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(*Z*)-3-(9-Anthryl)-2-(4-nitro-1*H*-imidazol-1-yl)-1-*p*-tolylprop-2-en-1-one

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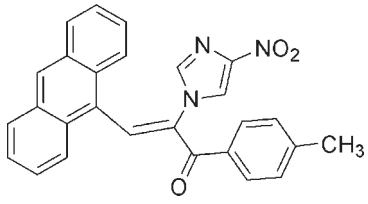
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.002 Å; R factor = 0.044; wR factor = 0.127; data-to-parameter ratio = 15.5.

In the title molecule, $C_{27}H_{19}N_3O_3$, the imidazole and benzene rings make dihedral angles of 64.72 (4) and 64.02 (4)°, respectively, with the anthracene ring system (r.m.s. deviation = 0.043 Å). The nitro group is coplanar with the imidazole ring [dihedral angle = 1.1 (1)°]. The crystal packing is stabilized by weak π–π interactions with centroid–centroid distances of 3.7342 (10) and 3.7627 (9) Å.

Related literature

For the crystal structures of the chloro and bromo analogues, see: Wang *et al.* (2009); Lu *et al.* (2009). For general background to chalcones, see: Vogel *et al.* (2008). For the synthesis, see: Erhardt *et al.* (1985).



Experimental

Crystal data

$C_{27}H_{19}N_3O_3$
M_r = 433.45
Triclinic, $P\overline{1}$
a = 7.9335 (9) Å
b = 11.2626 (13) Å
c = 13.0291 (15) Å
α = 75.454 (2)°
β = 85.763 (2)°
γ = 71.059 (2)°
V = 1065.8 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 K
0.36 × 0.23 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997)
T_{min} = 0.968, T_{max} = 0.991
12116 measured reflections
4621 independent reflections
3646 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.127
S = 1.05
4621 reflections
299 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; 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: CI2921).

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supporting information

Acta Cryst. (2009). E**65**, o2619 [https://doi.org/10.1107/S1600536809039221]

(*Z*)-3-(9-Anthryl)-2-(4-nitro-1*H*-imidazol-1-yl)-1-*p*-tolylprop-2-en-1-one

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S1. Comment

Chalcones or 1,3-diaryl-2-propen-1-ones are natural or synthetic compounds belonging to the flavonoid family (Vogel *et al.*, 2008). They exhibit diverse kinds of biological activities. Hence, chalcones are considered as an important class of therapeutic agents. A series of chalcone derivatives containing a imidazole ring have been synthesized in our lab and crystal structues of some of them have been reported (Lu *et al.*, 2009; Wang *et al.*, 2009). We report here the crystal structure of the title compound.

In the molecular structure of the title compound (Fig. 1), the imidazole and benzene ring of the tolyl group form dihedral angles of 64.72 (4)° and 64.02 (4)°, respectively, with the anthracene ring system (r.m.s. deviation 0.043 Å). The nitro group is coplanar with the imidazole ring [dihedral angle 1.1 (1)°].

The crystal structure is stabilized by weak π-π interactions between imidazole and benzene ring of the tolyl group (centroid to centroid distance = 3.7627 (9) Å) and those between the rings of the anthracene ring system (centroid to centroid distance = 3.7342 (10) Å).

S2. Experimental

The title compound was synthesized according to the procedure of Erhardt *et al.* (1985). Single crystals suitable for X-ray analysis was grown from a chloroform solution by slow evaporation at room temperature.

S3. Refinement

H atoms were placed at calculated positions with C-H = 0.93 Å (aromatic) and 0.96 Å (methyl). The U_{iso}(H) values were set equal to 1.2U_{eq}($C_{aromatic}$) and 1.5U_{eq}(C_{methyl}).

