Three new 2-methyl-4-styrylquinoline derivatives have been synthesized in high yields using Friedländer reactions between chalcones [1-(2-aminophenyl)-3-arylprop-2-en-1-ones] and acetone, and characterized using IR, $^1$H and $^{13}$C NMR spectroscopy, and mass spectrometry, and by crystal structure analysis. In (E)-4-(4-fluorostyryl)-2-methylquinoline, C$_{18}$H$_{14}$FN, (I), the molecules are joined into cyclic centrosymmetric dimers by C—H····N hydrogen bonds and these dimers are linked into sheets by π–π stacking interactions. The molecules of (E)-2-methyl-4-[4-(trifluoromethyl)styryl]quinoline, C$_{19}$H$_{14}$F$_3$N, (II), are linked into cyclic centrosymmetric dimers by C—H····π hydrogen bonds and these dimers are linked into chains by a single π–π stacking interaction. There are no significant hydrogen bonds in the structure of (E)-4-(2,6-dichlorostyryl)-2-methylquinoline, C$_{18}$H$_{13}$Cl$_2$N, (III), but molecules related by translation along [010] form stacks with an intermolecular spacing of only 3.8628 (2) Å. Comparisons are made with the structures of some related compounds.

1. Introduction

The quinoline nucleus constitutes a privileged scaffold because of the wide spectrum of promising biological activity exhibited by its derivatives (Kumar et al., 2009). Among quinoline derivatives, 2-styrylquinolines have been studied extensively, mainly because of their potential as inhibitors of HIV-1 integrase (Leonard & Roy, 2008; Mahajan et al., 2018; Mousnier et al., 2004) and as antimicrobial (Kamal et al., 2015), antifungal (Cieslik et al., 2012) and anticancer agents (Mrozek-Wileczkiewicz et al., 2015, 2019).

Accordingly, considerable efforts have been made in the development of effective methods for accessing new compounds containing the styrylquinoline scaffold (Musiol, 2020). Unlike 2-styrylquinolines, the 4-styrylquinoline regioisomers have been studied much less, with few published reports related to their synthesis and biological evaluation, which is probably due, at least in part, to a lack of generally applicable methodologies for their synthesis. In general, the published syntheses of 4-styrylquinolines have involved Heck coupling between 4-haloquinolines and different aryl–vinyl compounds (Omar & Hormi, 2009), and Knoevenagel-type condensation reactions between 4-methylquinolines and aromatic aldehydes using expensive and toxic heavy-metal catalysts (Jamal et al., 2016) or microwave irradiation (Lee et al., 2009). The use of palladium catalysts in the cross-coupling reaction between
To expand further both the synthetic utility of 1-(2-aminophenyl)-3-arylprop-2-en-1-ones and the flexibility of our approach, we report here the synthesis, characterization and molecular and supramolecular structures of a matched set of three closely-related quinoline derivatives, namely, (E)-4-(4-fluorostyryl)-2-methylquinoline, (I), (E)-2-methyl-4-[4-(trifluoromethyl)styryl]quinoline, (II), and (E)-4-(2,6-dichlorostyryl)-2-methylquinoline, (III) (Scheme 1 and Figs. 1–3), which differ only in the nature of the substituents at the C4 and C2/C6 positions on the benzene ring of the styryl fragment. Using our synthetic approach (Meléndez et al., 2020), (E)-1-(2-aminophenyl)-3-arylprop-2-en-1-ones of type (A) (Scheme 1) were subjected to Friedländer annulation with an excess of acetone in glacial acetic acid at 373 K, to provide the products (I)–(III) with yields in the range 77–94% (Scheme 1). These new 2-methylquinoline derivatives are intended for use as key precursors in the further development of more complex molecules of possible biological value, such as the bis-styrylquinolines (IV) (Scheme 2), (4-styrylquinolin-2-yl)chalcones (V) and the molecular hybrids of types (VI) and (VII).

2. Experimental

2.1. Synthesis and crystallization

For the synthesis of compounds (I)–(III), a mixture of the appropriate 1-(2-aminophenyl)-3-arylprop-2-en-1-ones (A) (Meléndez et al., 2020; see Scheme 1) (1.0 mmol) and acetone (12.0 mmol) in glacial acetic acid (3 ml) was stirred magnetically and heated at 353 K until the reactions were complete, as judged by the complete consumption of (A) (as monitored by thin-layer chromatography, TLC); the reaction times for completion were 15 h for (I), 19 h for (II) and 14 h for (III). Each reaction mixture was then neutralized with a saturated aqueous sodium carbonate solution and extracted with ethyl acetate (3 × 50 ml). The combined organic layers were washed with water and dried over anhydrous sodium sulfate, and the solvent was then removed under reduced pressure. In each case, the resulting crude product was purified by flash chromatography on silica-gel using hexane–ethyl acetate mixtures as eluent (compositions ranged from 7:1 to 2:1 v/v) to give the required solid compounds (I)–(III). Crystallization from hexane–ethyl acetate (10:1 v/v) at ambient temperature and in the presence of air gave crystals suitable for single-crystal X-ray diffraction; these were yellow for (I) and (III), and colourless for (II).

![Scheme 1](image1)

![Scheme 2](image2)
Table 1
Experimental details.

Experiments were carried out at 100 K with Mo Ka radiation using a Bruker D8 Venture diffractometer. Absorption was corrected for by multi-scan methods (SADABS; Bruker, 2016). H-atom parameters were constrained.

| Crystal data | (I) | (II) | (III) |
|--------------|-----|------|-------|
| Chemical formula | C18H14FN | C19H14F3NC | C18H13Cl2N |
| M_r | 263.30 | 313.31 | 314.19 |
| Crystal system, space group | Monoclinic, P2_1/c | Monoclinic, C2/c | Monoclinic, C2/c |
| a, b, c (Å) | 13.5921 (7), 12.7103 (6), 7.6215 (3) | 17.2969 (10), 10.8096 (7), 16.1495 (8) | 30.5651 (15), 3.8629 (2), 25.5357 (13) |
| β (°) | 103.133 (2) | 91.440 (2) | 110.497 (2) |
| V (Å³) | 1282.25 (10) | 3013.8 (3) | 2824.1 (2) |
| Z | 4 | 8 | 8 |
| μ (mm⁻¹) | 0.09 | 0.11 | 0.45 |
| Crystal size (mm) | 0.20 × 0.08 × 0.07 | 0.16 × 0.14 × 0.12 | 0.20 × 0.10 × 0.06 |

Data collection

| | (I) | (II) | (III) |
|---|------|------|-------|
| T_{min}, T_{max} | 0.934, 0.994 | 0.888, 0.987 | 0.897, 0.973 |
| No. of measured, independent and observed [I > 2σ(I)] reflections | 38068, 2949, 2342 | 46287, 3750, 2921 | 28110, 3208, 2930 |
| R_{int} (sin θ/λ)_{max} (Å⁻¹) | 0.079 | 0.085 | 0.042 |
| Refinement | | | |
| R(F²) > 2σ(F²), wR(F²), S | 0.042, 0.100, 1.05 | 0.047, 0.121, 1.03 | 0.031, 0.079, 1.07 |
| No. of reflections | 2949 | 3750 | 3208 |
| No. of parameters | 182 | 209 | 191 |
| Δρ_{max}, Δρ_{min} (e Å⁻³) | 0.26, −0.22 | 0.33, −0.30 | 0.33, −0.26 |

Computer programs: APEX3 (Bruker, 2018), SAINT (Bruker, 2017), SHELXT2014 (Sheldrick, 2015a), SHELXL2014 (Sheldrick, 2015b) and PLATON (Spek, 2020).

