6	36	35
-9	-6	11	13
10	-6	35	36
-10	6	23	19
-10	-6	15	12
11	-6	13	10
-11	6	15	14
12	-6	53	52
-12	6	22	24
13	-6	14	13
-13	6	24	24
14	-6	15	10
-14	6	24	23
0	7	17	18
0	-7	29	29
1	7	30	30
1	-7	56	59
-1	7	80	80
-1	-7	28	26
2	7	106	104
2	-7	18	21
-2	7	24	26
-2	-7	10*	4
3	7	26	27
3	-7	11	14
-3	7	42	45
-3	-7	49	50
4	7	10*	0
4	-7	12	1
-4	7	24	22
-4	-7	70	68
5	7	16	10
5	-7	66	65
-5	7	71	73
-5	-7	64	68
6	7	10*	5
6	-7	37	40
-6	7	11*	11
-6	-7	23	22
7	7	16	14
7	-7	41	57
-7	7	80	78
-7	-7	32	28
8	-7	100	98
-8	7	63	64
-8	-7	16	11
9	-7	105	104
-9	7	93	90
10	-7	11*	7
-10	7	74	74
11	-7	52	51
-11	7	12	9
12	-7	16	15
13	-7	9*	6
-13	7	9*	4
0	8	18	18
0	-8	70	70
1	8	52	54
1	-8	29	28
-1	8	15	17
-1	-8	81	78
2	8	22	22
2	-8	33	35
-2	8	10*	5
-2	-8	30	30
3	8	10*	2
3	-8	27	36
-3	8	26	26
-3	-8	10*	6
4	8	30	28
4	-8	10*	6
-4	8	15	15
-4	-8	42	42
5	-8	18	13
-5	8	75	76
-5	-8	12	16
6	-8	11	4
-6	8	81	80
-6	-8	9*	12
7	-8	14	10
-7	8	10*	8
8	-8	15	17
-8	8	17	14
9	-8	23	23
-9	8	10*	3
10	-8	25	26
-10	8	10*	1
11	-8	15	15
-11	8	29	29
12	-8	20	19
0	9	9*	2
0	-9	36	37
1	9	23	20
1	-9	19	22
-1	9	10*	3
-1	-9	47	45
2	-9	29	28
-2	9	20	22
-2	-9	9*	1
3	-9	16	11
-3	9	10*	2
-3	-9	33	28
4	-9	10*	6
-4	9	18	23
5	-9	10*	3
-5	9	10*	0
6	-9	10*	5
-6	9	23	21
7	-9	35	38
-7	9	9*	6
8	-9	55	52
-8	9	9*	10
9	-9	18	15
10	-9	12	11

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-8	-7	10	8
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12	-7	13	10
13	-7	9*	5
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1	8	17	14
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10	-8	10*	4
11	-8	41	39
12	-8	9*	8
0	-9	10*	4
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-1	-9	9*	6
2	-9	10*	4
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3	-9	20	18
-3	-9	26	28
4	-9	10*	11
5	-9	14	16
6	-9	27	24
7	-9	10*	3
8	-9	12	10
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12	0	101	99
-12	0	37	36
13	0	12	12
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-8	1	42	46
-8	-1	134	136
9	1	33	28
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8	3	86	86
8	-3	121	121
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10	-7	24	24
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11	-7	41	39
12	-7	9*	5
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10	-8	20	24
11	-8	51	49
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7	-9	18	14
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9	-9	14	13

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6	0	93	97
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7	0	54	52
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11	0	48	45
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12	0	21	16
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13	0	19	19
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3	-1	76	76
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10	1	41	43
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Table 6 (*cont.*)

