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Crystal structure of 4,4′-diethynylbiphenyl

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The title compound, $C_{16}H_{10}$, crystallizes with four unique molecules, designated 1–4, in the asymmetric unit of the monoclinic unit cell. None of the molecules is planar, with the benzene rings of molecules 1–4 inclined to one another at angles of 42.41 (4), 24.07 (6), 42.59 (4) and 46.88 (4)°, respectively. In the crystal, weak C—H···π(ring) interactions, augmented by even weaker C≡C—H···π(alkyne) contacts, generate a three-dimensional network structure with interlinked columns of molecules formed along the *c*-axis direction.

Keywords: crystal structure; 4,4′-diethynylbiphenyl; C—H···π(ring) interactions; C≡C—H···π contacts

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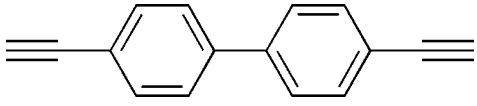
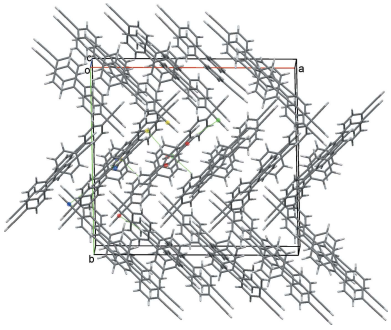
1. Chemical context

Donor–acceptor (*D*–*A*) dyads with the innate ability to generate long-lived charge separation in their excited states have elicited a great deal of current interest. Their applications cover fields ranging from artificial photosynthesis to solar cell technology (Rogozina *et al.*, 2013; Fukuzumi *et al.*, 2014). We have produced a variety of such dyads based on ferrocene as the donor and with a variety of acceptors (see for example: Flood *et al.*, 2007; Cuffe *et al.*, 2005; McAdam *et al.*, 2003). More recently, we have been interested in expanding the range of donor–acceptor dyads by interpolating a potentially conductive spacer between the donor and the acceptor to yield donor–spacer–acceptor (*D*–*S*–*A*) dyads. Biphenyl is a conductive spacer that we have used with some recent success, joined to a ferrocene donor through an alkene unit and to an acceptor *via* an alkyne link (McAdam *et al.*, 2010; Tagg *et al.*, 2015). We are interested in further developing the chemistry of biphenyl as a potential spacer, with alkyne links to both the donor and the acceptor. Surprisingly, the molecular and crystal structure of the precursor molecule, 4,4′-diethynylbiphenyl (Liu, Liu *et al.*, 2005), has not been previously studied and we report its structure here.





2. Structural commentary

The title compound, (I), crystallizes with four unique molecules in the asymmetric unit, identified by the leading digits 1–4 in the numbering schemes, Fig. 1. Each molecule comprises a central biphenyl ring system symmetrically substituted at the 4 and 4′ positions by terminal alkyne units. None of the molecules is planar, with the two benzene rings of each molecule inclined to one another at angles of 42.41 (4), 24.07 (6), 42.59 (4) and 46.88 (4)° for molecules 1–4, respectively. Bond distances and angles in the biphenyl ring systems

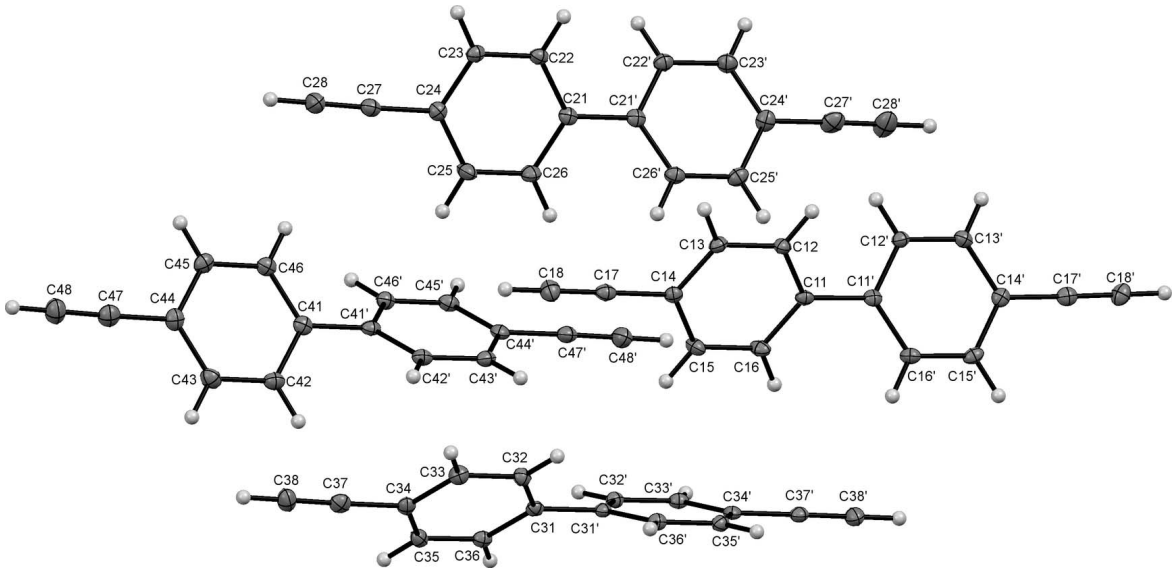


Figure 1
The asymmetric unit of (I), showing the numbering schemes for the four unique molecules designated as types 1–4 with the types discriminated by the leading characters in the atom labels.

are not unusual and compare well, both internally, over the four unique molecules, and with those observed in related systems (see for example: O'Brien *et al.*, 2010, Butler *et al.*, 2008; Muller, *et al.*, 2006, Nitsche *et al.*, 2003). The C*n*4—C*n*7 and C*n*4′—C*n*7′ distances (*n* = 1–4) [mean 1.445 (2) Å] are generally somewhat long, enough indeed to raise alerts in the *checkCIF* procedure. However analysis in *Vista* (Groom & Allen, 2014) of comparable values for eight other biphenyl systems, with terminal alkyne functions in the 4-position, provides a mean value of 1.442 (16) Å, not at all dissimilar to the values observed here (see for example: Langley *et al.*, 1998; Mague *et al.*, 1997; McAdam *et al.*, 2010; Laliberté *et al.*, 2006).