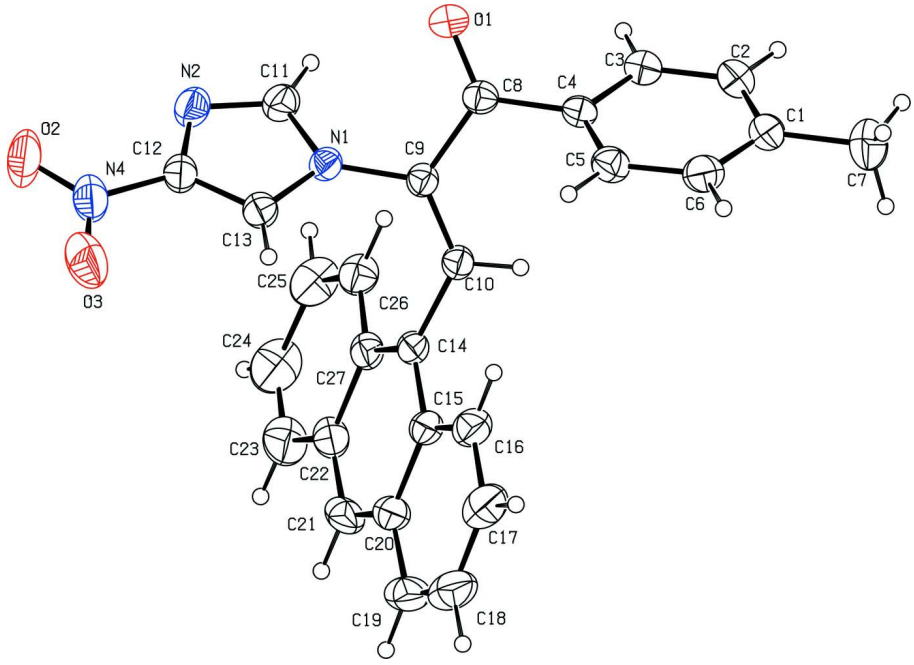

Figure 1

The molecular structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

(*Z*)-3-(9-Anthryl)-2-(4-nitro-1*H*-imidazol-1-yl)-1-*p*- tolylprop-2-en-1-one

Crystal data

$C_{27}H_{19}N_3O_3$
$M_r = 433.45$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.9335\ (9)$ Å
$b = 11.2626\ (13)$ Å
$c = 13.0291\ (15)$ Å
$\alpha = 75.454\ (2)°$
$\beta = 85.763\ (2)°$
$\gamma = 71.059\ (2)°$
$V = 1065.8\ (2)$ Å^3
$Z = 2$
$F(000) = 452$
$D_x = 1.351$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5053 reflections
$\theta = 2.2–28.1°$
$\mu = 0.09$ mm^{-1}
$T = 298$ K
Plate, yellow
0.36 × 0.23 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997)
$T_{min} = 0.968$, $T_{max} = 0.991$
12116 measured reflections
4621 independent reflections
3646 reflections with $I > 2\sigma(I)$
$R_{int} = 0.030$
$\theta_{max} = 27.0°$, $\theta_{min} = 2.2°$
$h = -10\rightarrow10$
$k = -14\rightarrow14$
$l = -16\rightarrow16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.127$
$S = 1.05$
4621 reflections
299 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
$w = 1/[\sigma^2(F_o^2) + (0.0696P)^2 + 0.061P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.012$
$\Delta\rho_{max} = 0.18$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.8022 (2)	0.80103 (14)	0.10371 (11)	0.0625 (4)
C2	0.9235 (2)	0.68461 (16)	0.09495 (12)	0.0655 (4)
H2	1.0443	0.6760	0.0895	0.079*
C3	0.86855 (18)	0.58070 (13)	0.09409 (10)	0.0542 (3)
H3	0.9521	0.5032	0.0871	0.065*
C4	0.68960 (16)	0.59098 (11)	0.10360 (9)	0.0443 (3)
C5	0.56700 (18)	0.70796 (12)	0.11149 (10)	0.0525 (3)
H5	0.4464	0.7164	0.1176	0.063*
C6	0.6231 (2)	0.81227 (13)	0.11031 (11)	0.0604 (4)
H6	0.5394	0.8911	0.1140	0.073*
C7	0.8646 (3)	0.91345 (19)	0.10604 (18)	0.1030 (7)
H7A	0.9884	0.8938	0.0878	0.155*
H7B	0.8486	0.9288	0.1759	0.155*
H7C	0.7964	0.9893	0.0559	0.155*
C8	0.63944 (15)	0.47439 (11)	0.10306 (9)	0.0429 (3)
C9	0.53578 (15)	0.42485 (10)	0.19465 (9)	0.0401 (3)
C10	0.51789 (15)	0.46279 (11)	0.28466 (9)	0.0424 (3)
H10	0.5567	0.5329	0.2825	0.051*
C11	0.55904 (19)	0.21206 (12)	0.15682 (10)	0.0547 (3)
H11	0.6800	0.1879	0.1413	0.066*
C12	0.29544 (19)	0.21363 (13)	0.18201 (9)	0.0522 (3)
C13	0.29627 (17)	0.32641 (12)	0.20011 (9)	0.0479 (3)
H13	0.2010	0.3902	0.2198	0.057*
C14	0.44576 (16)	0.41062 (12)	0.38765 (9)	0.0442 (3)
C15	0.31154 (16)	0.49758 (13)	0.43426 (9)	0.0497 (3)

