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3-Benzyl-2,4,6-triphenylpyrylium tetrafluoroborate

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.003 Å
R factor = 0.055
wR factor = 0.142
Data-to-parameter ratio = 12.7

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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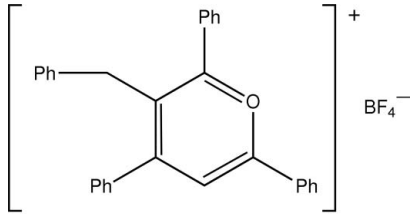
The central OC_5 ring in the cation of the title compound, $C_{30}H_{23}O^+\cdot BF_4^-$, has considerable aromatic character but the pendant aromatic rings are not coplanar. The crystal structure comprises undulating layers of cations separated by BF_4^- anions with significant intermolecular interactions between them.

Comment

The structure of the title compound, (I) (Fig. 1 and Table 1), shows significant twisting of the pendant aromatic rings out of the central plane. The dihedral angles between the O1/C1–C5 ring and the C6–C11, C12–C17 and C25–C30 rings are 28.14 (10), 56.70 (11) and 83.44 (10)°, respectively. Within the central ring, which formally carries a positive charge, the two O—C distances are equal within experimental error and the C—C distances lie in the relatively narrow range 1.361 (3)–1.414 (3) Å. These observations strongly suggest substantial delocalization of π-electron density over this ring.



(I)

In the crystal structure there are a number of intermolecular interactions linking the ions. The primary interactions operating in the crystal structure are illustrated in Fig. 2. Here, B—F···H contacts are highlighted as golden dashed lines. The first contact occurs between the two components of the asymmetric unit so that C20—H20···F4 is 2.49 Å, C20···F4 is 3.355 (3) Å and the angle at H20 is 152°. The second F···H contact involves the $C8^i$ and F3 atoms so that $C8^i$—$H8^i$···F3 is 2.55 Å, $C8^i$···F3 is 3.321 (3) Å and the angle at H8 is 139 Å [symmetry code: (i) $1-x, 1-y, -z$]. The remaining two F atoms serve to link two central O1/C1–C5 rings. The parameters associated with these interactions are B1—F1···ring centroid(O1/C1–C5) = 3.091 (2) Å and angle at F1 = 114.52 (15)°, and B1—F2···ring centroid(O1/C1–C5)^{ii} = 3.080 (2) Å and angle at F2 = 118.59 (17)° [symmetry code: (ii) $1-x, \frac{1}{2}+y, \frac{1}{2}-z$]. Formally, these might be considered as F···ring centroid(O1/C1–C5) interactions, but as seen in the B—F···ring centroid(O1/C1–C5) angles there is significant bending in the angles so that F1 approaches atoms O1 and C1 at 2.9508 (24) and 2.9766 (28) Å, respectively, with the other F1···C distances being greater than 3.3 Å. A similar situation pertains for the interactions involving atom F2. Thus, the

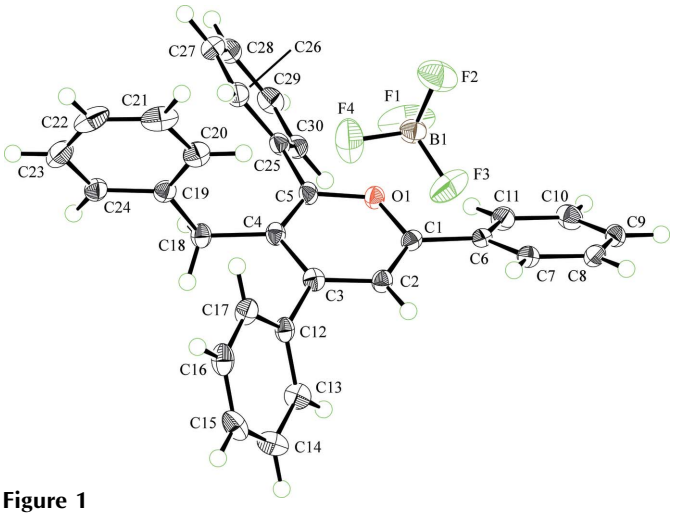


Figure 1
The asymmetric unit of (I) showing 50% probability displacement ellipsoids and the atom-numbering scheme.