3. Results and discussion

All compounds were fully characterized by standard spectroscopic and analytical methods. In the IR spectra of (I)–(III), the absence of any N—H stretching bands around 3275–3285 cm⁻¹, which are characteristic in the spectra of (2-aminoxyphenyl)chalcone precursors, was used for monitoring the formation of the quinoline ring. The formation of the 4-styrylquinoline scaffold was confirmed by a detailed analysis of the ¹H, ¹³C and 2D NMR spectra, which showed no signals arising from the H atoms of the amino group; neither were there any signals from the carbonyl groups which had been present in the precursor chalcones. Instead, the ¹³C spectra of the products contained signals from a new C₂=CH(—H) unit (C-3) in the range δ 117.9–118.5, and two new quaternary aromatic C atoms at δ 158.7–158.8 (C-2) and 142.2–142.8 (C-4). As in the spectra of the precursor chalcones, the ¹H spectra of compounds (I)–(III) contained signals from the trans vinylic protons —CH₂=CH—, appearing as doublets (see Section 2.1). Finally, definitive confirmation of the molecular constitutions and the regio- and stereochemistry for compounds (I)–(III) was established by means of single-crystal X-ray diffraction.

2.2. Refinement

Crystal data, data collection and refinement details are summarized in Table 1. A small number of bad outlier reflections [636 for (I), 204 and 336 for (II), and 16,0 and 339 for (III)] were omitted from the data sets. All H atoms were located in difference maps and then treated as riding atoms in geometrically idealized positions, with C—H distances of 0.95 (alkenic and aromatic) and 0.98 Å (CH₃), and with Uiso(H) = kUeq(C), where k = 1.5 for the methyl groups, which were permitted to rotate but not to tilt, and 1.2 for all other H atoms.

16.1 Hz, 1H, H₆—C==N, 7.72 (dd, J = 8.3, 6.9, 1.4 Hz, 1H, H₇), 7.72 (d, J = 8.5 Hz, 2H, H₂', H₆'), 7.68 (d, J = 8.5 Hz, 2H, H₃', H₅'), 7.54 (dd, J = 8.3, 6.8, 1.3 Hz, 1H, H₆), 7.50 (d, J = 0.7 Hz, 1H, H₃), 7.32 (d, J = 16.1 Hz, 1H, H₂=CH), 2.79 (s, 3H, 2-CH₃); δ (¹³C) 158.8 (C₂), 148.5 (C₈a), 142.3 (C₄), 140.0 (C₁'), 133.2 (C₁=CH₃), 130.3 (d, J = 32.4 Hz, C₄'), 129.5 (C₇), 129.4 (C₈), 127.2 (C₂', C₆', C₅', C₇'), 125.9 (q, J = 3.7 Hz, 4-CF₃), 125.4 (C₆), 124.7 (C₄a), 123.1 (C₅), 122.7 (H₆—C==N), 118.2 (C₃), 25.4 (2-CH₃). HRMS (ESI⁺) m/z found for [M + H⁺] 314.115, C₁₈H₁₄FN requires 313.1078.

Compound (III): yield 0.25 g (94%), m.p. 410–412 K, Rᵣ = 0.31 (12.5% ethyl acetate–hexane). FT–IR (ATR, cm⁻¹): 1629 (C≡N), 1593 (C=C(aryl)), 1554 (C=C(aryl)), 1505 (C=C(aryl)), 959 (C═H(aryl)). NMR (CDCl₃): δ(H) 8.10 (dd, J = 8.5, 1.4 Hz, 1H, H₅), 8.06 (dd, J = 8.5, 1.4 Hz, 1H, H₈), 7.85 (dd, J = 16.5, 0.87 Hz, 1H, H₆—C==N, 7.70 (dd, J = 8.4, 6.9, 1.4 Hz, 1H, H₇), 7.53 (dd, J = 8.4, 6.9, 1.3 Hz, 1H, H₆), 7.53 (s, 1H, H₃), 7.41 (d, J = 8.0 Hz, 2H, H₂', H₆'), 7.18 (dd, J = 8.4, 7.7 Hz, 1H, H₄'), 7.26 (d, J = 16.5 Hz, 1H, H₂=CH₃), 2.80 (s, 3H, 2-CH₃). δ (¹³C) 158.8 (C₂), 148.4 (C₈a), 142.2 (C₄), 137.2 (C₁'), 134.7 (C₂', C₆'), 133.8 (C₃'), 132.4 (H₆—C≡N), 130.1 (C₄'), 129.3 (C₇), 129.4 (C₈), 127.4 (C₅'), 125.9 (C₆), 124.8 (C₄a), 123.6 (C₅), 118.5 (C₃), 25.5 (2-CH₃). HRMS (ESI⁺) m/z found for [M + H⁺] 314.0500, C₁₈H₁₃Cl₂N requires 313.0425.
and thus we report here also the molecular and supramolecular structures for all three examples (Figs. 1–3).

These new 2-methylquinoline derivatives (I)–(III) are intended for use as key precursors in the further development of more complex molecules of possible biological value, such as the bis-styrylquinolines (IV) (Scheme 2), (4-styrylquinolin-2-yl)chalcones of the type (V), and the molecular hybrids of types (VI) and (VII), and the work reported here can be regarded as a continuation of an earlier crystallographic study which reported the structures of 2-methyl-4-styrylquinolines having either acetyl or carboethoxy functionalities at position C3 (Rodríguez et al., 2020).

The molecules of compounds (I)–(III) exhibit no internal symmetry, as indicated by the key torsion angles (Table 2). They are thus not superimposable upon their mirror images and hence they are all conformationally chiral (Moss, 1996; Flack & Bernardinelli, 1999). The space groups (Table 1) confirm that the crystals of each compound contain equal numbers of the two conformational enantiomers; for each compound, the reference molecule was selected as one having a positive sign for the torsion angle C3—C4—C41—C42 (Table 2). Only in compound (II) is the styryl fragment involved in direction-specific intermolecular interactions, as discussed below, and hence there appears to be no simple interpretation of the conformational differences in compounds (I)–(III), other than to note that the barriers to rotation about the C—C single bonds are generally quite low, typically a few kJ mol\(^{-1}\) (Alkorta & Elguero, 1998).

The supramolecular assembly in compounds (I)–(III) is very simple (Table 3). There is a single hydrogen bond in the structure of (I). In the structure of (II), there is a C—H···π(arene) hydrogen bond, but for the intermolecular C—

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**Table 2**

Selected torsion angles (°) for compounds (I)–(III).

| Parameter | (I)      | (II)     | (III)     |
|-----------|----------|----------|-----------|
| C3—C4—C41—C42 | 38.8 (2) | 28.1 (2) | 39.5 (2)  |
| C41—C42—C421—C422 | −174.47 (15) | −175.59 (15) | 139.58 (15) |

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**Figure 1**
The molecular structure of compound (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

**Figure 2**
The molecular structure of compound (II), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

**Figure 3**
The molecular structure of compound (III), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.
H···N contact, the H···N distance exceeds the sum, 2.70 Å, of the van der Waals radii for these atoms (Rowland & Taylor, 1996); hence, this is just a normal intermolecular contact with no associated attractive interaction which could be regarded as structurally significant. The C—H···N contact in compound (III) involves a methyl group (Table 3), where the C—H bonds are of low acidity. More significantly, methyl groups are, in general, likely to be undergoing very fast rotation about the adjacent C—C bond in the solid state (Riddell & Rogerson, 1996, 1997). For methyl groups bonded to planar fragments such as aryl rings, the sixfold barrier to rotation is usually very small, only a few J mol\(^{-1}\) rather than the typical order of magnitude in kJ mol\(^{-1}\) (Naylor & Wilson, 1957; Tannenbaum et al., 1956). Hence, this contact cannot be regarded as structurally significant. There are π–π stacking interactions in each structure.

