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(2*E*)-Methyl 2-{2-[6-(2-cyanophenoxy)-pyrimidin-4-yloxy]phenyl}-3-methoxyacrylate

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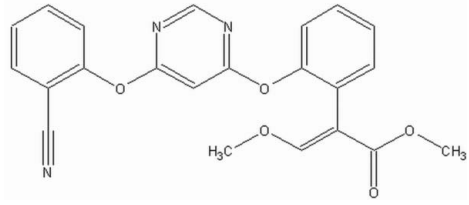
Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.007 Å; disorder in main residue; R factor = 0.079; wR factor = 0.220; data-to-parameter ratio = 7.7.

The title compound, $C_{22}H_{16}N_3O_5$, also known as azoxystrobin, possesses fungicidal properties. The dihedral angles between the cyanophenoxy and oxophenyl rings and the central pyrimidinyl ring are 80.5 (2) and 76.0 (1)°, respectively. The crystal structure is stabilized by aromatic π–π staching interactions between the pyrimide rings, the centroid–centroid distance being 3.914 (9) Å.

Related literature

For related structures, see: Lewis *et al.* (1991); Anderson *et al.* (1983); Zenei *et al.* (1988). For related literature, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{22}H_{16}N_3O_5$
M_r = 402.38
Monoclinic, $C2/c$
a = 28.946 (6) Å
b = 10.803 (2) Å
c = 13.302 (3) Å
β = 94.61 (3)°
V = 4146.1 (15) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 292 (2) K
0.08 × 0.07 × 0.02 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997*a*)
T_{min} = 0.948, T_{max} = 0.998
9000 measured reflections
2169 independent reflections
1733 reflections with $I > 2\sigma(I)$
R_{int} = 0.055
θ_{max} = 20.8°

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.079
$wR(F^2)$ = 0.220
S = 1.14
2169 reflections
283 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*b*); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2388).

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supplementary materials

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(2*E*)-Methyl 2-{2-[6-(2-cyanophenoxy)pyrimidin-4-yloxy]phenyl}-3-methoxyacrylate

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Comment

An important aspect in the rational design of bioactive molecules involves relating chemical structure to biological activity (Lewis *et al.*, 1991). The conformation of the molecule is found to influence the levels of biological activity. Correlation of the results obtained from X-ray crystallography with biological activity has aided in the chemical design of few active agrochemicals. The activity of a series of triazolyl ketone herbicides (Anderson *et al.*, 1983) has been investigated along with the fungicidal activities of *N*-phenyl succinamides (Zenei *et al.*, 1988).

The title compound, (I), has been shown to have fungicidal properties and its structure is reported here, Fig. 1. Bond lengths and angles observed in the structure are normal (Allen *et al.*, 1987). The crystal structure is stabilized by aromatic stacking π···π interactions (Fig. 2) between the pyrimidyl rings, the centroid to centroid distance being 3.914 (9)Å (Symmetry Code: −*x* + 1/2, −*y* + 3 /2, −*z* + 1).

Experimental

The title compound was obtained from Rallis India, Bangalore. Single crystals of the compound were grown by the slow evaporation method from acetone at 278 K.

Refinement

Despite repeated attempts to grow a better quality crystal with improved morphology, the crystals obtained were small and weakly diffracting so that the extent of diffraction observed is poor. The carbonyl oxygen atom is disordered over two sites O4 and O4A, with the occupancy factor for the major disorder component, O4, refining to 0.517 (11). All the hydrogen atoms were placed in calculated positions and allowed to ride on the parent atoms with C—H = 0.93 − 0.96Å and U_{eq}(H) = 1.2 or 1.5 U_{eq}(C).

Figures

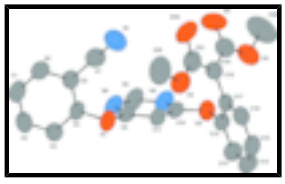

Fig. 1. Molecular structure of (I), showing 50% ellipsoidal probability.