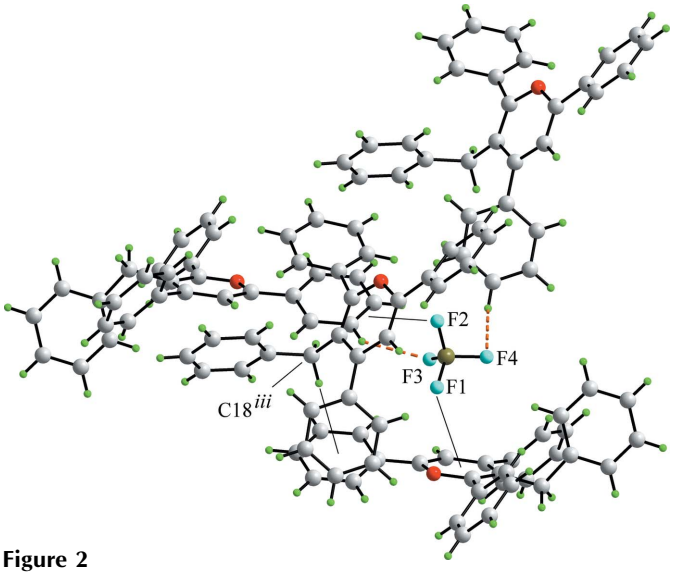


Figure 2
Environment about the BF_4^- anion in (I) (Crystal Impact, 2006). Color code: O (red), C (grey), B (brown) and H (green).

F2···O1^{ii}, F2···C1^{ii} and F2···C5^{ii} distances are 2.9270 (22), 3.1280 (28) and 3.1845 (26) Å, respectively, the remaining F2···C^{ii} distances being greater than 3.5 Å. The only other significant intermolecular contact in the structure of (I) is also illustrated in Fig. 2, *i.e.* a C18^{iii}—H18*A*^{iii}···ring centroid(C6–C11) contact with an H18*A*^{iii}···ring centroid distance of 2.98 Å and an angle of 152° at the H18*A*^{iii} atom. The global crystal structure may be described as comprising undulating layers of cations interspersed with anions (see Fig. 3).

Experimental

The title compound was isolated as a by-product in the preparation of 2-(4-hyroxyphenyl)-4,6-diphenylpyrylium tetrafluoroborate from 1,3-diphenylpropenone and 4-hydroxyphenylethanone in the presence of boron trifluoride etherate (Aliaga *et al.*, 1997). The two products were separated by fractional crystallization from acetic acid. The title compound, recrystallized from AcOH, had melting point and spectroscopic properties in agreement with literature values (Marton *et al.*, 1999).

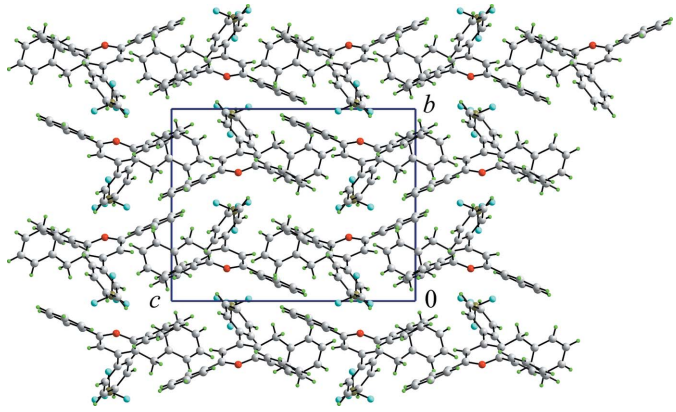


Figure 3
Packing diagram for (I), viewed approximately down the *a* axis (Crystal Impact, 2006). Color code as for Fig. 2.

Crystal data

$C_{30}H_{23}O^+\cdot BF^{4-}$
M_r = 486.29
Monoclinic, $P2_1/c$
a = 10.6170 (3) Å
b = 13.2065 (3) Å
c = 17.1985 (5) Å
β = 102.784 (1)°
V = 2351.68 (11) Å^3
Z = 4
D_x = 1.374 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 120 (2) K
Block, pale yellow
0.24 × 0.10 × 0.08 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.834, T_{max} = 1
25644 measured reflections
4136 independent reflections
3347 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.142
S = 1.05
4136 reflections
325 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0667P)^2 + 2.1496P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.80 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.341 (3)	C2—C3	1.397 (3)
O1—C5	1.350 (3)	C3—C4	1.414 (3)
C1—C2	1.361 (3)	C4—C5	1.381 (3)
C1—O1—C5	122.38 (17)		

All H atoms were allowed to ride on their parent atoms in the riding-model approximation at C—H distances of 0.95–0.99 Å, and with U_{iso}(H) = 1.2U_{eq}(C). Evidence of some disorder in the position of the BF_4^- anion can be noted from Fig. 1. However, multiple positions could not be resolved.

