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3-(Benzotriazol-2-yl)-1-(biphenyl-4-yl)-propan-1-one

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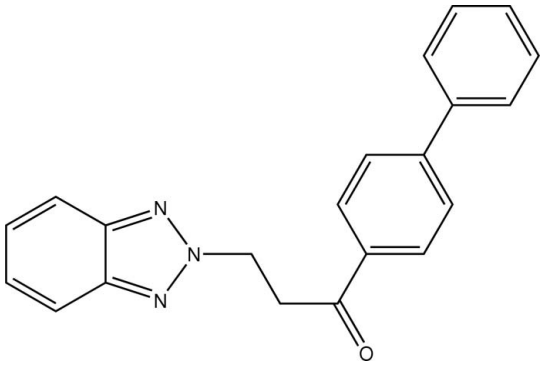
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; R factor = 0.053; wR factor = 0.125; data-to-parameter ratio = 14.4.

In the molecule of the title compound, $C_{21}H_{17}N_3O$, the nearly planar benzotriazole ring system is oriented with respect to the planar rings C (benzoyl) and D (terminal phenyl) at dihedral angles of 58.52 (1) and 77.16 (1)°, respectively. In the crystal structure, intermolecular C—H···N hydrogen bonds link the molecules into centrosymmetric dimers.

Related literature

For general background, see: Allen *et al.* (1987). For related literature, see: Wang *et al.* (2005).



Experimental

Crystal data

$C_{21}H_{17}N_3O$
M_r = 327.38
Monoclinic, $P2_1/c$
a = 13.313 (3) Å
b = 10.661 (3) Å
c = 13.629 (3) Å
β = 116.739 (4)°
V = 1727.5 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 294 (2) K
0.43 × 0.13 × 0.06 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.967, T_{max} = 0.995
9149 measured reflections
3259 independent reflections
2061 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.125
S = 1.06
3259 reflections
226 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C15—H15A···N1^{i}	0.96	2.61	3.567 (3)	171

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); 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, 1999); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2263).

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supplementary materials

Acta Cryst. (2007). E**63**, o3091 [**doi:10.1107/S1600536807026566**]

3-(Benzotriazol-2-yl)-1-(biphenyl-4-yl)propan-1-one

K. Cheng, H.-Q. Zhang, N.-N. Tian and J. Wan

Comment

Recently we have reported the structure of 2-(2*H*-benzotriazol-2-yl)-1 -phenylethanone (Wang *et al.*, 2005). As part of our ongoing studies on new benzotriazole derivatives with higher anti-inflammatory properties, the title compound, (I), was synthesized and we herein report its crystal structure.

In the molecule of the title compound, (I), (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The benzotriazole system is essentially planar, with a dihedral angle of 0.13 (1)° between the planar rings A (C16—C21) and B (N1—N3/C16/C21). The dihedral angles between the nearly planar benzotriazole ring system and planar rings C (C7—C12) and D (C1—C6) are 58.52 (1)° and 77.16 (1)°, respectively. The rings C and D are oriented at a dihedral angle of 30.73 (1)°.

In the crystal structure, intermolecular C—H···N hydrogen bonds (Table 1) link the molecules into centrosymmetric dimers (Fig. 2), in which they may be effective in the stabilization of the structure.

Experimental

The title compound was prepared according to the literature method (Wang *et al.*, 2005). Single crystals suitable for X-ray diffracion were obtained by slow evaporation of an ethyl acetate solution at room temperature over a period of 5 d.

Refinement

H atoms were positioned geometrically, with C—H = 0.93 and 0.96 Å for aromatic and methylene H atoms, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C).

Figures

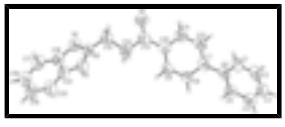

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

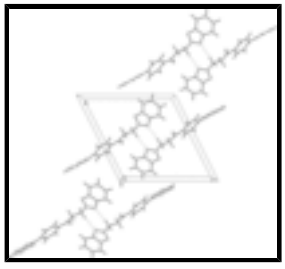

Fig. 2. A packing diagram for (I). Hydrogen bonds are shown as dashed lines.