In the structure of (I), inversion-related pairs of molecules are linked by almost linear C—H···N hydrogen bonds (Table 3) to form centrosymmetric dimers characterized by an \(R_2^2(8)\) motif (Etter, 1990; Etter et al., 1990; Bernstein et al., 1995) (Fig. 4). Dimers of this type are linked into sheets by π–π stacking interactions; the quinoline units of the molecule at \((x, y, z)\), makes dihedral angles of 9.21 (7)° with the corresponding rings of the molecules at \((-x + \frac{1}{2}, -y + 1, -z + 1\); \((ii) -x + \frac{1}{2}, y = \frac{1}{2}, -z + \frac{1}{2}\); \((iii) -x + 1, -y + 1, -z + 1\); \((iv) -x + 1, -y + 2, -z + 1\).
operations leads to the formation of a sheet of π-stacked dimers lying parallel to (100) (Fig. 4).

In the structure of compound (II), inversion-related pairs of molecules are linked by a C—H⋯π(arene) hydrogen bond to form centrosymmetric dimers (Fig. 5), and these dimers are linked into chains by a single π–π stacking interaction; the heteroaromatic rings in the molecules at (x, y, z) and (−x + 1, y, −z + ½) are strictly parallel, with an interplanar spacing of 3.5058 (6) Å and a ring-centroid separation of 3.6845 (9) Å, corresponding to a ring-centroid offset of 1.1335 (12) Å. By this means, the hydrogen-bonded dimers are linked into a chain running parallel to [001] (Fig. 5).

Although there are no hydrogen bonds in the structure of compound (III), the molecules which are related by translation along the [010] direction are stacked precisely in register with a spacing equal to the unit-cell vector b = 3.8629 (2) Å (Fig. 6). Eight stacks of this kind pass through each unit cell (Fig. 7), but there are no direction-specific interactions between adjacent stacks.

We have previously reported (Rodríguez et al., 2020) the synthesis and structures of a number of 4-styrylquinoline derivatives carrying either acetyl or carboethoxy substituents at position C-3. Of these, three closely related acetyl derivatives carrying either acetyl or carboethoxy substituents have been recorded in the Cambridge Structural Database (CSD; Groom et al., 2016), but it is striking that the majority of these compounds were found to be isomorphous, with their molecules linked into simple C(6) chains by a single C—H⋯O hydrogen bond. By contrast, the matching set of carboethoxy derivatives all exhibited different crystallization characteristics and different modes of supramolecular assembly, with one forming C(13) chains and the other two forming cyclic centrosymmetric dimers involving C—H⋯O hydrogen bonds in one case and C—H⋯π hydrogen bonds in the other. In addition, two other examples carrying acyl substituents have been reported (Meléndez et al., 2020) on a proof-of-structure basis without detailed structure analysis or description, but subsequent re-examination (Rodríguez et al., 2020) found a complex sheet structure in one of them, but no significant intermolecular interactions in the other.

The structures of a number of other styrylquinolines are recorded in the Cambridge Structural Database (CSD; Groom et al., 2016), but it is striking that the majority of these structures are of 2-styrylquinoline derivatives, along with those of a small number of 8-styrylquinolines. This may reflect, at least in part, a lack of efficient, straightforward and versatile routes to other isomeric styrylquinolines. The structure of 2-styrylquinoline itself has been reported three times (Valle et al., 1986; Gulakova et al., 2011; Kuz’mina et al., 2011), as have those of 2-[2-(4-methoxyphenyl)vinyl]quinoline (Gulakova et al., 2011; Kuz’mina et al., 2011; Das et al., 2019) and 2-[2-(3,4-methoxyphenyl)vinyl]quinolone (Gulakova et al., 2011; Kuz’mina et al., 2011; Sharma et al., 2021). There are two reports on the structure of 2-[2-(3-nitrophenyl)vinyl]quinolone (Gulakova et al., 2011; Kuz’mina et al., 2011) and one on the structure of 4-phenyl-2-styrylquinoline (Makela et al., 2021). In all of these 2-styrylquinolines, the molecular skeleton is planar, in marked contrast to the nonplanar conformations of the 4-styrylquinoline derivatives (I)–(III) reported here, and of those reported previously (Rodríguez et al., 2020). In both 8-styrylquinoline and 8-[2-(biphenyl-4-yl)vinyl]-2-methylquinoline, the styrylquinoline fragment is planar (Sharma et al., 2015), as found in 2-styrylquinolines but again in marked contrast to 4-styrylquinolines. It is not easy to see why 4-styrylquinolines should adopt nonplanar conformations, while molecules of the 2-styryl and 8-styryl isomers appear consistently to adopt planar forms.

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Synthesis and spectroscopic and structural characterization of three new 2-methyl-4-styrylquinolines formed using Friedländer reactions between (2-aminophenyl)chalcones and acetone

Diana Rocío Vera, Juan P. Mantilla, Alirio Palma, Justo Cobo and Christopher Glidewell

Computing details
For all structures, data collection: APEX3 (Bruker, 2018); cell refinement: SAINT (Bruker, 2017); data reduction: SAINT (Bruker, 2017); program(s) used to solve structure: SHELXT2014 (Sheldrick, 2015a); program(s) used to refine structure: SHELXL2014 (Sheldrick, 2015b); molecular graphics: PLATON (Spek, 2020); software used to prepare material for publication: SHELXL2014 (Sheldrick, 2015b) and PLATON (Spek, 2020).

(E)-4-[2-(4-Fluorophenyl)ethenyl]-2-methylquinoline (I)

Crystal data
C_{18}H_{14}FN

$M_r = 263.30$

Monoclinic, $P2_1/c$

$a = 13.5921$ (7) Å

$b = 12.7103$ (6) Å

$c = 7.6215$ (3) Å

$\beta = 103.133$ (2)°

$V = 1282.25$ (10) Å³

$Z = 4$

$F(000) = 552$

$D_\lambda = 1.364$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2950 reflections

$\theta = 2.2$–$27.5$°

$\mu = 0.09$ mm⁻¹

$T = 100$ K

Needle, yellow

$0.20 \times 0.08 \times 0.07$ mm

Data collection

Bruker D8 Venture diffractometer

Radiation source: INCOATEC high brilliance microfocus sealed tube

Multilayer mirror monochromator

$\phi$ and $\omega$ scans

Absorption correction: multi-scan

(SADABS; Bruker, 2016)

$T_{\text{min}} = 0.934$, $T_{\text{max}} = 0.994$

38068 measured reflections

2949 independent reflections

2342 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.079$

$\theta_{\text{max}} = 27.5$°, $\theta_{\text{min}} = 2.2$°

$h = -17$→$17$

$k = -16$→$16$

$l = -9$→$9$

Refinement
Refinement on $F^2$
Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.042$

