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Methyl 2,2-diphenyl-2-(prop-2-yn-1-yloxy)acetate

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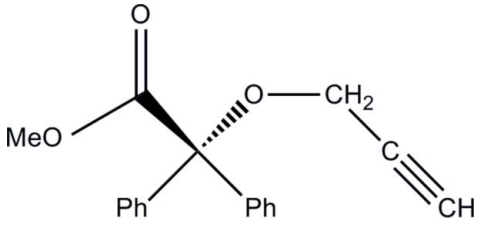
Key indicators: single-crystal X-ray study; T = 130 K; mean σ(C–C) = 0.002 Å; R factor = 0.048; wR factor = 0.117; data-to-parameter ratio = 18.2.

The molecular structure of the title compound, $C_{18}H_{16}O_3$, exhibits a new R_2–C(COOMe)(OCH_2CCH) group. The C—O—C—C torsion angle is 153.3 (1)°. The dihedral angles are 79.89 (5)° between phenyl/phenyl planes, and 73.13 (5) and 79.05 (8)° for the two COOMe/phenyl plane pairs.

Related literature

For related literature on the background of this work, see: Ferguson *et al.* (1995); Ohkuma *et al.* (2000). For related structures, see: Narayanan *et al.* (2011); Shah *et al.* (2011); Siddaraju *et al.* (2010); Zhang *et al.* (2008); Zhang *et al.* (2011).



Experimental

Crystal data

$C_{18}H_{16}O_3$
M_r = 280.31
Monoclinic, $P2_1/c$
a = 12.6771 (17) Å
b = 9.2410 (13) Å
c = 12.7055 (18) Å
β = 93.090 (3)°
V = 1486.3 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 130 K
0.37 × 0.22 × 0.10 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.969, T_{max} = 0.992
13808 measured reflections
3545 independent reflections
2623 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.117
S = 1.02
3545 reflections
195 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and local programs.

HPS is grateful to the University of Mysore for research facilities. HSY thanks R. L. Fine Chemicals, Bangalore, India, for the gift of a sample of the title compound.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NC2267).

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supporting information

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S1. Experimental

The title compound was obtained as a gift sample from R. L. Fine Chem., Bengaluru, India. X-ray quality crystals were obtained from toluene by slow evaporation (m.p. 318 K).

S2. Refinement

H atoms were clearly identified in difference syntheses, idealized and refined riding on the C atoms with C—H = 0.95–0.99 Å, and with isotropic displacement parameters U_{iso}(H) = 1.2U(C_{eq}) or 1.5U(–CH_3 H atoms). All CH_3 H atoms were allowed to rotate but not to tip. H6 was refined freely.

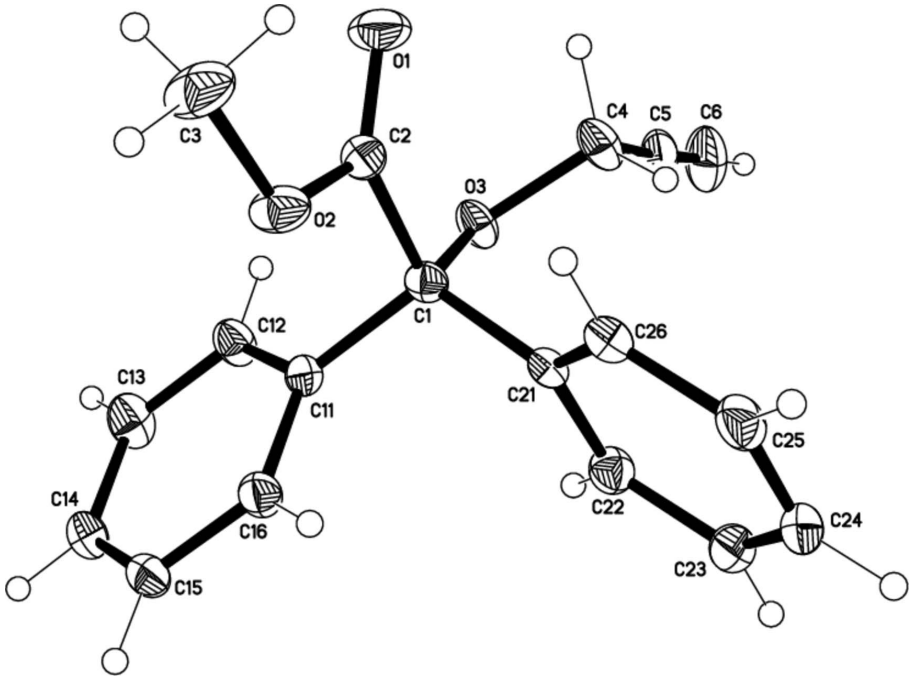

Figure 1

Molecular structure with labeling and displacement ellipsoids drawn at the 50% probability level.

