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2-(3,4-Dimethoxyphenyl)-3-hydroxybut-2-enenitrile

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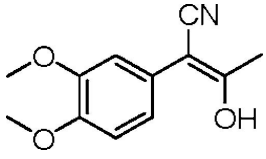
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.002 Å; R factor = 0.046; wR factor = 0.147; data-to-parameter ratio = 14.9.

The title compound, $C_{12}H_{13}NO_3$, adopts its enol tautomeric form and crystallizes with two molecules in the asymmetric unit, with similar conformations. In the crystal structure, molecules interact *via* O—H···N hydrogen bonds, leading to infinite chains.

Related literature

For background literature, see: Jung *et al.* (2002); Kumar *et al.* (2005).



Experimental

Crystal data

$C_{12}H_{13}NO_3$
M_r = 219.23
Triclinic, $P\overline{1}$
a = 8.5316 (13) Å
b = 11.1801 (17) Å
c = 11.8021 (18) Å
α = 82.777 (3)°
β = 81.232 (2)°
γ = 85.712 (3)°
V = 1102.0 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 294 (2) K
0.26 × 0.24 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.976, T_{max} = 0.981
6372 measured reflections
4428 independent reflections
3078 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.147
S = 1.03
4428 reflections
297 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N2^{i}	0.91 (2)	1.93 (2)	2.835 (2)	173.7 (19)
O4—H4···N1^{ii}	0.91 (2)	1.89 (2)	2.793 (2)	174.3 (19)

Symmetry codes: (i) $-x, -y+1, -z+1$; (ii) $-x+1, -y+1, -z$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); 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: HB2405).

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supplementary materials

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2-(3,4-Dimethoxyphenyl)-3-hydroxybut-2-enenitrile

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Comment

5-Aminopyrazoles posses many biological properties such as antibacterial (Kumar *et al.*, 2005) and herbicidal activities (Jung *et al.*, (2002). They can be prepared from substituted acetonitriles reacting with substituted hydrazines.

The title compound, (I), (Fig. 1) was obtained as part of our studies in this area and the X-ray analysis reveals that (I) is a enol with a conjugated system. There are two molecules in the asymmetric unit and intermolecular O—H···N hydrogen bonds (Table 1) help to stablize the crystal packing.

Experimental

A mixture of 2-(3,4-dimethoxyphenyl)acetonitrile (1.77 g, 10 mmol), 3,4,5-trimethoxybenzaldehyde (0.88 g, 10 mmol), and NaOEt (0.68 g, 10 mmol) in ethanol (5 ml) was stirred at room temperature and monitored by TLC. After completion of the reaction, 2 ml water was added and evaporated *in vacuo*. the product was purified through flash column chromatography and 50 mg of the title compound was dissolved in 100 ml absolute methanol and crystals suitable for X-ray analysis were grown by slow evaporation over a period of 15 d.

Refinement

The O-bound H atoms were located in difference maps and their positions were freely refined with U_{iso}(H) = 1.2U_{eq}(O).

The C-bound H atoms were positioned geometrically (C—H = 0.93–0.96 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Figures

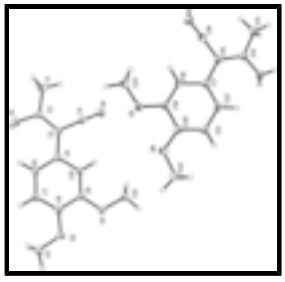

Fig. 1. The molecular structure of (I), drawn with 30% probability ellipsoids (arbitrary spheres for the H atoms).

Fig. 2. The reaction scheme for the formation of (I).