$wR(F^2) = 0.100$

$S = 1.05$

2949 reflections

182 parameters

0 restraints

Primary atom site location: dual

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma(F_c^2) + (0.0315P)^2 + 0.8512P]$ where $P = (F_c^2 + 2F_s^2)/3$
(Δ/σ)_{max} < 0.001
Δρ_{max} = 0.26 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

|     | x        | y        | z        | Uiso* / Ueq |
|-----|----------|----------|----------|-------------|
| N1  | 0.38298(9) | 0.09596(10) | 0.33198(16) | 0.0184(3)   |
| C2  | 0.29100(11) | 0.11467(12) | 0.23444(19) | 0.0176(3)   |
| C3  | 0.25558(11) | 0.21776(12) | 0.18306(19) | 0.0176(3)   |
| H3  | 0.1892    | 0.2272    | 0.1115    | 0.021*      |
| C4  | 0.31611(11) | 0.30404(11) | 0.23560(19) | 0.0167(3)   |
| C4A | 0.41653(10) | 0.28596(11) | 0.33921(19) | 0.0163(3)   |
| C5  | 0.48647(11) | 0.36772(12) | 0.4033(2)  | 0.0191(3)   |
| H5  | 0.4685    | 0.4386    | 0.3719    | 0.023*      |
| C6  | 0.57984(11) | 0.34538(12) | 0.5101(2)  | 0.0204(3)   |
| H6  | 0.6260    | 0.4008    | 0.5523    | 0.024*      |
| C7  | 0.60735(11) | 0.24060(12) | 0.5574(2)  | 0.0204(3)   |
| H7  | 0.6716    | 0.2261    | 0.6336    | 0.024*      |
| C8  | 0.54267(11) | 0.15932(12) | 0.4950(2)  | 0.0196(3)   |
| H8  | 0.5628    | 0.0889    | 0.5257    | 0.024*      |
| C8A | 0.44577(11) | 0.18016(12) | 0.38490(19) | 0.0170(3)   |
| C21 | 0.22304(12) | 0.02127(12) | 0.1834(2)  | 0.0225(3)   |
| H21A| 0.1914    | 0.0036    | 0.2830    | 0.034*      |
| H21B| 0.2628    | −0.0388   | 0.1578    | 0.034*      |
| H21C| 0.1705    | 0.0381    | 0.0759    | 0.034*      |
| C41 | 0.27793(11) | 0.41183(11) | 0.19305(19) | 0.0174(3)   |
| H41 | 0.3216    | 0.4626    | 0.1597    | 0.021*      |
| C42 | 0.18432(11) | 0.44098(11) | 0.19947(19) | 0.0173(3)   |
| H42 | 0.1420    | 0.3877    | 0.2295    | 0.021*      |
| C421| 0.13959(10) | 0.54644(11) | 0.16520(18) | 0.0163(3)   |
| C422| 0.04269(11) | 0.56378(12) | 0.1940(2)  | 0.0191(3)   |
| H422| 0.0077    | 0.5074    | 0.2345    | 0.023*      |
| C423| −0.00317(11) | 0.66179(12) | 0.1644(2)  | 0.0199(3)   |
| H423| −0.0691   | 0.6729    | 0.1835    | 0.024*      |
| C424| 0.04914(11) | 0.74221(11) | 0.10693(19) | 0.0187(3)   |
| F424| 0.00528(7)  | 0.83934(7)  | 0.08198(12) | 0.0255(2)   |
| C425| 0.14458(11) | 0.72940(12) | 0.0748(2)  | 0.0192(3)   |
| H425| 0.1785    | 0.7863    | 0.0333    | 0.023*      |
| C426| 0.18939(11) | 0.63090(12) | 0.10502(19) | 0.0181(3)   |
| H426| 0.2551    | 0.6206    | 0.0845    | 0.022*      |
Atomic displacement parameters (Å²)

|       | $U^{11}$  | $U^{22}$  | $U^{33}$  | $U^{12}$  | $U^{13}$  | $U^{23}$  |
|-------|-----------|-----------|-----------|-----------|-----------|-----------|
| N1    | 0.0183 (6) | 0.0176 (6) | 0.0200 (6) | 0.0012 (5) | 0.0059 (5) | 0.0007 (5) |
| C2    | 0.0186 (7) | 0.0177 (7) | 0.0181 (7) | -0.0004 (6) | 0.0075 (6) | -0.0006 (5) |
| C3    | 0.0159 (7) | 0.0197 (7) | 0.0177 (7) | 0.0016 (6) | 0.0050 (5) | 0.0006 (5) |
| C4    | 0.0171 (7) | 0.0175 (7) | 0.0167 (7) | 0.0023 (6) | 0.0066 (5) | 0.0014 (5) |
| C4A   | 0.0164 (7) | 0.0177 (7) | 0.0157 (7) | 0.0010 (5) | 0.0058 (5) | -0.0003 (5) |
| C5    | 0.0200 (7) | 0.0164 (7) | 0.0215 (7) | 0.0020 (6) | 0.0058 (6) | -0.0019 (6) |
| C6    | 0.0171 (7) | 0.0220 (8) | 0.0221 (7) | -0.0019 (6) | 0.0046 (6) | -0.0052 (6) |
| C7    | 0.0158 (7) | 0.0255 (8) | 0.0198 (7) | 0.0038 (6) | 0.0038 (6) | -0.0014 (6) |
| C8    | 0.0184 (7) | 0.0207 (8) | 0.0205 (7) | 0.0047 (6) | 0.0057 (6) | 0.0015 (6) |
| C8A   | 0.0180 (7) | 0.0172 (7) | 0.0172 (7) | 0.0014 (5) | 0.0071 (5) | -0.0002 (5) |
| C21   | 0.0231 (8) | 0.0182 (8) | 0.0259 (8) | -0.0017 (6) | 0.0048 (6) | -0.0010 (6) |
| C41   | 0.0179 (7) | 0.0164 (7) | 0.0175 (7) | -0.0003 (6) | 0.0035 (5) | 0.0007 (5) |
| C42   | 0.0178 (7) | 0.0161 (7) | 0.0179 (7) | -0.0013 (5) | 0.0041 (5) | 0.0008 (5) |
| C421  | 0.0152 (7) | 0.0169 (7) | 0.0159 (7) | 0.0003 (5) | 0.0016 (5) | -0.0012 (5) |
| C422  | 0.0178 (7) | 0.0195 (8) | 0.0204 (7) | -0.0013 (6) | 0.0051 (6) | 0.0011 (5) |
| C423  | 0.0168 (7) | 0.0239 (8) | 0.0192 (7) | 0.0040 (6) | 0.0049 (6) | -0.0008 (6) |
| C424  | 0.0221 (8) | 0.0153 (7) | 0.0173 (7) | 0.0060 (6) | 0.0016 (6) | -0.0006 (5) |
| F424  | 0.0298 (5) | 0.0174 (5) | 0.0296 (5) | 0.0095 (4) | 0.0076 (4) | 0.0024 (4) |
| C425  | 0.0201 (7) | 0.0162 (7) | 0.0207 (7) | -0.0014 (6) | 0.0030 (6) | 0.0002 (5) |
| C426  | 0.0152 (7) | 0.0195 (7) | 0.0193 (7) | 0.0002 (5) | 0.0030 (5) | -0.0001 (6) |