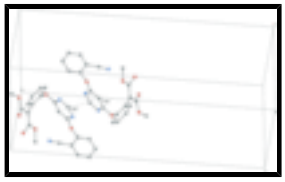

Fig. 2. Part of the packing diagram for (I), highlighting the π···π intermolecular interactions (dotted line).

(2E)-Methyl 2-{2-[6-(2-cyanophenoxy)pyrimidin-4-yloxy]phenyl}-3-methoxyacrylate

Crystal data

$C_{22}H_{16}N_3O_5$	F_{000} = 1672
M_r = 402.38	D_x = 1.289 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 565 reflections
a = 28.946 (6) Å	θ = 1.2–19.6º
b = 10.803 (2) Å	μ = 0.09 mm^{-1}
c = 13.302 (3) Å	*T* = 292 (2) K
β = 94.61 (3)º	Plate, colorless
V = 4146.1 (15) Å^3	0.08 × 0.07 × 0.02 mm
Z = 8	

Data collection

Bruker SMART CCD area-detector diffractometer	2169 independent reflections
Radiation source: fine-focus sealed tube	1733 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.055
T = 292(2) K	θ_{max} = 20.8º
φ and ω scans	θ_{min} = 1.4º
Absorption correction: multi-scan (SADABS; Sheldrick, 1997a)	*h* = −28→28
T_{min} = 0.948, T_{max} = 0.998	*k* = −10→10
9000 measured reflections	*l* = −13→13

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.079	H-atom parameters constrained
$wR(F^2)$ = 0.220	$w = 1/[\sigma^2(F_o^2) + (0.1574P)^2 + 9.0867P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.14	$(\Delta/\sigma)_{max}$ = <0.001
2169 reflections	$\Delta\rho_{max}$ = 0.31 e Å^{-3}
283 parameters	$\Delta\rho_{min}$ = −0.39 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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}	Occ. (<1)
O1	0.72469 (11)	0.4309 (3)	0.3502 (2)	0.0658 (10)	
O2	0.62147 (10)	0.1461 (3)	0.4936 (2)	0.0648 (9)	
O3	0.51541 (13)	0.2021 (4)	0.4877 (3)	0.0971 (13)	
O4	0.5153 (3)	0.4039 (9)	0.4684 (6)	0.103 (4)	0.517 (11)
O4A	0.5367 (3)	0.4936 (7)	0.2981 (7)	0.106 (4)	0.483 (11)
O5	0.58850 (14)	0.3775 (3)	0.2208 (3)	0.0872 (12)	
N1	0.63577 (19)	0.6404 (5)	0.4033 (4)	0.1047 (17)	
N2	0.72237 (14)	0.4148 (3)	0.5245 (3)	0.0660 (12)	
N3	0.67012 (15)	0.2677 (4)	0.5918 (3)	0.0707 (12)	
C1	0.7935 (2)	0.7708 (5)	0.3623 (4)	0.0715 (15)	
C2	0.81804 (17)	0.6609 (5)	0.3512 (4)	0.0713 (14)	
C3	0.79544 (16)	0.5464 (4)	0.3512 (3)	0.0631 (13)	
C4	0.74871 (16)	0.5440 (4)	0.3622 (3)	0.0530 (12)	
C5	0.72374 (15)	0.6540 (4)	0.3753 (3)	0.0575 (13)	
C6	0.74707 (18)	0.7679 (5)	0.3748 (3)	0.0650 (13)	
C7	0.6746 (2)	0.6477 (5)	0.3900 (4)	0.0736 (15)	
C8	0.70679 (15)	0.3777 (4)	0.4317 (3)	0.0519 (12)	
C9	0.7029 (2)	0.3558 (5)	0.5980 (4)	0.0783 (16)	
C10	0.65564 (15)	0.2350 (4)	0.4959 (3)	0.0517 (12)	
C11	0.67341 (14)	0.2847 (4)	0.4135 (3)	0.0527 (12)	
C12	0.60626 (15)	0.0952 (4)	0.3966 (3)	0.0565 (12)	
C13	0.62339 (17)	−0.0210 (5)	0.3743 (4)	0.0727 (14)	
C14	0.60929 (19)	−0.0757 (5)	0.2829 (4)	0.0801 (16)	
C15	0.57760 (18)	−0.0146 (5)	0.2143 (4)	0.0806 (16)	
C16	0.56032 (16)	0.1001 (5)	0.2397 (4)	0.0687 (14)	
C17	0.57395 (14)	0.1586 (4)	0.3327 (3)	0.0561 (12)	
C18	0.55490 (15)	0.2839 (4)	0.3569 (4)	0.0621 (14)	
C19	0.52730 (19)	0.3029 (6)	0.4364 (5)	0.0782 (16)	
C20	0.4827 (3)	0.2207 (9)	0.5632 (7)	0.155 (3)	
C21	0.5617 (2)	0.3891 (6)	0.2961 (5)	0.0779 (16)	
C22	0.5905 (2)	0.4881 (7)	0.1568 (6)	0.123 (3)	
H1	0.8088	0.8464	0.3611	0.086*	
H2	0.8497	0.6639	0.3438	0.086*	