3-(Benzotriazol-2-yl)-1-(biphenyl-4-yl)propan-1-one

Crystal data

$C_{21}H_{17}N_3O$	F_{000} = 688
M_r = 327.38	D_x = 1.259 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 1501 reflections
a = 13.313 (3) Å	θ = 2.6–21.5º
b = 10.661 (3) Å	μ = 0.08 mm^{-1}
c = 13.629 (3) Å	T = 294 (2) K
β = 116.739 (4)º	Needle, colorless
V = 1727.5 (7) Å^3	0.43 × 0.13 × 0.06 mm
Z = 4	

Data collection

Siemens SMART 1000 CCD area-detector diffractometer	3259 independent reflections
Radiation source: fine-focus sealed tube	2061 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.032
Detector resolution: 8.33 pixels mm^{-1}	θ_{max} = 25.7º
T = 294(2) K	θ_{min} = 1.7º
ω scans	h = −11→16
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	k = −13→12
T_{min} = 0.967, T_{max} = 0.995	l = −16→13
9149 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.053	H-atom parameters constrained
$wR(F^2)$ = 0.125	$w = 1/[\sigma^2(F_o^2) + (0.0491P)^2 + 0.0564P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.06	$(\Delta/\sigma)_{max} < 0.001$
3259 reflections	$\Delta\rho_{max}$ = 0.12 e Å^{-3}
226 parameters	$\Delta\rho_{min}$ = −0.14 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}
O1	0.55783 (13)	−0.10605 (15)	0.30143 (12)	0.0812 (5)
N1	0.35490 (14)	0.09972 (16)	−0.06672 (13)	0.0606 (5)
N2	0.33680 (13)	0.07937 (15)	0.02037 (13)	0.0574 (4)
N3	0.24092 (14)	0.12146 (17)	0.01559 (14)	0.0665 (5)
C1	0.79900 (17)	0.1402 (2)	0.84539 (16)	0.0695 (6)
H1B	0.7912	0.0536	0.8374	0.083*
C2	0.85160 (18)	0.1910 (3)	0.94937 (17)	0.0778 (7)
H2A	0.8774	0.1386	1.0104	0.093*
C3	0.86613 (19)	0.3174 (3)	0.96371 (18)	0.0820 (7)
H3B	0.9021	0.3513	1.0340	0.098*
C4	0.8269 (2)	0.3943 (2)	0.87297 (19)	0.0885 (8)
H4A	0.8365	0.4807	0.8818	0.106*
C5	0.77336 (19)	0.3433 (2)	0.76876 (18)	0.0771 (7)
H5A	0.7474	0.3963	0.7081	0.093*
C6	0.75742 (16)	0.2154 (2)	0.75232 (16)	0.0594 (5)
C7	0.69832 (16)	0.1610 (2)	0.64056 (15)	0.0572 (5)
C8	0.61326 (17)	0.2260 (2)	0.55468 (16)	0.0629 (6)
H8A	0.5921	0.3049	0.5679	0.076*
C9	0.55970 (17)	0.1758 (2)	0.45025 (16)	0.0615 (6)
H9A	0.5041	0.2219	0.3941	0.074*
C10	0.58771 (16)	0.05743 (19)	0.42801 (16)	0.0550 (5)
C11	0.67031 (19)	−0.0089 (2)	0.51349 (18)	0.0695 (6)
H11A	0.6892	−0.0892	0.5006	0.083*
C12	0.72515 (19)	0.0418 (2)	0.61747 (17)	0.0707 (6)
H12A	0.7811	−0.0043	0.6732	0.085*
C13	0.53522 (17)	0.0009 (2)	0.31687 (17)	0.0590 (5)
C14	0.45417 (17)	0.07756 (19)	0.22105 (14)	0.0618 (6)
H14A	0.4900	0.1555	0.2176	0.074*
H14B	0.3889	0.0980	0.2319	0.074*
C15	0.41685 (17)	0.00770 (19)	0.11401 (15)	0.0600 (5)
H15A	0.4822	−0.0116	0.1029	0.072*
H15B	0.3825	−0.0710	0.1183	0.072*
C16	0.26081 (17)	0.16226 (19)	−0.13612 (15)	0.0543 (5)