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduc-

tion: *DENZO* and *COLLECT*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976) and *DIAMOND* (Crystal Impact, 2006); software used to prepare material for publication: *SHELXL97*.

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supporting information

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Crystal data

$C_{30}H_{23}O^{+}\cdot BF_4^{-}$
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$Z = 4$
$F(000) = 1008$
$D_x = 1.374$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å
Cell parameters from 5538 reflections
$\theta = 2.9–27.5°$
$\mu = 0.10$ mm^{-1}
$T = 120$ K
Block, pale yellow
0.24 × 0.10 × 0.08 mm

Data collection

Bruker-Nonius 95mm CCD camera on κ-goniostat diffractometer
Radiation source: Bruker-Nonius FR591 rotating anode
Graphite monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ and ω scans
Absorption correction: multi scan (SADABS; Sheldrick, 2003)
$T_{min} = 0.834$, $T_{max} = 1$
25644 measured reflections
4136 independent reflections
3347 reflections with $I > 2\sigma(I)$
$R_{int} = 0.042$
$\theta_{max} = 25.0°$, $\theta_{min} = 3.0°$
$h = -12\rightarrow12$
$k = -15\rightarrow15$
$l = -20\rightarrow20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.142$
$S = 1.05$
4136 reflections
325 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0667P)^2 + 2.1496P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.80$ e Å^{-3}
$\Delta\rho_{min} = -0.40$ 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. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
F1	0.57576 (17)	0.50732 (15)	0.27361 (13)	0.0707 (7)
F2	0.71621 (18)	0.63183 (12)	0.25861 (12)	0.0559 (5)
F3	0.70332 (18)	0.48944 (15)	0.18351 (10)	0.0588 (5)
F4	0.78734 (18)	0.48523 (15)	0.31391 (11)	0.0636 (5)
O1	0.40466 (14)	0.33118 (11)	0.27331 (9)	0.0202 (3)
C1	0.4465 (2)	0.31678 (16)	0.20605 (13)	0.0190 (5)
C2	0.5580 (2)	0.26442 (16)	0.20922 (13)	0.0201 (5)
H2	0.5889	0.2550	0.1620	0.024*
C3	0.6273 (2)	0.22436 (16)	0.28119 (13)	0.0200 (5)
C4	0.5820 (2)	0.24083 (16)	0.35153 (13)	0.0193 (5)
C5	0.4691 (2)	0.29537 (16)	0.34461 (13)	0.0195 (5)
C6	0.3624 (2)	0.36022 (16)	0.13507 (13)	0.0187 (5)
C7	0.4156 (2)	0.38924 (16)	0.07108 (13)	0.0216 (5)
H7	0.5057	0.3818	0.0744	0.026*
C8	0.3370 (2)	0.42882 (17)	0.00296 (13)	0.0245 (5)
H8	0.3727	0.4482	−0.0408	0.029*
C9	0.2061 (2)	0.44013 (17)	−0.00133 (14)	0.0260 (5)
H9	0.1523	0.4681	−0.0479	0.031*
C10	0.1527 (2)	0.41098 (18)	0.06188 (15)	0.0281 (6)
H10	0.0627	0.4188	0.0584	0.034*
C11	0.2304 (2)	0.37063 (17)	0.12982 (14)	0.0242 (5)
H11	0.1938	0.3500	0.1729	0.029*
C12	0.7417 (2)	0.16057 (17)	0.27859 (13)	0.0207 (5)
C13	0.7277 (2)	0.07825 (18)	0.22708 (15)	0.0268 (5)
H13	0.6450	0.0621	0.1954	0.032*
C14	0.8336 (2)	0.01974 (19)	0.22177 (16)	0.0324 (6)
H14	0.8229	−0.0366	0.1866	0.039*
C15	0.9547 (2)	0.04247 (18)	0.26704 (15)	0.0305 (6)
H15	1.0270	0.0019	0.2633	0.037*
C16	0.9694 (2)	0.12461 (19)	0.31768 (15)	0.0298 (6)
H16	1.0528	0.1412	0.3483	0.036*
C17	0.8643 (2)	0.18334 (19)	0.32446 (14)	0.0271 (5)
H17	0.8755	0.2391	0.3603	0.033*
C18	0.6405 (2)	0.18787 (17)	0.42883 (13)	0.0213 (5)
H18A	0.6771	0.1228	0.4156	0.026*