C16	0.23060 (19)	0.62857 (14)	0.38169 (12)	0.0604 (4)
H16	0.2649	0.6593	0.3130	0.072*
C17	0.1035 (2)	0.71059 (18)	0.42967 (15)	0.0772 (5)
H17	0.0528	0.7965	0.3936	0.093*
C18	0.0482 (2)	0.6666 (2)	0.53315 (16)	0.0844 (6)
H18	−0.0377	0.7238	0.5655	0.101*
C19	0.1187 (2)	0.5429 (2)	0.58552 (13)	0.0770 (5)
H19	0.0799	0.5152	0.6538	0.092*
C20	0.25212 (18)	0.45250 (17)	0.53893 (10)	0.0587 (4)
C21	0.3253 (2)	0.32471 (18)	0.59118 (10)	0.0668 (4)
H21	0.2843	0.2958	0.6585	0.080*
C22	0.4581 (2)	0.23721 (15)	0.54715 (10)	0.0609 (4)
C23	0.5358 (3)	0.10705 (19)	0.60296 (13)	0.0849 (5)
H23	0.4934	0.0776	0.6698	0.102*
C24	0.6697 (3)	0.02531 (18)	0.56107 (15)	0.0961 (6)
H24	0.7168	−0.0604	0.5983	0.115*
C25	0.7395 (3)	0.06850 (16)	0.46106 (13)	0.0800 (5)
H25	0.8346	0.0116	0.4339	0.096*
C26	0.6691 (2)	0.19203 (13)	0.40416 (11)	0.0588 (4)
H26	0.7175	0.2190	0.3386	0.071*
C27	0.52314 (18)	0.28088 (13)	0.44281 (9)	0.0495 (3)
N1	0.46726 (13)	0.32578 (9)	0.18306 (7)	0.0428 (2)
N2	0.45809 (17)	0.14128 (11)	0.15594 (9)	0.0602 (3)
N4	0.1423 (2)	0.17060 (15)	0.18753 (10)	0.0718 (4)
O1	0.69016 (12)	0.41643 (9)	0.03388 (7)	0.0576 (3)
O2	0.1606 (2)	0.06711 (14)	0.16772 (11)	0.1051 (5)
O3	0.00028 (18)	0.24220 (15)	0.21342 (12)	0.0975 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0851 (10)	0.0617 (9)	0.0534 (8)	−0.0413 (8)	0.0181 (7)	−0.0175 (7)
C2	0.0631 (9)	0.0805 (10)	0.0669 (9)	−0.0393 (8)	0.0181 (7)	−0.0256 (8)
C3	0.0561 (8)	0.0585 (8)	0.0523 (7)	−0.0224 (6)	0.0110 (6)	−0.0185 (6)
C4	0.0526 (7)	0.0487 (7)	0.0330 (6)	−0.0207 (5)	0.0039 (5)	−0.0070 (5)
C5	0.0549 (7)	0.0518 (7)	0.0487 (7)	−0.0175 (6)	0.0043 (6)	−0.0088 (6)
C6	0.0793 (10)	0.0476 (7)	0.0520 (8)	−0.0192 (7)	0.0090 (7)	−0.0113 (6)
C7	0.1274 (17)	0.0883 (13)	0.1247 (16)	−0.0694 (13)	0.0351 (14)	−0.0441 (12)
C8	0.0430 (6)	0.0459 (6)	0.0378 (6)	−0.0122 (5)	−0.0015 (5)	−0.0083 (5)
C9	0.0436 (6)	0.0390 (6)	0.0385 (6)	−0.0150 (5)	−0.0023 (5)	−0.0078 (5)
C10	0.0473 (6)	0.0432 (6)	0.0399 (6)	−0.0189 (5)	−0.0012 (5)	−0.0094 (5)
C11	0.0663 (8)	0.0466 (7)	0.0539 (7)	−0.0195 (6)	0.0048 (6)	−0.0160 (6)
C12	0.0684 (9)	0.0562 (8)	0.0393 (6)	−0.0335 (7)	−0.0051 (6)	−0.0049 (5)
C13	0.0509 (7)	0.0533 (7)	0.0419 (6)	−0.0211 (6)	−0.0030 (5)	−0.0089 (5)
C14	0.0501 (7)	0.0566 (7)	0.0347 (6)	−0.0276 (6)	−0.0006 (5)	−0.0122 (5)
C15	0.0491 (7)	0.0693 (9)	0.0428 (6)	−0.0290 (6)	0.0004 (5)	−0.0216 (6)
C16	0.0582 (8)	0.0705 (9)	0.0604 (8)	−0.0221 (7)	0.0010 (6)	−0.0276 (7)
C17	0.0632 (9)	0.0857 (11)	0.0916 (12)	−0.0160 (8)	−0.0031 (8)	−0.0463 (10)