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5	-3	11*	12
-5	3	29	30
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6	-3	27	27
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7	-3	44	43
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9	-3	10*	2
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10	-3	9*	7
0	4	10*	9
0	-4	51	49
1	4	16	17
1	-4	35	35
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-1	-4	14	9
2	4	9*	2
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-2	4	10*	2
-2	-4	55	57
3	-4	12	8
-3	4	39	38
-3	-4	14	9
4	-4	10*	9
-4	4	11	11
-4	-4	33	33
5	-4	10*	3
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-6	4	10*	2
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-7	4	15	14
-7	-4	51	50
8	-4	23	24
-8	-4	66	67
9	-4	28	27
-9	-4	17	19
10	-4	26	27
0	-5	10*	10
1	-5	22	25
-1	-5	42	41
2	-5	15	12
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3	-5	61	61
-3	-5	21	19
4	-5	35	31
-4	-5	11*	12
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9	-5	11	13
0	-6	26	27
1	-6	11	16
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-5	-6	9*	3
6	-6	10*	2
-6	-6	47	50
7	-6	36	36
8	-6	15	17
9	-6	9*	13
0	-7	43	43
1	-7	10*	2
-1	-7	26	24
2	-7	10*	6
-2	-7	31	32
3	-7	42	41
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4	-7	11	8
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5	-7	96	103
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0	-8	55	57
1	-8	33	32
2	-8	15	12
3	-8	9*	10
4	-8	39	41
***** H= 9 *****			
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-3	0	13	11
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1	1	29	27
1	-1	51	48
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2	1	11*	9
2	-1	31	35
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-2	-1	48	49
3	1	10*	0
3	-1	10*	9
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4	1	15	17
4	-1	12	14
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-5	-1	11*	11
6	-1	10*	2
-6	1	39	42
-6	-1	47	46
7	-1	42	41
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-8	-1	28	31
-9	-1	22	22
0	2	11*	9
0	-2	39	39
1	2	36	35
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2	2	11	11
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6	-3	24	21
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8	-3	9*	0
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0	-4	41	43
1	-4	19	18
-1	-4	10*	5
2	-4	10*	4
-2	-4	16	14
3	-4	11*	10
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4	-4	17	20
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5	-4	10*	10
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6	-4	27	27
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7	-4	14	11
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8	-4	14	16
0	-5	48	49
1	-5	43	45
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2	-7	9*	5
3	-7	29	31
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-5	0	25	26
0	1	11	11
0	-1	38	36
1	1	37	39
1	-1	10*	0
-1	1	9*	9
-1	-1	23	25
2	-1	9*	5
-2	1	21	17
-2	-1	31	32
3	-1	33	32
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0	-2	19	19
1	-2	30	29
-1	-2	15	12
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5	-2	10	7
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3	-4	13	14
-3	-4	20	24
4	-4	12	15
-4	-4	9*	9
5	-4	9*	8
0	-5	25	25
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2	-5	49	47
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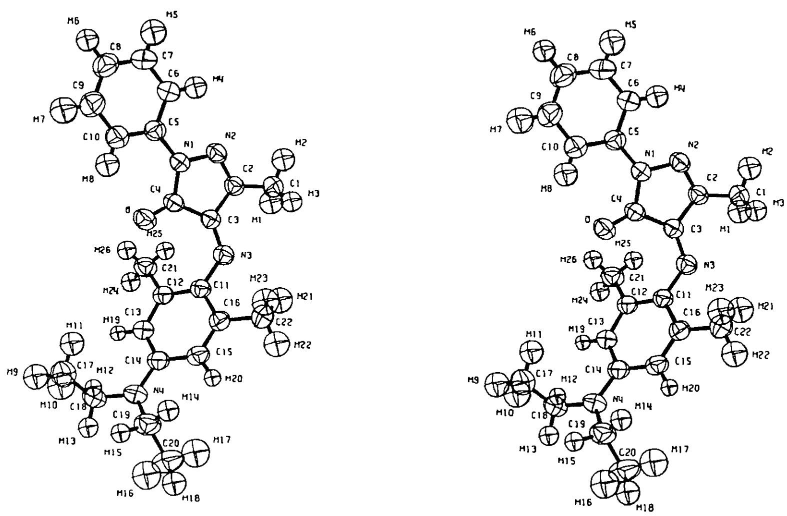
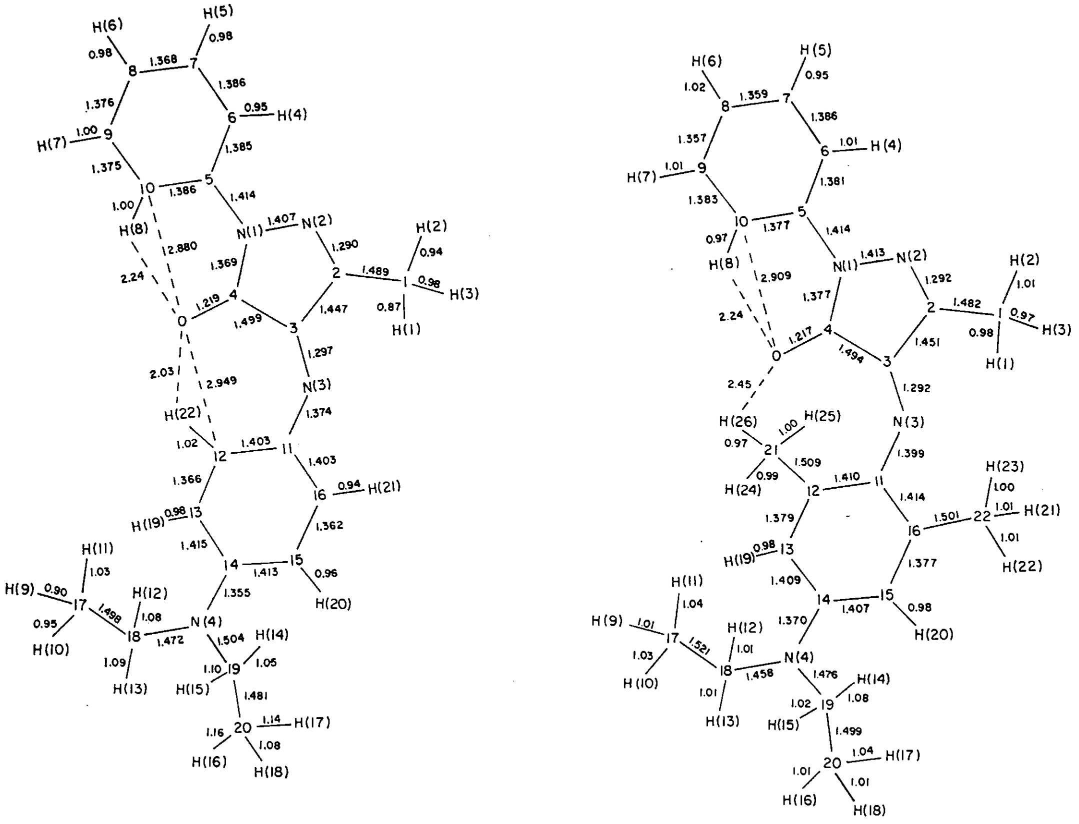