Methyl 2,2-diphenyl-2-(prop-2-yn-1-yloxy)acetate

Crystal data

$C_{18}H_{16}O_3$
M_r = 280.31
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 12.6771 (17) Å
b = 9.2410 (13) Å
c = 12.7055 (18) Å
β = 93.090 (3)°

V = 1486.3 (4) Å^3
Z = 4
F(000) = 592
D_x = 1.253 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1710 reflections

θ = 2.7–23.4°
μ = 0.09 mm^{-1}
T = 130 K
Prism, colourless
0.37 × 0.22 × 0.10 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.969, T_{max} = 0.992

13808 measured reflections
3545 independent reflections
2623 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 27.9°, θ_{min} = 1.6°
h = −14→16
k = −12→12
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.117
S = 1.02
3545 reflections
195 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0487P)^2 + 0.3727P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
O1	0.79582 (9)	0.45794 (12)	0.41949 (10)	0.0378 (3)
O2	0.66203 (9)	0.37609 (11)	0.51072 (9)	0.0296 (3)
O3	0.78724 (8)	0.22289 (11)	0.28970 (8)	0.0247 (3)
C1	0.72467 (12)	0.21809 (15)	0.38023 (11)	0.0203 (3)
C2	0.73393 (12)	0.36505 (15)	0.43855 (12)	0.0233 (3)
C3	0.66088 (16)	0.51182 (17)	0.56825 (15)	0.0393 (5)
H3A	0.7287	0.5250	0.6078	0.059*
H3B	0.6038	0.5100	0.6173	0.059*
H3C	0.6494	0.5920	0.5185	0.059*
C4	0.90005 (12)	0.22196 (19)	0.31004 (13)	0.0299 (4)
H4A	0.9188	0.1639	0.3738	0.036*

