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[4-(Allyloxy)phenyl](phenyl)methanone

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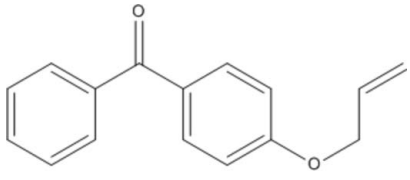
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.049; wR factor = 0.133; data-to-parameter ratio = 9.6.

The structure of the title compound, $C_{16}H_{14}O_2$, features a dihedral angle of 54.4 (3)° between the aromatic rings. The allyl group is rotated by 37.4 (4)° relative to the adjacent benzene ring. The crystal packing is characterized by numerous C—H···O and C—H···π interactions. Most of these interactions occur in layers along (011). The layers are linked by C—H···π interactions along [100], forming a three-dimensional network.

Related literature

For more details of the synthesis, see: Prucker *et al.* (1999). For photoreactive properties of benzophenone derivates, see: Shirahata & Kishimoto (1984); Dorman & Prestwich (1994); Beckett & Porter (1963); Kubo *et al.* (2010); Balakirev *et al.* (2005); Ferreira *et al.* (1995); Matsushita *et al.* (1992). For related structures, see: Schlemper (1982); Norment & Karle (1962); Guo *et al.* (1992).



Experimental

Crystal data

$C_{16}H_{14}O_2$
M_r = 238.27
Monoclinic, $P2_1$
a = 6.0141 (5) Å
b = 7.8839 (8) Å
c = 13.5992 (14) Å
β = 94.442 (6)°
V = 642.86 (11) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 K
0.12 × 0.08 × 0.06 mm

Data collection

Nonius KappaCCD diffractometer
1609 measured reflections
1603 independent reflections
1021 reflections with $I > 2\sigma(I)$
R_{int} = 0.065

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.133
S = 1.01
1603 reflections
167 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

*Cg*1 and *Cg*2 are the centroids of the C1–C6 and C8–C13 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···*Cg*1^{i}	0.93	2.83	3.651 (3)	147
C14—H14*B*···*Cg*2^{ii}	0.97	2.96	3.630 (3)	127
C10—H10···O2^{ii}	0.93	2.89	3.528 (4)	127
C2—H2···O1^{iii}	0.93	2.85	3.698 (4)	152
C14—H14*B*···O1^{iv}	0.97	2.85	3.596 (4)	134

Symmetry codes: (i) $-x+1, y+\frac{1}{2}, -z+2$; (ii) $-x+2, y+\frac{1}{2}, -z+1$; (iii) $x+1, y, z$; (iv) $-x+1, y+\frac{1}{2}, -z+1$.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SHELXS2013* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012), *DIAMOND* (Brandenburg, 2006), *Mercury* (Macrae *et al.*, 2008) and *PARST* (Nardelli, 1995).

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Supporting information for this paper is available from the IUCr electronic archives (Reference: LD2129).

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supporting information

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[4-(Allyloxy)phenyl](phenyl)methanone

Richard F. D'Vries, Carlos D. Grande, Manuel N. Chaur, Javier A. Ellena and Rigoberto C. Advincula

S1. Introduction

The title compound $C_{16}H_{14}O_2$, is based on a photoreactive benzophenone derivative that can be bound to SiO_2 surfaces *via* a silane anchor. This substrate is a compound that has a benzophenone moiety which exhibits a known photoreactivity and is particularly useful in photopolymerizable organopolysiloxane and silicone resins Prucker *et al.*, (1999); Shirahata & Kishimoto, (1984); Dorman & Prestwich, (1994); Beckett & Porter, (1963). When triggered by UV light (λ = 365 nm), a biradical triplet state is formed, which is able of abstracting a proton from any neighboring aliphatic C—H group to form a C—C bond (Ferreira *et al.*, (1995); Balakirev *et al.*, (2005); Kubo *et al.* (2010)) and as a result of the photochemical reaction, a thin layer of the polymer is covalently bound to the surface (Prucker *et al.* (1999); Shirahata & Kishimoto, (1984); Dorman & Prestwich, (1994); Matsushita *et al.* (1992)). This molecule can be also copolymerized with other polymer molecules and will not migrate out through its double bond.