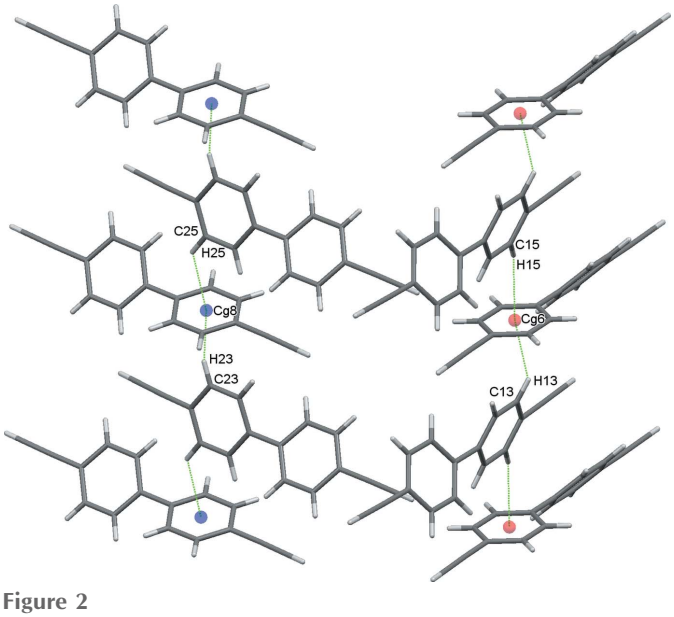


Figure 2
Complementary chains of 1, 3 and 2, 4 molecules extending along the *c*-axis direction. In this and subsequent figures, C—H···π(ring) contacts are drawn as dotted lines with ring centroids shown as coloured spheres.

The C≡C distances are also generally reasonable, with the exception of C27′—C28′, 1.130 (2) Å, which is unusually short compared to more typical C≡C distances of 1.181 (14) Å (Allen *et al.* 1987). There is no obvious explanation for this, except to note that the adjacent C27′—C24′ distance 1.4507 (19) Å is the longest of those reported here.

3. Supramolecular features

The absence of donor and acceptor components, to provide classical hydrogen bonding or even C—H···*E* (*E* = O, N, halogen) contacts, challenge the packing in this system. There has been considerable speculation on the factors influencing the formation of structures with $Z' > 1$ (Desiraju, 2007; Steed & Steed, 2015; Anderson & Steed 2007, Nichol & Clegg, 2007), and the nature, extent and degree of the intermolecular contacts are clearly contributory factors. In this instance, the packing in the structure is profoundly influenced by an extensive series of weak edge-to-face C—H···π(ring) interactions (Table 1) augmented by still weaker C≡C—H···π(alkyne) contacts. It is likely that the inherent weakness

Table 1
C—H···π interactions (Å, °).

*Cg*1, *Cg*3, *Cg*4, *Cg*6 and *Cg*8 are the centroids of the C11–C16, C21–C26, C21′–C26′, C31′–C36′ and C41′–C46′ rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13···*Cg*6^{i}	0.95	2.73	3.4910 (13)	137
C15—H15···*Cg*6	0.95	2.70	3.4782 (13)	140
C16′—H16′···*Cg*1^{ii}	0.95	2.92	3.5375 (12)	124
C23—H23···*Cg*8^{i}	0.95	2.71	3.4809 (13)	139
C25—H25···*Cg*8	0.95	2.76	3.4976 (14)	136
C33′—H33′···*Cg*4^{iii}	0.95	2.88	3.6153 (13)	135
C36—H36···*Cg*3^{iii}	0.95	2.87	3.6112 (12)	135

Symmetry codes: (i) $x, y, z-1$; (ii) $-x+1, -y+1, -z+1$; (iii) $x, y, z+1$.

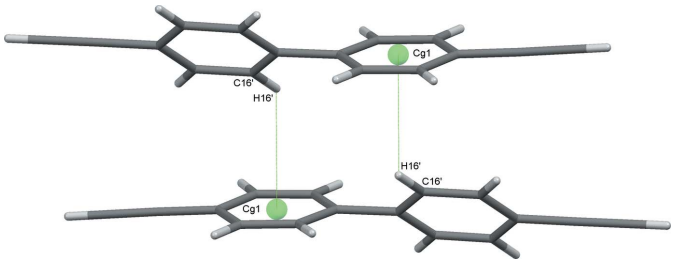


Figure 3
Inversion dimers formed through C—H···π(ring) contacts between molecules of type 1.

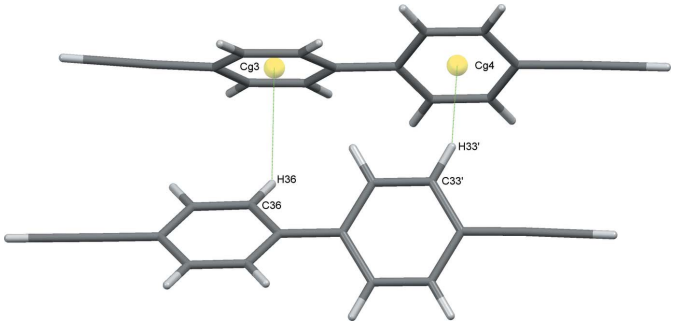


Figure 4
Dimers formed through C—H···π(ring) contacts between molecules of types 2 and 4.

of these contacts may influence the adoption of a $Z' > 1$ structure.

A complementary set of C—H···π contacts, involving in one case molecules 1 and 3 and in the second molecules 2 and 4, sandwiches a molecule of 1 between two molecules of 3 and a molecule of 2 between two molecules of 4. These contacts generate infinite chains approximately along the *c*-axis direction. The two chains lie approximately orthogonal to one another, Fig. 2. Weak C16′—H16′···*Cg*1 contacts form inversion dimers between two adjacent 1 molecules, Fig. 3, and dimers also result from C—H···π contacts involving both rings of adjacent 2 and 3 molecules, Fig. 4; both these sets of contacts contribute to the overall packing. In addition to these C—H···π(ring) interactions, one further set of somewhat unusual contacts is formed, again involving all four molecules in the structure. These are weak C≡C—H···π(alkyne) contacts (Desiraju & Steiner, 1999) involving the relatively acidic C—H donors of the alkyne substituents. These again involve pairs of molecules with C18—H18···C37≡C38 and C38′—H38′···C17′≡C18′ contacts generating one set of zigzag chains along *b* with an adjacent and complementary zigzag produced by C28—H28···C47≡C48 and C48′—H48′···C27′≡C28′ interactions, These chains generate layers of molecules in the *ac* plane, Fig. 5. The contacts display the classic T shape, found also in the neutron structure of acetylene (McMullan *et al.*, 1992), but not perfectly so. The H*n*8···C*n*7 distances are consistently slightly shorter [mean of the four distances = 2.77 (3) Å] than the H*n*8···C*n*8 equivalents [mean 2.97 (4) Å]. The mean H*n*8···C≡C centroid distance is 2.82 (4) Å and these values all fall well within projected ranges for such contacts (Desiraju & Steiner, 1999).

