1982). Table 1 shows atomic positional parameters and Table 2 the bond lengths and angles. Fig. 1 shows an *ORTEP* plot of the molecule and Fig. 2 shows the contents of the unit cell.

Related literature. Pyrromethene–BF_2 complexes are of interest because of their pronounced fluorescence (Vos de Wael, Pardoen, van Koeveringe & Lugtenburg, 1977). The structures of BF_2 complexes of 1,2,3,4-tetrahydro-1,10-phenanthroline (Klebe, Hensen & Fuess, 1983) and octaethyl-21*H*,24*H*-bilin-1,9-dione (Bonfiglio *et al.*, 1983), which forms a similar *s*-indacene ring system, have been reported.

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1-(1-Chlorovinyl)-2,7-dimethoxynaphthalene

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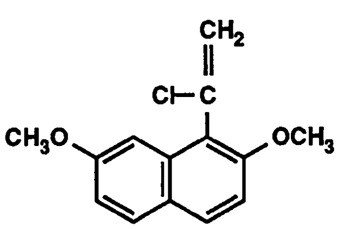
Abstract. $C_{14}H_{13}ClO_2$, $M_r = 248{\cdot}71$, monoclinic, $P2_1/n$, $a = 11{\cdot}291\,(1)$, $b = 7{\cdot}343\,(1)$, $c = 15{\cdot}223\,(2)$ Å, $\beta = 90{\cdot}899\,(8)°$, $V = 1262{\cdot}0\,(5)$ Å^3, $Z = 4$, $D_x = 1{\cdot}309$ g cm^{-3}, $\lambda(\text{Cu } K\alpha) = 1{\cdot}54184$ Å, $\mu = 26{\cdot}0$ cm^{-1}, $F(000) = 520$, $T = 299$ K, $R = 0{\cdot}041$ for 2405 observations (of 2516 unique data). The average deviation from planarity is 0·019 (2) Å with a maximum of 0·035 (1) Å for the fused rings. The dihedral angle between the naphthalene system and the chlorovinyl group is 101·93 (4)°. The methoxy group *ortho* to the chlorovinyl adopts a conformation with the methyl group *anti* to the neighboring α carbon of the ring, with a C—C—O—C torsion angle of −175·6 (2)°. The other methoxy group has the methyl *syn* to the neighboring α carbon, with a C—C—O—C torsion angle of 1·9 (3)°.

Experimental. The title compound (1) was prepared by the reaction of phosphorous trichloride and phosphorous pentachloride on 1-acetyl-2,7-dimethoxynaphthalene in benzene at room temperature (Buckle & Rockewell, 1985). Colorless irregular crystals of (1) were isolated by recrystallization from ether/hexane. Crystal size 0·68 × 0·60 × 0·52 mm, mounted on a glass fiber in random orientation on an Enraf–Nonius CAD-4 κ-axis diffractometer equipped with a graphite monochromator, $\lambda(\text{Cu } K\alpha) = 1{\cdot}54184$ Å. Cell dimensions from setting angles of 25 reflections having $25 < \theta < 29°$. Space group determined to be $P2_1/n$ from systematic absences $h0l$ with $h + 1$ odd, $0k0$ with k odd.



(1)

Data having $2 < 2\theta < 150°$, $0 \leq h \leq 14$, $0 \leq k \leq 9$, $-19 \leq l \leq 19$ were collected using ω–2θ scans designed for $I = 25\sigma(I)$, subject to max. scan time =

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Table 1. *Fractional atomic coordinates and equivalent isotropic temperature factors*

