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4-[(*E*)-(3-Chloro-4-methylphenyl)iminomethyl]-2-methoxy-3-nitrophenyl acetate

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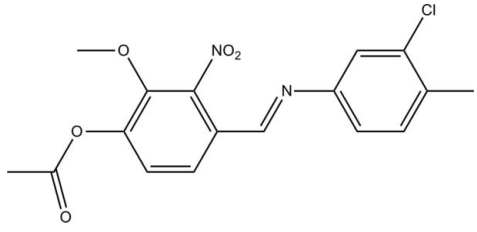
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.045; wR factor = 0.122; data-to-parameter ratio = 13.5.

The title compound, $C_{17}H_{15}ClN_2O_5$, displays a *trans*-configuration with respect to the C=N double bond. The molecule is twisted, the dihedral angle between the mean planes of the two benzene rings being 18.70 (12)°. The nitro, methoxy and acetyl groups are oriented at 80.70 (11), 35.2 (2) and 72.35 (10)°, respectively, to the benzene ring to which they are bonded. The crystal structure is stabilized by weak C—H···O hydrogen-bonding contacts.

Related literature

For background to Schiff bases in coordination chemistry, see: Bhatia *et al.* (1981); Costamagna *et al.* (1992). For a related structure, see: Qian & Liu (2010).



Experimental

Crystal data

$C_{17}H_{15}ClN_2O_5$ M_r = 362.76
Triclinic, $P\overline{1}$
a = 7.035 (6) Å
b = 7.672 (6) Å
c = 17.272 (14) Å
α = 83.477 (8)°
β = 84.994 (8)°
γ = 66.697 (7)°
V = 849.7 (12) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.26 mm^{-1}
T = 296 K
0.26 × 0.23 × 0.21 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.936, T_{max} = 0.948
5579 measured reflections
3083 independent reflections
2207 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.122
S = 1.05
3083 reflections
229 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12···O1^{i}	0.93	2.58	3.431 (3)	153

Symmetry code: (i) $x+1, y-1, z$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2498).

References

Bhatia, S. C., Bindlish, J. M., Saini, A. R. & Jain, P. C. (1981). *J. Chem. Soc. Dalton Trans.* pp. 1773–1779.
Bruker (2004). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Costamagna, J., Vargas, J., Latorre, R., Alvarado, A. & Mena, G. (1992). *Coord. Chem. Rev.* **119**, 67–88.
Qian, S.-S. & Liu, T. (2010). *Acta Cryst.* E**66**, o18.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2012). E**68**, o303 [doi:10.1107/S1600536811055590]

4-[(*E*)-(3-Chloro-4-methylphenyl)iminomethyl]-2-methoxy-3-nitrophenyl acetate

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S1. Comment

Schiff bases play an important role in the development of coordination chemistry related to catalysis and enzymatic reactions, magnetism and molecular architectures (Costamagna *et al.*, 1992; Bhatia *et al.*, 1981). As an extension of work on the structural characterization of Schiff base compounds, we report the synthesis and crystal structure of the title compound in this article.

The title compound (Fig. 1) assumes an E conformation about the C═N double bond. The molecule is twisted, with the dihedral angle between the two benzene rings being 18.70 (12)°. The nitro (N2/O1/O2), methoxy (O3/C15) and ethanone (O4/O5/C16/C17) groups are oriented with respect to the benzene ring (C8–C13) to which they are bonded, at 80.70 (11), 35.2 (2) and 72.35 (10) °, respectively. The crystal structure is stabilized by π-π interactions [centroid-centroid distance = 3.886 (4) Å] and weak C12—H12···O1 hydrogen bonding contacts.

The bond lengths and bond angles in the title compound are comparable to the corresponding bond lengths and bond angles observed in a closely related compound (Qian & Liu, 2010).

S2. Experimental

4-Formyl-2-methoxy-3-nitrophenyl acetate (0.0995 g) and 3-chloro-4-methylaniline (0.0706 g) were dissolved in methanol (20 mL). The mixture was stirred at room temperature for 45 mins to give a clear solution. The solution was allowed to stand in the air for 3 days. Yellow block-shaped single crystals of the title compound suitable for X-ray diffraction analysis were obtained at the bottom of the vessel.