C18	0.0562 (9)	0.1257 (17)	0.0902 (13)	−0.0252 (10)	0.0098 (9)	−0.0667 (13)
C19	0.0564 (9)	0.1382 (17)	0.0592 (9)	−0.0450 (10)	0.0129 (7)	−0.0491 (11)
C20	0.0508 (7)	0.0984 (11)	0.0442 (7)	−0.0399 (7)	0.0042 (6)	−0.0274 (7)
C21	0.0708 (9)	0.1096 (13)	0.0367 (7)	−0.0552 (9)	0.0048 (6)	−0.0134 (8)
C22	0.0771 (10)	0.0761 (9)	0.0401 (7)	−0.0446 (8)	−0.0072 (6)	−0.0034 (6)
C23	0.1265 (16)	0.0850 (12)	0.0485 (8)	−0.0569 (12)	−0.0116 (9)	0.0089 (8)
C24	0.151 (2)	0.0634 (10)	0.0639 (11)	−0.0333 (12)	−0.0260 (12)	0.0091 (9)
C25	0.1040 (13)	0.0594 (9)	0.0676 (10)	−0.0148 (9)	−0.0201 (9)	−0.0081 (8)
C26	0.0715 (9)	0.0565 (8)	0.0480 (7)	−0.0221 (7)	−0.0097 (6)	−0.0065 (6)
C27	0.0603 (8)	0.0576 (8)	0.0378 (6)	−0.0308 (6)	−0.0062 (5)	−0.0065 (5)
N1	0.0501 (6)	0.0427 (5)	0.0385 (5)	−0.0179 (4)	−0.0008 (4)	−0.0105 (4)
N2	0.0837 (9)	0.0513 (6)	0.0546 (7)	−0.0321 (6)	0.0017 (6)	−0.0150 (5)
N4	0.0921 (10)	0.0831 (9)	0.0569 (7)	−0.0572 (9)	−0.0091 (7)	−0.0046 (7)
O1	0.0656 (6)	0.0654 (6)	0.0495 (5)	−0.0253 (5)	0.0130 (4)	−0.0253 (5)
O2	0.1427 (12)	0.1039 (10)	0.1091 (10)	−0.0885 (10)	−0.0031 (9)	−0.0309 (8)
O3	0.0747 (8)	0.1167 (11)	0.1149 (11)	−0.0555 (8)	0.0020 (7)	−0.0195 (8)

Geometric parameters (Å, º)