$B_{eq} = (8\pi^2/3)\sum_i\sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	B_{eq}(Å^2)
Cl(1)	0·72000 (4)	0·16796 (6)	0·41091 (3)	5·339 (9)
O1	0·6591 (1)	0·5721 (2)	0·49995 (7)	4·75 (2)
O2	1·11695 (9)	0·4128 (2)	0·18145 (8)	5·09 (2)
C1	0·8071 (1)	0·5125 (2)	0·39940 (8)	3·37 (2)
C2	0·7713 (1)	0·6074 (2)	0·47243 (9)	3·79 (3)
C3	0·8481 (2)	0·7311 (2)	0·5154 (1)	4·41 (3)
C4	0·9589 (2)	0·7582 (2)	0·4833 (1)	4·45 (3)
C5	0·9978 (1)	0·6705 (2)	0·4076 (1)	3·87 (3)
C6	1·1110 (1)	0·7031 (2)	0·3709 (1)	4·73 (3)
C7	1·1463 (1)	0·6184 (3)	0·2974 (1)	4·80 (3)
C8	1·0717 (1)	0·4889 (2)	0·25549 (9)	4·08 (3)
C9	0·9620 (1)	0·4503 (2)	0·28868 (9)	3·58 (2)
C10	0·9223 (1)	0·5416 (2)	0·36457 (8)	3·32 (2)
C11	0·7255 (1)	0·3797 (2)	0·35761 (9)	3·49 (2)
C12	0·6607 (2)	0·4061 (2)	0·2851 (1)	4·61 (3)
C13	0·6139 (2)	0·6747 (3)	0·5711 (1)	5·70 (4)
C14	1·0441 (2)	0·2894 (3)	0·1343 (1)	6·07 (4)

Table 2. *Bond distances* (Å) *and angles* (°)

Cl(1)—C11	1·755 (1)	C1—C10	1·428 (2)
C5—C10	1·427 (2)	O1—C2	1·366 (2)
C1—C11	1·479 (2)	C6—C7	1·346 (2)
O1—C13	1·420 (2)	C2—C3	1·410 (2)
C7—C8	1·415 (2)	O2—C8	1·365 (2)
C3—C4	1·365 (2)	C8—C9	1·374 (2)
O2—C14	1·412 (2)	C4—C5	1·397 (2)
C9—C10	1·415 (2)	C1—C2	1·378 (2)
C5—C6	1·422 (2)	C11—C12	1·329 (2)

C2—O1—C13	118·6 (1)	C3—C4—C5	122·0 (1)
C8—C9—C10	120·1 (1)	C8—O2—C14	117·4 (1)
C4—C5—C6	122·8 (1)	C1—C10—C5	118·1 (1)
C2—C1—C10	120·3 (1)	C4—C5—C10	119·4 (1)
C1—C10—C9	122·3 (1)	C2—C1—C11	119·5 (1)
C6—C5—C10	117·8 (1)	C5—C10—C9	119·6 (1)
C10—C1—C11	120·2 (1)	C5—C6—C7	121·8 (2)
Cl(1)—C11—C1	114·31 (9)	O1—C2—C1	115·9 (1)
C6—C7—C8	120·2 (1)	Cl(1)—C11—C12	119·4 (1)
O1—C2—C3	123·1 (1)	O2—C8—C7	114·8 (1)
C1—C11—C12	126·3 (1)	C1—C2—C3	121·0 (1)
O2—C8—C9	124·8 (1)	C2—C3—C4	119·2 (1)
C7—C8—C9	120·4 (1)		

90 s, scan rates varied 0·61–3·30° min^{-1}. Three reflections (400, 020, 004) were measured every 166 min, and their intensities exhibited only random fluctuations during data collection. Lorentz and polarization corrections were applied. An empirical absorption correction based on a series of ψ scans was applied to the data. Relative transmission coefficients ranged from 0·697 to 0·997 with an average value of 0·846. The extinction coefficient was refined in the least squares to $g = 6{\cdot}9\,(5) \times 10^{-6}$, where the correction factor $(1 + gI_c)^{-1}$ was applied to F_c. $R_{\rm int}$ = 0·019 for averaging 0*kl* and 0*k*$\bar{l}$. Structure solved by direct methods using *MULTAN* (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982), and successive difference Fourier syntheses. The structure was refined by weighted full-matrix least squares; non-H atoms refined anisotropically; H atoms refined isotropically.