2-(3,4-Dimethoxyphenyl)-3-hydroxybut-2-enenitrile

Crystal data

$C_{12}H_{13}NO_3$	$Z = 4$
$M_r = 219.23$	$F_{000} = 464$
Triclinic, $P\overline{1}$	$D_x = 1.321$ Mg m^{-3}
Hall symbol: -P 1	Melting point: 478-480 K
$a = 8.5316$ (13) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 11.1801$ (17) Å	Cell parameters from 2572 reflections
$c = 11.8021$ (18) Å	$\theta = 2.4$–26.2º
$\alpha = 82.777$ (3)º	$\mu = 0.10$ mm^{-1}
$\beta = 81.232$ (2)º	$T = 294$ (2) K
$\gamma = 85.712$ (3)º	Prism, orange
$V = 1102.0$ (3) Å^3	0.26 × 0.24 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer	4428 independent reflections
Radiation source: fine-focus sealed tube	3078 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.017$
$T = 294$(2) K	$\theta_{max} = 26.4$º
φ and ω scans	$\theta_{min} = 1.8$º
Absorption correction: multi-scan (SADABS; Bruker, 1997)	$h = -10 \rightarrow 10$
$T_{min} = 0.976$, $T_{max} = 0.981$	$k = -13 \rightarrow 9$
6372 measured reflections	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0789P)^2 + 0.2254P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.046$	$(\Delta/\sigma)_{max} = 0.003$
$wR(F^2) = 0.147$	$\Delta\rho_{max} = 0.43$ e Å^{-3}
$S = 1.03$	$\Delta\rho_{min} = -0.39$ e Å^{-3}
4428 reflections	Extinction correction: SHELXL97
297 parameters	Extinction coefficient: 0.019 (3)
Hydrogen site location: inferred from neighbouring sites	

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 $F^2 > 2\text{sigma}(F^2)$ 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}
C1	−0.0117 (2)	0.27079 (18)	0.68305 (17)	0.0500 (5)
H1A	−0.0933	0.2146	0.6899	0.075*
H1B	0.0173	0.3008	0.6033	0.075*
H1C	−0.0503	0.3369	0.7262	0.075*
C2	0.13047 (19)	0.20862 (15)	0.72932 (14)	0.0367 (4)
C3	0.27142 (19)	0.18544 (15)	0.66240 (13)	0.0348 (4)
C4	0.27460 (19)	0.22417 (16)	0.54200 (15)	0.0415 (4)
C5	0.42067 (18)	0.12585 (14)	0.69735 (13)	0.0340 (4)
C6	0.4403 (2)	0.08622 (16)	0.81096 (14)	0.0435 (4)
H6	0.3560	0.0959	0.8697	0.052*
C7	0.5842 (2)	0.03238 (17)	0.83791 (15)	0.0459 (4)
H7	0.5942	0.0061	0.9146	0.055*
C8	0.71225 (19)	0.01707 (16)	0.75376 (14)	0.0408 (4)
C9	0.69499 (19)	0.05794 (15)	0.63854 (14)	0.0380 (4)
C10	0.55151 (18)	0.11012 (14)	0.61176 (13)	0.0363 (4)
H10	0.5412	0.1355	0.5350	0.044*
C11	0.8792 (2)	−0.07909 (19)	0.88671 (16)	0.0570 (5)
H11A	0.8578	−0.0153	0.9352	0.086*
H11B	0.9864	−0.1115	0.8881	0.086*
H11C	0.8071	−0.1417	0.9145	0.086*
C12	0.8223 (2)	0.09421 (19)	0.44412 (15)	0.0545 (5)
H12A	0.7447	0.0550	0.4131	0.082*
H12B	0.9246	0.0827	0.3989	0.082*
H12C	0.7933	0.1790	0.4421	0.082*
N1	0.27990 (19)	0.25311 (16)	0.44499 (14)	0.0607 (5)
O1	0.11331 (15)	0.17462 (12)	0.84264 (10)	0.0505 (3)
H1	0.015 (3)	0.1997 (17)	0.8758 (18)	0.061*
O2	0.85876 (14)	−0.03284 (12)	0.77157 (10)	0.0549 (4)
O3	0.82865 (14)	0.04373 (12)	0.56009 (10)	0.0519 (4)
C13	0.4089 (2)	0.77590 (16)	−0.23875 (14)	0.0442 (4)
H13A	0.4517	0.8497	−0.2774	0.066*
H13B	0.3063	0.7933	−0.1962	0.066*
H13C	0.3989	0.7227	−0.2947	0.066*