Fig. 3. Stereoscopic view of the HPAD molecule showing the 50% probability thermal ellipsoids.

the *p*-phenylenediamine and the pyrazolinone rings, the *B–D* angle, is 56·6°. When the substituent is hydrogen, as in UPAD, the overcrowding is much less severe but is still sufficient to result in a *B–D* angle equal to 13·9°. As will be seen below, this angle in UPAD is also influenced by the formation of an intramolecular C–H···O hydrogen bond. It is important to notice from the comparison of planes *B*, *C*, and *D* that the *B–D* dihedral angle is composed primarily of a twist at the *N*-phenyl bond with a much smaller twist at the *N*-pyrazolinyl bond. The *B–D* angles found here are close to those found for two similar molecules: 55° for the crowded *anti*-2,6-dimethyl-4-chloro-*N*-methylbenzaldoxime (III) (Jensen & Jerslev, 1969), and 5° for the uncrowded *anti*-4-chloro-*N*-methylbenzaldoxime (IV) (Folting, Lipscomb & Jerslev, 1964).

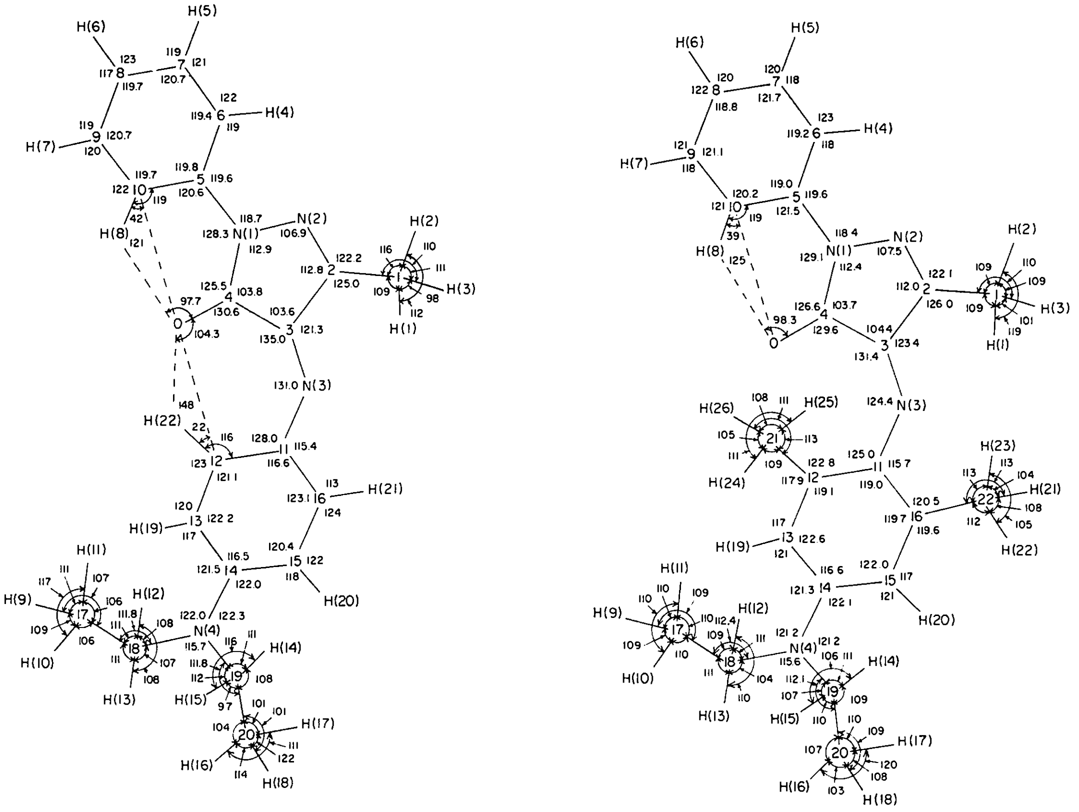


(I) (II)

Fig. 4. Intramolecular distances. Molecule (I) is UPAD, (II) is HPAD.

Table 7. *Estimated standard deviations for bond distances and angles*

	Molecule	Bond or angle	Average	Range
Distances				
	UPAD	Heavy–Heavy	0·003 Å	0·002–0·004 Å
		Methyl C–H	0·034	0·025–0·044
		All other C–H	0·022	0·019–0·025
	HPAD	Heavy–Heavy	0·002	0·002–0·003
		All C–H	0·019	0·014–0·022
Angles				
	UPAD	Heavy–Heavy–Heavy	0·20°	0·16–0·26°
		Heavy–Heavy–Hydrogen		
		Methyl hydrogen atoms	1·9	1·6–2·3
		H(4)–H(8)	1·3	1·2–1·5
		All other	1·2	1·1–1·3
		H–C–H		
		Methyl	2·7	2·5–3·1
		Methylene	1·7	—
	HPAD	Heavy–Heavy–Heavy		
		C(5)–C(10) phenyl	0·19	0·17–0·20