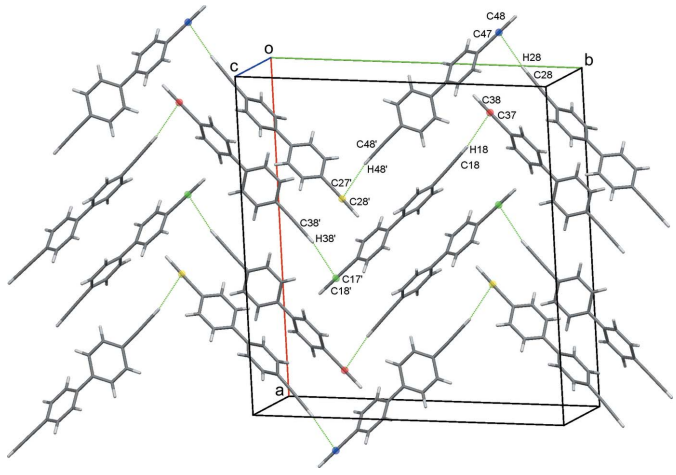


Figure 5
Zigzag chains of molecules generated by C—H···C≡C contacts between molecules of types 1 and 3 and molecules of types 2 and 4. The centroids of the C≡C bonds are drawn as coloured spheres and the C—H···C≡C contacts are shown as dotted lines.

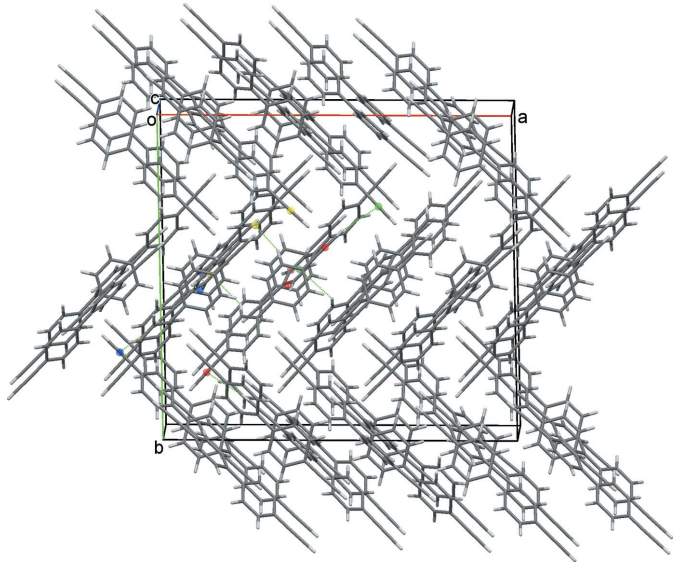


Figure 6
Overall packing for (I) viewed along the *c* axis. Representative C—H···π(ring) and C—H···π(alkyne) contacts are drawn as dotted lines.

The overall effect of this plethora of weak interactions is to stack molecules into 'multiple-decker sandwich' columns, linked together along the *c*-axis direction, Fig. 6.

4. Database survey

Structures of 4-4′-disubstituted biphenyls abound with 2891 hits on the CSD (Groom & Allen, 2014). However, those with 4,4′-alkyne substituents are far less plentiful with only 29 entries. These fall into two distinct categories. First compounds with one or both of the alkyne substituents on the biphenyls bound to carbon or silicon atoms, 14 entries (see for example: Zhou *et al.*, 2012; McAdam *et al.*, 2010; O'Brien *et al.*, 2010, Zeng *et al.*, 2007; Muller, *et al.*, 2006; Nitsche *et al.*, 2003). Second, the well represented class of organometallic acetyl-

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{16}H_{10}$
M_r	202.24
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	85
a, b, c (Å)	23.4263 (5), 21.1181 (5), 9.2989 (2)
β (°)	100.731 (1)
V (Å^3)	4519.89 (17)
Z	16
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.07
Crystal size (mm)	0.46 × 0.40 × 0.07
Data collection	
Diffractometer	Bruker–Nonius APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2011)
T_{min}, T_{max}	0.887, 0.980
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	77658, 8885, 7147
R_{int}	0.030
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.036, 0.103, 1.03
No. of reflections	8885
No. of parameters	577
No. of restraints	42
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.29, −0.16

Computer programs: , *APEX2* and *SAINT* (Bruker, 2011), *SHELXS* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *TITAN2000* (Hunter & Simpson, 1999), *Mercury* (Macrae *et al.*, 2008), *enCIFer* (Allen *et al.*, 2004), *PLATON* (Spek, 2009) and *publCIF* (Westrip 2010).

ides, also referred to as ethynyl compounds. These have either the terminal hydrogen atoms of the alkyne groups both replaced by a transition metal complex moiety (see for example: Shanmugaraju *et al.*, 2011; Gao *et al.*, 2007; Ibn Ghazala *et al.*, 2006; Liu, Poon *et al.*, 2005) or, much less frequently, only a single terminal hydrogen atom is replaced to afford ethynyl complexes with terminal C≡C–H substituents (Zeng *et al.*, 2013; Saha *et al.*, 2005).

5. Synthesis and crystallization

The title compound (I) was prepared by a literature procedure (Liu, Liu *et al.*, 2005) and recrystallized from dichloromethane/hexane (1:1) to give pale-yellow plates suitable for X-ray analysis.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All hydrogen atoms were refined using a riding model with d(C—H) = 0.95 Å, $U_{iso} = 1.2U_{eq}$(C) for both the aromatic and terminal alkyne H atoms. Two low angle reflections with $F_o << F_c$, with intensities likely to have been attenuated by the beam-stop, were removed for the final refinement cycles.