H4B	0.9261	0.3219	0.3222	0.036*
C5	0.94840 (13)	0.15941 (18)	0.21894 (14)	0.0302 (4)
C6	0.99076 (16)	0.1114 (2)	0.14631 (16)	0.0432 (5)
H6	1.0260 (19)	0.068 (3)	0.0870 (19)	0.073 (7)*
C11	0.60998 (11)	0.20274 (15)	0.33670 (11)	0.0199 (3)
C12	0.57858 (12)	0.25763 (17)	0.23856 (13)	0.0271 (4)
H12A	0.6288	0.3037	0.1969	0.032*
C13	0.47418 (13)	0.24566 (19)	0.20079 (13)	0.0326 (4)
H13A	0.4534	0.2830	0.1332	0.039*
C14	0.40033 (13)	0.17983 (17)	0.26091 (13)	0.0291 (4)
H14A	0.3292	0.1700	0.2343	0.035*
C15	0.43066 (12)	0.12818 (17)	0.36029 (13)	0.0279 (4)
H15A	0.3798	0.0853	0.4028	0.033*
C16	0.53494 (12)	0.13889 (16)	0.39776 (13)	0.0247 (3)
H16A	0.5554	0.1023	0.4657	0.030*
C21	0.76008 (11)	0.09067 (15)	0.45070 (11)	0.0198 (3)
C22	0.76063 (12)	−0.04599 (16)	0.40361 (13)	0.0255 (3)
H22A	0.7343	−0.0573	0.3327	0.031*
C23	0.79918 (13)	−0.16498 (17)	0.45948 (14)	0.0307 (4)
H23A	0.7992	−0.2575	0.4269	0.037*
C24	0.83784 (13)	−0.14904 (17)	0.56317 (14)	0.0312 (4)
H24A	0.8648	−0.2305	0.6015	0.037*
C25	0.83705 (13)	−0.01480 (18)	0.61038 (13)	0.0294 (4)
H25A	0.8628	−0.0040	0.6815	0.035*
C26	0.79855 (12)	0.10528 (16)	0.55403 (12)	0.0239 (3)
H26A	0.7988	0.1977	0.5868	0.029*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0357 (7)	0.0252 (6)	0.0539 (8)	−0.0100 (5)	0.0158 (6)	−0.0027 (5)
O2	0.0363 (7)	0.0233 (6)	0.0304 (6)	−0.0054 (5)	0.0122 (5)	−0.0064 (4)
O3	0.0162 (5)	0.0372 (6)	0.0210 (6)	0.0001 (4)	0.0048 (4)	0.0035 (4)
C1	0.0200 (8)	0.0221 (7)	0.0192 (7)	−0.0014 (6)	0.0044 (6)	0.0010 (6)
C2	0.0222 (8)	0.0225 (7)	0.0252 (8)	−0.0003 (6)	0.0006 (6)	0.0029 (6)
C3	0.0522 (12)	0.0246 (8)	0.0424 (11)	−0.0033 (8)	0.0146 (9)	−0.0111 (7)
C4	0.0174 (8)	0.0434 (10)	0.0292 (9)	−0.0015 (7)	0.0042 (7)	0.0028 (7)
C5	0.0207 (8)	0.0364 (9)	0.0338 (9)	0.0061 (7)	0.0034 (7)	0.0106 (7)
C6	0.0339 (11)	0.0559 (12)	0.0407 (11)	0.0179 (9)	0.0090 (9)	0.0058 (9)
C11	0.0183 (8)	0.0195 (7)	0.0222 (8)	0.0014 (5)	0.0029 (6)	−0.0005 (5)
C12	0.0207 (8)	0.0349 (8)	0.0259 (8)	−0.0001 (6)	0.0036 (7)	0.0052 (7)
C13	0.0283 (9)	0.0455 (10)	0.0237 (8)	0.0029 (7)	−0.0016 (7)	0.0074 (7)
C14	0.0191 (8)	0.0317 (8)	0.0361 (9)	0.0006 (6)	−0.0028 (7)	0.0011 (7)
C15	0.0195 (8)	0.0289 (8)	0.0355 (9)	−0.0009 (6)	0.0042 (7)	0.0077 (7)
C16	0.0211 (8)	0.0271 (8)	0.0261 (8)	0.0005 (6)	0.0026 (6)	0.0065 (6)
C21	0.0143 (7)	0.0222 (7)	0.0231 (8)	−0.0017 (5)	0.0022 (6)	0.0003 (6)
C22	0.0241 (8)	0.0262 (8)	0.0260 (8)	0.0000 (6)	−0.0011 (7)	−0.0031 (6)
C23	0.0254 (9)	0.0236 (8)	0.0430 (10)	0.0013 (6)	0.0001 (8)	−0.0024 (7)

C24	0.0214 (8)	0.0296 (8)	0.0418 (10)	0.0013 (6)	−0.0044 (7)	0.0100 (7)
C25	0.0231 (9)	0.0364 (9)	0.0277 (9)	−0.0020 (7)	−0.0068 (7)	0.0050 (7)
C26	0.0194 (8)	0.0263 (7)	0.0260 (8)	−0.0031 (6)	−0.0001 (6)	−0.0008 (6)

Geometric parameters (Å, º)