		All other	0·14	0·13–0·15
		Heavy–Heavy–Hydrogen	1·1	0·9–1·3
		H–C–H	1·5	1·3–1·8



(I) (II)

Fig. 5. Intramolecular angles. Molecule (I) is UPAD, (II) is HPAD.

Table 8. *Equations of least-squares planes for UPAD and distances* (Å) *of atoms from these planes*

X, Y and Z are expressed in Å units relative to the Cartesian axial system defined by the a, b and c^* axes. The planes were calculated by the method of Schomaker, Waser, Marsh & Bergman (1959) as modified by Blow (1960).

Plane A: $0{\cdot}3569X+0{\cdot}3338Y+0{\cdot}8725Z=5{\cdot}3105$
B: $0{\cdot}3044X+0{\cdot}0607Y+0{\cdot}9506Z=4{\cdot}0722$
C: $0{\cdot}2591X+0{\cdot}1235Y+0{\cdot}9579Z=4{\cdot}0842$
D: $0{\cdot}1241X+0{\cdot}2208Y+0{\cdot}9674Z=3{\cdot}5971$
E: $-0{\cdot}0592X+0{\cdot}3170Y+0{\cdot}9466Z=2{\cdot}6649$

Plane *A*			
C(5)	0·007	*H(4)	0·015
C(6)	−0·002	*H(5)	−0·018
C(7)	−0·003	*H(6)	−0·037
C(8)	0·003	*H(7)	0·072
C(9)	0·002	*H(8)	0·010
C(10)	−0·007	*N(1)	0·040
*C(4)	0·390	*N(2)	−0·272

Plane *B*			
N(1)	0·000	*C(10)	−0·261
N(2)	−0·003	*O	0·065
C(2)	0·004	*C(1)	0·033
C(3)	−0·004	*N(3)	0·029
C(4)	0·002	*C(11)	−0·024
*C(5)	0·048	*C(12)	−0·327
*C(6)	0·415		

Plane *C*	
N(3)	0·000
C(3)	0·000
C(11)	0·000
*C(2)	−0·064
*C(4)	0·111
*C(12)	−0·197
*C(16)	0·173

Plane *D*			
C(11)	−0·001	*H(19)	−0·011
C(12)	0·013	*H(20)	−0·029
C(13)	−0·012	*H(21)	−0·132
C(14)	0·000	*H(22)	0·108
C(15)	0·012	*C(17)	1·003
C(16)	−0·012	*C(18)	−0·265
N(3)	−0·051	*C(19)	0·256
*N(4)	−0·006	*C(20)	−1·002

Plane *E*	
N(4)	−0·001
C(14)	0·000
C(18)	0·000
C(19)	0·000
*C(13)	0·236
*C(15)	−0·238
*C(17)	1·391
*C(20)	−1·368

* Not included in the calculation of the plane.