S2. Experimental

Synthesis of (4-Allyloxy-phenyl)-phenyl-methanone. This compound was synthesized by a procedure already reported. A mixture of 4-hydroxybenzophenone (39.6 g, 0.2 mol) and allyl bromide (26.6 g, 0.22 mol) were dissolved in 120 mL of acetone and 28 g of potassium carbonate. The mixture was heated to reflux for 8 h and then cooled down to room temperature. Water (80 mL) was added and the resulting solution was extracted twice with 100 mL of diethyl ether. The combined organic phases were washed with 100 mL of aqueous NaOH (10%) and dried over Na_2SO_4, and the solvent was evaporated. The resulting yellowish product was purified from methanol to yield 40 g (89%) of pure product as confirmed by NMR. FTIR (KBr): 3081, 3059, 3022, 2939, 2865, 1650, 1600 cm^{-1}. ^1H NMR ($CDCl_3$, δ(ppm): 4.6 (m, 2H, OCH_2), 5.3-5.5 (m, 2H, CH_2=), 6.1 (m, 1H,=CH-), 7.21 (2H, m); 7.44 (2H, m); 7.56 (1H, m); 7.77 (2H, m); 7.88 (2H, m). ^{13}C NMR: δ(ppm) in $CDCl_3$: 195.13 (C=O), 162.14 (OCarom), 149.12, 137.60, 135.94, 132.78, 131.93, 130.19, 128.35, 118.29, 115.91, 69.34 (OCH_2).

S2.1. Refinement

All H atoms were placed in idealized positions, with C—H bond lengths fixed to 0.93 (aromatic C—H) or 0.97 Å (terminal methylene), and refined as riding with displacement parameters calculated as Uiso(H) = xUeq(carrier C) where x = 1.2.

S3. Results and discussion

The compound $C_{16}H_{14}O_2$ is a benzophenone derivate formed by two aromatic rings linked by a ketone funtion. The presence of the ketone funtion and an allyloxy group make of this molecule particularly useful in photopolymerizable organopolysiloxane and silicone resins, and a excellent substrate for selective catalysis. The rings are twisted with a torsion angle formed between C6—C1—C7—C8 of 136.59 (31)°. The allyloxy group presents a torsion angle of -7.99

(42)° (C10—C11—O2—C14) relative to the aromatic ring. The molecules interact *via* supramolecular weak interactions C5—H5···π = 3.651 (3) , C14—H14B···O1 = 3.596 (4) and C10—H10··O2 = 3.528 (4) Å giving rise to supramolecular layers in the plane (011). C14—H14B···π = 3.698 (2) Å interaction join the layers along [100] to obtain the supramolecular crystal packing.

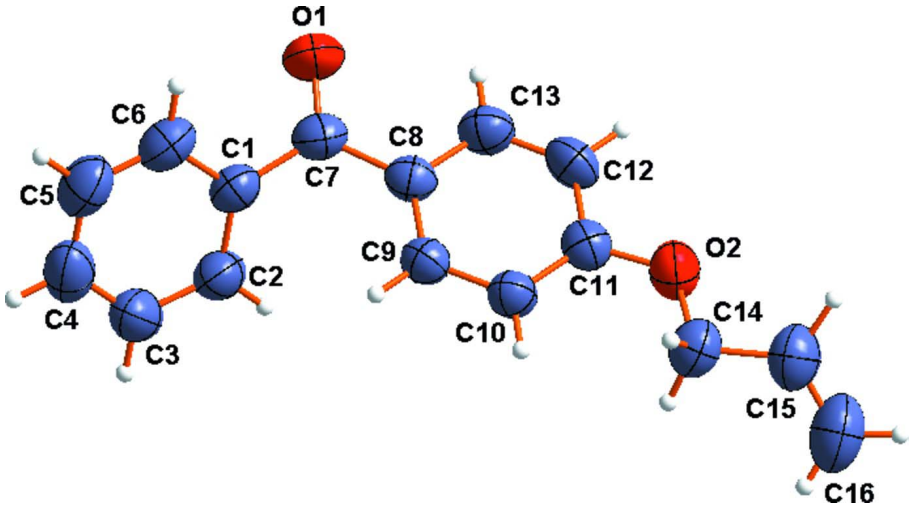

Figure 1

The *ORTEP* structure of the title compound with displacement ellipsoid plot drawn at the 50% probability level.