C1—C2	1.378 (2)	C13—H13	0.93
C1—C6	1.383 (2)	C14—C27	1.4085 (18)
C1—C7	1.509 (2)	C14—C15	1.4099 (17)
C2—C3	1.3779 (19)	C15—C16	1.414 (2)
C2—H2	0.93	C15—C20	1.4327 (18)
C3—C4	1.3852 (18)	C16—C17	1.361 (2)
C3—H3	0.93	C16—H16	0.93
C4—C5	1.3835 (18)	C17—C18	1.405 (3)
C4—C8	1.4923 (16)	C17—H17	0.93
C5—C6	1.3814 (18)	C18—C19	1.339 (3)
C5—H5	0.93	C18—H18	0.93
C6—H6	0.93	C19—C20	1.429 (2)
C7—H7A	0.96	C19—H19	0.93
C7—H7B	0.96	C20—C21	1.377 (2)
C7—H7C	0.96	C21—C22	1.390 (2)
C8—O1	1.2133 (13)	C21—H21	0.93
C8—C9	1.4933 (16)	C22—C23	1.415 (2)
C9—C10	1.3289 (15)	C22—C27	1.4426 (18)
C9—N1	1.4332 (14)	C23—C24	1.344 (3)
C10—C14	1.4772 (15)	C23—H23	0.93
C10—H10	0.93	C24—C25	1.411 (3)
C11—N2	1.3029 (17)	C24—H24	0.93
C11—N1	1.3657 (16)	C25—C26	1.355 (2)
C11—H11	0.93	C25—H25	0.93
C12—C13	1.3510 (17)	C26—C27	1.418 (2)
C12—N2	1.3551 (18)	C26—H26	0.93
C12—N4	1.4381 (18)	N4—O2	1.2174 (17)
C13—N1	1.3563 (15)	N4—O3	1.2346 (18)

C2—C1—C6	118.62 (13)	C14—C15—C20	119.28 (13)
C2—C1—C7	120.37 (15)	C16—C15—C20	117.91 (12)
C6—C1—C7	121.01 (15)	C17—C16—C15	121.32 (15)
C1—C2—C3	120.94 (14)	C17—C16—H16	119.3
C1—C2—H2	119.5	C15—C16—H16	119.3
C3—C2—H2	119.5	C16—C17—C18	120.57 (18)
C2—C3—C4	120.40 (13)	C16—C17—H17	119.7
C2—C3—H3	119.8	C18—C17—H17	119.7
C4—C3—H3	119.8	C19—C18—C17	120.34 (16)
C5—C4—C3	118.92 (12)	C19—C18—H18	119.8
C5—C4—C8	123.45 (11)	C17—C18—H18	119.8
C3—C4—C8	117.62 (11)	C18—C19—C20	121.48 (16)
C6—C5—C4	120.24 (13)	C18—C19—H19	119.3
C6—C5—H5	119.9	C20—C19—H19	119.3
C4—C5—H5	119.9	C21—C20—C19	122.36 (14)
C5—C6—C1	120.85 (13)	C21—C20—C15	119.29 (13)
C5—C6—H6	119.6	C19—C20—C15	118.35 (15)
C1—C6—H6	119.6	C20—C21—C22	122.53 (12)
C1—C7—H7A	109.5	C20—C21—H21	118.7
C1—C7—H7B	109.5	C22—C21—H21	118.7
H7A—C7—H7B	109.5	C21—C22—C23	121.93 (14)
C1—C7—H7C	109.5	C21—C22—C27	119.26 (13)
H7A—C7—H7C	109.5	C23—C22—C27	118.78 (16)
H7B—C7—H7C	109.5	C24—C23—C22	121.12 (16)
O1—C8—C4	121.31 (10)	C24—C23—H23	119.4
O1—C8—C9	120.52 (11)	C22—C23—H23	119.4
C4—C8—C9	118.02 (10)	C23—C24—C25	120.55 (16)
C10—C9—N1	121.36 (10)	C23—C24—H24	119.7
C10—C9—C8	122.61 (10)	C25—C24—H24	119.7
N1—C9—C8	115.87 (9)	C26—C25—C24	120.61 (18)
C9—C10—C14	129.89 (10)	C26—C25—H25	119.7
C9—C10—H10	115.1	C24—C25—H25	119.7
C14—C10—H10	115.1	C25—C26—C27	121.12 (14)
N2—C11—N1	112.40 (13)	C25—C26—H26	119.4
N2—C11—H11	123.8	C27—C26—H26	119.4
N1—C11—H11	123.8	C14—C27—C26	123.60 (11)
C13—C12—N2	112.85 (11)	C14—C27—C22	118.59 (13)
C13—C12—N4	125.76 (14)	C26—C27—C22	117.70 (12)
N2—C12—N4	121.39 (13)	C13—N1—C11	106.73 (10)
C12—C13—N1	104.50 (11)	C13—N1—C9	125.53 (10)
C12—C13—H13	127.7	C11—N1—C9	127.71 (11)
N1—C13—H13	127.7	C11—N2—C12	103.51 (11)
C27—C14—C15	121.01 (11)	O2—N4—O3	124.53 (15)
C27—C14—C10	120.56 (11)	O2—N4—C12	118.72 (16)
C15—C14—C10	118.04 (11)	O3—N4—C12	116.74 (13)
C14—C15—C16	122.80 (11)		