H18B	0.5698	0.1715	0.4558	0.026*
C19	0.7452 (2)	0.24305 (17)	0.48847 (13)	0.0213 (5)
C20	0.7977 (2)	0.33477 (18)	0.47235 (15)	0.0278 (5)
H20	0.7641	0.3688	0.4235	0.033*
C21	0.8997 (2)	0.3768 (2)	0.52801 (17)	0.0366 (6)
H21	0.9354	0.4395	0.5166	0.044*
C22	0.9499 (2)	0.3289 (2)	0.59937 (16)	0.0376 (7)
H22	1.0217	0.3571	0.6359	0.045*
C23	0.8946 (2)	0.2396 (2)	0.61708 (15)	0.0344 (6)
H23	0.9263	0.2073	0.6669	0.041*
C24	0.7929 (2)	0.19681 (18)	0.56234 (13)	0.0249 (5)
H24	0.7552	0.1355	0.5751	0.030*
C25	0.3994 (2)	0.31854 (16)	0.40788 (13)	0.0207 (5)
C26	0.4613 (2)	0.36439 (17)	0.47898 (14)	0.0247 (5)
H26	0.5509	0.3796	0.4884	0.030*
C27	0.3916 (2)	0.38770 (18)	0.53592 (14)	0.0284 (5)
H27	0.4333	0.4201	0.5841	0.034*
C28	0.2617 (2)	0.36415 (18)	0.52307 (14)	0.0277 (6)
H28	0.2147	0.3797	0.5626	0.033*
C29	0.2000 (2)	0.31797 (18)	0.45261 (15)	0.0278 (5)
H29	0.1109	0.3017	0.4440	0.033*
C30	0.2680 (2)	0.29533 (17)	0.39466 (14)	0.0239 (5)
H30	0.2253	0.2642	0.3462	0.029*
B1	0.6920 (3)	0.5292 (2)	0.25495 (17)	0.0271 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0457 (10)	0.0742 (13)	0.1045 (17)	−0.0265 (9)	0.0432 (11)	−0.0448 (12)
F2	0.0666 (12)	0.0319 (9)	0.0727 (13)	−0.0064 (8)	0.0231 (10)	−0.0016 (8)
F3	0.0723 (12)	0.0718 (13)	0.0360 (10)	−0.0067 (10)	0.0199 (9)	−0.0175 (9)
F4	0.0644 (12)	0.0754 (13)	0.0489 (11)	0.0126 (10)	0.0083 (9)	0.0235 (10)
O1	0.0210 (8)	0.0222 (8)	0.0177 (8)	0.0011 (6)	0.0051 (6)	0.0023 (6)
C1	0.0221 (11)	0.0188 (11)	0.0171 (11)	−0.0036 (9)	0.0061 (9)	−0.0006 (9)
C2	0.0204 (11)	0.0231 (11)	0.0180 (11)	0.0003 (9)	0.0065 (9)	0.0015 (9)
C3	0.0183 (11)	0.0196 (11)	0.0224 (12)	−0.0035 (9)	0.0048 (9)	0.0017 (9)
C4	0.0196 (11)	0.0191 (11)	0.0186 (11)	−0.0028 (9)	0.0030 (9)	0.0028 (9)
C5	0.0229 (11)	0.0174 (11)	0.0178 (11)	−0.0026 (9)	0.0035 (9)	0.0038 (9)
C6	0.0210 (11)	0.0173 (11)	0.0168 (11)	0.0012 (9)	0.0021 (9)	−0.0022 (9)
C7	0.0223 (11)	0.0205 (11)	0.0217 (12)	0.0008 (9)	0.0042 (10)	−0.0008 (9)
C8	0.0332 (13)	0.0218 (12)	0.0180 (12)	−0.0020 (10)	0.0046 (10)	−0.0011 (9)
C9	0.0310 (13)	0.0194 (11)	0.0217 (12)	0.0014 (10)	−0.0071 (10)	−0.0012 (9)
C10	0.0199 (11)	0.0271 (13)	0.0349 (14)	0.0039 (10)	0.0012 (11)	−0.0013 (11)
C11	0.0217 (11)	0.0269 (12)	0.0242 (13)	0.0025 (10)	0.0055 (10)	−0.0008 (10)
C12	0.0207 (11)	0.0239 (12)	0.0186 (11)	−0.0003 (9)	0.0066 (9)	0.0058 (9)
C13	0.0216 (11)	0.0277 (13)	0.0314 (13)	−0.0040 (10)	0.0064 (10)	−0.0005 (10)
C14	0.0325 (14)	0.0236 (12)	0.0440 (16)	0.0005 (10)	0.0150 (12)	−0.0025 (11)
C15	0.0262 (13)	0.0280 (13)	0.0415 (15)	0.0067 (10)	0.0167 (11)	0.0132 (11)