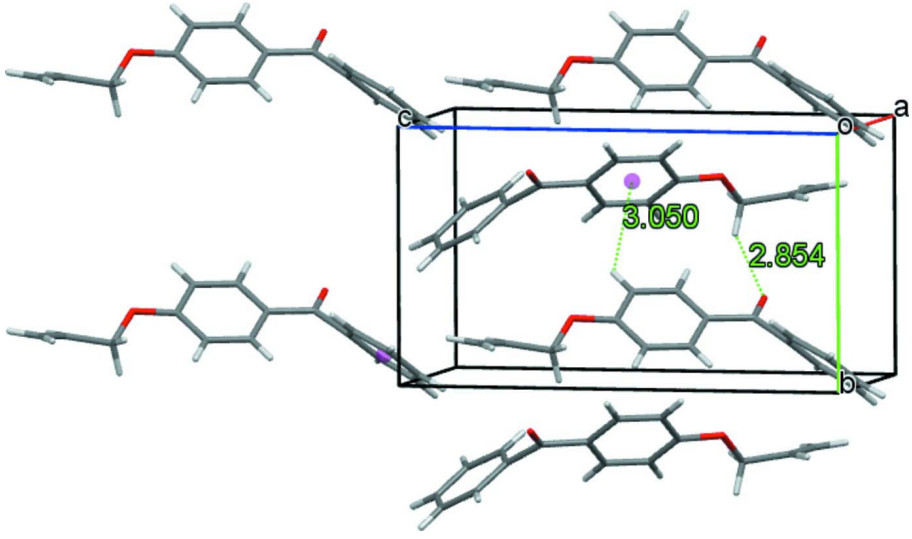

Figure 2

Crystal packing view of the title compound along [100] direction. The hydrogen bonds are shown as dashed lines.

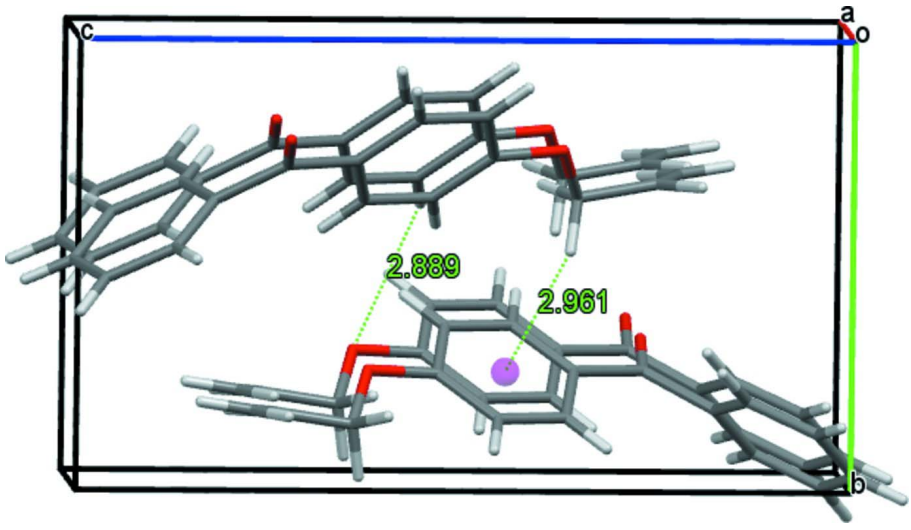

Figure 3

Crystal packing view of the title compound along [001] direction. The hydrogen bonds are shown as dashed lines.

[4-(Allyloxy)phenyl](phenyl)methanone

Crystal data

$C_{16}H_{14}O_2$
$M_r = 238.27$
Monoclinic, $P2_1$
Hall symbol: P 2yb
$a = 6.0141\ (5)$ Å
$b = 7.8839\ (8)$ Å
$c = 13.5992\ (14)$ Å
$\beta = 94.442\ (6)°$
$V = 642.86\ (11)$ Å^3
$Z = 2$
$F(000) = 252$
$D_x = 1.231$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1583 reflections
$\theta = 3.0–27.9°$
$\mu = 0.08$ mm^{-1}
$T = 293$ K
Prism, colourless
0.12 × 0.08 × 0.06 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: Enraf–Nonius FR590
Horizonally mounted graphite crystal monochromator
Detector resolution: 9 pixels mm^{-1}
CCD rotation images, thick slices scans
1609 measured reflections
1603 independent reflections
1021 reflections with $I > 2\sigma(I)$
$R_{int} = 0.065$
$\theta_{max} = 27.8°$, $\theta_{min} = 3.0°$
$h = 0.000000 \rightarrow 7.000000$
$k = 0.00000 \rightarrow 10.000000$
$l = -17.00000 \rightarrow 17.000000$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.133$
$S = 1.01$
1603 reflections
167 parameters
1 restraint
0 constraints
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0858P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}

Special details

Experimental. The absence of some reflections of the data sets is due to merged them. The 001 reflection was removed because it intensity was affect by the beam stop.