C14	0.51762 (19)	0.71690 (15)	−0.15769 (14)	0.0361 (4)
C15	0.47497 (18)	0.69111 (15)	−0.04146 (13)	0.0347 (4)
C16	0.3143 (2)	0.72645 (16)	0.00098 (14)	0.0416 (4)
C17	0.57160 (19)	0.62988 (14)	0.04565 (13)	0.0340 (4)
C18	0.50094 (19)	0.61017 (14)	0.16094 (13)	0.0366 (4)
H18	0.3956	0.6370	0.1807	0.044*
C19	0.58282 (19)	0.55206 (15)	0.24623 (13)	0.0377 (4)
C20	0.74174 (19)	0.51091 (15)	0.21806 (14)	0.0378 (4)
C21	0.8120 (2)	0.53047 (17)	0.10525 (15)	0.0476 (5)
H21	0.9174	0.5040	0.0855	0.057*
C22	0.7286 (2)	0.58899 (17)	0.01980 (15)	0.0458 (5)
H22	0.7793	0.6009	−0.0560	0.055*
C23	0.3598 (2)	0.56599 (19)	0.39341 (16)	0.0517 (5)
H23A	0.3456	0.6518	0.3748	0.078*
H23B	0.3316	0.5452	0.4750	0.078*
H23C	0.2932	0.5262	0.3530	0.078*
C24	0.9679 (2)	0.39793 (19)	0.28011 (18)	0.0584 (5)
H24A	0.9636	0.3387	0.2286	0.088*
H24B	1.0046	0.3595	0.3494	0.088*
H24C	1.0396	0.4581	0.2435	0.088*
N2	0.18624 (19)	0.75399 (16)	0.03788 (14)	0.0599 (5)
O4	0.66561 (14)	0.68852 (12)	−0.20565 (11)	0.0493 (3)
H4	0.678 (2)	0.7112 (17)	−0.2832 (19)	0.059*
O5	0.52107 (14)	0.52857 (13)	0.35992 (10)	0.0561 (4)
O6	0.81370 (14)	0.45353 (12)	0.30797 (10)	0.0516 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0338 (9)	0.0654 (12)	0.0469 (11)	0.0104 (8)	−0.0044 (8)	−0.0008 (9)
C2	0.0340 (9)	0.0433 (9)	0.0302 (9)	0.0032 (7)	−0.0028 (7)	0.0003 (7)
C3	0.0313 (8)	0.0427 (9)	0.0279 (8)	0.0034 (7)	−0.0019 (7)	−0.0009 (7)
C4	0.0308 (9)	0.0561 (11)	0.0336 (10)	0.0085 (7)	−0.0025 (7)	0.0004 (8)
C5	0.0309 (8)	0.0402 (9)	0.0289 (8)	0.0021 (7)	−0.0022 (7)	−0.0014 (6)
C6	0.0335 (9)	0.0630 (11)	0.0296 (9)	0.0084 (8)	0.0002 (7)	−0.0006 (8)
C7	0.0425 (10)	0.0656 (12)	0.0261 (9)	0.0059 (8)	−0.0057 (7)	0.0041 (8)
C8	0.0326 (9)	0.0536 (10)	0.0337 (9)	0.0051 (7)	−0.0071 (7)	0.0031 (7)
C9	0.0290 (8)	0.0507 (10)	0.0307 (9)	0.0042 (7)	0.0006 (7)	−0.0005 (7)
C10	0.0335 (9)	0.0489 (10)	0.0231 (8)	0.0047 (7)	−0.0020 (7)	0.0017 (7)
C11	0.0497 (11)	0.0770 (14)	0.0410 (11)	0.0142 (10)	−0.0170 (9)	0.0082 (9)
C12	0.0423 (10)	0.0804 (14)	0.0328 (10)	0.0138 (9)	0.0017 (8)	0.0055 (9)
N1	0.0502 (10)	0.0902 (13)	0.0336 (9)	0.0182 (9)	−0.0030 (7)	0.0076 (8)
O1	0.0365 (7)	0.0771 (9)	0.0312 (7)	0.0129 (6)	0.0028 (5)	0.0012 (6)
O2	0.0359 (7)	0.0865 (10)	0.0362 (7)	0.0166 (6)	−0.0078 (5)	0.0080 (6)
O3	0.0327 (7)	0.0836 (9)	0.0312 (7)	0.0171 (6)	0.0006 (5)	0.0070 (6)
C13	0.0428 (10)	0.0577 (11)	0.0293 (9)	0.0046 (8)	−0.0080 (7)	0.0054 (7)
C14	0.0335 (9)	0.0447 (9)	0.0283 (8)	0.0032 (7)	−0.0048 (7)	0.0002 (7)
C15	0.0306 (8)	0.0442 (9)	0.0266 (8)	0.0046 (7)	−0.0030 (6)	0.0006 (7)