C16	0.0207 (12)	0.0403 (15)	0.0281 (13)	0.0013 (11)	0.0046 (10)	0.0096 (11)
C17	0.0250 (12)	0.0340 (13)	0.0220 (12)	0.0013 (10)	0.0044 (10)	0.0009 (10)
C18	0.0211 (11)	0.0238 (11)	0.0195 (12)	−0.0002 (9)	0.0055 (9)	0.0038 (9)
C19	0.0197 (11)	0.0253 (12)	0.0200 (12)	0.0033 (9)	0.0066 (9)	−0.0013 (9)
C20	0.0268 (12)	0.0302 (13)	0.0285 (13)	−0.0028 (10)	0.0104 (11)	−0.0017 (11)
C21	0.0319 (14)	0.0358 (15)	0.0476 (17)	−0.0100 (11)	0.0205 (13)	−0.0147 (13)
C22	0.0247 (13)	0.0554 (18)	0.0333 (15)	−0.0026 (12)	0.0080 (11)	−0.0216 (13)
C23	0.0291 (13)	0.0493 (16)	0.0233 (13)	0.0099 (12)	0.0024 (11)	−0.0080 (12)
C24	0.0264 (12)	0.0281 (12)	0.0207 (12)	0.0063 (10)	0.0065 (10)	−0.0008 (10)
C25	0.0241 (11)	0.0189 (11)	0.0204 (12)	0.0032 (9)	0.0077 (9)	0.0043 (9)
C26	0.0250 (12)	0.0252 (12)	0.0239 (13)	0.0013 (10)	0.0052 (10)	0.0016 (10)
C27	0.0354 (14)	0.0281 (13)	0.0214 (12)	0.0036 (11)	0.0055 (11)	−0.0022 (10)
C28	0.0337 (13)	0.0281 (13)	0.0257 (13)	0.0072 (10)	0.0158 (11)	0.0035 (10)
C29	0.0248 (12)	0.0268 (13)	0.0342 (14)	0.0019 (10)	0.0115 (11)	0.0035 (11)
C30	0.0253 (12)	0.0234 (12)	0.0234 (12)	0.0012 (9)	0.0061 (10)	0.0009 (10)
B1	0.0270 (14)	0.0263 (14)	0.0298 (15)	0.0001 (11)	0.0099 (12)	−0.0016 (12)

Geometric parameters (Å, º)

F1—B1	1.373 (3)	C14—H14	0.9500
F2—B1	1.378 (3)	C15—C16	1.378 (4)
F3—B1	1.366 (3)	C15—H15	0.9500
F4—B1	1.392 (3)	C16—C17	1.385 (3)
O1—C1	1.341 (3)	C16—H16	0.9500
O1—C5	1.350 (3)	C17—H17	0.9500
C1—C2	1.361 (3)	C18—C19	1.521 (3)
C1—C6	1.461 (3)	C18—H18A	0.9900
C2—C3	1.397 (3)	C18—H18B	0.9900
C2—H2	0.9500	C19—C24	1.400 (3)
C3—C4	1.414 (3)	C19—C20	1.386 (3)
C3—C12	1.488 (3)	C20—C21	1.392 (4)
C4—C5	1.381 (3)	C20—H20	0.9500
C4—C18	1.509 (3)	C21—C22	1.378 (4)
C5—C25	1.476 (3)	C21—H21	0.9500
C6—C11	1.391 (3)	C22—C23	1.382 (4)
C6—C7	1.397 (3)	C22—H22	0.9500
C7—C8	1.382 (3)	C23—C24	1.386 (3)
C7—H7	0.9500	C23—H23	0.9500
C8—C9	1.384 (3)	C24—H24	0.9500
C8—H8	0.9500	C25—C30	1.398 (3)
C9—C10	1.387 (3)	C25—C26	1.392 (3)
C9—H9	0.9500	C26—C27	1.387 (3)
C10—C11	1.380 (3)	C26—H26	0.9500
C10—H10	0.9500	C27—C28	1.383 (3)
C11—H11	0.9500	C27—H27	0.9500
C12—C13	1.389 (3)	C28—C29	1.385 (3)
C12—C17	1.397 (3)	C28—H28	0.9500
C13—C14	1.384 (3)	C29—C30	1.386 (3)