O1—C2	1.1965 (18)	C12—H12A	0.9500
O2—C2	1.3312 (18)	C13—C14	1.381 (2)
O2—C3	1.4522 (18)	C13—H13A	0.9500
O3—C1	1.4327 (17)	C14—C15	1.385 (2)
O3—C4	1.4396 (18)	C14—H14A	0.9500
C1—C21	1.532 (2)	C15—C16	1.384 (2)
C1—C11	1.534 (2)	C15—H15A	0.9500
C1—C2	1.548 (2)	C16—H16A	0.9500
C3—H3A	0.9800	C21—C26	1.382 (2)
C3—H3B	0.9800	C21—C22	1.398 (2)
C3—H3C	0.9800	C22—C23	1.384 (2)
C4—C5	1.458 (2)	C22—H22A	0.9500
C4—H4A	0.9900	C23—C24	1.388 (2)
C4—H4B	0.9900	C23—H23A	0.9500
C5—C6	1.179 (3)	C24—C25	1.378 (2)
C6—H6	0.98 (2)	C24—H24A	0.9500
C11—C12	1.385 (2)	C25—C26	1.394 (2)
C11—C16	1.391 (2)	C25—H25A	0.9500
C12—C13	1.388 (2)	C26—H26A	0.9500
C2—O2—C3	116.02 (12)	C14—C13—C12	120.41 (15)
C1—O3—C4	116.32 (11)	C14—C13—H13A	119.8
O3—C1—C21	109.60 (11)	C12—C13—H13A	119.8
O3—C1—C11	105.57 (11)	C13—C14—C15	119.54 (15)
C21—C1—C11	112.45 (11)	C13—C14—H14A	120.2
O3—C1—C2	109.03 (11)	C15—C14—H14A	120.2
C21—C1—C2	112.47 (12)	C16—C15—C14	120.13 (15)
C11—C1—C2	107.43 (11)	C16—C15—H15A	119.9
O1—C2—O2	124.42 (14)	C14—C15—H15A	119.9
O1—C2—C1	124.47 (14)	C15—C16—C11	120.51 (14)
O2—C2—C1	111.08 (12)	C15—C16—H16A	119.7
O2—C3—H3A	109.5	C11—C16—H16A	119.7
O2—C3—H3B	109.5	C26—C21—C22	119.02 (13)
H3A—C3—H3B	109.5	C26—C21—C1	123.87 (13)
O2—C3—H3C	109.5	C22—C21—C1	116.90 (13)
H3A—C3—H3C	109.5	C23—C22—C21	120.55 (15)
H3B—C3—H3C	109.5	C23—C22—H22A	119.7
O3—C4—C5	108.41 (13)	C21—C22—H22A	119.7
O3—C4—H4A	110.0	C22—C23—C24	119.95 (15)
C5—C4—H4A	110.0	C22—C23—H23A	120.0
O3—C4—H4B	110.0	C24—C23—H23A	120.0
C5—C4—H4B	110.0	C25—C24—C23	119.87 (15)

H4A—C4—H4B	108.4	C25—C24—H24A	120.1
C6—C5—C4	177.6 (2)	C23—C24—H24A	120.1
C5—C6—H6	178.2 (14)	C24—C25—C26	120.22 (15)
C12—C11—C16	119.06 (14)	C24—C25—H25A	119.9
C12—C11—C1	120.77 (13)	C26—C25—H25A	119.9
C16—C11—C1	120.11 (13)	C21—C26—C25	120.38 (14)
C11—C12—C13	120.32 (15)	C21—C26—H26A	119.8
C11—C12—H12A	119.8	C25—C26—H26A	119.8
C13—C12—H12A	119.8		

C4—O3—C1—C21	−52.38 (16)	C11—C12—C13—C14	0.4 (3)
C4—O3—C1—C11	−173.72 (12)	C12—C13—C14—C15	1.3 (3)
C4—O3—C1—C2	71.12 (15)	C13—C14—C15—C16	−1.8 (2)
C3—O2—C2—O1	0.2 (2)	C14—C15—C16—C11	0.7 (2)
C3—O2—C2—C1	−178.05 (13)	C12—C11—C16—C15	1.1 (2)
O3—C1—C2—O1	−10.3 (2)	C1—C11—C16—C15	178.21 (13)
C21—C1—C2—O1	111.46 (17)	O3—C1—C21—C26	119.93 (15)
C11—C1—C2—O1	−124.27 (16)	C11—C1—C21—C26	−122.97 (15)
O3—C1—C2—O2	167.95 (11)	C2—C1—C21—C26	−1.5 (2)
C21—C1—C2—O2	−70.27 (16)	O3—C1—C21—C22	−54.88 (16)
C11—C1—C2—O2	54.00 (15)	C11—C1—C21—C22	62.22 (17)
C1—O3—C4—C5	153.28 (13)	C2—C1—C21—C22	−176.34 (13)
O3—C1—C11—C12	−28.55 (17)	C26—C21—C22—C23	−0.1 (2)
C21—C1—C11—C12	−148.02 (14)	C1—C21—C22—C23	175.02 (14)
C2—C1—C11—C12	87.70 (16)	C21—C22—C23—C24	−0.1 (2)
O3—C1—C11—C16	154.35 (13)	C22—C23—C24—C25	0.4 (2)
C21—C1—C11—C16	34.87 (18)	C23—C24—C25—C26	−0.6 (2)
C2—C1—C11—C16	−89.40 (15)	C22—C21—C26—C25	−0.2 (2)
C16—C11—C12—C13	−1.6 (2)	C1—C21—C26—C25	−174.87 (14)
C1—C11—C12—C13	−178.74 (14)	C24—C25—C26—C21	0.5 (2)