C16	0.0402 (10)	0.0548 (11)	0.0264 (9)	0.0104 (8)	−0.0056 (7)	0.0014 (7)
C17	0.0331 (8)	0.0408 (9)	0.0261 (8)	0.0025 (7)	−0.0033 (6)	−0.0004 (6)
C18	0.0298 (8)	0.0492 (10)	0.0272 (8)	0.0083 (7)	−0.0015 (7)	0.0000 (7)
C19	0.0350 (9)	0.0516 (10)	0.0241 (8)	0.0035 (7)	−0.0026 (7)	−0.0005 (7)
C20	0.0318 (8)	0.0510 (10)	0.0287 (8)	0.0047 (7)	−0.0074 (7)	0.0022 (7)
C21	0.0297 (9)	0.0719 (12)	0.0356 (10)	0.0119 (8)	−0.0009 (7)	0.0018 (8)
C22	0.0347 (9)	0.0694 (12)	0.0269 (9)	0.0095 (8)	0.0013 (7)	0.0052 (8)
C23	0.0391 (10)	0.0775 (13)	0.0313 (9)	0.0137 (9)	0.0012 (8)	0.0041 (8)
C24	0.0365 (10)	0.0782 (14)	0.0547 (12)	0.0152 (9)	−0.0115 (9)	0.0097 (10)
N2	0.0429 (9)	0.0914 (13)	0.0384 (9)	0.0233 (8)	−0.0026 (7)	−0.0009 (8)
O4	0.0370 (7)	0.0786 (9)	0.0244 (6)	0.0107 (6)	0.0021 (5)	0.0080 (6)
O5	0.0376 (7)	0.0963 (10)	0.0253 (6)	0.0189 (6)	0.0001 (5)	0.0099 (6)
O6	0.0355 (7)	0.0800 (9)	0.0339 (7)	0.0143 (6)	−0.0086 (5)	0.0081 (6)

Geometric parameters (Å, °)

C1—C2	1.494 (2)	C13—C14	1.494 (2)
C1—H1A	0.9600	C13—H13A	0.9600
C1—H1B	0.9600	C13—H13B	0.9600
C1—H1C	0.9600	C13—H13C	0.9600
C2—O1	1.3325 (19)	C14—O4	1.3352 (19)
C2—C3	1.361 (2)	C14—C15	1.364 (2)
C3—C4	1.429 (2)	C15—C16	1.431 (2)
C3—C5	1.483 (2)	C15—C17	1.484 (2)
C4—N1	1.145 (2)	C16—N2	1.147 (2)
C5—C6	1.389 (2)	C17—C22	1.384 (2)
C5—C10	1.403 (2)	C17—C18	1.399 (2)
C6—C7	1.390 (2)	C18—C19	1.380 (2)
C6—H6	0.9300	C18—H18	0.9300
C7—C8	1.376 (2)	C19—O5	1.365 (2)
C7—H7	0.9300	C19—C20	1.403 (2)
C8—O2	1.3654 (19)	C20—O6	1.3722 (19)
C8—C9	1.405 (2)	C20—C21	1.372 (2)
C9—O3	1.3678 (19)	C21—C22	1.390 (2)
C9—C10	1.380 (2)	C21—H21	0.9300
C10—H10	0.9300	C22—H22	0.9300
C11—O2	1.424 (2)	C23—O5	1.419 (2)
C11—H11A	0.9600	C23—H23A	0.9600
C11—H11B	0.9600	C23—H23B	0.9600
C11—H11C	0.9600	C23—H23C	0.9600
C12—O3	1.421 (2)	C24—O6	1.422 (2)
C12—H12A	0.9600	C24—H24A	0.9600
C12—H12B	0.9600	C24—H24B	0.9600
C12—H12C	0.9600	C24—H24C	0.9600
O1—H1	0.91 (2)	O4—H4	0.91 (2)
C2—C1—H1A	109.5	C14—C13—H13A	109.5
C2—C1—H1B	109.5	C14—C13—H13B	109.5
H1A—C1—H1B	109.5	H13A—C13—H13B	109.5
C2—C1—H1C	109.5	C14—C13—H13C	109.5