C13—H13	0.9500	C29—H29	0.9500
C14—C15	1.381 (4)	C30—H30	0.9500
C1—O1—C5	122.38 (17)	C16—C17—H17	120.0
O1—C1—C2	119.2 (2)	C12—C17—H17	120.0
O1—C1—C6	114.02 (18)	C4—C18—C19	117.97 (18)
C2—C1—C6	126.7 (2)	C4—C18—H18A	107.8
C1—C2—C3	120.7 (2)	C19—C18—H18A	107.8
C1—C2—H2	119.6	C4—C18—H18B	107.8
C3—C2—H2	119.6	C19—C18—H18B	107.8
C2—C3—C4	119.20 (19)	H18A—C18—H18B	107.2
C2—C3—C12	117.49 (19)	C24—C19—C20	118.8 (2)
C4—C3—C12	123.20 (19)	C24—C19—C18	117.8 (2)
C5—C4—C3	117.36 (19)	C20—C19—C18	123.3 (2)
C5—C4—C18	119.88 (19)	C19—C20—C21	119.8 (2)
C3—C4—C18	122.05 (19)	C19—C20—H20	120.1
O1—C5—C4	121.08 (19)	C21—C20—H20	120.1
O1—C5—C25	111.18 (18)	C22—C21—C20	121.2 (2)
C4—C5—C25	127.68 (19)	C22—C21—H21	119.4
C11—C6—C7	119.9 (2)	C20—C21—H21	119.4
C11—C6—C1	120.9 (2)	C21—C22—C23	119.2 (2)
C7—C6—C1	119.14 (19)	C21—C22—H22	120.4
C8—C7—C6	119.8 (2)	C23—C22—H22	120.4
C8—C7—H7	120.1	C22—C23—C24	120.2 (2)
C6—C7—H7	120.1	C22—C23—H23	119.9
C9—C8—C7	119.8 (2)	C24—C23—H23	119.9
C9—C8—H8	120.1	C19—C24—C23	120.6 (2)
C7—C8—H8	120.1	C19—C24—H24	119.7
C8—C9—C10	120.6 (2)	C23—C24—H24	119.7
C8—C9—H9	119.7	C30—C25—C26	119.9 (2)
C10—C9—H9	119.7	C30—C25—C5	118.7 (2)
C11—C10—C9	120.0 (2)	C26—C25—C5	121.4 (2)
C11—C10—H10	120.0	C27—C26—C25	119.7 (2)
C9—C10—H10	120.0	C27—C26—H26	120.2
C6—C11—C10	119.9 (2)	C25—C26—H26	120.2
C6—C11—H11	120.1	C26—C27—C28	120.4 (2)
C10—C11—H11	120.1	C26—C27—H27	119.8
C13—C12—C17	118.9 (2)	C28—C27—H27	119.8
C13—C12—C3	119.3 (2)	C29—C28—C27	120.0 (2)
C17—C12—C3	121.7 (2)	C29—C28—H28	120.0
C12—C13—C14	120.3 (2)	C27—C28—H28	120.0
C12—C13—H13	119.8	C28—C29—C30	120.3 (2)
C14—C13—H13	119.8	C28—C29—H29	119.9
C15—C14—C13	120.7 (2)	C30—C29—H29	119.9
C15—C14—H14	119.7	C25—C30—C29	119.7 (2)
C13—C14—H14	119.7	C25—C30—H30	120.1
C14—C15—C16	119.3 (2)	C29—C30—H30	120.1
C14—C15—H15	120.4	F1—B1—F3	113.1 (2)

C16—C15—H15	120.4	F1—B1—F2	111.4 (2)
C17—C16—C15	120.9 (2)	F3—B1—F2	111.5 (2)
C17—C16—H16	119.6	F1—B1—F4	106.8 (2)
C15—C16—H16	119.6	F3—B1—F4	107.5 (2)
C16—C17—C12	119.9 (2)	F2—B1—F4	106.2 (2)