H3	0.8118	0.4733	0.3439	0.076*
H6	0.7310	0.8413	0.3829	0.078*
H9	0.7136	0.3790	0.6631	0.094*
H11	0.6639	0.2584	0.3485	0.063*
H13	0.6441	−0.0614	0.4203	0.087*
H14	0.6208	−0.1530	0.2669	0.096*
H15	0.5683	−0.0506	0.1525	0.097*
H16	0.5392	0.1398	0.1943	0.082*
H20A	0.4989	0.2502	0.6244	0.233*
H20B	0.4677	0.1438	0.5760	0.233*
H20C	0.4599	0.2806	0.5392	0.233*
H22A	0.5659	0.5436	0.1705	0.185*
H22B	0.5872	0.4640	0.0871	0.185*
H22C	0.6198	0.5288	0.1711	0.185*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.076 (2)	0.063 (2)	0.056 (2)	−0.0193 (17)	−0.0109 (16)	−0.0068 (16)
O2	0.063 (2)	0.065 (2)	0.063 (2)	−0.0096 (17)	−0.0157 (16)	0.0085 (16)
O3	0.069 (2)	0.116 (3)	0.107 (3)	0.010 (2)	0.009 (2)	0.009 (3)
O4	0.092 (6)	0.115 (7)	0.102 (6)	0.036 (5)	0.000 (4)	−0.027 (5)
O4A	0.120 (7)	0.058 (6)	0.134 (8)	0.004 (5)	−0.021 (5)	−0.006 (5)
O5	0.089 (3)	0.068 (3)	0.100 (3)	0.003 (2)	−0.016 (2)	0.023 (2)
N1	0.068 (3)	0.112 (4)	0.132 (5)	0.013 (3)	−0.004 (3)	0.011 (3)
N2	0.087 (3)	0.053 (2)	0.053 (3)	−0.008 (2)	−0.028 (2)	0.000 (2)
N3	0.097 (3)	0.058 (3)	0.053 (3)	−0.007 (2)	−0.017 (2)	0.007 (2)
C1	0.085 (4)	0.061 (3)	0.067 (3)	−0.018 (3)	−0.010 (3)	0.005 (2)
C2	0.054 (3)	0.078 (4)	0.079 (3)	−0.010 (3)	−0.013 (2)	0.009 (3)
C3	0.056 (3)	0.061 (3)	0.070 (3)	0.001 (3)	−0.011 (2)	0.008 (2)
C4	0.057 (3)	0.052 (3)	0.046 (3)	−0.010 (2)	−0.019 (2)	0.001 (2)
C5	0.054 (3)	0.064 (3)	0.051 (3)	−0.002 (3)	−0.017 (2)	0.002 (2)
C6	0.072 (4)	0.059 (3)	0.062 (3)	0.004 (3)	−0.011 (2)	0.002 (2)
C7	0.072 (4)	0.071 (4)	0.075 (3)	0.009 (3)	−0.014 (3)	0.003 (3)
C8	0.056 (3)	0.046 (3)	0.050 (3)	0.008 (2)	−0.015 (2)	0.000 (2)
C9	0.118 (4)	0.061 (3)	0.050 (3)	−0.018 (3)	−0.027 (3)	0.006 (3)
C10	0.055 (3)	0.041 (3)	0.056 (3)	0.005 (2)	−0.018 (2)	0.005 (2)
C11	0.051 (3)	0.051 (3)	0.053 (3)	−0.005 (2)	−0.019 (2)	−0.005 (2)
C12	0.052 (3)	0.051 (3)	0.064 (3)	−0.004 (2)	−0.009 (2)	0.001 (2)
C13	0.069 (3)	0.065 (4)	0.082 (4)	0.002 (3)	−0.012 (3)	0.002 (3)
C14	0.079 (4)	0.058 (3)	0.101 (4)	0.004 (3)	−0.008 (3)	−0.004 (3)
C15	0.074 (4)	0.073 (4)	0.093 (4)	−0.020 (3)	−0.003 (3)	−0.019 (3)
C16	0.045 (3)	0.072 (4)	0.086 (4)	−0.004 (2)	−0.018 (2)	−0.007 (3)
C17	0.043 (3)	0.056 (3)	0.066 (3)	−0.006 (2)	−0.014 (2)	−0.001 (2)
C18	0.046 (3)	0.068 (4)	0.068 (3)	0.000 (2)	−0.020 (3)	−0.009 (3)
C19	0.057 (3)	0.085 (4)	0.089 (4)	0.005 (3)	−0.020 (3)	−0.008 (4)
C20	0.114 (6)	0.220 (10)	0.137 (7)	0.023 (6)	0.040 (6)	0.028 (6)
C21	0.067 (4)	0.079 (4)	0.084 (4)	−0.010 (3)	−0.024 (3)	−0.002 (3)