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C16	1.2957 (8)	0.3081 (6)	0.2215 (3)	0.1064 (13)
H16A	1.4203	0.317	0.2662	0.128*
H16B	1.3132	0.2899	0.155	0.128*
H15	0.960 (6)	0.322 (7)	0.199 (3)	0.119 (14)*
C1	0.5814 (4)	0.3364 (4)	0.8323 (2)	0.0589 (7)
C2	0.7988 (4)	0.3074 (4)	0.8703 (2)	0.0660 (8)
H2	0.8946	0.2419	0.8356	0.079*
C3	0.8714 (5)	0.3768 (5)	0.9602 (2)	0.0780 (9)
H3	1.0159	0.3552	0.9867	0.094*
C4	0.7337 (6)	0.4775 (5)	1.0114 (2)	0.0846 (10)
H4	0.7851	0.5244	1.0717	0.102*
C5	0.5206 (6)	0.5084 (5)	0.9730 (3)	0.0825 (9)
H5	0.4277	0.5779	1.0068	0.099*
C6	0.4430 (5)	0.4374 (5)	0.8849 (2)	0.0732 (8)
H6	0.2967	0.457	0.8601	0.088*
C7	0.4818 (4)	0.2537 (4)	0.7404 (2)	0.0618 (7)
C8	0.6023 (4)	0.2502 (3)	0.64903 (19)	0.0551 (6)
C9	0.7921 (4)	0.3450 (4)	0.63562 (19)	0.0558 (6)
H9	0.8546	0.4107	0.6874	0.067*
C10	0.8906 (4)	0.3438 (3)	0.54670 (18)	0.0577 (6)
H10	1.0187	0.4071	0.5394	0.069*
C11	0.7969 (4)	0.2475 (4)	0.46872 (19)	0.0570 (6)
C12	0.6079 (4)	0.1514 (4)	0.4819 (2)	0.0666 (8)
H12	0.5458	0.0852	0.4302	0.08*
C13	0.5125 (4)	0.1529 (4)	0.5696 (2)	0.0656 (7)
H13	0.3855	0.0881	0.5767	0.079*
C14	1.0531 (5)	0.3498 (4)	0.3553 (2)	0.0700 (8)
H14A	1.1858	0.3269	0.3984	0.084*
H14B	1.0095	0.4668	0.3647	0.084*
C15	1.0986 (7)	0.3210 (6)	0.2518 (2)	0.0848 (10)
O1	0.2952 (3)	0.1918 (4)	0.74038 (17)	0.0906 (8)
O2	0.8762 (3)	0.2378 (3)	0.37801 (13)	0.0715 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C16	0.136 (3)	0.105 (3)	0.082 (2)	0.012 (3)	0.032 (2)	−0.009 (2)

C1	0.0556 (14)	0.0588 (16)	0.0637 (14)	−0.0029 (13)	0.0135 (12)	0.0036 (14)
C2	0.0571 (15)	0.0756 (19)	0.0663 (17)	0.0002 (13)	0.0116 (13)	0.0027 (15)
C3	0.0674 (16)	0.103 (3)	0.0636 (17)	−0.0109 (17)	0.0026 (14)	0.0057 (17)
C4	0.098 (2)	0.093 (2)	0.0655 (18)	−0.0230 (19)	0.0192 (18)	−0.0085 (18)
C5	0.089 (2)	0.077 (2)	0.084 (2)	0.0005 (18)	0.0283 (18)	−0.0107 (18)
C6	0.0629 (15)	0.0760 (19)	0.083 (2)	0.0060 (15)	0.0220 (14)	0.0025 (18)
C7	0.0487 (14)	0.0666 (16)	0.0700 (16)	0.0002 (13)	0.0041 (12)	0.0027 (14)
C8	0.0513 (13)	0.0511 (14)	0.0624 (15)	0.0022 (12)	0.0006 (11)	0.0025 (13)
C9	0.0535 (13)	0.0560 (14)	0.0570 (14)	−0.0015 (12)	−0.0011 (11)	−0.0035 (13)
C10	0.0563 (13)	0.0584 (15)	0.0584 (15)	−0.0056 (13)	0.0038 (12)	0.0000 (14)
C11	0.0617 (14)	0.0521 (13)	0.0568 (15)	0.0042 (13)	0.0017 (12)	0.0011 (14)
C12	0.0700 (16)	0.0608 (16)	0.0671 (18)	−0.0082 (14)	−0.0076 (14)	−0.0089 (15)
C13	0.0603 (15)	0.0614 (16)	0.0751 (19)	−0.0101 (14)	0.0055 (14)	−0.0019 (16)
C14	0.0773 (18)	0.0667 (18)	0.0672 (17)	0.0032 (15)	0.0133 (14)	−0.0003 (16)
C15	0.099 (2)	0.092 (2)	0.0645 (17)	0.001 (2)	0.0139 (18)	0.0056 (18)
O1	0.0605 (12)	0.121 (2)	0.0911 (15)	−0.0256 (13)	0.0138 (11)	−0.0100 (15)
O2	0.0857 (13)	0.0694 (12)	0.0600 (11)	−0.0070 (11)	0.0099 (9)	−0.0039 (11)

