0·0423 for 2569 reflections, $wR = 0·0351$ ($R_{\rm all} = 0·0492$, $wR_{\rm all} = 0·0357$) and a goodness of fit = 1·892. The maximum $|\Delta/\sigma| < 0·1$ in the final refinement cycle and the minimum and maximum peaks in the final ΔF map were −0·20 and 0·30 e Å^{-3}, respectively. Differentiation between enantiomorphs was not possible on the basis of the X-ray diffraction results (wR for enantiomorph was 0·0351). The scattering factors for the non-H atoms were obtained from Cromer & Mann (1968), with anomalous-dispersion corrections from the work of Cromer & Liberman (1970), while scattering factors for the H atoms were taken from Stewart, Davidson & Simpson (1965). The linear absorption coefficient was calculated using values in *International Tables for X-ray Crystallography* (1974). Atomic positional and thermal parameters for the non-H atoms are listed in Table 1, while the bond lengths and angles for the non-H atoms are listed in Table 2.* The atomic labelling scheme is shown in Fig. 1. Fig. 1 was generated using the Nicolet XRD *SHELXTL-PLUS* software package (Sheldrick, 1987). The least-squares-planes program was supplied by Cordes (1983); other computer programs from reference 11 of Gadol & Davis (1982).

Related literature. The crystal structure of the α-phenylethyl analog of (1) has been previously reported and references cited therein (Lynch, Li & Martin, 1988).

The authors would like to thank the Robert A. Welch Foundation (F-652) and the National Institutes of Health (G. M. 25439 to SFM) for support for this work.

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* Tables of anisotropic thermal parameters, positional and thermal parameters for the H atoms, bond distances and angles involving the H atoms, torsion angles, least-squares planes, structure-factor amplitudes and a unit-cell packing diagram have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52597 (28 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Acta Cryst. (1990). **C46**, 1157–1158

Structure of 1,2-Bis(2-methyl-4-quinazolinyl)ethylene

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(*Received* 29 *November* 1989; *accepted* 23 *January* 1990)

Abstract. $C_{20}H_{16}N_4$, $M_r = 312·38$, monoclinic, $P2_1/n$, $a = 9·654\,(1)$, $b = 7·544\,(1)$, $c = 11·018\,(1)$ Å, $\beta = 99·84\,(1)°$, $V = 790·6$ Å^3, $Z = 2$, $D_x = 1·312$ g cm^{-3}, Cu $K\alpha$, $\lambda = 1·54184$ Å, $\mu = 5·964$ cm^{-1}, $F(000) = 328$, $T = 293$ K. The final R value converged to 0·049 for 907 significant [$I > 3\sigma(I)$] reflections. In the asymmetric unit is a half molecule completed by an inversion center in the ethylene bond. The resulting planar molecule is the *trans* isomer.

Experimental. The product was obtained by oxidation of 2,4-dimethylquinazoline with SeO_2 (Kepez, 1989). To clarify which of the methyl groups is oxidated we decided to perform a structure determination. A yellow single crystal of approximate dimensions 0·40 × 0·15 × 0·25 mm was mounted on a glass fiber. The systematic absences indicated space

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0108-2701/90/061157-02$03.00

Table 1. *Data-collection and structure-refinement parameters*

Crystal shape	Parallelepiped
Diffractometer used	CAD-4, Enraf–Nonius
Method of intensity measurement	ω/θ scan
No. and θ range (°) of reflections for lattice parameters	25; 12–26
Method used for absorption correction	*DIFABS* (Walker & Stuart, 1983)
Minimum absorption correction	0·717
Maximum absorption correction	1·463
Average absorption correction	0·998
Maximum value of $(\sin\theta)/\lambda$ reached in intensity measurement (Å^{-1})	0·587
Range of h, k and l	$0\rightarrow11$, $0\rightarrow8$, $-12\rightarrow12$
Standard reflections	$\bar{3}\bar{3}2$, $10\bar{5}$
Interval, standard reflections measured	1 h, loss of intensity
Total No. of reflections measured; θ range (°)	1547; 65 (418 unobserved reflections)
No. of observed reflections	907 with $I > 3\sigma(I)$
Methods used to solve structure	Direct methods
Use of F or F^2 in LS refinement	F
Method of locating H atoms	From difference electron density map, positions included in refinement with fixed $B_{iso} = 4$ Å^2
Weighting scheme	$1/\sigma_F^2$
Parameters refined	134
Value of R	0·049
Value of wR	0·045
Ratio of max. LS shift to e.s.d. (Δ/σ)	0·002
Max. height in final ΔF map (e Å^{-3})	0·162
Error in an observation of unit weight	0·634
Secondary-extinction coefficient	6·77 (1) × 10^{-6} (Zachariasen, 1963)
Source of atomic scattering factors	*International Tables for X-ray Crystallography* (1974)
Computer used	DEC MicroVAX 3500

