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4-(Diphenylmethoxy)-3-ethoxybenzaldehyde

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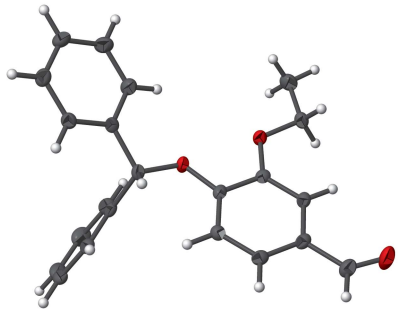
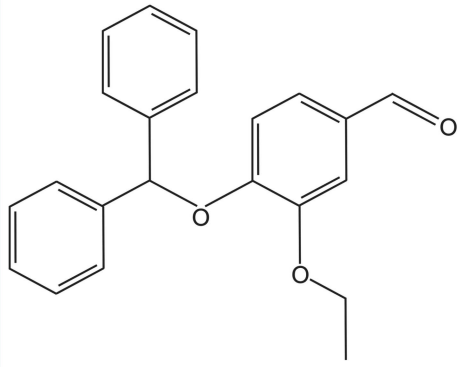
In the title compound, $C_{22}H_{20}O_3$, the dihedral angle between the aromatic rings linked by the methine group is 81.265 (4)° and the ethoxy side chain adopts an extended conformation [C—O—C—C = 177.24 (10)°]. In the crystal, weak C—H···π and C—H···O interactions link the molecules into sheets.

3D view



Chemical scheme



Structure description

The preparation of Schiff bases (Omidi & Kakanejadifard, 2020) is nowadays an interesting topic, because of their various application and properties (*e.g.*, Kizilkaya *et al.*, 2020). As part of our studies in this area, the title aldehyde, $C_{22}H_{20}O_3$, was prepared as a precursor to new Schiff bases and we now describe its crystal structure (Fig. 1).

As expected, the C2—O2, C20—O2, C1—O1 and C7—O1 bond lengths reveal single bond character while C22═O3 is a double bond. The dihedral angle between the C1–C6 and C8–C13 aromatic rings connected by the C7 methine group is 81.265 (4)°. In the crystal, weak C—H···O (Table 1) and C—H···π interactions [C20^{iii}—H1*c*20^{iii}···*Cg*3 = 3.05 Å and C5^{iv}—H1*c*5^{iv}···*Cg*3 = 2.89 Å; symmetry codes: (iii) $\frac{1}{2}-x,\frac{1}{2}+y,z$; (iv) $x-\frac{1}{2},y,\frac{1}{2}-z$; *Cg*3 is the centroid of the C14–C19 ring] are observed. These link the molecules into sheets lying perpendicular to the *c*-axis direction (Fig. 2).

Synthesis and crystallization

3-Ethoxy-4-hydroxy benzaldehyde (0.20 mmol) and potassium carbonate (0.40 mmol) were mixed in dimethylformamide (25 ml) and stirred for 0.5 h. A solution of diphenylbromomethane (0.2 mmol) in ethanol (20 ml) was added dropwise and the mixture was stirred at 80°C for 24 h. After that, the solution was concentrated under reduced pressure. The cream precipitate of the title compound formed by adding cold water (250 ml) was filtered off and washed several times with cold ethanol. Colourless slabs were recrystallized from the mixed solvents of chloroform and ethanol (1:1).

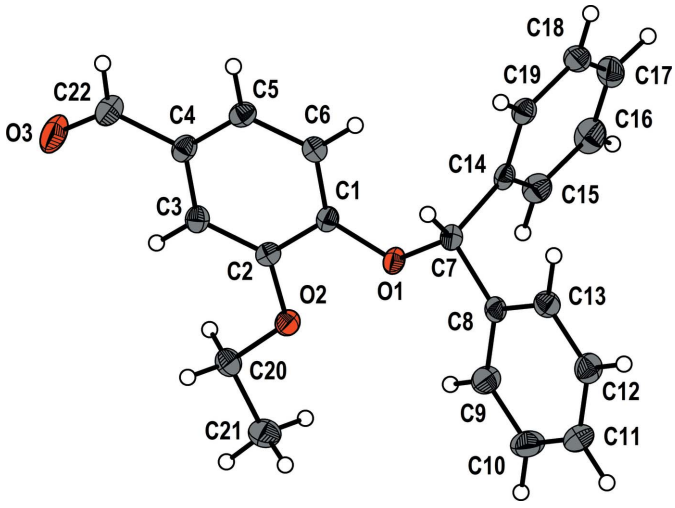


Figure 1
The molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

The authors are grateful to Golestan University. CzechNanoLab project LM2018110 funded by MEYS CR is gratefully acknowledged for the financial support of the measurements at LNSM Research Infrastructure.