Acknowledgements

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References

Allen, F. H., Johnson, O., Shields, G. P., Smith, B. R. & Towler, M. (2004). *J. Appl. Cryst.* **37**, 335–338.
Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Anderson, K. M. & Steed, J. W. (2007). *CrystEngComm*, **9**, 328–330.
Bruker (2011). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Butler, P., Manning, A. R., McAdam, C. J. & Simpson, J. (2008). *J. Organomet. Chem.* **693**, 381–392.
Cuffe, L., Hudson, R. D. A., Gallagher, J., Jennings, S., McAdam, C. J., Connelly, R. B. T., Manning, A. R., Robinson, B. H. & Simpson, J. (2005). *Organometallics*, **24**, 2051–2060.
Desiraju, G. R. (2007). *CrystEngComm*, **9**, 91–92.
Desiraju, G. R. & Steiner, T. (1999). *The Weak Hydrogen Bond in Structural Chemistry and Biology*, pp 169–175. New York: Oxford University Press Inc.
Flood, A. H., McAdam, C. J., Gordon, K. C., Kjaergaard, H. G., Manning, A. R., Robinson, B. H. & Simpson, J. (2007). *Polyhedron*, **26**, 448–455.
Fukuzumi, S., Ohkubo, K. & Suenobu, T. (2014). *Acc. Chem. Res.* **47**, 1455–1464.
Gao, L.-B., Kan, J., Fan, Y., Zhang, L.-Y., Liu, S.-H. & Chen, Z.-N. (2007). *Inorg. Chem.* **46**, 5651–5664.
Groom, C. R. & Allen, F. H. (2014). *Angew. Chem. Int. Ed.* **53**, 662–671.
Hunter, K. A. & Simpson, J. (1999). *TITAN2000*. University of Otago, New Zealand.
Ibn Ghazala, S., Paul, F., Toupet, L., Roisnel, T., Hapiot, P. & Lapinte, C. (2006). *J. Am. Chem. Soc.* **128**, 2463–2476.
Laliberté, D., Maris, T., Ryan, P. E. & Wuest, J. D. (2006). *Cryst. Growth Des.* **6**, 1335–1340.
Langley, P. J., Hulliger, J., Thaimattam, R. & Desiraju, G. R. (1998). *New J. Chem.* **22**, 1307–1309.
Liu, L., Liu, Z., Xu, W., Xu, H., Zhang, D. & Zhu, D. (2005). *Tetrahedron*, **61**, 3813–3817.
Liu, L., Poon, S.-Y. & Wong, W.-Y. (2005). *J. Organomet. Chem.* **690**, 5036–5048.
Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.
Mague, J. T., Foroozesh, M., Hopkins, N. E., Gan, L. L.-S. & Alworth, W. L. (1997). *J. Chem. Crystallogr.* **27**, 183–189.
McAdam, C. J., Morgan, J. L., Robinson, B. H., Simpson, J., Rieger, P. H. & Rieger, A. L. (2003). *Organometallics*, **22**, 5126–5136.
McAdam, C. J., Robinson, B. H., Simpson, J. & Tagg, T. (2010). *Organometallics*, **29**, 2474–2483.
McMullan, R. K., Kvick, Å. & Popelier, P. (1992). *Acta Cryst.* B**48**, 726–731.
Muller, T., Seichter, W. & Weber, E. (2006). *New J. Chem.* **30**, 751–758.
Nichol, G. S. & Clegg, W. (2007). *CrystEngComm*, **9**, 959–960.
Nitsche, S. I., Weber, E., Seichter, W., Bathori, N., Beketov, K. M. & Roewer, G. (2003). *Silicon Chem.* **2**, 55–71.
O'Brien, Z. J., Karlen, S. D., Khan, S. & Garcia-Garibay, M. A. (2010). *J. Org. Chem.* **75**, 2482–2491.
Rogozina, M. V., Ionkin, V. N. & Ivanov, A. I. (2013). *J. Phys. Chem. A*, **117**, 4564–4573.

Saha, R., Qaium, M. A., Debnath, D., Younus, M., Chawdhury, N., Sultana, N., Kociok-Köhn, G., Ooi, L., Raithby, P. R. & Kijima, M. (2005). *Dalton Trans.* pp. 2760–2765.
Shanmugaraju, S., Joshi, S. A. & Mukherjee, P. S. (2011). *Inorg. Chem.* **50**, 11736–11745.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Steed, K. M. & Steed, J. W. (2015). *Chem. Rev.* **115**, 2895–2933.
Tagg, T., Kjaergaard, H. G., Lane, J. R., McAdam, C. J., Robinson, B. H. & Simpson, J. (2015). *Organometallics*, **34**, 2662–2666.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.
Zeng, X., Wang, C., Bryce, M. R., Batsanov, A. S., Sirichantaropass, S., García-Suárez, V. M., Lambert, C. J. & Sage, I. (2007). *Eur. J. Org. Chem.* pp. 5244–5249.
Zeng, L.-Z., Wu, Y.-Y., Tian, G.-X. & Li, Z. (2013). *Acta Cryst.* E**69**, m607.
Zhou, H., Maris, T. & Wuest, J. D. (2012). *J. Phys. Chem. C*, **116**, 13052–13062.

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Computing details

Data collection: *APEX2* (Bruker, 2011); cell refinement: *APEX2* (Bruker, 2011) and *SAINT* (Bruker, 2011); data reduction: *SAINT* (Bruker, 2011); program(s) used to solve structure: *SHELXS* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015) and *TITAN2000* (Hunter & Simpson, 1999); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL2014* (Sheldrick, 2015), *enCIFer* (Allen *et al.*, 2004), *PLATON* (Spek, 2009) and *publCIF* (Westrip 2010).

4,4′-Diethynylbiphenyl

Crystal data

$C_{16}H_{10}$
M_r = 202.24
Monoclinic, $P2_1/c$
a = 23.4263 (5) Å
b = 21.1181 (5) Å
c = 9.2989 (2) Å
β = 100.731 (1)°
V = 4519.89 (17) Å^3
Z = 16
$F(000)$ = 1696
D_x = 1.189 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 8416 reflections
θ = 4.9–62.5°
μ = 0.07 mm^{-1}
T = 85 K
Plate, pale yellow
0.46 × 0.40 × 0.07 mm

Data collection

Bruker–Nonius APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2011)
T_{min} = 0.887, T_{max} = 0.980
77658 measured reflections
8885 independent reflections
7147 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 26.0°, θ_{min} = 1.3°
h = −28→28
k = −26→26
l = −11→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.103
S = 1.03
8885 reflections
577 parameters
42 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0471P)^2 + 1.454P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Special details

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

Refinement. Two low angle reflections with F_o << Fc with intensities affected by the beam-stop were removed for the final refinement cycles.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C18	0.26084 (6)	0.61801 (6)	0.27932 (15)	0.0318 (3)
H18	0.2298	0.6477	0.2663	0.038*
C17	0.29917 (5)	0.58137 (6)	0.29541 (13)	0.0240 (3)
C16	0.40471 (6)	0.45861 (6)	0.46859 (13)	0.0252 (3)
H16	0.4152	0.4381	0.5606	0.030*
C15	0.36119 (5)	0.50352 (6)	0.44947 (13)	0.0253 (3)
H15	0.3417	0.5130	0.5278	0.030*
C14	0.34553 (5)	0.53520 (5)	0.31607 (13)	0.0206 (2)
C13	0.37510 (5)	0.52063 (6)	0.20294 (13)	0.0226 (3)
H13	0.3657	0.5423	0.1121	0.027*
C12	0.41799 (5)	0.47484 (6)	0.22237 (12)	0.0221 (2)
H12	0.4372	0.4650	0.1438	0.027*
C11	0.43363 (5)	0.44272 (5)	0.35501 (12)	0.0196 (2)
C11′	0.47811 (5)	0.39198 (5)	0.37373 (12)	0.0197 (2)
C12′	0.47908 (5)	0.34774 (5)	0.26198 (12)	0.0214 (2)
H12′	0.4516	0.3511	0.1732	0.026*
C13′	0.51937 (5)	0.29931 (6)	0.27899 (13)	0.0229 (3)
H13′	0.5192	0.2696	0.2023	0.027*
C15′	0.56013 (5)	0.33806 (5)	0.52006 (13)	0.0231 (3)
H15′	0.5880	0.3351	0.6082	0.028*
C16′	0.51939 (5)	0.38625 (5)	0.50273 (12)	0.0222 (2)
H16′	0.5195	0.4159	0.5796	0.027*
C14′	0.56056 (5)	0.29371 (5)	0.40853 (13)	0.0212 (2)
C17′	0.60326 (5)	0.24352 (6)	0.42461 (13)	0.0242 (3)
C18′	0.63815 (6)	0.20297 (6)	0.43483 (14)	0.0294 (3)
H18′	0.6663	0.1702	0.4431	0.035*
C28	0.01222 (6)	0.61620 (7)	−0.10611 (15)	0.0359 (3)
H28	−0.0189	0.6457	−0.1243	0.043*
C27	0.05092 (6)	0.57953 (6)	−0.08355 (14)	0.0277 (3)
C24	0.09698 (5)	0.53344 (6)	−0.05973 (13)	0.0231 (3)
C25	0.12721 (6)	0.51937 (6)	0.08080 (14)	0.0292 (3)
H25	0.1184	0.5417	0.1626	0.035*
C26	0.16983 (6)	0.47332 (6)	0.10195 (13)	0.0280 (3)
H26	0.1901	0.4647	0.1983	0.034*
C23	0.11208 (5)	0.50095 (6)	−0.17817 (13)	0.0227 (3)
H23	0.0931	0.5109	−0.2750	0.027*
C22	0.15419 (5)	0.45468 (5)	−0.15572 (13)	0.0217 (2)