Geometric parameters (Å, º)

|       |          |          |          |          |          |          |
|-------|-----------|-----------|-----------|-----------|-----------|-----------|
| N1—C2 | 1.3227 (19) | C21—H21A | 0.9800    |          |          |          |
| N1—C8A| 1.3712 (19) | C21—H21B | 0.9800    |          |          |          |
| C2—C3 | 1.420 (2)   | C21—H21C | 0.9800    |          |          |          |
| C2—C21| 1.500 (2)   | C41—C42  | 1.337 (2) |          |          |          |
| C3—C4 | 1.375 (2)   | C41—H41  | 0.9500    |          |          |          |
| C3—H3 | 0.9500     | C42—C42  | 1.471 (2) |          |          |          |
| C4—C4A| 1.432 (2)   | C42—H42  | 0.9500    |          |          |          |
| C4—C41| 1.475 (2)   | C421—C426| 1.401 (2) |          |          |          |
| C4A—C5| 1.418 (2)   | C421—C422| 1.401 (2) |          |          |          |
| C4A—C8A| 1.423 (2)  | C422—C423| 1.388 (2) |          |          |          |
| C5—C6 | 1.373 (2)   | C422—H422| 0.9500    |          |          |          |
| C5—H5 | 0.9500     | C423—C424| 1.373 (2) |          |          |          |
| C6—C7 | 1.408 (2)   | C423—H423| 0.9500    |          |          |          |
| C6—H6 | 0.9500     | C424—F424| 1.3653 (16)|         |          |          |
| C7—C8 | 1.370 (2)   | C424—C425| 1.383 (2) |          |          |          |
| C7—H7 | 0.9500     | C425—C426| 1.388 (2) |          |          |          |
| C8—C8A| 1.417 (2)   | C425—H425| 0.9500    |          |          |          |
| C8—H8 | 0.9500     | C426—H426| 0.9500    |          |          |          |
| C2—N1—C8A| 118.08 (13) | C2—C21—H21B| 109.5 |          |          |          |
| N1—C2—C3| 122.60 (13) | H21A—C21—H21B| 109.5 |          |          |          |
| N1—C2—C21| 116.82 (13) | C2—C21—H21C| 109.5 |          |          |          |
C3—C2—C21 120.56 (13) H21A—C21—H21C 109.5
C4—C3—C2 120.85 (13) H21B—C21—H21C 109.5
C4—C3—H3 119.6 C42—C41—C4 122.66 (14)
C2—C3—H3 119.6 C42—C41—H41 118.7
C3—C4—C4A 117.71 (13) C4—C41—H41 118.7
C3—C4—C41 121.31 (13) C41—C42—C421 127.21 (14)
C4A—C4—C41 120.94 (13) C41—C42—H42 116.4
C5—C4A—C8A 118.70 (13) C42—C421—C42—H42 116.4
C5—C4A—C4 123.56 (13) C426—C421—C422 118.18 (13)
C8A—C4A—C4 117.71 (13) C426—C421—C42 123.07 (13)
C6—C5—C4A 120.64 (14) C421—C42—C421 121.28 (14)
C6—C5—H5 119.7 C423—C422—C421 121.28 (14)
C4A—C5—H5 119.7 C423—C422—C421 121.28 (14)
C5—C6—C7 120.23 (14) C421—C422—H422 119.4
C5—C6—H6 119.9 C422—C421—C426 118.45 (13)
C7—C6—H6 119.9 C422—C421—C422 118.63 (13)
C8—C7—C6 120.82 (14) C422—C421—C42 121.0
C8—C7—H7 119.6 C422—C421—C421 121.26 (13)
C6—C7—H7 119.6 C422—C421—C422 121.26 (13)
C7—C8—C8A 120.11 (14) C422—C421—C423 122.92 (14)
C7—C8—H8 119.9 C422—C421—C424 122.92 (14)
C8A—C8—H8 119.9 C422—C421—C425 122.92 (14)
N1—C8A—C8 117.46 (13) C422—C421—C426 122.92 (14)
N1—C8A—C4A 123.03 (13) C422—C421—C421 122.92 (14)
C8—C8A—C4A 119.48 (13) C422—C421—C422 122.92 (14)
C2—C21—H21A 109.5 C422—C421—C423 122.92 (14)
C8A—N1—C2—C3 0.1 (2) C422—C421—C424 122.92 (14)
C8A—N1—C2—C21 −178.20 (13) C422—C421—C425 122.92 (14)
N1—C2—C3—C4 −0.9 (2) C422—C421—C426 122.92 (14)
N1—C2—C3—C4 177.35 (13) C422—C421—H422 122.92 (14)
C2—C3—C4—C4A 1.7 (2) C422—C421—H423 122.92 (14)
C2—C3—C4—C41 −175.99 (13) C422—C421—H424 122.92 (14)
C3—C4—C4A—C5 −179.48 (13) C422—C421—H425 122.92 (14)
C4A—C4—C4A—C5 1.8 (2) C422—C421—H426 122.92 (14)
C4—C4—C4A—C5 176.49 (14) C424—C422—C421—C426 5.5 (2)
C4—C4—C4A—C5 −176.49 (14) C424—C422—C421—C422 −147.47 (15)
C4A—C4—C4A—C5 175.96 (13) C424—C422—C421—C423 −0.2 (2)
C8A—C4A—C8A 0.1 (2) C424—C422—C421—C423 179.79 (14)
C4A—C5—C6 176.49 (14) C424—C422—C421—C424 −0.4 (2)
C4A—C5—C6 176.49 (14) C424—C422—C421—C425 1.0 (2)
C4A—C5—C6 176.49 (14) C424—C422—C421—C426 4.0 (2)
C4—C5—C6 176.49 (14) C424—C422—C421—C427 5.0 (2)
C4—C5—C6 −174.47 (15) C424—C422—C421—C427 5.0 (2)
C4—C5—C6 −174.47 (15) C424—C422—C421—C428 5.0 (2)
C4—C5—C6 −174.47 (15) C424—C422—C421—C429 5.0 (2)
C4—C5—C6 −174.47 (15) C424—C422—C421—C430 5.0 (2)
C4—C5—C6 −174.47 (15) C424—C422—C421—C431 5.0 (2)
C4—C5—C6 −174.47 (15) C424—C422—C421—C432 5.0 (2)
C4—C5—C6 −174.47 (15) C424—C422—C421—C433 5.0 (2)
C4—C5—C6 −174.47 (15) C424—C422—C421—C434 5.0 (2)
C4—C5—C6 −174.47 (15) C424—C422—C421—C435 5.0 (2)
Hydrogen-bond geometry (Å, °)

| D—H···A       | D—H  | H···A  | D···A  | D—H···A |
|---------------|-------|--------|--------|---------|
| C8—H8···N1i   | 0.95  | 2.62   | 3.561  | 2 (2)   | 170     |

Symmetry code: (i) −x+1, −y, −z+1.

(E)-2-Methyl-4-(2-[4-(trifluoromethyl)phenyl]ethenyl)quinoline (II)

Crystal data

C$_{19}$H$_{14}$F$_{3}$N

$F(000) = 1296$

$D_c = 1.381$ Mg m$^{-3}$

Monoclinic, $C2/c$

$\theta = 2.2$–$28.3^\circ$

$\mu = 0.11$ mm$^{-1}$

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

$\theta = 2.2$–$28.3^\circ$

$T = 100$ K

$F(000) = 1296$

Cell parameters from 3752 reflections

$V = 3013.8$ (3) Å$^3$

$Z = 8$

$\chi = 0.11$ mm$^{-1}$

$T = 100$ K

Block, colourless

0.16 × 0.14 × 0.12 mm

Data collection

Bruker D8 Venture diffractometer

3750 independent reflections

Absorption correction: multi-scan (SADABS; Bruker, 2016)

$\mu = 0.11$ mm$^{-1}$

$\theta = 2.2$–$28.3^\circ$

$h = -22$→$22$

$k = -14$→$14$

$l = -21$→$20$

$T_{\text{min}} = 0.888$, $T_{\text{max}} = 0.987$

Refinement

Refinement on $F^2$

$R[F^2 > 2\sigma(F^2)] = 0.047$

$wR(F^2) = 0.121$

$S = 1.03$

3750 reflections

209 parameters

0 restraints

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\AA^2$)

|      | x       | y       | z       | $U_{\text{iso}}$ or $U_{eq}$ |
|------|---------|---------|---------|-----------------------------|
| N1   | 0.35530 (8) | 0.65666 (13) | 0.70993 (8) | 0.0214 (3) |
| C2   | 0.40811 (9) | 0.73252 (15) | 0.68089 (10) | 0.0220 (3) |
| C3   | 0.47497 (9) | 0.69044 (15) | 0.64043 (10) | 0.0208 (3) |