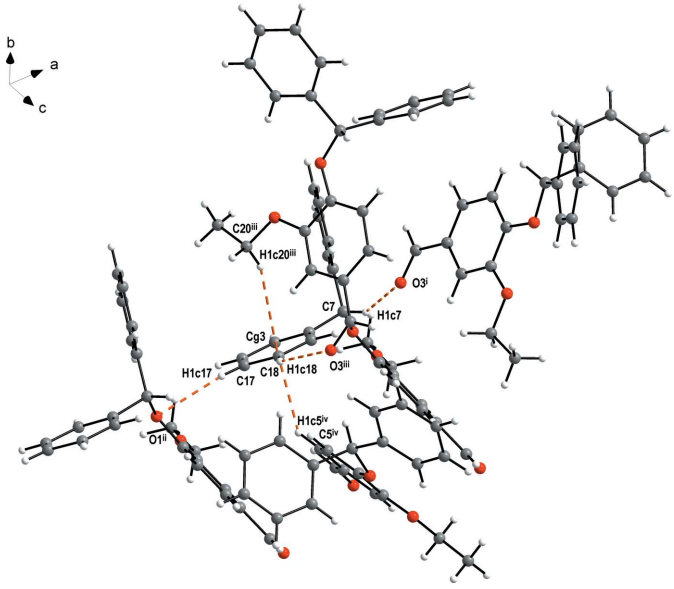


Figure 2
Partial packing diagram showing the hydrogen bonds in the title compound. Hydrogen atoms not involved in hydrogen bonding were omitted for clarity. Symmetry codes: (i) $-x+1, y+\frac{1}{2}, -z+1$; (ii) $x-1, y, z$; (iii) $-x+\frac{1}{2}, y+\frac{1}{2}, z$.

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H1*c*7···O3^{i}	0.96	2.52	3.3794 (15)	148
C17—H1*c*17···O1^{ii}	0.96	2.57	3.4440 (15)	152
C18—H1*c*18···O3^{iii}	0.96	2.53	3.2906 (16)	136

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{22}H_{20}O_3$
M_r	332.4
Crystal system, space group	Orthorhombic, *Pbca*
Temperature (K)	120
a, *b*, *c* (Å)	8.1123 (4), 15.8713 (9), 27.6155 (14)
V (Å^3)	3555.6 (3)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	0.83 × 0.32 × 0.26
Data collection	
Diffractometer	Rigaku Oxford Diffraction Xcalibur, AtlasS2, Gemini ultra
Absorption correction	Analytical (*CrysAlis PRO*; Rigaku OD, 2015)
T_{min}, T_{max}	0.958, 0.982
No. of measured, independent and observed [$I > 3\sigma(I)$] reflections	16215, 4454, 3284
R_{int}	0.028
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.695
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.040, 0.107, 1.44
No. of reflections	4454
No. of parameters	227
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.22, −0.20

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SUPERFLIP* (Palatinus & Chapuis, (2007), *JANA2006* (Petříček *et al.*, 2014) and *DIAMOND* (Brandenburg, 1999).

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full crystallographic data

IUCrData (2021). **6**, x210356 [https://doi.org/10.1107/S2414314621003564]

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Crystal data

$C_{22}H_{20}O_3$
M_r = 332.4
Orthorhombic, *Pbca*
Hall symbol: -P -2xab;-2ybc;-2zac
a = 8.1123 (4) Å
b = 15.8713 (9) Å
c = 27.6155 (14) Å
V = 3555.6 (3) Å^3
Z = 8
F(000) = 1408
D_x = 1.242 Mg m^{-3}
Mo *Kα* radiation, λ = 0.71073 Å
Cell parameters from 4539 reflections
θ = 3.9–29.2°
μ = 0.08 mm^{-1}
T = 120 K
Plate, colourless
0.83 × 0.32 × 0.26 mm

Data collection

Rigaku Oxford Diffraction Xcalibur, AtlasS2, Gemini ultra diffractometer
Radiation source: X-ray tube
Graphite monochromator
Detector resolution: 5.1783 pixels mm^{-1}
ω scans
Absorption correction: analytical (CrysalisPro; Rigaku OD, 2015)
T_{min} = 0.958, T_{max} = 0.982
16215 measured reflections
4454 independent reflections
3284 reflections with $I > 3\sigma(I)$
R_{int} = 0.028
θ_{max} = 29.6°, θ_{min} = 3.6°
h = −11→8
k = −20→20
l = −37→37