The function minimized was $\sum w(|F_o| - |F_c|)^2$ and weights were assigned as $w = 4F_o^2{\rm Lp}[S^2(C + R^2B) + (0{\cdot}02F_o^2)^2]^{-1}$, where S = scan rate, C = total integrated peak count, R = scan time/background counting time, B = total background count, Lp = Lorentz–polarization factor, using Enraf–Nonius *SDP* (Frenz & Okaya, 1980), scattering factors from Cromer & Waber (1974), anomalous coefficients from Cromer (1974). Of 2516 unique data, 2405 reflections having $I > 3\sigma(I)$ were used in the refinement. The final cycle included 207 variables and converged (largest Δ/σ = 0·01) with R = 0·041, wR = 0·066, R(all) = 0·042, and S = 4·51. The max. residual density was 0·32 e Å^{-3}, min. −0·31 e Å^{-3}. Table 1 presents the final coordinates* and equivalent isotropic thermal parameters, and Table 2 presents bond distances and angles. Fig. 1 illustrates the molecule and the numbering scheme, and Fig. 2 shows the unit cell.

Related literature. Crystal structures of 2,7-dimethoxynaphthalene: Prince, Fronczek & Gandour

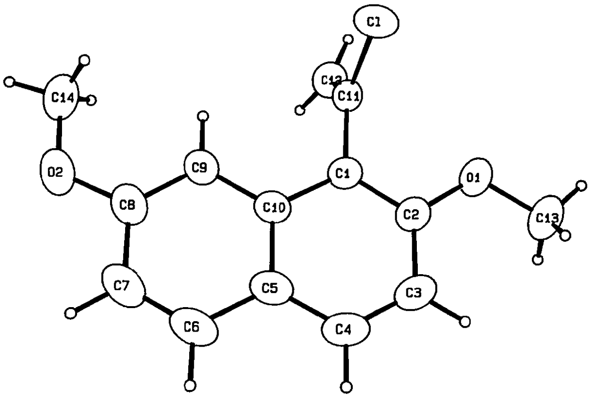

Fig. 1. Numbering scheme and thermal ellipsoids drawn at the 40% probability level. H atoms are drawn as circles with arbitrary radius.

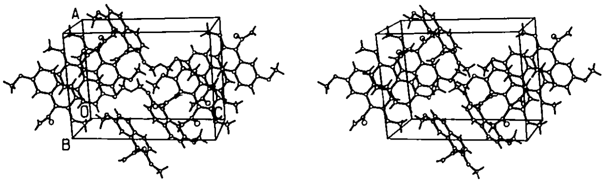

Fig. 2. Stereoview of the unit cell.

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* Lists of H-atom coordinates, bond distances and angles involving H atoms, anisotropic thermal parameters, least-squares-planes data and structure-factor amplitudes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52575 (17 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Acta Cryst. (1990). C**46**, 1152–1153

Structure of 2-(5-Methylthien-2-yl)-2,5-dihydro-3*H*-pyrazolo[4,3-*c*]quinolin-3-one

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Abstract. $C_{15}H_{11}N_3OS$, $M_r = 281{\cdot}33$, monoclinic, $P2_1/c$, $a = 13{\cdot}550\,(4)$, $b = 8{\cdot}723\,(2)$, $c = 14{\cdot}052\,(2)$ Å, $\beta = 130{\cdot}88\,(1)°$, $V = 1255{\cdot}8\,(6)$ Å^3, $Z = 4$, $D_x = 1{\cdot}488$ Mg m^{-3}, $\lambda(\mathrm{Cu}\ K\alpha) = 1{\cdot}54178$ Å, $\mu = 2{\cdot}22$ mm^{-1}, $F(000) = 584$, $T = 295$ K, $R = 0{\cdot}076$ for 1474 reflections. The molecule is almost planar. The intermolecular hydrogen bond NH···O, 2·750 (8) Å, is formed between N at position 5 of one pyrazoloquinoline skeleton and C═O at position 3 of another related by a twofold screw axis.