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\AA^2$)

Acta Cryst. (2022). C78, 524-530
|    | \(U_{11}^i\)         | \(U_{22}^i\)         | \(U_{33}^i\)         | \(U_{12}^i\)         | \(U_{13}^i\)         | \(U_{23}^i\)         |
|----|-----------------------|-----------------------|-----------------------|-----------------------|-----------------------|-----------------------|
| N1 | 0.0182 (7)            | 0.0233 (7)            | 0.0229 (7)            | 0.0019 (5)            | 0.0041 (5)            | −0.0005 (5)           |
| C2 | 0.0196 (8)            | 0.0223 (8)            | 0.0245 (8)            | 0.0015 (6)            | 0.0053 (6)            | 0.0003 (6)            |
| C3 | 0.0168 (7)            | 0.0223 (8)            | 0.0236 (8)            | −0.0009 (6)           | 0.0048 (6)            | 0.0016 (6)            |
| C4 | 0.0154 (7)            | 0.0235 (8)            | 0.0162 (7)            | 0.0020 (6)            | 0.0002 (5)            | −0.0001 (6)           |
| C4A| 0.0160 (7)            | 0.0218 (8)            | 0.0150 (7)            | 0.0001 (6)            | −0.0010 (5)           | 0.0004 (6)            |
| C5 | 0.0208 (8)            | 0.0224 (8)            | 0.0216 (7)            | 0.0016 (6)            | 0.0010 (6)            | −0.0013 (6)           |
| C6 | 0.0270 (9)            | 0.0213 (8)            | 0.0241 (8)            | −0.0028 (7)           | −0.0003 (6)           | 0.0003 (6)            |
| C7 | 0.0226 (8)            | 0.0278 (9)            | 0.0233 (8)            | −0.0066 (7)           | 0.0022 (6)            | 0.0012 (6)            |
| C8 | 0.0174 (7)            | 0.0280 (9)            | 0.0210 (7)            | −0.0021 (6)           | 0.0033 (6)            | −0.0005 (6)           |
| C8A| 0.0171 (7)            | 0.0228 (8)            | 0.0163 (7)            | 0.0005 (6)            | 0.0004 (6)            | 0.0004 (6)            |

Atomic displacement parameters (Å²)
supporting information

C21 0.0306 (10) 0.0227 (9) 0.0448 (11) 0.0030 (7) 0.0160 (8) −0.0003 (8)
C41 0.0173 (7) 0.0210 (7) 0.0186 (7) 0.0030 (6) 0.0013 (6) 0.0000 (6)
C42 0.0187 (7) 0.0225 (8) 0.0205 (7) 0.0012 (6) 0.0015 (6) −0.0019 (6)
C421 0.0217 (8) 0.0169 (7) 0.007 (6) 0.0013 (5) 0.0111 (6)
C422 0.0233 (8) 0.0254 (8) −0.0014 (6) 0.0020 (6) −0.0057 (6)
C423 0.0175 (8) 0.0277 (8) −0.0042 (6) 0.0021 (6) −0.0033 (6)
C424 0.0160 (7) 0.0189 (7) 0.0014 (6) 0.0013 (6) 0.0017 (6)
C425 0.0193 (7) 0.0217 (8) 0.0197 (7) −0.0003 (6) 0.0018 (6) −0.0021 (6)
C426 0.0158 (7) 0.0218 (8) 0.0220 (7) −0.0025 (6) 0.0010 (6) −0.0010 (6)
C427 0.0201 (8) 0.0248 (8) 0.0251 (8) −0.0019 (6) 0.0041 (6) −0.0024 (6)
F471 0.0287 (6) 0.0367 (6) 0.0522 (7) 0.0131 (5) 0.0118 (5) 0.0077 (5)
F472 0.0307 (6) 0.0758 (9) 0.0318 (6) −0.0015 (6) 0.0096 (5) −0.0237 (6)
F473 0.0274 (6) 0.0328 (6) 0.0578 (7) −0.0076 (5) 0.0212 (5) −0.0055 (5)

Geometric parameters (Å, °)

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| N1—C2 | 1.321 (2) | C21—H21C | 0.9800 |
| N1—C8A | 1.368 (2) | C41—C42 | 1.334 (2) |
| C2—C3 | 1.416 (2) | C41—H41 | 0.9500 |
| C2—C21 | 1.507 (2) | C42—C421 | 1.468 (2) |
| C3—C4 | 1.375 (2) | C42—H42 | 0.9500 |
| C3—H3 | 0.9500 | C421—C426 | 1.399 (2) |
| C4—C4A | 1.432 (2) | C421—C422 | 1.400 (2) |
| C4—C41 | 1.471 (2) | C421—C423 | 1.388 (2) |
| C4A—C5 | 1.419 (2) | C422—C42 | 0.9500 |
| C4A—C8A | 1.422 (2) | C42—C424 | 1.389 (2) |
| C5—C6 | 1.369 (2) | C423—C424 | 1.392 (2) |
| C5—H5 | 0.9500 | C424—C425 | 1.491 (2) |
| C6—C7 | 1.411 (2) | C424—C427 | 1.383 (2) |
| C6—H6 | 0.9500 | C425—C426 | 1.383 (2) |
| C7—C8 | 1.368 (2) | C425—H425 | 0.9500 |
| C7—H7 | 0.9500 | C426—H426 | 0.9500 |
| C8—C8A | 1.418 (2) | C427—F473 | 1.3350 (19) |
| C8—H8 | 0.9500 | C427—F47 | 1.335 (2) |
| C21—H21A | 0.9800 | C427—F471 | 1.347 (2) |
| C21—H21B | 0.9800 |   |   |