H22	0.1634	0.4327	−0.2377	0.026*
C21	0.18383 (5)	0.43917 (5)	−0.01531 (13)	0.0212 (2)
C21′	0.22840 (5)	0.38863 (5)	0.00710 (13)	0.0219 (2)
C22′	0.22770 (5)	0.33988 (6)	−0.09553 (13)	0.0247 (3)
H22′	0.1977	0.3390	−0.1798	0.030*
C23′	0.26965 (5)	0.29318 (6)	−0.07676 (14)	0.0278 (3)
H23′	0.2686	0.2610	−0.1486	0.033*
C25′	0.31418 (5)	0.34058 (6)	0.15210 (14)	0.0269 (3)
H25′	0.3433	0.3405	0.2381	0.032*
C26′	0.27264 (5)	0.38763 (6)	0.13152 (13)	0.0240 (3)
H26′	0.2740	0.4200	0.2030	0.029*
C24′	0.31377 (5)	0.29291 (6)	0.04756 (14)	0.0270 (3)
C27′	0.35848 (6)	0.24449 (7)	0.06802 (16)	0.0352 (3)
C28′	0.39403 (7)	0.20760 (7)	0.08536 (18)	0.0447 (4)
H28′	0.4239	0.1766	0.0999	0.054*
C38	0.11161 (6)	0.79841 (6)	0.69494 (16)	0.0334 (3)
H38	0.0828	0.8306	0.6771	0.040*
C37	0.14702 (5)	0.75884 (6)	0.71693 (14)	0.0274 (3)
C34	0.19066 (5)	0.70967 (5)	0.74066 (13)	0.0231 (3)
C35	0.18803 (5)	0.66086 (6)	0.84074 (13)	0.0240 (3)
H35	0.1577	0.6605	0.8958	0.029*
C36	0.22913 (5)	0.61314 (5)	0.86027 (13)	0.0218 (2)
H36	0.2265	0.5800	0.9277	0.026*
C33	0.23589 (5)	0.70960 (6)	0.66094 (13)	0.0250 (3)
H33	0.2381	0.7423	0.5920	0.030*
C32	0.27727 (5)	0.66226 (6)	0.68221 (13)	0.0229 (3)
H32	0.3080	0.6631	0.6285	0.027*
C31	0.27464 (5)	0.61318 (5)	0.78158 (12)	0.0199 (2)
C31′	0.31938 (5)	0.56270 (5)	0.80312 (12)	0.0192 (2)
C32′	0.30445 (5)	0.49923 (5)	0.81532 (12)	0.0209 (2)
H32′	0.2648	0.4881	0.8105	0.025*
C33′	0.34629 (5)	0.45206 (6)	0.83436 (12)	0.0220 (2)
H33′	0.3352	0.4091	0.8416	0.026*
C35′	0.41999 (5)	0.53127 (6)	0.83133 (12)	0.0225 (2)
H35′	0.4597	0.5424	0.8375	0.027*
C36′	0.37810 (5)	0.57790 (6)	0.81118 (12)	0.0211 (2)
H36′	0.3892	0.6208	0.8027	0.025*
C34′	0.40476 (5)	0.46768 (6)	0.84285 (12)	0.0206 (2)
C37′	0.44936 (5)	0.41951 (6)	0.86414 (12)	0.0237 (3)
C38′	0.48707 (6)	0.38135 (6)	0.88180 (14)	0.0302 (3)
H38′	0.5173	0.3507	0.8960	0.036*
C48	−0.13344 (6)	0.79702 (7)	0.30586 (17)	0.0402 (3)
H48	−0.1621	0.8292	0.2858	0.048*
C47	−0.09783 (6)	0.75706 (6)	0.33069 (15)	0.0324 (3)
C44	−0.05457 (5)	0.70779 (6)	0.35722 (14)	0.0272 (3)
C45	−0.05343 (5)	0.66035 (6)	0.25252 (14)	0.0264 (3)
H45	−0.0811	0.6610	0.1637	0.032*
C46	−0.01241 (5)	0.61263 (6)	0.27733 (13)	0.0241 (3)