Experimental. Needle-like yellow crystals were obtained from ethanol. Crystal dimensions 0·7 × 0·1 × 0·02 mm. Rigaku AFC-5 diffractometer, graphite-monochromatized Cu $K\alpha$. Unit-cell parameters were refined by 2θ angles for 20 reflections in the range $30 < 2\theta < 40°$. Intensities were measured up to $2\theta = 130°$ in h 0/15, k −10/0 and l −16/12, $R_{\mathrm{int}} = 0{\cdot}035$, ω–2θ scans, ω-scan width $(1{\cdot}0 + 0{\cdot}2\tan\theta)°$, three standard reflections monitored every 100 measurements showed no significant change. 2130 unique reflections were measured, 1480 intensities were observed $[F_o > 3\sigma(F_o)]$. Structure solved by *MULTAN*84 (Main, Germain & Woolfson, 1984) and refined by block-diagonal least squares to minimize $\sum(w|\Delta F|^2)$. Absorption corrections by an empirical method (Walker & Stuart, 1983) applied after isotropic refinement (max. and min. transmission factors 1·44 and 0·75). H atoms located on a difference density map. Positional parameters for all atoms and anisotropic thermal parameters for non-H atoms refined. Temperature factor of each H atom set equal to B_{eq} of the bonded atom. $w = [\sigma^2(F_o) + 0{\cdot}00440|F_o|^2]^{-1}$, $w = 0$ for four reflections with $w^{1/2}|\Delta F| \geq 4$ and two very strong ones. Final $R = 0{\cdot}076$, $wR = 0{\cdot}100$ and $S = 1{\cdot}137$. The relatively large R value is assumed to be due to the poor quality of intensity data collected using a very small crystal. Highest peak in the final difference map 0·3 e Å^{-3}. Max. Δ/σ in the final cycle 0·08. Atomic scattering

Table 1. *Atomic coordinates* ($\times 10^4$) *and equivalent isotropic temperature factors* (Å^2 × 10) *with e.s.d.'s in parentheses*

	x	y	z	B_{eq}*
N(1)	5685 (4)	6725 (5)	803 (4)	27 (2)
N(2)	6644 (4)	5991 (5)	852 (4)	24 (2)
C(3)	6551 (5)	6273 (7)	−171 (5)	27 (2)
C(4)	4977 (5)	8085 (7)	−1988 (5)	27 (2)
N(5)	3991 (4)	9056 (6)	−2457 (4)	29 (2)
C(6)	2423 (5)	10356 (7)	−2474 (5)	29 (2)
C(7)	1878 (5)	10626 (7)	−1932 (5)	32 (3)
C(8)	2344 (6)	9894 (7)	−841 (6)	36 (3)
C(9)	3355 (5)	8860 (7)	−264 (5)	29 (3)
C(10)	3930 (5)	8548 (6)	−791 (4)	24 (2)
C(11)	3436 (5)	9307 (6)	−1911 (5)	26 (2)
C(12)	5006 (5)	7520 (6)	−262 (4)	23 (2)
C(13)	5489 (5)	7308 (6)	−911 (4)	24 (2)
O(14)	7276 (4)	5669 (5)	−338 (4)	34 (2)
C(15)	7566 (5)	5036 (6)	1886 (5)	27 (2)
S(16)	7516 (1)	4763 (2)	3055 (1)	29 (1)
C(17)	8820 (5)	3516 (7)	3826 (5)	32 (3)
C(18)	9278 (6)	3363 (7)	3230 (6)	34 (3)
C(19)	8585 (5)	4233 (7)	2113 (5)	25 (2)
C(20)	9324 (6)	2719 (8)	5021 (6)	42 (3)

$*B_{\mathrm{eq}} = \frac{4}{3}\sum_i\sum_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j$.

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