Table 2. *Atomic positional and equivalent isotropic displacement parameters*

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

	x	y	z	U_{eq}(Å^2)
N1	0·5446 (2)	0·3391 (3)	0·3389 (2)	0·037 (1)
N3	0·7750 (2)	0·4582 (3)	0·3481 (2)	0·034 (1)
C2	0·6436 (3)	0·4168 (4)	0·2892 (2)	0·035 (2)
C4	0·8091 (3)	0·4173 (4)	0·4659 (2)	0·028 (1)
C5	0·7377 (3)	0·2908 (4)	0·6577 (3)	0·040 (2)
C6	0·6334 (3)	0·2174 (5)	0·7107 (3)	0·049 (2)
C7	0·4993 (3)	0·1844 (5)	0·6417 (3)	0·048 (2)
C8	0·4715 (3)	0·2245 (4)	0·5197 (3)	0·041 (2)
C9	0·5760 (3)	0·3016 (4)	0·4609 (2)	0·031 (1)
C10	0·7103 (3)	0·3359 (4)	0·5309 (2)	0·029 (1)
C21	0·6104 (3)	0·4649 (5)	0·1555 (3)	0·051 (2)
C41	0·9533 (3)	0·4582 (4)	0·5278 (2)	0·032 (1)

Table 3. *Bond distances* (Å) *and angles* (°) *with e.s.d.'s*

Symmetry operator: (i) $-x+2$, $-y+1$, $-z+1$.

N1—C2	1·317 (4)	C5—C6	1·365 (5)
N1—C9	1·356 (3)	C5—C10	1·418 (4)
N3—C2	1·359 (3)	C6—C7	1·407 (4)
N3—C4	1·319 (3)	C7—C8	1·359 (4)
C2—C21	1·498 (4)	C8—C9	1·415 (4)
C4—C10	1·427 (4)	C9—C10	1·414 (3)
C4—C41	1·475 (3)	C41—C41^i	1·332 (4)

C2—N1—C9	116·7 (2)	C6—C7—C8	120·2 (3)
C2—N3—C4	118·1 (2)	C7—C8—C9	120·5 (2)
N1—C2—N3	126·0 (2)	N1—C9—C8	119·0 (2)
N1—C2—C21	117·9 (2)	N1—C9—C10	122·0 (3)
N3—C2—C21	116·1 (3)	C8—C9—C10	119·0 (2)
N3—C4—C10	121·3 (2)	C4—C10—C5	124·7 (2)
N3—C4—C41	117·6 (2)	C4—C10—C9	115·8 (2)
C10—C4—C41	121·2 (2)	C5—C10—C9	119·6 (3)
C6—C5—C10	119·4 (2)	C4—C41—C41^i	123·2 (2)
C5—C6—C7	121·3 (3)		

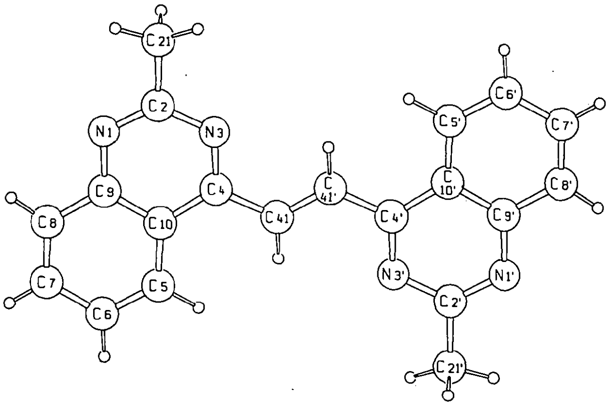

Fig. 1. Plot of the molecule and numbering scheme.

group $P2_1/n$. During the exposure time of 21·8 h the total loss in intensity was 14·9%. A linear decay correction was applied using the slope of the least-squares line through the standards' plot of intensity *vs* time. In the final full-matrix least-squares refinement, all non-H atoms were assigned anisotropic atomic displacement parameters. A summary of data-collection and structure-refinement parameters is given in Table 1. Final atomic coordinates are listed in Table 2, distances and angles in Table 3.* All calculations were performed with *MOLEN* (Enraf–Nonius, 1989). A graphic representation (Keller, 1988) of the molecule is shown in Fig. 1.

Related literature. The synthesis of the compound has recently been published by Kepez (1989).

We thank the Scientific and Technical Research Council of Turkey for a research grant (MA). We are also grateful to Professor Dr J. Strähle, University of Tübingen, Federal Republic of Germany, for providing the laboratory facilities, and Dr M. Kepez, Erciyes University, Kayseri, Turkey, for the crystals.

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* Lists of structure factors, H-atom positions, torsion angles, and anisotropic atomic displacement parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52636 (9 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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