Table 9. *Equations of least-squares planes for HPAD and distances* (Å) *of atoms from these planes*

X, *Y* and *Z* are expressed in Å units relative to the Cartesian axial system defined by **b** × **c***, **b**, and **c***. The planes were calculated by the method of Schomaker *et al.* (1959) as modified by Blow (1960).

Plane *A*: $0{\cdot}7686X+0{\cdot}4143Y-0{\cdot}4875Z=4{\cdot}2811$
B: $0{\cdot}7900X+0{\cdot}3524Y-0{\cdot}5017Z=3{\cdot}4920$
C: $0{\cdot}8958X+0{\cdot}2764Y-0{\cdot}3482Z=3{\cdot}5368$
D: $0{\cdot}9404X-0{\cdot}2885Y+0{\cdot}1802Z=0{\cdot}6084$
E: $0{\cdot}8705X-0{\cdot}4730Y+0{\cdot}1360Z=-0{\cdot}7741$
F: $0{\cdot}9099X-0{\cdot}3369Y+0{\cdot}2420Z=\ 0{\cdot}2528$
G: $0{\cdot}9573X-0{\cdot}2543Y+0{\cdot}1374Z=\ 0{\cdot}7567$

Plane *A*

C(5)	−0·005	*H(4)	−0·035
C(6)	−0·002	*H(5)	−0·038
C(7)	0·009	*H(6)	−0·025
C(8)	−0·007	*H(7)	0·015
C(9)	0·000	*H(8)	0·027
C(10)	0·006	*N(1)	−0·003
*C(4)	0·089	*N(2)	−0·031

Plane *B*

N(1)	0·003	*C(10)	0·074
N(2)	−0·009	*O	0·067
C(2)	0·012	*C(1)	0·050
C(3)	−0·009	*N(3)	0·148
C(4)	0·004	*C(11)	0·062
*C(5)	0·074	*C(12)	−0·982
*C(6)	0·163		

Plane *C*

N(3)	0·000
C(3)	0·000
C(11)	0·000
*C(2)	−0·075
*C(4)	0·311
*C(12)	−0·865
*C(16)	0·848

Plane *D*

C(11)	0·056	*H(19)	−0·096
C(12)	−0·016	*H(20)	−0·053
C(13)	−0·038	*C(22)	−0·089
C(14)	0·051	*C(21)	−0·167
C(15)	−0·012	*C(17)	1·696
C(16)	−0·041	*C(18)	0·292
*N(3)	0·081	*C(19)	0·546
*N(4)	0·169	*C(20)	−0·639

Plane *E*

N(4)	−0·089
C(14)	0·032
C(18)	0·029
C(19)	0·028
*C(13)	0·194
*C(15)	−0·022
*C(17)	1·475
*C(20)	−1·310

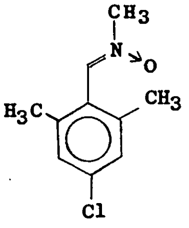
Plane *F*

C(11)	−0·006
C(12)	0·025
C(13)	0·003
C(14)	−0·009
C(21)	−0·013
*C(15)	−0·173
*C(16)	−0·205
*N(3)	0·008
*N(4)	0·112

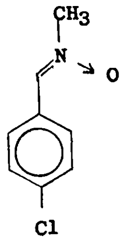
Plane *G*

C(11)	0·007
C(14)	0·001
C(15)	0·007
C(16)	−0·021
C(22)	0·007
*C(12)	−0·135
*C(13)	−0·156
*N(3)	0·040
*N(4)	0·117

* Not included in the calculation of the plane.