H46	−0.0127	0.5804	0.2060	0.029*
C43	−0.01289 (6)	0.70624 (6)	0.48626 (15)	0.0297 (3)
H43	−0.0132	0.7379	0.5586	0.036*
C42	0.02873 (5)	0.65901 (6)	0.50944 (14)	0.0270 (3)
H42	0.0572	0.6591	0.5968	0.032*
C41	0.02949 (5)	0.61109 (6)	0.40583 (13)	0.0229 (3)
C41′	0.07433 (5)	0.56078 (6)	0.42969 (12)	0.0219 (2)
C42′	0.13294 (5)	0.57601 (6)	0.47849 (13)	0.0232 (3)
H42′	0.1439	0.6189	0.4983	0.028*
C43′	0.17498 (5)	0.52946 (6)	0.49820 (13)	0.0243 (3)
H43′	0.2146	0.5407	0.5293	0.029*
C45′	0.10123 (5)	0.45009 (6)	0.42502 (13)	0.0246 (3)
H45′	0.0902	0.4071	0.4081	0.030*
C46′	0.05956 (5)	0.49710 (6)	0.40248 (13)	0.0238 (3)
H46′	0.0201	0.4860	0.3678	0.029*
C44′	0.15977 (5)	0.46576 (6)	0.47284 (12)	0.0235 (3)
C47′	0.20428 (5)	0.41762 (6)	0.49536 (13)	0.0273 (3)
C48′	0.24191 (6)	0.37986 (7)	0.51539 (15)	0.0350 (3)
H48′	0.2723	0.3494	0.5316	0.042*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C18	0.0334 (7)	0.0309 (7)	0.0326 (7)	0.0041 (6)	0.0103 (6)	0.0050 (6)
C17	0.0262 (6)	0.0268 (6)	0.0198 (6)	−0.0057 (5)	0.0062 (5)	−0.0005 (5)
C16	0.0370 (7)	0.0220 (6)	0.0173 (6)	0.0024 (5)	0.0065 (5)	0.0022 (5)
C15	0.0341 (7)	0.0238 (6)	0.0201 (6)	0.0014 (5)	0.0105 (5)	−0.0016 (5)
C14	0.0213 (6)	0.0183 (5)	0.0217 (6)	−0.0030 (4)	0.0029 (5)	−0.0019 (4)
C13	0.0224 (6)	0.0276 (6)	0.0167 (6)	−0.0015 (5)	0.0011 (4)	0.0023 (5)
C12	0.0215 (6)	0.0288 (6)	0.0165 (6)	−0.0005 (5)	0.0049 (4)	−0.0005 (5)
C11	0.0216 (6)	0.0191 (6)	0.0175 (6)	−0.0044 (5)	0.0027 (4)	−0.0024 (4)
C11′	0.0213 (6)	0.0200 (6)	0.0186 (6)	−0.0041 (5)	0.0056 (4)	0.0019 (4)
C12′	0.0213 (6)	0.0251 (6)	0.0173 (6)	−0.0016 (5)	0.0023 (4)	−0.0001 (5)
C13′	0.0251 (6)	0.0231 (6)	0.0212 (6)	−0.0023 (5)	0.0062 (5)	−0.0031 (5)
C15′	0.0248 (6)	0.0234 (6)	0.0196 (6)	−0.0051 (5)	0.0001 (5)	0.0040 (5)
C16′	0.0282 (6)	0.0212 (6)	0.0171 (6)	−0.0036 (5)	0.0035 (5)	−0.0008 (4)
C14′	0.0205 (6)	0.0199 (6)	0.0238 (6)	−0.0033 (5)	0.0055 (5)	0.0040 (5)
C17′	0.0251 (6)	0.0244 (6)	0.0235 (6)	−0.0072 (5)	0.0057 (5)	0.0016 (5)
C18′	0.0274 (7)	0.0271 (7)	0.0332 (7)	−0.0001 (6)	0.0040 (5)	0.0067 (5)
C28	0.0371 (8)	0.0381 (8)	0.0313 (7)	0.0090 (6)	0.0027 (6)	−0.0049 (6)
C27	0.0301 (7)	0.0304 (7)	0.0230 (6)	−0.0038 (6)	0.0059 (5)	−0.0044 (5)
C24	0.0226 (6)	0.0218 (6)	0.0255 (6)	−0.0029 (5)	0.0060 (5)	−0.0006 (5)
C25	0.0363 (7)	0.0318 (7)	0.0215 (6)	0.0038 (6)	0.0102 (5)	−0.0031 (5)
C26	0.0340 (7)	0.0316 (7)	0.0186 (6)	0.0034 (6)	0.0052 (5)	0.0021 (5)
C23	0.0207 (6)	0.0264 (6)	0.0208 (6)	−0.0054 (5)	0.0033 (5)	−0.0003 (5)
C22	0.0215 (6)	0.0242 (6)	0.0201 (6)	−0.0050 (5)	0.0056 (5)	−0.0034 (5)
C21	0.0216 (6)	0.0214 (6)	0.0219 (6)	−0.0058 (5)	0.0071 (5)	0.0005 (5)
C21′	0.0228 (6)	0.0224 (6)	0.0219 (6)	−0.0054 (5)	0.0074 (5)	0.0018 (5)

C22′	0.0246 (6)	0.0253 (6)	0.0236 (6)	−0.0029 (5)	0.0026 (5)	−0.0011 (5)
C23′	0.0295 (7)	0.0240 (6)	0.0294 (7)	−0.0028 (5)	0.0040 (5)	−0.0046 (5)
C25′	0.0259 (6)	0.0271 (6)	0.0262 (6)	−0.0045 (5)	0.0006 (5)	0.0016 (5)
C26′	0.0271 (6)	0.0230 (6)	0.0223 (6)	−0.0048 (5)	0.0055 (5)	−0.0021 (5)
C24′	0.0252 (6)	0.0215 (6)	0.0336 (7)	−0.0021 (5)	0.0039 (5)	0.0005 (5)
C27′	0.0338 (7)	0.0306 (7)	0.0380 (8)	−0.0095 (6)	−0.0016 (6)	−0.0062 (6)
C28′	0.0388 (8)	0.0274 (7)	0.0606 (10)	0.0002 (7)	−0.0095 (7)	−0.0131 (7)
C38	0.0267 (7)	0.0301 (7)	0.0433 (8)	0.0003 (6)	0.0065 (6)	−0.0079 (6)
C37	0.0266 (6)	0.0254 (6)	0.0298 (7)	−0.0073 (5)	0.0043 (5)	−0.0049 (5)
C34	0.0206 (6)	0.0208 (6)	0.0265 (6)	−0.0021 (5)	0.0011 (5)	−0.0059 (5)
C35	0.0208 (6)	0.0262 (6)	0.0259 (6)	−0.0041 (5)	0.0069 (5)	−0.0061 (5)
C36	0.0231 (6)	0.0218 (6)	0.0208 (6)	−0.0048 (5)	0.0043 (5)	−0.0016 (5)
C33	0.0264 (6)	0.0231 (6)	0.0254 (6)	−0.0023 (5)	0.0044 (5)	0.0013 (5)
C32	0.0215 (6)	0.0249 (6)	0.0232 (6)	−0.0027 (5)	0.0068 (5)	−0.0006 (5)
C31	0.0193 (5)	0.0210 (6)	0.0188 (6)	−0.0041 (5)	0.0018 (4)	−0.0043 (4)
C31′	0.0202 (6)	0.0246 (6)	0.0130 (5)	−0.0022 (5)	0.0035 (4)	−0.0009 (4)
C32′	0.0190 (5)	0.0259 (6)	0.0181 (6)	−0.0037 (5)	0.0042 (4)	−0.0005 (5)
C33′	0.0258 (6)	0.0224 (6)	0.0178 (6)	−0.0028 (5)	0.0039 (5)	0.0003 (5)
C35′	0.0193 (6)	0.0300 (6)	0.0183 (6)	−0.0026 (5)	0.0039 (4)	−0.0004 (5)
C36′	0.0221 (6)	0.0220 (6)	0.0196 (6)	−0.0045 (5)	0.0046 (5)	−0.0004 (5)
C34′	0.0229 (6)	0.0267 (6)	0.0123 (5)	0.0017 (5)	0.0031 (4)	−0.0004 (4)
C37′	0.0253 (6)	0.0303 (7)	0.0154 (6)	−0.0024 (5)	0.0037 (5)	−0.0008 (5)
C38′	0.0328 (7)	0.0335 (7)	0.0236 (6)	0.0073 (6)	0.0041 (5)	0.0007 (5)
C48	0.0328 (8)	0.0351 (8)	0.0517 (9)	0.0024 (6)	0.0056 (7)	−0.0063 (7)
C47	0.0305 (7)	0.0281 (7)	0.0381 (8)	−0.0055 (6)	0.0048 (6)	−0.0034 (6)
C44	0.0239 (6)	0.0240 (6)	0.0346 (7)	−0.0037 (5)	0.0075 (5)	0.0007 (5)
C45	0.0227 (6)	0.0272 (6)	0.0288 (7)	−0.0063 (5)	0.0034 (5)	0.0004 (5)
C46	0.0237 (6)	0.0239 (6)	0.0256 (6)	−0.0071 (5)	0.0071 (5)	−0.0033 (5)
C43	0.0320 (7)	0.0257 (7)	0.0319 (7)	−0.0025 (5)	0.0076 (6)	−0.0062 (5)
C42	0.0289 (6)	0.0278 (6)	0.0233 (6)	−0.0037 (5)	0.0028 (5)	−0.0025 (5)
C41	0.0222 (6)	0.0226 (6)	0.0252 (6)	−0.0062 (5)	0.0079 (5)	0.0001 (5)
C41′	0.0247 (6)	0.0260 (6)	0.0160 (5)	−0.0046 (5)	0.0061 (5)	−0.0013 (5)
C42′	0.0265 (6)	0.0242 (6)	0.0191 (6)	−0.0052 (5)	0.0042 (5)	−0.0019 (5)
C43′	0.0231 (6)	0.0323 (7)	0.0173 (6)	−0.0058 (5)	0.0030 (5)	−0.0017 (5)
C45′	0.0285 (6)	0.0242 (6)	0.0224 (6)	−0.0048 (5)	0.0080 (5)	−0.0025 (5)
C46′	0.0220 (6)	0.0271 (6)	0.0229 (6)	−0.0045 (5)	0.0061 (5)	−0.0024 (5)
C44′	0.0269 (6)	0.0291 (6)	0.0153 (6)	0.0006 (5)	0.0060 (5)	−0.0006 (5)
C47′	0.0293 (7)	0.0333 (7)	0.0192 (6)	−0.0042 (6)	0.0046 (5)	−0.0034 (5)
C48′	0.0377 (8)	0.0360 (8)	0.0300 (7)	0.0065 (6)	0.0032 (6)	−0.0031 (6)