H1A—C1—H1C	109.5	H13A—C13—H13C	109.5
H1B—C1—H1C	109.5	H13B—C13—H13C	109.5
O1—C2—C3	120.05 (15)	O4—C14—C15	119.68 (14)
O1—C2—C1	116.31 (15)	O4—C14—C13	115.77 (14)
C3—C2—C1	123.64 (15)	C15—C14—C13	124.55 (15)
C2—C3—C4	114.95 (14)	C14—C15—C16	115.05 (14)
C2—C3—C5	128.93 (15)	C14—C15—C17	128.79 (15)
C4—C3—C5	116.11 (14)	C16—C15—C17	116.15 (14)
N1—C4—C3	178.38 (19)	N2—C16—C15	178.22 (18)
C6—C5—C10	117.49 (14)	C22—C17—C18	117.27 (14)
C6—C5—C3	123.81 (14)	C22—C17—C15	123.91 (14)
C10—C5—C3	118.69 (14)	C18—C17—C15	118.81 (14)
C5—C6—C7	120.86 (16)	C19—C18—C17	121.97 (14)
C5—C6—H6	119.6	C19—C18—H18	119.0
C7—C6—H6	119.6	C17—C18—H18	119.0
C8—C7—C6	121.50 (16)	O5—C19—C18	125.13 (14)
C8—C7—H7	119.3	O5—C19—C20	115.04 (14)
C6—C7—H7	119.3	C18—C19—C20	119.82 (15)
O2—C8—C7	125.90 (15)	O6—C20—C21	125.57 (15)
O2—C8—C9	115.71 (14)	O6—C20—C19	115.94 (14)
C7—C8—C9	118.37 (15)	C21—C20—C19	118.49 (14)
O3—C9—C10	124.74 (15)	C20—C21—C22	121.35 (16)
O3—C9—C8	115.17 (14)	C20—C21—H21	119.3
C10—C9—C8	120.07 (15)	C22—C21—H21	119.3
C9—C10—C5	121.70 (15)	C17—C22—C21	121.10 (16)
C9—C10—H10	119.2	C17—C22—H22	119.5
C5—C10—H10	119.2	C21—C22—H22	119.5
O2—C11—H11A	109.5	O5—C23—H23A	109.5
O2—C11—H11B	109.5	O5—C23—H23B	109.5
H11A—C11—H11B	109.5	H23A—C23—H23B	109.5
O2—C11—H11C	109.5	O5—C23—H23C	109.5
H11A—C11—H11C	109.5	H23A—C23—H23C	109.5
H11B—C11—H11C	109.5	H23B—C23—H23C	109.5
O3—C12—H12A	109.5	O6—C24—H24A	109.5
O3—C12—H12B	109.5	O6—C24—H24B	109.5
H12A—C12—H12B	109.5	H24A—C24—H24B	109.5
O3—C12—H12C	109.5	O6—C24—H24C	109.5
H12A—C12—H12C	109.5	H24A—C24—H24C	109.5
H12B—C12—H12C	109.5	H24B—C24—H24C	109.5
C2—O1—H1	109.7 (13)	C14—O4—H4	110.4 (13)
C8—O2—C11	117.32 (14)	C19—O5—C23	117.69 (13)
C9—O3—C12	117.45 (13)	C20—O6—C24	117.18 (14)
O1—C2—C3—C4	178.90 (15)	O4—C14—C15—C16	179.39 (15)
C1—C2—C3—C4	−0.6 (2)	C13—C14—C15—C16	−0.8 (3)
O1—C2—C3—C5	−1.0 (3)	O4—C14—C15—C17	−1.8 (3)
C1—C2—C3—C5	179.46 (17)	C13—C14—C15—C17	178.01 (16)
C2—C3—C5—C6	−2.2 (3)	C14—C15—C17—C22	0.8 (3)
C4—C3—C5—C6	177.82 (16)	C16—C15—C17—C22	179.58 (17)
C2—C3—C5—C10	179.03 (17)	C14—C15—C17—C18	−178.36 (17)

C4—C3—C5—C10	−0.9 (2)	C16—C15—C17—C18	0.5 (2)
C10—C5—C6—C7	−0.4 (3)	C22—C17—C18—C19	−0.2 (3)
C3—C5—C6—C7	−179.17 (17)	C15—C17—C18—C19	178.93 (15)
C5—C6—C7—C8	0.4 (3)	C17—C18—C19—O5	−179.21 (16)
C6—C7—C8—O2	178.91 (17)	C17—C18—C19—C20	0.0 (3)
C6—C7—C8—C9	0.3 (3)	O5—C19—C20—O6	−0.3 (2)
O2—C8—C9—O3	−1.0 (2)	C18—C19—C20—O6	−179.62 (15)
C7—C8—C9—O3	177.74 (16)	O5—C19—C20—C21	179.60 (16)
O2—C8—C9—C10	−179.79 (16)	C18—C19—C20—C21	0.3 (3)
C7—C8—C9—C10	−1.1 (3)	O6—C20—C21—C22	179.56 (17)
O3—C9—C10—C5	−177.60 (15)	C19—C20—C21—C22	−0.4 (3)
C8—C9—C10—C5	1.1 (3)	C18—C17—C22—C21	0.2 (3)
C6—C5—C10—C9	−0.3 (3)	C15—C17—C22—C21	−178.94 (17)
C3—C5—C10—C9	178.48 (15)	C20—C21—C22—C17	0.1 (3)
C7—C8—O2—C11	3.5 (3)	C18—C19—O5—C23	0.4 (3)
C9—C8—O2—C11	−177.88 (16)	C20—C19—O5—C23	−178.84 (16)
C10—C9—O3—C12	4.8 (3)	C21—C20—O6—C24	−7.4 (3)
C8—C9—O3—C12	−173.95 (17)	C19—C20—O6—C24	172.52 (16)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N2^{i}	0.91 (2)	1.93 (2)	2.835 (2)	173.7 (19)
O4—H4···N1^{ii}	0.91 (2)	1.89 (2)	2.793 (2)	174.3 (19)