(III)



(IV)

Table 10. *Dihedral angles between the various planes in the molecules*

Planes	UPAD	HPAD
A–B	16·6°	3·8°
B–C	4·5	11·5
C–D	9·6	45·6
D–E	11·9	11·6
B–D	13·9	56·6
F–G		8·1

A striking feature of the structures is the presence of short intramolecular C–H···O contacts. The H(8)···O separation in both compounds is 2·24 Å and the H(22)···O separation in UPAD is exceedingly short, 2·03 Å. These distances would be even shorter if the true C–H distance of 1·08 Å (Sutton, 1965) were used instead of the typically shortened values determined by X-rays. For comparison, the crowded H(26)···O distance of 2·45 Å in HPAD conforms to the minimum expected van der Waals separation of 2·4 Å. Hydrogen bonds of the C–H···O type have been claimed by a number of authors and the evidence was recently reviewed by Donohue (1968), who concluded that such bonds do not exist. The H(8)···O distance, the large departure of the C(10)–H(8)···O angle from 180°, and the angular distortion at N(1) in both UPAD and HPAD seem to indicate that this is not a hydrogen bond. On the other hand, in UPAD the C(12)–H(22)···O angle (148°) is reasonably close to 180° and the H(22)···O distance is so short that we believe this must be a hydrogen bond. The infrared spectra of the dye crystals suspended in a mineral oil mull revealed that the C=O stretching frequency occurs at 1689 cm^{-1} for HPAD but is shifted to 1665 cm^{-1} for UPAD, a

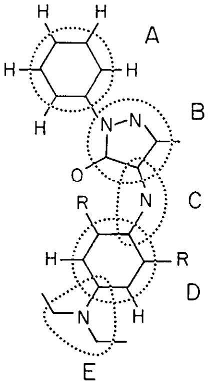


Fig. 6. Definition of the planes of Tables 8 and 9.

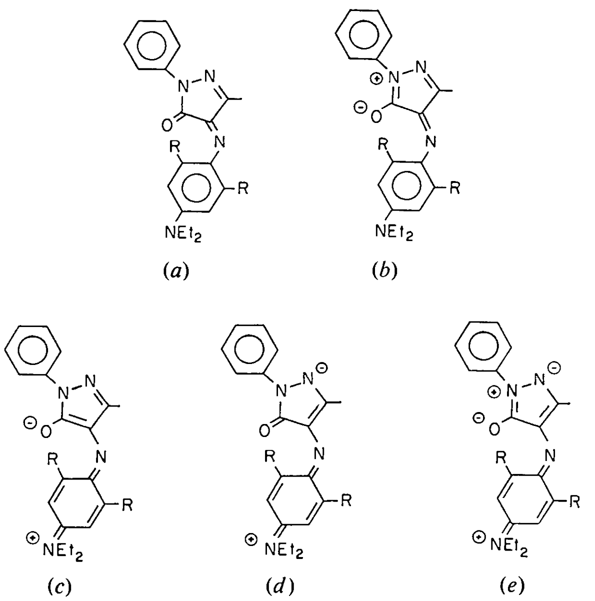


Fig. 7. Most probable structures contributing to the resonance hybrid of a pyrazolinone azomethine dye.

decrease of 24 cm^{-1} and excellent confirmation of the hydrogen bond.

The most probable canonical structures contributing to the resonance hybrid of a pyrazolinone azomethine dye are drawn in Fig. 7. The structure in Fig. 7(*a*) does not involve charge separation and should be the dominant contributor. The contributions from structures in Fig. 7(*c*), (*d*), and (*e*), in which the *p*-phenylenediamine ring is quinoid, should be sensitive to the nature of R and would be expected to be more important for UPAD than for HPAD. Brown *et al.* (1951) have argued that 7(*c*) is less important than 7(*d*) and (*e*) because the polarization of the lactam system to structure 7(*b*) facilitates the accumulation of negative charge on N(2), as in 7(*d*) and (*e*). The observed bond lengths follow this oversimplified picture quite well.