S3. Refinement

All H atoms were placed in geometrical positions and constrained to ride on their parent atoms with C—H distances in the range 0.93–0.96 Å, in a riding mode, with U_{iso}(H) = kU_{eq}(C), where k = 1.5 for methyl and 1.2 for all other H atoms.

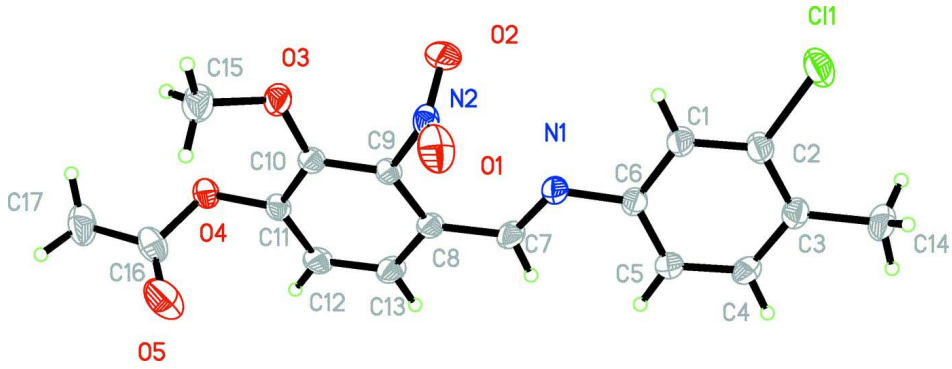

Figure 1

The structure of the title molecule showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

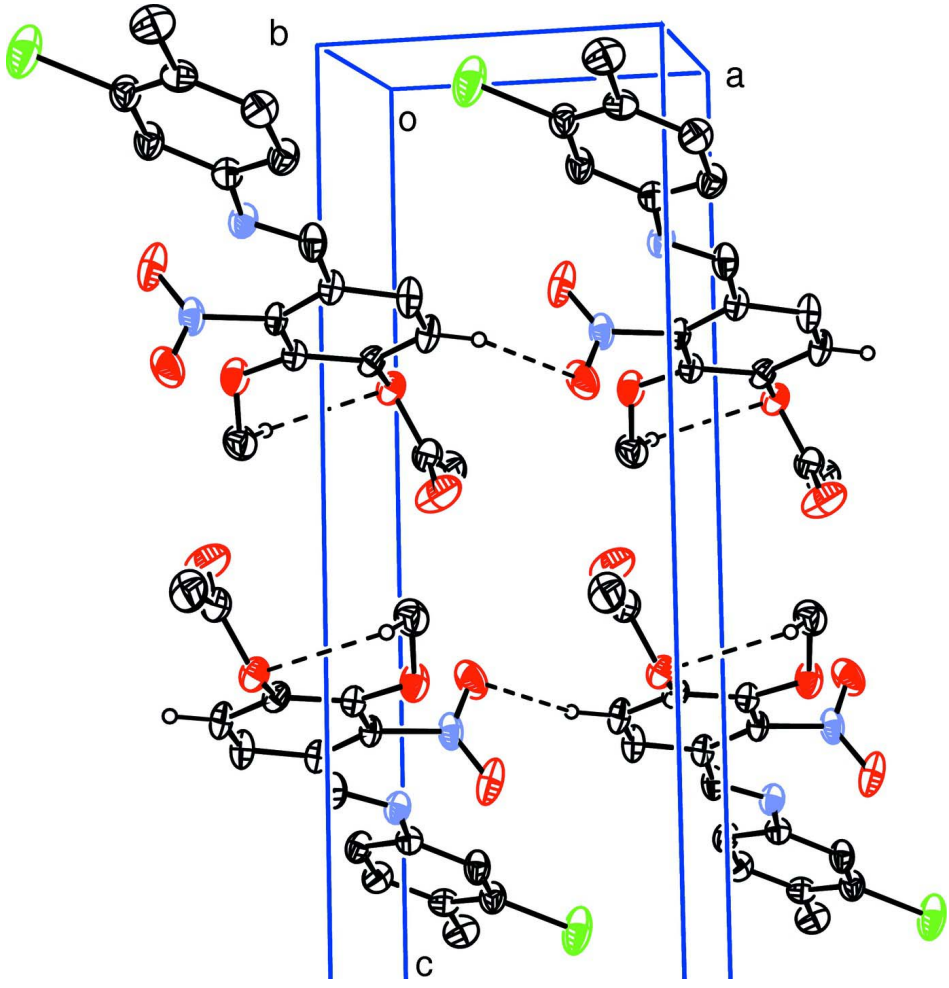

Figure 2

The packing diagram for the title compound; hydrogen-bonding interactions are represented by dashed lines.