C17	0.22998 (18)	0.2101 (2)	−0.24210 (16)	0.0661 (6)
H17A	0.2765	0.2018	−0.2762	0.079*
C18	0.1295 (2)	0.2687 (2)	−0.29181 (17)	0.0703 (6)
H18A	0.1064	0.3010	−0.3621	0.084*
C19	0.05804 (19)	0.2828 (2)	−0.24106 (19)	0.0817 (7)
H19A	−0.0104	0.3239	−0.2788	0.098*
C20	0.08668 (19)	0.2378 (2)	−0.13857 (19)	0.0810 (7)
H20A	0.0397	0.2478	−0.1052	0.097*
C21	0.19040 (17)	0.1756 (2)	−0.08537 (16)	0.0597 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0986 (12)	0.0610 (10)	0.0841 (10)	0.0134 (9)	0.0412 (9)	−0.0008 (8)
N1	0.0585 (11)	0.0736 (12)	0.0594 (10)	−0.0082 (9)	0.0351 (9)	−0.0082 (9)
N2	0.0525 (11)	0.0679 (12)	0.0571 (10)	−0.0043 (8)	0.0293 (9)	−0.0063 (8)
N3	0.0532 (11)	0.0909 (14)	0.0656 (11)	0.0038 (10)	0.0359 (9)	0.0010 (9)
C1	0.0594 (14)	0.0866 (17)	0.0596 (14)	−0.0049 (12)	0.0242 (11)	0.0152 (12)
C2	0.0593 (15)	0.111 (2)	0.0594 (15)	−0.0005 (14)	0.0233 (12)	0.0180 (14)
C3	0.0654 (16)	0.114 (2)	0.0615 (15)	0.0160 (15)	0.0238 (12)	−0.0047 (15)
C4	0.0904 (19)	0.0851 (19)	0.0749 (17)	0.0225 (14)	0.0239 (15)	−0.0023 (14)
C5	0.0817 (17)	0.0790 (18)	0.0615 (14)	0.0207 (13)	0.0242 (13)	0.0091 (12)
C6	0.0499 (13)	0.0743 (16)	0.0558 (13)	0.0069 (11)	0.0253 (10)	0.0095 (11)
C7	0.0530 (13)	0.0676 (15)	0.0559 (12)	0.0074 (11)	0.0287 (10)	0.0151 (10)
C8	0.0616 (14)	0.0674 (14)	0.0587 (13)	0.0142 (11)	0.0260 (11)	0.0041 (11)
C9	0.0563 (13)	0.0694 (15)	0.0567 (12)	0.0135 (11)	0.0236 (10)	0.0096 (11)
C10	0.0542 (13)	0.0543 (13)	0.0626 (13)	0.0042 (10)	0.0316 (11)	0.0086 (10)
C11	0.0799 (17)	0.0571 (14)	0.0724 (15)	0.0127 (12)	0.0351 (13)	0.0114 (11)
C12	0.0732 (16)	0.0695 (16)	0.0658 (15)	0.0193 (12)	0.0281 (12)	0.0222 (12)
C13	0.0580 (14)	0.0565 (14)	0.0725 (14)	0.0006 (11)	0.0382 (12)	0.0032 (11)
C14	0.0624 (14)	0.0616 (14)	0.0638 (13)	0.0015 (10)	0.0305 (11)	−0.0027 (10)
C15	0.0571 (13)	0.0639 (14)	0.0656 (13)	0.0001 (10)	0.0336 (11)	−0.0012 (11)
C16	0.0496 (12)	0.0627 (13)	0.0538 (12)	−0.0103 (10)	0.0262 (10)	−0.0117 (10)
C17	0.0610 (15)	0.0825 (16)	0.0598 (13)	−0.0152 (12)	0.0318 (12)	−0.0128 (11)
C18	0.0637 (16)	0.0892 (17)	0.0538 (13)	−0.0132 (13)	0.0226 (12)	−0.0072 (11)
C19	0.0549 (15)	0.114 (2)	0.0686 (15)	0.0011 (13)	0.0209 (12)	0.0015 (14)
C20	0.0594 (15)	0.120 (2)	0.0724 (16)	0.0075 (14)	0.0372 (13)	0.0055 (14)
C21	0.0488 (13)	0.0769 (15)	0.0561 (12)	−0.0071 (11)	0.0260 (11)	−0.0037 (11)

Geometric parameters (Å, °)