The contribution of the quinoid forms to both dyes is evident from the systematic variation of the bond lengths in the *p*-phenylenediamine region. Bonds C(11)–C(12), C(13)–C(14), C(14)–C(15), and C(16)–C(11) are longer and bonds N(3)–C(11), N(4)–C(14), C(12)–C(13), and C(15)–C(16) are shorter than the usual value for phenyl C–C bonds (1·394 Å, Sutton, 1965) and the idealized value for sp^2–sp^2 C–N bonds (1·45 Å, Lide, 1962). The shortened bonds in UPAD are from 0·013 to 0·025 Å shorter than those in HPAD and show the greater contribution of quinoid structures to the more planar UPAD molecule. The shortness of the N(4)–C(14) bonds compared with the N(3)–C(11) bonds occurs because N(4) is conjugated only through C(14), whereas N(3) is conjugated through both C(3) and C(11) and the p_z electron is largely utilized in the double bond with C(3). Bond lengths in the pyrazolinone ring and between the ring and its four substituent atoms are very similar for both dyes and indicate the dominance of structure 7(*a*). The N(2)–C(2) and N(3)–C(3) distances agree very well with the value 1·29 Å expected for C=N (Pauling, 1960). The C(4)–O distances are comparable to C=O separations (1·21 Å) found in aliphatic and conjugated aldehydes and ketones (Sutton, 1965) but are longer than the 1·189 Å found for the unconjugated C=O of the five-membered ring of androsterone (High & Kraut, 1966). The C(3)–C(4) bonds are slightly longer than the 1·488 Å expected (Dewar & Schmeising, 1960) for the sp^2–sp^2 C–C single bond and indicate that the contribution of 7(*c*) to the structures must be small. The shortening of the N(1)–C(4) and C(2)–C(3) bonds from the usual single-bond distances conforms to contributions from 7(*b*), (*d*), and (*e*). The N(1)–N(2) and N(1)–C(5) separations are considerably less than the idealized single-bond values, indicating that canonical structures other than those shown in Fig. 7 are undoubtedly important. Similar N–N distances (1·407, 1·413, 1·416, 1·419 Å) have been found in the structures of four other pyrazolinones (Vijayan & Viswamitra, 1967, 1968; Smith, 1969; Smith & Barrett, 1969); in one of these (Smith, 1969) similar *N*-phenyl bonds (1·412, 1·415 Å) have also been found.

The C–C bonds in the 1-phenyl group are all shorter than the usual 1·394 Å, probably because of the lack of thermal correction. The sp^2–sp^3 C(1)–C(2) distances are a little shorter than the normal 1·501 Å (Lide, 1962) while the C(12)–C(21) and C(16)–C(22) bonds in HPAD agree very well. Some of the N–C and the C–C bonds of the ethyl groups deviate from the expected values of 1·47 and 1·526 Å because of the thermal motion and the structure determination problem in this region for UPAD. As is typical of X-ray structures, the C–H distances are generally less than the true 1·08 Å separation.

Most of the angles in UPAD and HPAD are similar and normal in value. The angles at C(4), N(1), and N(2) in the pyrazolinone system are also strikingly close to those we have observed in $C_{16}H_{12}N_4OS$ (Smith, 1969) and $C_9H_8N_2O_2$ (Smith & Barrett, 1969) where the intramolecular overcrowding was less severe than in the present compounds and the conjugation was somewhat different. The overcrowding caused by the interaction of the C(12) substituent with oxygen has caused the angles C(4)–C(3)–N(3), C(3)–N(3)–C(11), and N(3)–C(11)–C(12) to be larger than normal for both dyes. In HPAD, where the strain has been relieved by a large deviation from planarity, these angles have not been enlarged as much as in UPAD, where the C–H···O hydrogen bond and the conjugation have forced a more planar structure. The C(18)–N(4)–C(19) angles can be compared to the 116·7° found by Hanson (1965) in an *N*,*N*,*N'*,*N'*-tetramethyl-*p*-phenylenediamine complex.

Carter, McPhail & Sim (1966) noted that within a benzene ring the valency angles at carbon atoms bearing substituents with strong electron-withdrawing power were significantly larger than 120°. Likewise, at carbon atoms bearing strong electron-releasing substituents, the angles were consistently less than 120°. They suggested that the fraction of *s* character in the carbon σ orbital directed toward the substituent atom would be greater or less than $\frac{1}{3}$ depending on whether the substituent was electron-releasing or electron-withdrawing. If the orbital had more then $\frac{1}{3}$ *s* character, the carbon σ orbitals directed toward the *ortho* carbon atoms would have less than $\frac{1}{3}$ *s* character and the ring angle should be less than 120°; if the orbital had less than $\frac{1}{3}$ *s* character, the reverse should be true. At C(11) and C(14) in UPAD and at C(14) in HPAD, where the substituents are electron-releasing, the phenyl angles are low. The situation at C(11) of HPAD is complicated by the mildly electron-releasing methyl groups on the *ortho* carbon atoms C(12) and C(16), but the angles at C(11), C(12), and C(16) are smaller than those at C(13) and C(15), where the substituents are hydrogen.