C2—N1—C8A | 117.72 (14) | H21A—C21—H21C | 109.5 |
N1—C2—C3 | 122.85 (15) | H21B—C21—H21C | 109.5 |
N1—C2—C21 | 116.62 (14) | C42—C41—C4 | 124.49 (15) |
C3—C2—C21 | 120.53 (15) | C42—C41—H41 | 117.8 |
C4—C3—C2 | 120.99 (15) | C4—C41—H41 | 117.8 |
C4—C3—H3 | 119.5 | C41—C42—C421 | 126.36 (15) |
C2—C3—H3 | 119.5 | C41—C42—H42 | 116.8 |
C3—C4—C4A | 117.40 (14) | C421—C42—H42 | 116.8 |
C3—C4—C41 | 121.69 (14) | C426—C421—C422 | 118.27 (14) |
C4A—C4—C41 | 120.90 (14) | C426—C421—C42 | 123.05 (14) |
C5—C4A—C8A | 118.29 (14) | C422—C421—C42 | 118.68 (14) |
C5—C4A—C4 124.02 (14) C423—C422—C421 121.30 (15)
C8A—C4A—C4 117.69 (14) C423—C422—H422 119.4
C6—C5—C4A 120.77 (15) C421—C422—H422 119.4
C6—C5—H5 119.6 C422—C423—C424 119.29 (15)
C4A—C5—C4 119.6 C422—C423—H423 120.4
C5—C6—C7 120.90 (16) C424—C423—H423 120.4
C5—C6—H6 119.5 C423—C424—C425 120.34 (14)
C7—C6—H6 119.5 C423—C424—C427 120.88 (14)
C8—C7—C6 119.67 (15) C425—C424—C427 118.77 (14)
C8—C7—H7 120.2 C426—C425—C424 119.97 (15)
C6—C7—H7 120.2 C426—C425—H425 120.0
C7—C8—C8A 120.89 (15) C424—C425—H425 120.0
C7—C8—H8 119.6 C425—C426—C421 120.83 (14)
C8A—C8—H8 119.6 C425—C426—H426 119.6
N1—C8A—C8 117.23 (14) C421—C426—H426 119.6
N1—C8A—C4A 123.33 (14) F473—C427—F472 106.26 (14)
C8—C8A—C4A 119.44 (15) F473—C427—F471 105.69 (14)
C2—C21—H21A 109.5 F472—C427—C424 113.47 (14)
C2—C21—H21B 109.5 F472—C427—C424 112.81 (14)
H21A—C21—H21B 109.5 F471—C427—C424 112.17 (13)
C2—C21—H21C 109.5 F471—C427—C424 112.17 (13)
C8A—N1—C2—C3 0.7 (2) C4—C4A—C8A—C8 178.87 (14)
C8A—N1—C2—C21 179.91 (15) C4—C4A—C8A—C8 28.1 (2)
N1—C2—C3—C4 −1.3 (3) C4A—C4—C41—C42 −153.27 (16)
C21—C2—C3—C4 179.50 (16) C4—C41—C42—C421 −179.85 (15)
C2—C3—C4—C4A 0.6 (2) C41—C42—C421—C426 4.6 (3)
C2—C3—C4—C41 179.28 (15) C41—C42—C421—C422 −175.68 (16)
C3—C4—C4A—C5 −178.50 (15) C426—C421—C422—C423 0.2 (2)
C41—C4—C4A—C5 2.8 (2) C42—C421—C422—C423 −179.59 (15)
C3—C4—C4A—C8A 0.6 (2) C421—C422—C423—C424 0.1 (3)
C41—C4—C4A—C8A −178.12 (13) C422—C423—C424—C425 −0.2 (2)
C8A—C4A—C5—C6 1.3 (2) C422—C423—C424—C425 −178.80 (15)
C4—C4A—C5—C6 −179.65 (15) C423—C424—C425—C426 0.0 (2)
C4A—C5—C6—C7 0.4 (2) C427—C424—C425—C426 178.65 (15)
C5—C6—C7—C8 −1.3 (3) C424—C425—C426—C421 0.3 (2)
C6—C7—C8—C8A 0.5 (2) C422—C421—C426—C425 −0.3 (2)
C2—N1—C8A—C8 −179.51 (14) C42—C421—C426—C425 179.40 (15)
C2—N1—C8A—C4A 0.6 (2) C423—C424—C427—F473 −16.7 (2)
C7—C8—C8A—N1 −178.81 (15) C425—C424—C427—F473 164.64 (15)
C7—C8—C8A—C4A 1.1 (2) C423—C424—C427—F472 −137.61 (16)
C5—C4A—C8A—N1 177.91 (14) C425—C424—C427—F472 43.7 (2)
C4—C4A—C8A—N1 −1.2 (2) C423—C424—C427—F471 102.99 (18)
C5—C4A—C8A—C8 −2.0 (2) C425—C424—C427—F471 −75.67 (19)
Hydrogen-bond geometry (Å, °)

| D—H···A       | D—H  | H···A  | D···A     | D—H···A |
|---------------|-------|--------|-----------|---------|
| C426—H426···Cg1i | 0.95  | 2.86   | 3.3627 (17) | 114     |

Symmetry code: (i) −x+1, −y+1, −z+1.

(E)-4-[2-(2,6-dichlorophenyl)ethenyl]-2-methylquinoline (III)

Crystal data

C18H13Cl2N

Mr = 314.19

Monoclinic, C2/c

a = 30.5651 (15) Å

b = 3.8629 (2) Å

c = 25.5357 (13) Å

β = 110.497 (2)°

V = 2824.1 (2) Å³

Z = 8

F(000) = 1296

Dc = 1.478 Mg m⁻³

Mo Kα radiation, λ = 0.71073 Å

Cell parameters from 3210 reflections

θ = 2.6–27.5°

µ = 0.45 mm⁻¹

T = 100 K

Needle, yellow

0.20 × 0.10 × 0.06 mm

Data collection

Bruker D8 Venture diffractometer

Radiation source: INCOATEC high brilliance microfocus sealed tube

Multilayer mirror monochromator

φ and ω scans

Absorption correction: multi-scan (SADABS; Bruker, 2016)

Tmin = 0.897, Tmax = 0.973

28110 measured reflections

3208 independent reflections

2930 reflections with I > 2σ(I)

Rint = 0.042

θmax = 27.5°, θmin = 2.6°

h = −38→38

k = −5→4

l = −33→33

Refinement

Refinement on F²

Least-squares matrix: full

R[F² > 2σ(F²)] = 0.031

wR(F²) = 0.079

S = 1.07

3208 reflections

191 parameters

0 restraints

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

w = 1/[σ²(Fo²) + (0.0342P)² + 4.0386P]

where P = (Foc² + 2Fc²)/3

(Δ/σ)max = 0.001

Δρmax = 0.33 e Å⁻³

Δρmin = −0.26 e Å⁻³

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

|   | x    | y    | z    | Uiso */U_eq |
|---|------|------|------|-------------|
| N1| 0.56531 (4) | 0.8852 (3) | 0.48948 (5) | 0.0130 (2) |
| C2| 0.54198 (5) | 0.7306 (3) | 0.44182 (6) | 0.0128 (3) |
| C3| 0.56318 (5) | 0.6274 (4) | 0.40297 (6) | 0.0137 (3) |
### Atomic displacement parameters (Å²)

|     | $U^{11}$    | $U^{22}$    | $U^{33}$    | $U^{12}$    | $U^{13}$    | $U^{23}$    |
|-----|-------------|-------------|-------------|-------------|-------------|-------------|
| N1  | 0.0133 (5)  | 0.0127 (6)  | 0.0132 (5)  | 0.0006 (4)  | 0.0048 (4)  | 0.0009 (4)  |
| C2  | 0.0125 (6)  | 0.0112 (6)  | 0.0143 (6)  | 0.0010 (5)  | 0.0043 (5)  | 0.0018 (5)  |
| C3  | 0.0145 (6)  | 0.0146 (7)  | 0.0108 (6)  | 0.0001 (5)  | 0.0028 (5)  | −0.0003 (5) |
| C4  | 0.0152 (6)  | 0.0113 (6)  | 0.0107 (6)  | 0.0022 (5)  | 0.0043 (5)  | 0.0022 (5)  |
| C4A | 0.0126 (6)  | 0.0113 (6)  | 0.0113 (6)  | 0.0009 (5)  | 0.0035 (5)  | 0.0026 (5)  |
| C5  | 0.0138 (6)  | 0.0144 (7)  | 0.0140 (6)  | 0.0016 (5)  | 0.0059 (5)  | 0.0027 (5)  |
| C6  | 0.0116 (6)  | 0.0146 (7)  | 0.0176 (7)  | −0.0002 (5) | 0.0034 (5)  | 0.0033 (5)  |
| C7  | 0.0169 (7)  | 0.0138 (7)  | 0.0120 (6)  | −0.0008 (5) | 0.0021 (5)  | −0.0001 (5) |
| C8  | 0.0174 (7)  | 0.0128 (6)  | 0.0116 (6)  | 0.0011 (5)  | 0.0006 (5)  | 0.0007 (5)  |
| C8A | 0.0133 (6)  | 0.0101 (6)  | 0.0119 (6)  | 0.0010 (5)  | 0.0044 (5)  | 0.0025 (5)  |
| C21 | 0.0135 (7)  | 0.0175 (7)  | 0.0178 (7)  | −0.0010 (5) | 0.0062 (5)  | −0.0023 (6) |
| C41 | 0.0145 (6)  | 0.0132 (7)  | 0.0138 (6)  | 0.0018 (5)  | 0.0054 (5)  | 0.0006 (5)  |
| C42 | 0.0120 (6)  | 0.0151 (7)  | 0.0140 (6)  | 0.0011 (5)  | 0.0055 (5)  | −0.0006 (5) |
### Geometric parameters (Å, \( ^\circ \))