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$\beta = 84.994$ (8)°
$\gamma = 66.697$ (7)°
$V = 849.7$ (12) Å^3
$Z = 2$
$F(000) = 376$
$D_x = 1.418$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3083 reflections
$\theta = 2.4$–25.5°
$\mu = 0.26$ mm^{-1}
$T = 296$ K
Block, yellow
0.26 × 0.23 × 0.21 mm

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Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
$T_{min} = 0.936$, $T_{max} = 0.948$
5579 measured reflections
3083 independent reflections
2207 reflections with $I > 2\sigma(I)$
$R_{int} = 0.022$
$\theta_{max} = 25.5°$, $\theta_{min} = 2.4°$
$h = -8 \rightarrow 8$
$k = -9 \rightarrow 9$
$l = -20 \rightarrow 17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.122$
$S = 1.05$
3083 reflections
229 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
$w = 1/[\sigma^2(F_o^2) + (0.0433P)^2 + 0.4254P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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}
Cl1	−0.50222 (11)	1.23475 (11)	0.05852 (6)	0.0880 (3)
O1	−0.3219 (3)	0.5157 (3)	0.34263 (13)	0.0728 (6)
O2	−0.3928 (3)	0.4212 (3)	0.23925 (14)	0.0733 (6)

O3	−0.2466 (2)	0.0650 (2)	0.34480 (11)	0.0563 (5)
O4	0.1492 (2)	−0.2520 (2)	0.35298 (10)	0.0472 (4)
O5	0.2885 (4)	−0.2451 (3)	0.46343 (13)	0.0891 (8)
N1	−0.0690 (3)	0.6082 (3)	0.20244 (12)	0.0450 (5)
N2	−0.2784 (3)	0.4109 (3)	0.28994 (14)	0.0490 (5)
C1	−0.2521 (3)	0.9075 (3)	0.13350 (15)	0.0491 (6)
H1	−0.3684	0.8771	0.1395	0.059*
C2	−0.2654 (4)	1.0797 (3)	0.09522 (15)	0.0491 (6)
C3	−0.0985 (4)	1.1342 (3)	0.08453 (14)	0.0459 (6)
C4	0.0867 (4)	1.0021 (4)	0.11302 (15)	0.0510 (6)
H4	0.2035	1.0317	0.1061	0.061*
C5	0.1053 (4)	0.8288 (3)	0.15121 (15)	0.0472 (6)
H5	0.2328	0.7443	0.1692	0.057*
C6	−0.0665 (3)	0.7799 (3)	0.16295 (13)	0.0405 (5)
C7	0.0954 (3)	0.4730 (3)	0.22155 (15)	0.0469 (6)
H7	0.2197	0.4885	0.2100	0.056*
C8	0.1029 (3)	0.2917 (3)	0.26103 (14)	0.0411 (5)
C9	−0.0705 (3)	0.2553 (3)	0.29035 (13)	0.0377 (5)
C10	−0.0619 (3)	0.0795 (3)	0.32370 (13)	0.0390 (5)
C11	0.1336 (3)	−0.0677 (3)	0.32809 (14)	0.0404 (5)
C12	0.3094 (3)	−0.0359 (3)	0.30170 (15)	0.0492 (6)
H12	0.4389	−0.1349	0.3063	0.059*
C13	0.2947 (3)	0.1401 (3)	0.26888 (16)	0.0505 (6)
H13	0.4148	0.1587	0.2515	0.061*
C14	−0.1131 (5)	1.3253 (4)	0.04590 (17)	0.0626 (8)
H14A	0.0227	1.3280	0.0397	0.094*
H14B	−0.2006	1.4239	0.0778	0.094*
H14C	−0.1706	1.3456	−0.0043	0.094*
C15	−0.2664 (4)	−0.0543 (4)	0.41121 (17)	0.0644 (8)
H15A	−0.2223	−0.1825	0.3972	0.097*
H15B	−0.4086	−0.0101	0.4301	0.097*
H15C	−0.1817	−0.0511	0.4513	0.097*
C16	0.2390 (4)	−0.3320 (4)	0.42227 (17)	0.0568 (7)
C17	0.2612 (5)	−0.5342 (4)	0.43672 (19)	0.0748 (9)
H17A	0.2924	−0.5781	0.4902	0.112*
H17B	0.3714	−0.6114	0.4033	0.112*
H17C	0.1340	−0.5434	0.4260	0.112*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0514 (4)	0.0650 (5)	0.1311 (8)	−0.0151 (3)	−0.0205 (4)	0.0421 (5)
O1	0.0657 (13)	0.0466 (11)	0.0789 (15)	0.0036 (9)	0.0188 (11)	−0.0090 (11)
O2	0.0380 (10)	0.0623 (12)	0.1146 (18)	−0.0145 (9)	−0.0277 (11)	0.0122 (11)
O3	0.0386 (9)	0.0504 (10)	0.0747 (13)	−0.0175 (8)	−0.0028 (8)	0.0165 (9)
O4	0.0476 (9)	0.0301 (8)	0.0579 (11)	−0.0087 (7)	−0.0108 (8)	0.0025 (7)
O5	0.121 (2)	0.0643 (14)	0.0713 (15)	−0.0178 (13)	−0.0387 (14)	−0.0035 (11)
N1	0.0378 (10)	0.0385 (11)	0.0580 (13)	−0.0158 (8)	−0.0069 (9)	0.0048 (9)