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.107
S = 1.44
4454 reflections
227 parameters
0 restraints
80 constraints
H-atom parameters constrained
Weighting scheme based on measured s.u.'s $w = 1/(\sigma^2(I) + 0.0016I^2)$
$(\Delta/\sigma)_{max}$ = 0.0004
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Extinction correction: B-C type 1 Gaussian isotropic [Becker, P. J. & Coppens, P. (1974). *Acta Cryst.* A**30**, 129–147]
Extinction coefficient: 13000 (2000)

Special details

Refinement. All hydrogen atoms were discernible in difference Fourier maps and could be refined to reasonable geometry, but according to common practice they were refined as riding atoms with C—H = 0.96 Å and U_{iso}(H) = 1.2U_{eq}(C).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.34686 (10)	0.62710 (5)	0.13059 (3)	0.0193 (2)
O2	0.52510 (10)	0.49847 (5)	0.11100 (3)	0.0203 (2)
O3	0.64458 (13)	0.36127 (6)	0.27937 (3)	0.0385 (3)
C1	0.38844 (13)	0.57930 (7)	0.16975 (4)	0.0170 (3)
C2	0.48965 (13)	0.50922 (7)	0.15898 (4)	0.0170 (3)
C3	0.54565 (14)	0.45894 (7)	0.19596 (4)	0.0195 (3)
C4	0.50097 (14)	0.47681 (7)	0.24410 (4)	0.0205 (3)
C5	0.40159 (14)	0.54531 (8)	0.25426 (4)	0.0206 (3)
C6	0.34409 (14)	0.59647 (8)	0.21712 (4)	0.0198 (3)
C7	0.27297 (14)	0.70813 (7)	0.13914 (4)	0.0171 (3)
C8	0.32021 (13)	0.76454 (7)	0.09687 (4)	0.0178 (3)
C9	0.39897 (15)	0.73419 (8)	0.05577 (4)	0.0261 (4)
C10	0.43962 (18)	0.78854 (9)	0.01835 (5)	0.0326 (4)
C11	0.40310 (16)	0.87355 (9)	0.02180 (5)	0.0297 (4)
C12	0.32477 (15)	0.90430 (9)	0.06254 (5)	0.0261 (4)
C13	0.28374 (14)	0.85001 (8)	0.10003 (4)	0.0218 (4)
C14	0.08714 (14)	0.70028 (7)	0.14420 (4)	0.0177 (3)
C15	−0.00177 (15)	0.65479 (8)	0.11019 (5)	0.0256 (4)
C16	−0.17290 (16)	0.65229 (9)	0.11241 (5)	0.0322 (4)
C17	−0.25477 (16)	0.69522 (8)	0.14866 (5)	0.0298 (4)
C18	−0.16734 (15)	0.73910 (8)	0.18332 (5)	0.0250 (4)
C19	0.00414 (14)	0.74156 (7)	0.18104 (4)	0.0199 (3)
C20	0.63310 (15)	0.43012 (8)	0.09834 (4)	0.0245 (4)
C21	0.64587 (17)	0.42893 (9)	0.04403 (5)	0.0316 (4)
C22	0.55991 (16)	0.42412 (8)	0.28389 (5)	0.0275 (4)
H1c3	0.615307	0.411587	0.188954	0.0233*
H1c5	0.37214	0.557585	0.287186	0.0248*
H1c6	0.273891	0.643544	0.22428	0.0237*
H1c7	0.312056	0.732024	0.168939	0.0205*
H1c9	0.425323	0.675383	0.053266	0.0313*
H1c10	0.493341	0.767159	−0.010079	0.0391*
H1c11	0.432179	0.911071	−0.004095	0.0357*