Fig. 8 and 9 are stereoscopic views of the molecular packing for both dyes. The approximately planar UPAD molecules lie in sheets which are parallel to the 103 planes and 3·72 Å apart. This explains the exceedingly high observed intensity for 103. The highly twisted HPAD molecules lie in sheets parallel to $01\bar{1}$. In these sheets the planes of the pyrazolinone rings and their substituents pack plane to plane in rows along **a** with the *p*-phenylenediamine part of adjacent molecules pointing in opposite directions in $01\bar{1}$. The rows then line up with each other by interlocking of the *p*-phenylenediamine ends. If we consider both compounds, the minimum intermolecular contacts are 2·40 Å for hydrogen–hydrogen, 3·375 Å for heavy–heavy and 2·71 Å for hydrogen–heavy, except for two shorter H···O contacts. These H···O contacts are 2·43 Å for H(15)···O $(-x, 1-y, -z)$ in HPAD and 2·54 Å for H(16)···O$(-\frac{1}{2}+x, \frac{3}{2}-y, 1+z)$ in UPAD. None of these contacts appears unusual.

Conclusions

The results show that UPAD contains a definite intramolecular C–H···O hydrogen bond. With the exception of this bond, the details of the molecular structures are close to what one would expect. The major component of twist at the azomethine linkages is in the *N*-phenyl bonds. The *N*-pyrazolinyl bonds, which are almost double bonds, have a much higher bond order than the *N*-phenyl bonds. This shows that the azomethine linkage is not an isoenergetic system, as suggested by Knott & Pauwels (1968) and the absorption spectra cannot be explained by analogy to the symmetric cyanine dyes. The structures reported here should provide a basis for the eventual explanation of why the *x*-band ground and excited states are closer together in HPAD than in UPAD.

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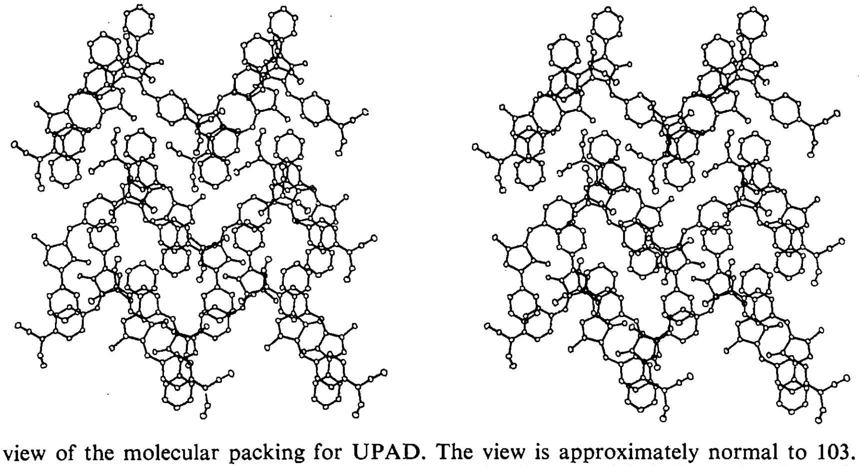

Fig. 8. Stereoscopic view of the molecular packing for UPAD. The view is approximately normal to 103. The *b* axis is horizontal, left to right, and the *a* axis is vertical, top to bottom, but is rotated 20° above the plane of the picture.

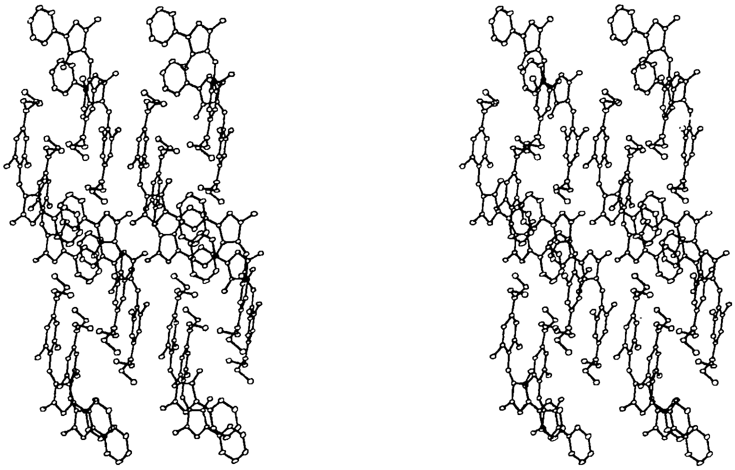

Fig. 9. Stereoscopic view of the molecular packing for HPAD. The view is approximately normal to $01\bar{1}$. The *a* axis is horizontal, left to right, and the *b* axis is vertical, bottom to top, but is rotated 35° below the plane of the picture.

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