N2	0.0326 (10)	0.0328 (11)	0.0714 (15)	−0.0065 (8)	0.0028 (11)	0.0088 (11)
C1	0.0351 (12)	0.0438 (14)	0.0662 (17)	−0.0165 (10)	−0.0007 (11)	0.0069 (12)
C2	0.0408 (13)	0.0429 (14)	0.0576 (16)	−0.0130 (10)	−0.0023 (11)	0.0067 (12)
C3	0.0551 (14)	0.0434 (13)	0.0429 (14)	−0.0247 (11)	−0.0005 (11)	0.0003 (11)
C4	0.0502 (14)	0.0562 (15)	0.0571 (16)	−0.0331 (12)	−0.0053 (12)	0.0024 (12)
C5	0.0400 (12)	0.0464 (14)	0.0578 (15)	−0.0200 (11)	−0.0085 (11)	0.0024 (12)
C6	0.0407 (12)	0.0370 (12)	0.0444 (13)	−0.0168 (10)	−0.0012 (10)	−0.0007 (10)
C7	0.0319 (12)	0.0392 (13)	0.0702 (17)	−0.0153 (10)	−0.0014 (11)	−0.0024 (12)
C8	0.0311 (11)	0.0332 (12)	0.0575 (15)	−0.0103 (9)	−0.0066 (10)	−0.0031 (10)
C9	0.0276 (10)	0.0284 (11)	0.0510 (14)	−0.0039 (8)	−0.0048 (10)	−0.0025 (10)
C10	0.0319 (11)	0.0354 (12)	0.0474 (14)	−0.0105 (9)	−0.0040 (10)	−0.0023 (10)
C11	0.0423 (12)	0.0276 (11)	0.0478 (14)	−0.0087 (9)	−0.0110 (10)	−0.0014 (10)
C12	0.0313 (12)	0.0365 (13)	0.0714 (17)	−0.0030 (10)	−0.0127 (11)	−0.0022 (12)
C13	0.0290 (11)	0.0395 (13)	0.0805 (19)	−0.0104 (10)	−0.0060 (11)	−0.0035 (12)
C14	0.0789 (19)	0.0525 (16)	0.0637 (18)	−0.0371 (15)	−0.0055 (15)	0.0103 (14)
C15	0.0564 (16)	0.0651 (18)	0.0666 (19)	−0.0235 (14)	0.0067 (14)	0.0065 (15)
C16	0.0533 (15)	0.0428 (15)	0.0562 (17)	−0.0006 (12)	−0.0052 (13)	0.0015 (13)
C17	0.0739 (19)	0.0481 (16)	0.084 (2)	−0.0107 (14)	−0.0018 (16)	0.0189 (15)