H1c12	0.298754	0.963157	0.06492	0.0313*
H1c13	0.22977	0.871597	0.128373	0.0261*
H1c15	0.055107	0.624903	0.085003	0.0307*
H1c16	−0.23405	0.620772	0.088795	0.0386*
H1c17	−0.373047	0.694527	0.149741	0.0357*
H1c18	−0.224467	0.767824	0.208906	0.0301*
H1c19	0.065108	0.772039	0.205141	0.0239*
H1c20	0.586452	0.377955	0.10939	0.0294*
H2c20	0.740136	0.439896	0.112063	0.0294*
H1c21	0.719041	0.384571	0.034222	0.0379*
H2c21	0.538733	0.419448	0.030313	0.0379*
H3c21	0.687979	0.482033	0.032892	0.0379*
H1c22	0.529438	0.440345	0.316162	0.033*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0248 (4)	0.0172 (4)	0.0158 (4)	0.0056 (3)	−0.0024 (3)	0.0000 (3)
O2	0.0249 (4)	0.0180 (4)	0.0180 (4)	0.0037 (3)	0.0006 (3)	−0.0005 (3)
O3	0.0567 (6)	0.0310 (6)	0.0277 (5)	0.0151 (5)	−0.0056 (4)	0.0064 (4)
C1	0.0164 (5)	0.0162 (6)	0.0185 (6)	−0.0025 (5)	−0.0032 (4)	0.0020 (4)
C2	0.0181 (5)	0.0164 (6)	0.0165 (5)	−0.0037 (5)	−0.0010 (4)	−0.0009 (4)
C3	0.0207 (6)	0.0160 (6)	0.0217 (6)	−0.0001 (5)	−0.0018 (5)	0.0006 (4)
C4	0.0219 (6)	0.0190 (6)	0.0205 (6)	−0.0036 (5)	−0.0029 (5)	0.0032 (5)
C5	0.0220 (6)	0.0219 (6)	0.0180 (6)	−0.0037 (5)	−0.0007 (5)	0.0006 (5)
C6	0.0188 (5)	0.0197 (6)	0.0208 (6)	0.0006 (5)	0.0000 (4)	−0.0005 (5)
C7	0.0197 (6)	0.0151 (6)	0.0164 (5)	0.0019 (5)	−0.0028 (4)	−0.0022 (4)
C8	0.0143 (5)	0.0208 (6)	0.0182 (5)	−0.0004 (5)	−0.0042 (4)	0.0004 (4)
C9	0.0328 (7)	0.0224 (7)	0.0230 (6)	0.0036 (6)	0.0031 (5)	0.0003 (5)
C10	0.0405 (8)	0.0327 (8)	0.0245 (7)	0.0045 (6)	0.0101 (6)	0.0017 (6)
C11	0.0326 (7)	0.0299 (7)	0.0267 (7)	−0.0012 (6)	0.0039 (5)	0.0093 (6)
C12	0.0280 (6)	0.0200 (7)	0.0304 (7)	0.0006 (5)	−0.0002 (5)	0.0033 (5)
C13	0.0218 (6)	0.0211 (6)	0.0225 (6)	0.0012 (5)	0.0008 (5)	−0.0010 (5)
C14	0.0190 (5)	0.0145 (6)	0.0195 (6)	−0.0008 (5)	−0.0033 (4)	0.0050 (4)
C15	0.0268 (7)	0.0270 (7)	0.0230 (7)	−0.0037 (5)	−0.0032 (5)	−0.0009 (5)
C16	0.0279 (7)	0.0352 (8)	0.0335 (8)	−0.0112 (6)	−0.0109 (6)	0.0019 (6)
C17	0.0178 (6)	0.0313 (7)	0.0402 (7)	−0.0048 (6)	−0.0016 (5)	0.0120 (6)
C18	0.0234 (6)	0.0210 (6)	0.0307 (7)	0.0010 (5)	0.0053 (5)	0.0076 (5)
C19	0.0222 (6)	0.0167 (6)	0.0208 (6)	−0.0010 (5)	−0.0011 (5)	0.0029 (5)
C20	0.0256 (6)	0.0223 (6)	0.0257 (6)	0.0064 (5)	0.0022 (5)	−0.0009 (5)
C21	0.0347 (7)	0.0333 (8)	0.0267 (7)	0.0066 (6)	0.0065 (6)	−0.0034 (6)
C22	0.0347 (7)	0.0257 (7)	0.0221 (7)	0.0013 (6)	−0.0025 (5)	0.0035 (5)

Geometric parameters (Å, º)