C6—C1—C2—C3	−0.8 (2)	C14—C15—C20—C19	178.69 (11)

C7—C1—C2—C3	179.16 (15)	C16—C15—C20—C19	−1.83 (17)
C1—C2—C3—C4	−0.9 (2)	C19—C20—C21—C22	−178.42 (12)
C2—C3—C4—C5	1.47 (19)	C15—C20—C21—C22	1.3 (2)
C2—C3—C4—C8	−179.46 (11)	C20—C21—C22—C23	178.14 (14)
C3—C4—C5—C6	−0.28 (18)	C20—C21—C22—C27	0.1 (2)
C8—C4—C5—C6	−179.29 (11)	C21—C22—C23—C24	−176.94 (16)
C4—C5—C6—C1	−1.5 (2)	C27—C22—C23—C24	1.1 (3)
C2—C1—C6—C5	2.0 (2)	C22—C23—C24—C25	1.6 (3)
C7—C1—C6—C5	−177.96 (14)	C23—C24—C25—C26	−2.0 (3)
C5—C4—C8—O1	127.74 (13)	C24—C25—C26—C27	−0.5 (2)
C3—C4—C8—O1	−51.28 (16)	C15—C14—C27—C26	−174.16 (11)
C5—C4—C8—C9	−56.71 (15)	C10—C14—C27—C26	−1.40 (18)
C3—C4—C8—C9	124.27 (12)	C15—C14—C27—C22	2.01 (17)
O1—C8—C9—C10	161.69 (12)	C10—C14—C27—C22	174.76 (11)
C4—C8—C9—C10	−13.90 (17)	C25—C26—C27—C14	179.39 (13)
O1—C8—C9—N1	−13.70 (16)	C25—C26—C27—C22	3.2 (2)
C4—C8—C9—N1	170.72 (10)	C21—C22—C27—C14	−1.75 (18)
N1—C9—C10—C14	5.68 (19)	C23—C22—C27—C14	−179.84 (13)
C8—C9—C10—C14	−169.46 (11)	C21—C22—C27—C26	174.64 (12)
N2—C12—C13—N1	0.92 (14)	C23—C22—C27—C26	−3.45 (19)
N4—C12—C13—N1	−178.45 (11)	C12—C13—N1—C11	−0.61 (13)
C9—C10—C14—C27	59.15 (18)	C12—C13—N1—C9	−178.63 (10)
C9—C10—C14—C15	−127.88 (14)	N2—C11—N1—C13	0.13 (14)
C27—C14—C15—C16	179.91 (11)	N2—C11—N1—C9	178.09 (10)
C10—C14—C15—C16	6.98 (17)	C10—C9—N1—C13	54.97 (16)
C27—C14—C15—C20	−0.64 (17)	C8—C9—N1—C13	−129.58 (11)
C10—C14—C15—C20	−173.57 (10)	C10—C9—N1—C11	−122.63 (14)
C14—C15—C16—C17	−178.85 (12)	C8—C9—N1—C11	52.83 (15)
C20—C15—C16—C17	1.70 (19)	N1—C11—N2—C12	0.41 (14)
C15—C16—C17—C18	−0.4 (2)	C13—C12—N2—C11	−0.83 (14)
C16—C17—C18—C19	−0.7 (2)	N4—C12—N2—C11	178.56 (11)
C17—C18—C19—C20	0.5 (2)	C13—C12—N4—O2	178.97 (13)
C18—C19—C20—C21	−179.54 (14)	N2—C12—N4—O2	−0.34 (19)
C18—C19—C20—C15	0.8 (2)	C13—C12—N4—O3	−1.7 (2)
C14—C15—C20—C21	−1.03 (17)	N2—C12—N4—O3	178.98 (13)
C16—C15—C20—C21	178.45 (12)		