| Bond/Angle | Length/Distance | Angle | Value |
|------------|-----------------|-------|-------|
| N1—C2      | 1.3186 (18)     | C21—H21A | 0.9800 |
| N1—C8A     | 1.3713 (17)     | C21—H21B | 0.9800 |
| C2—N1      | 1.4188 (19)     | C21—H21C | 0.9800 |
| C2—C3      | 1.5034 (18)     | C41—C42  | 1.3345 (19) |
| C3—C4      | 1.4730 (19)     | C41—H41  | 0.9500 |
| C3—H3      | 0.9500          | C42—C421 | 1.4791 (18) |
| C4—C3      | 1.366 (2)       | C42—C42  | 1.4735 (19) |
| C5—C4A     | 1.4336 (19)     | C42—H42  | 0.9500 |
| C6—C5      | 1.4130 (19)     | C42—H43  | 0.9500 |
| C7—C6      | 1.4100 (19)     | C42—H44  | 0.9500 |
| C8—C7      | 1.4159 (19)     | C42—H45  | 0.9500 |
| C8—H8      | 0.9500          | C42—H46  | 0.9500 |

| Bond/Angle | Length/Distance | Angle | Value |
|------------|-----------------|-------|-------|
| C2—N1—C8A | 117.80 (12)     | C2—C21—H21B | 109.5 |
| N1—C2—C3  | 122.74 (13)     | H21A—C21—H21B | 109.5 |
| N1—C2—C21 | 117.92 (12)     | C2—C21—H21C | 109.5 |
| C3—C2—C21 | 119.32 (12)     | H21A—C21—H21C | 109.5 |
| C4—C3—C2  | 120.99 (13)     | H21B—C21—H21C | 109.5 |
| C4—C3—H3  | 119.5           | C42—C41—C4  | 122.10 (13) |
| C2—C3—H3  | 119.5           | C42—C41—H41 | 119.0 |
| C3—C4—C4A | 117.69 (12)     | C4—C41—H41  | 119.0 |
| C3—C4—C4A | 121.40 (13)     | C41—C42—C41 | 126.85 (13) |
| C4A—C4—C4 | 120.91 (12)     | C41—C42—H42 | 116.6 |
| C5—C4A—C8A| 118.73 (12)     | C42—C42—H42 | 116.6 |
| C5—C4A—C4 | 123.91 (12)     | C42—C42—C422 | 114.95 (12) |
| C8A—C4A—C4| 117.34 (12)     | C42—C42—C42 | 125.20 (12) |
| C6—C5—C4A | 120.84 (13)     | C42—C42—C42 | 119.73 (12) |
| C6—C5—H5  | 119.6           | C42—C42—C42 | 123.63 (13) |
| C4A—C5—H5 | 119.6           | C42—C42—C42 | 117.44 (11) |
| C5—C6—C7  | 120.43 (13)     | C42—C42—C42 | 118.90 (10) |
| C5—C6—H6  | 119.8           | C42—C42—C42 | 118.79 (13) |
| Bond                        | Angle (°) | Bond                        | Angle (°) |
|-----------------------------|-----------|-----------------------------|-----------|
| C7—C6—H6                   | 119.8     | C422—C423—C424—H425—C426  | 120.6     |
| C8—C7—C6                   | 120.11 (13) | C424—C423—H423             | 120.6     |
| C8—C7—H7                   | 119.9     | C425—C424—C423             | 120.14 (13) |
| C6—C7—H7                   | 119.9     | C425—C424—H424             | 119.9     |
| C7—C8—C8A                  | 120.84 (13) | C426—C424—C423             | 120.1     |
| C7—C8—H8                   | 119.6     | C426—C424—C425             | 120.1     |
| C8A—C8—H8                  | 119.6     | N1—C8A—C4A                 | 122.76 (13) |
| N1—C8A—C4A                 | 117.54 (12) | C425—C426—H425             | 119.9     |
| N1—C8A—C4A                 | 123.43 (12) | C426—C425—H425             | 119.9     |
| C8—C8A—C4A                 | 119.04 (12) | C425—C426—C421             | 116.38 (10) |
| C2—C21—H21A                | 109.5     | C425—C426—Cl46             | 120.85 (10) |
| C8A—N1—C2—C3               | −0.4 (2)  | C5—C4A—C8A—C8             | 0.12 (19)  |
| C8A—N1—C2—C2—C21           | 178.35 (12) | C4—C4A—C8A—C8             | −178.67 (12) |
| N1—C2—C3—C4                | 0.6 (2)   | C3—C4—C41—C42             | 39.5 (2)   |
| C21—C2—C3—C4               | −178.06 (13) | C4A—C4—C41—C42            | −140.35 (15) |
| C2—C3—C4—C4A               | 0.0 (2)   | C4—C41—C42—C421           | −179.23 (13) |
| C2—C3—C4—C41               | −179.85 (13) | C41—C42—C421—C426         | −44.5 (2)   |
| C3—C4—C4A—C5               | −179.50 (13) | C41—C42—C421—C422         | 139.58 (15) |
| C41—C4—C4A—C5              | 0.3 (2)   | C42—C421—C422—C423        | 0.4 (2)    |
| C3—C4—C4A—C8A              | −0.78 (19) | C42—C421—C422—C423        | 176.74 (13) |
| C41—C4—C4A—C8A             | 179.06 (12) | C42—C421—C422—Cl42       | 178.52 (10) |
| C8A—C4A—C5—C6              | 1.1 (2)   | C42—C421—C422—Cl42       | −5.14 (18)  |
| C4—C4A—C5—C6               | 179.83 (13) | C42—C421—C422—C424        | −0.2 (2)   |
| C4A—C5—C6—C7               | −1.2 (2)  | Cl42—C422—C423—C424      | −178.36 (11) |
| C5—C6—C7—C8                | 0.0 (2)   | C422—C423—C424—C425       | −0.2 (2)   |
| C6—C7—C8—C8A               | 1.3 (2)   | C423—C424—C425—C426       | 0.5 (2)    |
| C2—N1—C8A—C8               | 179.24 (12) | C424—C425—C426—C421       | −0.3 (2)   |
| C2—N1—C8A—C4A              | −0.5 (2)  | C424—C425—C426—Cl46       | −179.35 (11) |
| C7—C8—C8A—C4A              | 178.89 (13) | C422—C421—C426—C425       | −0.2 (2)   |
| C7—C8—C8A—C4A              | −1.3 (2)  | C42—C421—C426—C425        | −176.27 (13) |
| C5—C4A—C8A—N1              | 179.88 (12) | C422—C421—C426—Cl46       | 178.89 (10) |
| C4—C4A—C8A—N1              | 1.1 (2)   | C42—C421—C426—Cl46        | 2.8 (2)    |