C22	0.116 (5)	0.111 (5)	0.137 (6)	−0.019 (4)	−0.030 (4)	0.033 (5)

Geometric parameters (Å, °)

O4—C19	1.230 (9)	C18—C21	1.418 (8)
O4A—C21	1.342 (10)	C4—C3	1.372 (7)
O1—C8	1.366 (5)	C2—C1	1.398 (7)
O1—C4	1.409 (6)	C2—C3	1.399 (7)
O2—C10	1.377 (5)	C2—H2	0.9300
O2—C12	1.439 (6)	N1—C7	1.154 (7)
N2—C9	1.329 (6)	C3—H3	0.9300
N2—C8	1.342 (6)	C13—C14	1.384 (7)
O5—C21	1.321 (7)	C13—H13	0.9300
O5—C22	1.471 (8)	C6—C1	1.367 (7)
O3—C19	1.345 (7)	C6—H6	0.9300
O3—C20	1.448 (8)	C14—C15	1.406 (8)
C10—N3	1.357 (6)	C14—H14	0.9300
C10—C11	1.358 (6)	C15—C16	1.388 (7)
N3—C9	1.342 (7)	C15—H15	0.9300
C17—C12	1.392 (6)	C9—H9	0.9300
C17—C16	1.417 (7)	C16—H16	0.9300
C17—C18	1.506 (7)	C1—H1	0.9300
C8—C11	1.401 (6)	C22—H22A	0.9600
C11—H11	0.9300	C22—H22B	0.9600
C12—C13	1.390 (7)	C22—H22C	0.9600
C5—C6	1.404 (7)	C20—H20A	0.9600
C5—C4	1.409 (7)	C20—H20B	0.9600
C5—C7	1.453 (8)	C20—H20C	0.9600
C18—C19	1.391 (8)		
C8—O1—C4	119.4 (3)	C12—C13—H13	120.4
C10—O2—C12	116.9 (3)	N1—C7—C5	178.3 (6)
C9—N2—C8	113.8 (4)	C1—C6—C5	119.9 (5)
C21—O5—C22	114.5 (5)	C1—C6—H6	120.0
C19—O3—C20	116.6 (6)	C5—C6—H6	120.0
N3—C10—C11	123.2 (4)	O5—C21—O4A	116.5 (6)
N3—C10—O2	111.7 (4)	O5—C21—C18	118.2 (5)
C11—C10—O2	125.2 (4)	O4A—C21—C18	124.3 (7)
C9—N3—C10	114.0 (4)	C13—C14—C15	120.0 (5)
C12—C17—C16	116.1 (4)	C13—C14—H14	120.0
C12—C17—C18	123.4 (4)	C15—C14—H14	120.0
C16—C17—C18	120.4 (4)	O4—C19—O3	116.9 (7)
N2—C8—O1	119.0 (4)	O4—C19—C18	126.0 (7)
N2—C8—C11	123.3 (4)	O3—C19—C18	116.8 (6)
O1—C8—C11	117.7 (4)	C16—C15—C14	119.4 (5)
C10—C11—C8	116.4 (4)	C16—C15—H15	120.3
C10—C11—H11	121.8	C14—C15—H15	120.3
C8—C11—H11	121.8	N2—C9—N3	129.4 (4)
C13—C12—C17	123.2 (4)	N2—C9—H9	115.3
C13—C12—O2	116.6 (4)	N3—C9—H9	115.3