Geometric parameters (Å, º)

Cl1—C2	1.743 (3)	C7—C8	1.461 (3)
O1—N2	1.221 (3)	C7—H7	0.9300
O2—N2	1.215 (3)	C8—C13	1.395 (3)
O3—C10	1.362 (3)	C8—C9	1.397 (3)
O3—C15	1.417 (3)	C9—C10	1.386 (3)
O4—C16	1.366 (3)	C10—C11	1.394 (3)
O4—C11	1.394 (3)	C11—C12	1.382 (3)
O5—C16	1.186 (3)	C12—C13	1.372 (3)
N1—C7	1.250 (3)	C12—H12	0.9300
N1—C6	1.419 (3)	C13—H13	0.9300
N2—C9	1.478 (3)	C14—H14A	0.9600
C1—C2	1.381 (3)	C14—H14B	0.9600
C1—C6	1.383 (3)	C14—H14C	0.9600
C1—H1	0.9300	C15—H15A	0.9600
C2—C3	1.386 (4)	C15—H15B	0.9600
C3—C4	1.386 (3)	C15—H15C	0.9600
C3—C14	1.508 (3)	C16—C17	1.490 (4)
C4—C5	1.378 (3)	C17—H17A	0.9600
C4—H4	0.9300	C17—H17B	0.9600
C5—C6	1.393 (3)	C17—H17C	0.9600
C5—H5	0.9300		
C10—O3—C15	120.89 (19)	O3—C10—C9	116.62 (18)
C16—O4—C11	117.65 (19)	O3—C10—C11	126.4 (2)
C7—N1—C6	121.1 (2)	C9—C10—C11	116.9 (2)
O2—N2—O1	125.6 (2)	C12—C11—C10	120.7 (2)
O2—N2—C9	118.1 (2)	C12—C11—O4	119.86 (19)

O1—N2—C9	116.3 (2)	C10—C11—O4	119.2 (2)
C2—C1—C6	120.3 (2)	C13—C12—C11	120.7 (2)
C2—C1—H1	119.9	C13—C12—H12	119.6
C6—C1—H1	119.9	C11—C12—H12	119.6
C1—C2—C3	122.8 (2)	C12—C13—C8	121.2 (2)
C1—C2—Cl1	118.53 (19)	C12—C13—H13	119.4
C3—C2—Cl1	118.66 (19)	C8—C13—H13	119.4
C4—C3—C2	115.7 (2)	C3—C14—H14A	109.5
C4—C3—C14	120.9 (2)	C3—C14—H14B	109.5
C2—C3—C14	123.4 (2)	H14A—C14—H14B	109.5
C5—C4—C3	122.8 (2)	C3—C14—H14C	109.5
C5—C4—H4	118.6	H14A—C14—H14C	109.5
C3—C4—H4	118.6	H14B—C14—H14C	109.5
C4—C5—C6	120.2 (2)	O3—C15—H15A	109.5
C4—C5—H5	119.9	O3—C15—H15B	109.5
C6—C5—H5	119.9	H15A—C15—H15B	109.5
C1—C6—C5	118.1 (2)	O3—C15—H15C	109.5
C1—C6—N1	116.1 (2)	H15A—C15—H15C	109.5
C5—C6—N1	125.7 (2)	H15B—C15—H15C	109.5
N1—C7—C8	123.6 (2)	O5—C16—O4	122.1 (3)
N1—C7—H7	118.2	O5—C16—C17	127.0 (3)
C8—C7—H7	118.2	O4—C16—C17	110.9 (3)
C13—C8—C9	116.4 (2)	C16—C17—H17A	109.5
C13—C8—C7	118.9 (2)	C16—C17—H17B	109.5
C9—C8—C7	124.71 (19)	H17A—C17—H17B	109.5
C10—C9—C8	124.07 (18)	C16—C17—H17C	109.5
C10—C9—N2	115.70 (19)	H17A—C17—H17C	109.5
C8—C9—N2	120.18 (19)	H17B—C17—H17C	109.5

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15*A*···O4	0.96	2.52	2.861 (4)	101
C12—H12···O1^{i}	0.93	2.58	3.431 (3)	153

Symmetry code: (i) *x*+1, *y*−1, *z*.