N1—C16	1.357 (2)	C10—C11	1.384 (3)
N2—N1	1.3309 (19)	C11—H11A	0.9300
N2—N3	1.327 (2)	C12—C11	1.380 (3)
N2—C15	1.458 (2)	C12—H12A	0.9300
N3—C21	1.359 (2)	C13—O1	1.222 (2)
C1—C2	1.378 (3)	C13—C10	1.481 (3)
C1—H1B	0.9300	C13—C14	1.506 (3)
C2—C3	1.362 (3)	C14—C15	1.509 (2)

C2—H2A	0.9300	C14—H14A	0.9700
C3—H3B	0.9300	C14—H14B	0.9700
C4—C3	1.376 (3)	C15—H15A	0.9700
C4—C5	1.382 (3)	C15—H15B	0.9700
C4—H4A	0.9300	C16—C17	1.408 (3)
C5—H5A	0.9300	C16—C21	1.400 (3)
C6—C1	1.388 (3)	C17—H17A	0.9300
C6—C5	1.382 (3)	C18—C17	1.350 (3)
C7—C6	1.482 (3)	C18—C19	1.413 (3)
C7—C12	1.393 (3)	C18—H18A	0.9300
C8—C7	1.393 (3)	C19—H19A	0.9300
C8—H8A	0.9300	C20—C19	1.359 (3)
C9—C8	1.381 (3)	C20—H20A	0.9300
C9—C10	1.387 (3)	C21—C20	1.404 (3)
C9—H9A	0.9300		
N2—N1—C16	102.77 (15)	C10—C11—H11A	119.4
N3—N2—N1	117.21 (16)	C11—C12—C7	121.25 (19)
N3—N2—C15	121.91 (16)	C11—C12—H12A	119.4
N1—N2—C15	120.80 (16)	C7—C12—H12A	119.4
N2—N3—C21	102.73 (16)	O1—C13—C10	121.09 (19)
C2—C1—C6	121.4 (2)	O1—C13—C14	119.52 (19)
C2—C1—H1B	119.3	C10—C13—C14	119.37 (18)
C6—C1—H1B	119.3	C13—C14—C15	111.48 (17)
C3—C2—C1	120.7 (2)	C13—C14—H14A	109.3
C3—C2—H2A	119.7	C15—C14—H14A	109.3
C1—C2—H2A	119.7	C13—C14—H14B	109.3
C2—C3—C4	119.2 (2)	C15—C14—H14B	109.3
C2—C3—H3B	120.4	H14A—C14—H14B	108.0
C4—C3—H3B	120.4	N2—C15—C14	112.38 (16)
C3—C4—C5	120.0 (2)	N2—C15—H15A	109.1
C3—C4—H4A	120.0	C14—C15—H15A	109.1
C5—C4—H4A	120.0	N2—C15—H15B	109.1
C4—C5—C6	121.7 (2)	C14—C15—H15B	109.1
C4—C5—H5A	119.2	H15A—C15—H15B	107.9
C6—C5—H5A	119.2	N1—C16—C21	108.58 (17)
C5—C6—C1	116.91 (19)	N1—C16—C17	130.15 (18)
C5—C6—C7	121.63 (18)	C21—C16—C17	121.3 (2)
C1—C6—C7	121.5 (2)	C18—C17—C16	116.6 (2)
C8—C7—C12	117.25 (19)	C18—C17—H17A	121.7
C8—C7—C6	121.58 (19)	C16—C17—H17A	121.7
C12—C7—C6	121.17 (18)	C17—C18—C19	122.4 (2)
C9—C8—C7	121.4 (2)	C17—C18—H18A	118.8
C9—C8—H8A	119.3	C19—C18—H18A	118.8
C7—C8—H8A	119.3	C20—C19—C18	121.7 (2)
C8—C9—C10	120.86 (19)	C20—C19—H19A	119.1
C8—C9—H9A	119.6	C18—C19—H19A	119.1
C10—C9—H9A	119.6	C19—C20—C21	117.0 (2)
C11—C10—C9	118.09 (19)	C19—C20—H20A	121.5
C11—C10—C13	118.94 (19)	C21—C20—H20A	121.5