C17—C12—O2	120.1 (4)	C15—C16—C17	122.0 (5)
C6—C5—C4	119.1 (4)	C15—C16—H16	119.0
C6—C5—C7	121.2 (4)	C17—C16—H16	119.0
C4—C5—C7	119.6 (4)	C6—C1—C2	120.4 (5)
C19—C18—C21	115.4 (5)	C6—C1—H1	119.8
C19—C18—C17	122.5 (5)	C2—C1—H1	119.8
C21—C18—C17	121.9 (5)	O5—C22—H22A	109.5
C3—C4—O1	119.1 (4)	O5—C22—H22B	109.5
C3—C4—C5	121.1 (4)	H22A—C22—H22B	109.5
O1—C4—C5	119.5 (4)	O5—C22—H22C	109.5
C1—C2—C3	120.6 (5)	H22A—C22—H22C	109.5
C1—C2—H2	119.7	H22B—C22—H22C	109.5
C3—C2—H2	119.7	O3—C20—H20A	109.5
C4—C3—C2	118.8 (4)	O3—C20—H20B	109.5
C4—C3—H3	120.6	H20A—C20—H20B	109.5
C2—C3—H3	120.6	O3—C20—H20C	109.5
C14—C13—C12	119.2 (5)	H20A—C20—H20C	109.5
C14—C13—H13	120.4	H20B—C20—H20C	109.5
C12—O2—C10—N3	−174.3 (3)	O1—C4—C3—C2	172.4 (4)
C12—O2—C10—C11	5.3 (6)	C5—C4—C3—C2	−1.2 (6)
C11—C10—N3—C9	1.4 (7)	C1—C2—C3—C4	0.0 (7)
O2—C10—N3—C9	−178.9 (4)	C17—C12—C13—C14	2.4 (7)
C9—N2—C8—O1	−179.3 (4)	O2—C12—C13—C14	178.8 (4)
C9—N2—C8—C11	−0.5 (6)	C4—C5—C6—C1	−0.4 (6)
C4—O1—C8—N2	−17.4 (6)	C7—C5—C6—C1	179.0 (4)
C4—O1—C8—C11	163.7 (4)	C22—O5—C21—O4A	6.3 (7)
N3—C10—C11—C8	−2.8 (6)	C22—O5—C21—C18	175.2 (5)
O2—C10—C11—C8	177.6 (4)	C19—C18—C21—O5	178.4 (4)
N2—C8—C11—C10	2.4 (6)	C17—C18—C21—O5	−5.2 (7)
O1—C8—C11—C10	−178.8 (4)	C19—C18—C21—O4A	−13.7 (8)
C16—C17—C12—C13	−2.5 (7)	C17—C18—C21—O4A	162.7 (6)
C18—C17—C12—C13	179.4 (4)	C12—C13—C14—C15	−0.7 (8)
C16—C17—C12—O2	−178.7 (4)	C20—O3—C19—O4	11.1 (9)
C18—C17—C12—O2	3.2 (6)	C20—O3—C19—C18	−173.6 (5)
C10—O2—C12—C13	101.8 (5)	C21—C18—C19—O4	−13.3 (8)
C10—O2—C12—C17	−81.7 (5)	C17—C18—C19—O4	170.4 (6)
C12—C17—C18—C19	−65.7 (6)	C21—C18—C19—O3	171.9 (4)
C16—C17—C18—C19	116.2 (5)	C17—C18—C19—O3	−4.5 (7)
C12—C17—C18—C21	118.1 (5)	C13—C14—C15—C16	−0.7 (8)
C16—C17—C18—C21	−59.9 (6)	C8—N2—C9—N3	−1.1 (8)
C8—O1—C4—C3	112.7 (4)	C10—N3—C9—N2	0.7 (8)
C8—O1—C4—C5	−73.5 (5)	C14—C15—C16—C17	0.6 (8)
C6—C5—C4—C3	1.4 (6)	C12—C17—C16—C15	1.0 (7)
C7—C5—C4—C3	−178.0 (4)	C18—C17—C16—C15	179.2 (4)
C6—C5—C4—O1	−172.2 (4)	C5—C6—C1—C2	−0.8 (7)
C7—C5—C4—O1	8.4 (6)	C3—C2—C1—C6	1.0 (7)