Geometric parameters (Å, º)

C16—C15	1.289 (5)	C8—C9	1.388 (4)
C16—H16A	0.93	C8—C13	1.399 (4)
C16—H16B	0.93	C9—C10	1.387 (4)
C1—C2	1.387 (3)	C9—H9	0.93
C1—C6	1.390 (4)	C10—C11	1.387 (4)
C1—C7	1.494 (4)	C10—H10	0.93
C2—C3	1.379 (4)	C11—O2	1.359 (3)
C2—H2	0.93	C11—C12	1.389 (4)
C3—C4	1.375 (5)	C12—C13	1.363 (4)
C3—H3	0.93	C12—H12	0.93
C4—C5	1.368 (5)	C13—H13	0.93
C4—H4	0.93	C14—O2	1.435 (3)
C5—C6	1.371 (5)	C14—C15	1.472 (4)
C5—H5	0.93	C14—H14A	0.97
C6—H6	0.93	C14—H14B	0.97
C7—O1	1.224 (3)	C15—H15	1.06 (4)
C7—C8	1.486 (4)		
C15—C16—H16A	120	C13—C8—C7	118.1 (2)
C15—C16—H16B	120	C8—C9—C10	121.5 (2)
H16A—C16—H16B	120	C8—C9—H9	119.3
C2—C1—C6	119.2 (3)	C10—C9—H9	119.3
C2—C1—C7	123.1 (3)	C11—C10—C9	119.6 (2)
C6—C1—C7	117.6 (2)	C11—C10—H10	120.2
C3—C2—C1	119.3 (3)	C9—C10—H10	120.2
C3—C2—H2	120.3	O2—C11—C10	125.1 (2)
C1—C2—H2	120.3	O2—C11—C12	115.7 (2)
C4—C3—C2	121.1 (3)	C10—C11—C12	119.2 (2)

C4—C3—H3	119.5	C13—C12—C11	120.8 (3)
C2—C3—H3	119.5	C13—C12—H12	119.6
C5—C4—C3	119.5 (3)	C11—C12—H12	119.6
C5—C4—H4	120.3	C12—C13—C8	121.1 (2)
C3—C4—H4	120.3	C12—C13—H13	119.4
C6—C5—C4	120.5 (3)	C8—C13—H13	119.4
C6—C5—H5	119.8	O2—C14—C15	107.8 (3)
C4—C5—H5	119.8	O2—C14—H14A	110.1
C5—C6—C1	120.4 (3)	C15—C14—H14A	110.1
C5—C6—H6	119.8	O2—C14—H14B	110.1
C1—C6—H6	119.8	C15—C14—H14B	110.1
O1—C7—C8	120.0 (3)	H14A—C14—H14B	108.5
O1—C7—C1	118.8 (3)	C16—C15—C14	124.2 (4)
C8—C7—C1	121.2 (2)	C16—C15—H15	119 (2)
C9—C8—C13	117.8 (2)	C14—C15—H15	117 (2)
C9—C8—C7	124.0 (2)	C11—O2—C14	118.6 (2)

Hydrogen-bond geometry (Å, º)

Cg1 and Cg2 are the centroids of the C1–C6 and C8–C13 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···*Cg*1^{i}	0.93	2.83	3.651 (3)	147
C14—H14*B*···*Cg*2^{ii}	0.97	2.96	3.630 (3)	127
C10—H10···O2^{ii}	0.93	2.89	3.528 (4)	127
C2—H2···O1^{iii}	0.93	2.85	3.698 (4)	152
C14—H14*B*···O1^{iv}	0.97	2.85	3.596 (4)	134

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+2; (ii) −*x*+2, *y*+1/2, −*z*+1; (iii) *x*+1, *y*, *z*; (iv) −*x*+1, *y*+1/2, −*z*+1.