Geometric parameters (Å, º)

C18—C17	1.1736 (18)	C38—C37	1.1684 (18)
C18—H18	0.9500	C38—H38	0.9500
C17—C14	1.4454 (17)	C37—C34	1.4450 (17)
C16—C15	1.3795 (17)	C34—C35	1.3977 (17)
C16—C11	1.3977 (16)	C34—C33	1.4018 (17)
C16—H16	0.9500	C35—C36	1.3823 (17)

C15—C14	1.3968 (17)	C35—H35	0.9500
C15—H15	0.9500	C36—C31	1.4009 (16)
C14—C13	1.3974 (16)	C36—H36	0.9500
C13—C12	1.3820 (17)	C33—C32	1.3809 (17)
C13—H13	0.9500	C33—H33	0.9500
C12—C11	1.3955 (16)	C32—C31	1.3976 (16)
C12—H12	0.9500	C32—H32	0.9500
C11—C11′	1.4821 (16)	C31—C31′	1.4820 (16)
C11′—C16′	1.3988 (16)	C31′—C32′	1.3953 (16)
C11′—C12′	1.4008 (16)	C31′—C36′	1.4009 (15)
C12′—C13′	1.3806 (16)	C32′—C33′	1.3854 (16)
C12′—H12′	0.9500	C32′—H32′	0.9500
C13′—C14′	1.4011 (17)	C33′—C34′	1.3968 (16)
C13′—H13′	0.9500	C33′—H33′	0.9500
C15′—C16′	1.3839 (17)	C35′—C36′	1.3783 (16)
C15′—C14′	1.3989 (17)	C35′—C34′	1.3986 (16)
C15′—H15′	0.9500	C35′—H35′	0.9500
C16′—H16′	0.9500	C36′—H36′	0.9500
C14′—C17′	1.4459 (17)	C34′—C37′	1.4452 (17)
C17′—C18′	1.1753 (18)	C37′—C38′	1.1843 (18)
C18′—H18′	0.9500	C38′—H38′	0.9500
C28—C27	1.1810 (19)	C48—C47	1.179 (2)
C28—H28	0.9500	C48—H48	0.9500
C27—C24	1.4394 (17)	C47—C44	1.4413 (18)
C24—C25	1.3974 (17)	C44—C43	1.3993 (18)
C24—C23	1.3979 (17)	C44—C45	1.4008 (18)
C25—C26	1.3815 (18)	C45—C46	1.3820 (17)
C25—H25	0.9500	C45—H45	0.9500
C26—C21	1.3963 (17)	C46—C41	1.3984 (17)
C26—H26	0.9500	C46—H46	0.9500
C23—C22	1.3765 (17)	C43—C42	1.3834 (18)
C23—H23	0.9500	C43—H43	0.9500
C22—C21	1.3988 (16)	C42—C41	1.3997 (17)
C22—H22	0.9500	C42—H42	0.9500
C21—C21′	1.4803 (17)	C41—C41′	1.4814 (17)
C21′—C22′	1.4019 (17)	C41′—C46′	1.3998 (17)
C21′—C26′	1.4023 (17)	C41′—C42′	1.4009 (16)
C22′—C23′	1.3803 (17)	C42′—C43′	1.3793 (17)
C22′—H22′	0.9500	C42′—H42′	0.9500
C23′—C24′	1.3999 (18)	C43′—C44′	1.4003 (17)
C23′—H23′	0.9500	C43′—H43′	0.9500
C25′—C26′	1.3790 (17)	C45′—C46′	1.3806 (17)
C25′—C24′	1.3982 (18)	C45′—C44′	1.4004 (17)
C25′—H25′	0.9500	C45′—H45′	0.9500
C26′—H26′	0.9500	C46′—H46′	0.9500
C24′—C27′	1.4507 (19)	C44′—C47′	1.4433 (18)
C27′—C28′	1.130 (2)	C47′—C48′	1.1776 (19)
C28′—H28′	0.9500	C48′—H48′	0.9500