C9—C10—C13	122.95 (18)	N3—C21—C16	108.71 (19)
C12—C11—C10	121.1 (2)	N3—C21—C20	130.34 (19)
C12—C11—H11A	119.4	C16—C21—C20	120.95 (19)
N2—N1—C16—C21	−0.1 (2)	C9—C8—C7—C6	178.93 (18)
N2—N1—C16—C17	179.73 (19)	C10—C9—C8—C7	1.2 (3)
N1—N2—N3—C21	−0.1 (2)	C8—C9—C10—C11	0.4 (3)
C15—N2—N3—C21	−176.82 (17)	C8—C9—C10—C13	−178.14 (18)
N3—N2—N1—C16	0.2 (2)	C9—C10—C11—C12	−1.4 (3)
C15—N2—N1—C16	176.90 (16)	C13—C10—C11—C12	177.18 (19)
N3—N2—C15—C14	−56.8 (2)	C7—C12—C11—C10	0.9 (3)
N1—N2—C15—C14	126.62 (17)	O1—C13—C14—C15	−3.4 (3)
N2—N3—C21—C16	0.0 (2)	C10—C13—C14—C15	175.54 (17)
N2—N3—C21—C20	−179.5 (2)	O1—C13—C10—C11	5.3 (3)
C6—C1—C2—C3	−1.2 (3)	C14—C13—C10—C11	−173.63 (18)
C1—C2—C3—C4	0.4 (3)	O1—C13—C10—C9	−176.23 (19)
C5—C4—C3—C2	0.1 (4)	C14—C13—C10—C9	4.9 (3)
C3—C4—C5—C6	0.1 (4)	C13—C14—C15—N2	179.00 (16)
C5—C6—C1—C2	1.3 (3)	N1—C16—C17—C18	179.9 (2)
C7—C6—C1—C2	−178.46 (19)	C21—C16—C17—C18	−0.2 (3)
C1—C6—C5—C4	−0.8 (3)	N1—C16—C21—N3	0.1 (2)
C7—C6—C5—C4	179.0 (2)	C17—C16—C21—N3	−179.81 (18)
C8—C7—C6—C5	−31.0 (3)	N1—C16—C21—C20	179.63 (19)
C12—C7—C6—C5	149.5 (2)	C17—C16—C21—C20	−0.2 (3)
C8—C7—C6—C1	148.8 (2)	C19—C18—C17—C16	0.3 (3)
C12—C7—C6—C1	−30.7 (3)	C17—C18—C19—C20	0.0 (4)
C8—C7—C12—C11	0.6 (3)	C21—C20—C19—C18	−0.5 (4)
C6—C7—C12—C11	−179.95 (19)	N3—C21—C20—C19	−180.0 (2)
C9—C8—C7—C12	−1.6 (3)	C16—C21—C20—C19	0.6 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15A···N1^{i}	0.96	2.61	3.567 (3)	171

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

Fig. 1

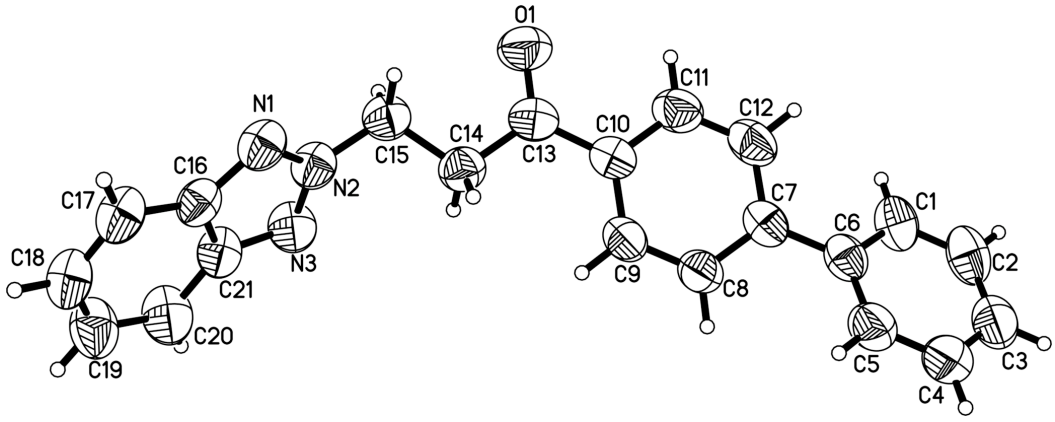
O1
C11
N1
C12
C10
C14
C15
C13
C16
N2
C7
C17
C6
C1
N3
C18
C9
C2
C21
C8
C20
C5
C3
C19
C4

Fig. 2