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

Fig. 1

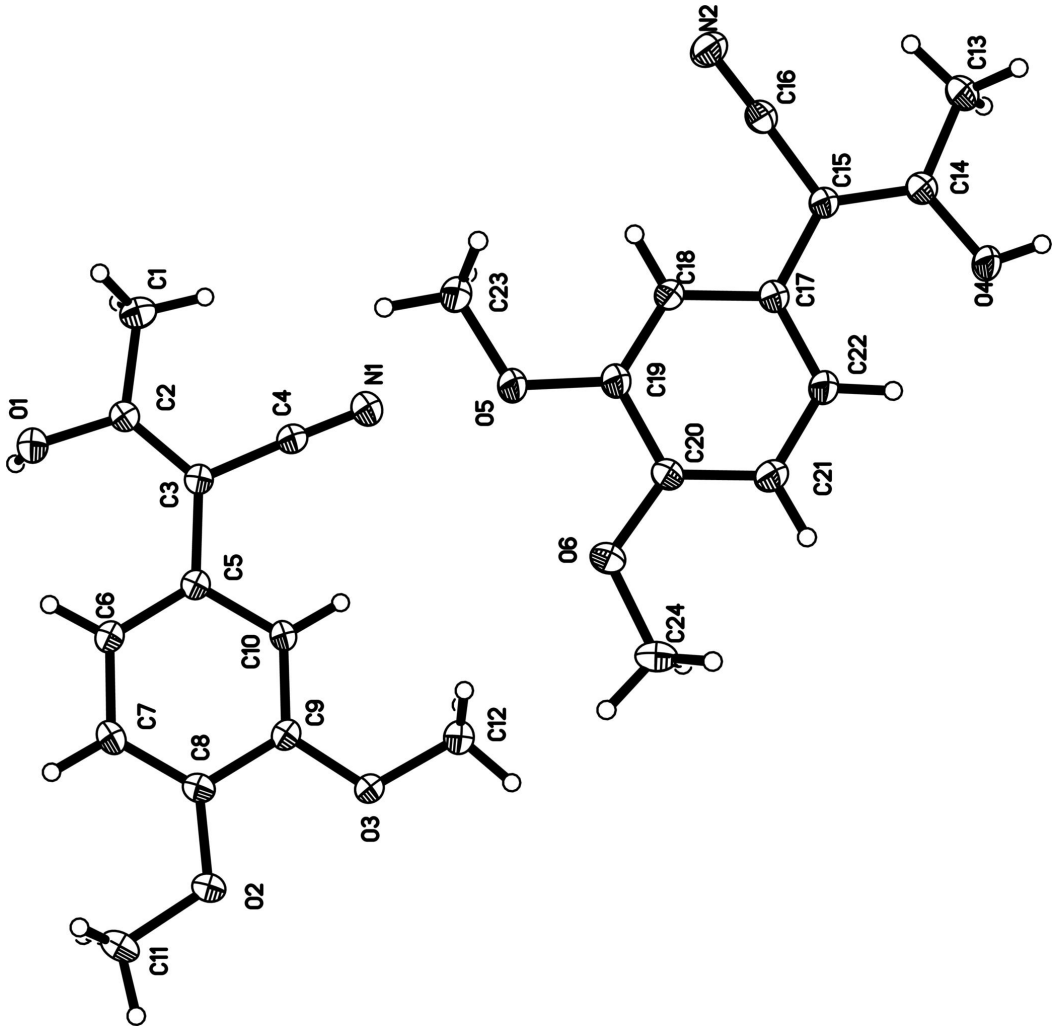
N2
C16
C13
C15
C14
O4
C18
C17
C23
C22
C19
O5
C20
C21
O6
C24
C1
O1
C2
C4
N1
C3
C5
C6
C10
C7
C9
C12
C8
O3
O2
C11

Fig. 2