Fig. 1

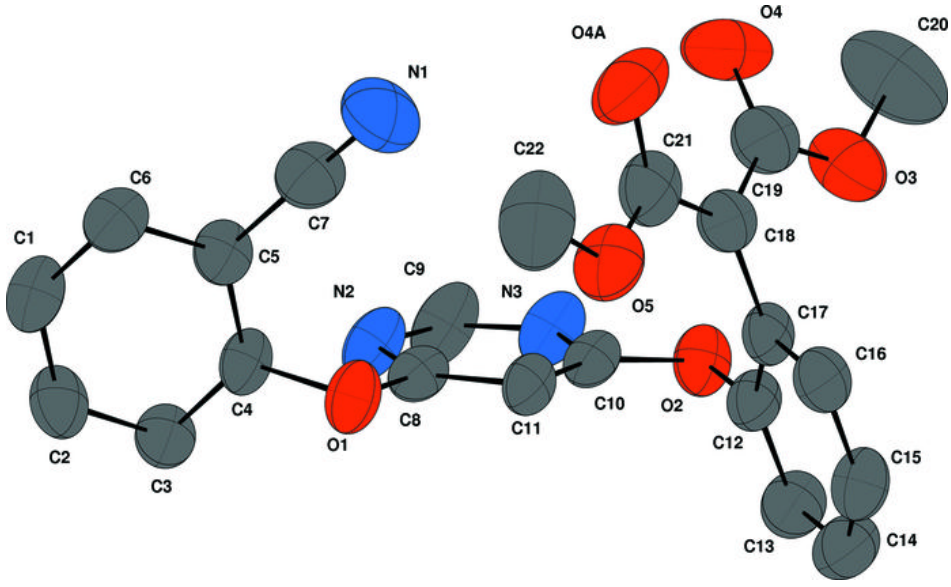
O4
C20
O4A
N1
C22
C21
O3
C6
C19
C7
C1
C18
C5
C9
N2
N3
O5
C17
C16
C4
C10
O2
C8
C11
C12
C2
O1
C15
C3
C13
C14

Fig. 2