C17—C18—H18	180.0	C37—C38—H38	180.0
C18—C17—C14	178.75 (13)	C38—C37—C34	178.73 (14)
C15—C16—C11	121.21 (11)	C35—C34—C33	118.87 (11)
C15—C16—H16	119.4	C35—C34—C37	120.93 (11)
C11—C16—H16	119.4	C33—C34—C37	120.19 (11)
C16—C15—C14	120.62 (11)	C36—C35—C34	120.60 (11)
C16—C15—H15	119.7	C36—C35—H35	119.7
C14—C15—H15	119.7	C34—C35—H35	119.7
C15—C14—C13	118.56 (11)	C35—C36—C31	120.68 (11)
C15—C14—C17	120.51 (11)	C35—C36—H36	119.7
C13—C14—C17	120.93 (10)	C31—C36—H36	119.7
C12—C13—C14	120.40 (11)	C32—C33—C34	120.30 (11)
C12—C13—H13	119.8	C32—C33—H33	119.8
C14—C13—H13	119.8	C34—C33—H33	119.8
C13—C12—C11	121.36 (11)	C33—C32—C31	121.03 (11)
C13—C12—H12	119.3	C33—C32—H32	119.5
C11—C12—H12	119.3	C31—C32—H32	119.5
C12—C11—C16	117.83 (11)	C32—C31—C36	118.51 (11)
C12—C11—C11′	121.22 (10)	C32—C31—C31′	120.38 (10)
C16—C11—C11′	120.92 (10)	C36—C31—C31′	121.11 (10)
C16′—C11′—C12′	118.31 (11)	C32′—C31′—C36′	118.30 (11)
C16′—C11′—C11	121.46 (10)	C32′—C31′—C31	121.36 (10)
C12′—C11′—C11	120.22 (10)	C36′—C31′—C31	120.34 (10)
C13′—C12′—C11′	120.95 (11)	C33′—C32′—C31′	121.27 (11)
C13′—C12′—H12′	119.5	C33′—C32′—H32′	119.4
C11′—C12′—H12′	119.5	C31′—C32′—H32′	119.4
C12′—C13′—C14′	120.52 (11)	C32′—C33′—C34′	120.02 (11)
C12′—C13′—H13′	119.7	C32′—C33′—H33′	120.0
C14′—C13′—H13′	119.7	C34′—C33′—H33′	120.0
C16′—C15′—C14′	120.40 (11)	C36′—C35′—C34′	120.73 (11)
C16′—C15′—H15′	119.8	C36′—C35′—H35′	119.6
C14′—C15′—H15′	119.8	C34′—C35′—H35′	119.6
C15′—C16′—C11′	121.01 (11)	C35′—C36′—C31′	120.72 (11)
C15′—C16′—H16′	119.5	C35′—C36′—H36′	119.6
C11′—C16′—H16′	119.5	C31′—C36′—H36′	119.6
C15′—C14′—C13′	118.81 (11)	C33′—C34′—C35′	118.94 (11)
C15′—C14′—C17′	120.96 (11)	C33′—C34′—C37′	121.18 (11)
C13′—C14′—C17′	120.22 (11)	C35′—C34′—C37′	119.87 (10)
C18′—C17′—C14′	178.63 (13)	C38′—C37′—C34′	178.12 (13)
C17′—C18′—H18′	180.0	C37′—C38′—H38′	180.0
C27—C28—H28	180.0	C47—C48—H48	180.0
C28—C27—C24	178.05 (14)	C48—C47—C44	178.56 (15)
C25—C24—C23	118.29 (11)	C43—C44—C45	118.61 (11)
C25—C24—C27	121.50 (11)	C43—C44—C47	121.32 (12)
C23—C24—C27	120.21 (11)	C45—C44—C47	120.08 (12)
C26—C25—C24	120.65 (11)	C46—C45—C44	120.54 (12)
C26—C25—H25	119.7	C46—C45—H45	119.7

C24—C25—H25	119.7	C44—C45—H45	119.7
C25—C26—C21	121.40 (11)	C45—C46—C41	121.01 (11)
C25—C26—H26	119.3	C45—C46—H46	119.5
C21—C26—H26	119.3	C41—C46—H46	119.5
C22—C23—C24	120.55 (11)	C42—C43—C44	120.63 (12)
C22—C23—H23	119.7	C42—C43—H43	119.7
C24—C23—H23	119.7	C44—C43—H43	119.7
C23—C22—C21	121.67 (11)	C43—C42—C41	120.86 (12)
C23—C22—H22	119.2	C43—C42—H42	119.6
C21—C22—H22	119.2	C41—C42—H42	119.6
C26—C21—C22	117.39 (11)	C46—C41—C42	118.33 (11)
C26—C21—C21′	121.63 (11)	C46—C41—C41′	120.66 (11)
C22—C21—C21′	120.98 (11)	C42—C41—C41′	120.99 (11)
C22′—C21′—C26′	117.62 (11)	C46′—C41′—C42′	118.25 (11)
C22′—C21′—C21	121.01 (11)	C46′—C41′—C41	121.16 (10)
C26′—C21′—C21	121.37 (11)	C42′—C41′—C41	120.58 (11)
C23′—C22′—C21′	121.39 (11)	C43′—C42′—C41′	120.79 (11)
C23′—C22′—H22′	119.3	C43′—C42′—H42′	119.6
C21′—C22′—H22′	119.3	C41′—C42′—H42′	119.6
C22′—C23′—C24′	120.41 (12)	C42′—C43′—C44′	120.62 (11)
C22′—C23′—H23′	119.8	C42′—C43′—H43′	119.7
C24′—C23′—H23′	119.8	C44′—C43′—H43′	119.7
C26′—C25′—C24′	120.59 (11)	C46′—C45′—C44′	120.07 (11)
C26′—C25′—H25′	119.7	C46′—C45′—H45′	120.0
C24′—C25′—H25′	119.7	C44′—C45′—H45′	120.0
C25′—C26′—C21′	121.30 (11)	C45′—C46′—C41′	121.30 (11)
C25′—C26′—H26′	119.4	C45′—C46′—H46′	119.3
C21′—C26′—H26′	119.4	C41′—C46′—H46′	119.3
C25′—C24′—C23′	118.66 (11)	C43′—C44′—C45′	118.94 (11)
C25′—C24′—C27′	120.33 (12)	C43′—C44′—C47′	119.87 (11)
C23′—C24′—C27′	121.01 (12)	C45′—C44′—C47′	121.19 (11)
C28′—C27′—C24′	178.68 (15)	C48′—C47′—C44′	177.80 (14)
C27′—C28′—H28′	180.0	C47′—C48′—H48′	180.0

Hydrogen-bond geometry (Å, º)

Cg1, Cg3, Cg4, Cg6 and Cg8 are the centroids of the C11–C16, C21–C26, C21′–C26′, C31′–C36′ and C41′–C46′ rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13···*Cg*6^{i}	0.95	2.73	3.4910 (13)	137
C15—H15···*Cg*6	0.95	2.70	3.4782 (13)	140
C16′—H16′···*Cg*1^{ii}	0.95	2.92	3.5375 (12)	124
C23—H23···*Cg*8^{i}	0.95	2.71	3.4809 (13)	139
C25—H25···*Cg*8	0.95	2.76	3.4976 (14)	136
C33′—H33′···*Cg*4^{iii}	0.95	2.88	3.6153 (13)	135
C36—H36···*Cg*3^{iii}	0.95	2.87	3.6112 (12)	135

Symmetry codes: (i) *x*, *y*, *z*−1; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) *x*, *y*, *z*+1.