O1—C1	1.3632 (13)	C11—C12	1.3813 (18)
O1—C7	1.4380 (13)	C11—H1c11	0.96
O2—C2	1.3662 (13)	C12—C13	1.3873 (18)
O2—C20	1.4377 (14)	C12—H1c12	0.96
O3—C22	1.2174 (16)	C13—H1c13	0.96
C1—C2	1.4142 (15)	C14—C15	1.3870 (17)
C1—C6	1.3838 (16)	C14—C19	1.3845 (16)
C2—C3	1.3736 (16)	C15—C16	1.3902 (18)
C3—C4	1.4067 (16)	C15—H1c15	0.96
C3—H1c3	0.96	C16—C17	1.3809 (19)
C4—C5	1.3821 (16)	C16—H1c16	0.96
C4—C22	1.4614 (17)	C17—C18	1.3807 (18)
C5—C6	1.3892 (16)	C17—H1c17	0.96
C5—H1c5	0.96	C18—C19	1.3931 (17)
C6—H1c6	0.96	C18—H1c18	0.96
C7—C8	1.5202 (16)	C19—H1c19	0.96
C7—C14	1.5192 (16)	C20—C21	1.5034 (17)

C7—H1c7	0.96	C20—H1c20	0.96
C8—C9	1.3885 (17)	C20—H2c20	0.96
C8—C13	1.3911 (17)	C21—H1c21	0.96
C9—C10	1.3865 (18)	C21—H2c21	0.96
C9—H1c9	0.96	C21—H3c21	0.96
C10—C11	1.3843 (19)	C22—H1c22	0.96
C10—H1c10	0.96		

C1—O1—C7	118.07 (8)	C11—C12—H1c12	120.04
C2—O2—C20	117.29 (9)	C13—C12—H1c12	120.04
O1—C1—C2	114.48 (9)	C8—C13—C12	120.52 (11)
O1—C1—C6	125.17 (10)	C8—C13—H1c13	119.74
C2—C1—C6	120.32 (10)	C12—C13—H1c13	119.74
O2—C2—C1	115.12 (9)	C7—C14—C15	119.76 (10)
O2—C2—C3	125.37 (10)	C7—C14—C19	120.76 (10)
C1—C2—C3	119.51 (10)	C15—C14—C19	119.40 (10)
C2—C3—C4	120.02 (10)	C14—C15—C16	120.29 (12)
C2—C3—H1c3	119.99	C14—C15—H1c15	119.86
C4—C3—H1c3	119.99	C16—C15—H1c15	119.86
C3—C4—C5	120.07 (11)	C15—C16—C17	119.88 (12)
C3—C4—C22	120.72 (11)	C15—C16—H1c16	120.06
C5—C4—C22	119.22 (11)	C17—C16—H1c16	120.06
C4—C5—C6	120.37 (11)	C16—C17—C18	120.30 (12)
C4—C5—H1c5	119.81	C16—C17—H1c17	119.85
C6—C5—H1c5	119.81	C18—C17—H1c17	119.85
C1—C6—C5	119.71 (11)	C17—C18—C19	119.70 (11)
C1—C6—H1c6	120.14	C17—C18—H1c18	120.15
C5—C6—H1c6	120.14	C19—C18—H1c18	120.15
O1—C7—C8	107.20 (8)	C14—C19—C18	120.39 (11)
O1—C7—C14	110.82 (9)	C14—C19—H1c19	119.8
O1—C7—H1c7	110.86	C18—C19—H1c19	119.8
C8—C7—C14	111.65 (9)	O2—C20—C21	107.10 (10)
C8—C7—H1c7	110.01	O2—C20—H1c20	109.47
C14—C7—H1c7	106.34	O2—C20—H2c20	109.47
C7—C8—C9	122.61 (10)	C21—C20—H1c20	109.47
C7—C8—C13	118.21 (10)	C21—C20—H2c20	109.47
C9—C8—C13	119.18 (11)	H1c20—C20—H2c20	111.74
C8—C9—C10	120.17 (12)	C20—C21—H1c21	109.47
C8—C9—H1c9	119.91	C20—C21—H2c21	109.47
C10—C9—H1c9	119.91	C20—C21—H3c21	109.47
C9—C10—C11	120.28 (12)	H1c21—C21—H2c21	109.47
C9—C10—H1c10	119.86	H1c21—C21—H3c21	109.47
C11—C10—H1c10	119.86	H2c21—C21—H3c21	109.47
C10—C11—C12	119.93 (12)	O3—C22—C4	125.21 (12)
C10—C11—H1c11	120.04	O3—C22—H1c22	117.39
C12—C11—H1c11	120.04	C4—C22—H1c22	117.4
C11—C12—C13	119.91 (12)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H1*c*7···O3^{i}	0.96	2.52	3.3794 (15)	148
C17—H1*c*17···O1^{ii}	0.96	2.57	3.4440 (15)	152
C18—H1*c*18···O3^{iii}	0.96	2.53	3.2906 (16)	136

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