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N-(3-Nitrophenyl)maleimide

Rodolfo Moreno-Fuquen,[a]* Hoover Valencia,[b] Zulay Diney Pardo,[a] Richard D'Vries[a] and Alan R. Kennedy[c]

[a]Departamento de Química, Facultad de Ciencias, Universidad del Valle, Apartado 25360, Santiago de Cali, Colombia, [b]Departamento de Química, Facultad de Ciencias, Universidad Tecnológica de Pereira, Pereira, Colombia, and [c]Department of Pure and Applied Chemistry, University of Strathclyde, Scotland

Correspondence e-mail: rodimo26@yahoo.es

Key indicators

Single-crystal X-ray study
T = 123 K
Mean σ(C–C) = 0.005 Å
R factor = 0.045
wR factor = 0.119
Data-to-parameter ratio = 7.7

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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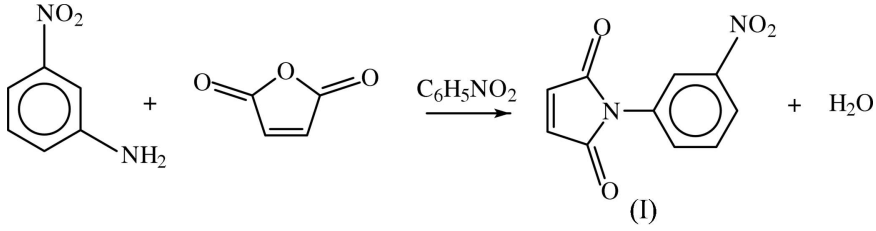
The title compound, $C_{10}H_6N_2O_4$, belongs to a series of *N*-arylmaleimides, which can be used as photoinitiators for free-radical polymerization. The dihedral angles between the planes of the benzene and imide rings are 56.2 (1) and 52.9 (1)° in the two independent molecules in the asymmetric unit.

Comment

There is considerable activity related to the use of *N*-substituted maleimides as photoionizers for free-radical polymerization, where the maleimide can produce the initiating radical species (Pyriadi & Nabeel, 1988; Andersson *et al.*, 1996; Hoyle *et al.*, 1999). In continuing the structural studies on *N*-substituted maleimide systems, to study the behaviour of C_{aryl}—N distance and imide/benzene interplanar angle, the crystal structure determination of *m*-nitrophenylmaleimide, $C_{10}H_6N_2O_4$, (I), was undertaken. The reactivity of *N*-aromatic maleimides in photopolymerization processes as a function of the angle between the maleimide and benzene rings has been analysed (Miller *et al.*, 2000). The *p*-nitrophenylmaleimide (*p*-NPM) system has been reported by our research group (Moreno-Fuquen *et al.*, 2003). This structure has a close analogy to the title compound and it has been used as a model for comparison.



(I)

A perspective view of the two independent molecules in the asymmetric unit of the title compound, showing the atomic numbering scheme, is given in Fig. 1. Focusing on the N—C_{aryl} bond length, in the title compound the N2—C5 and N4—C15 distances are 1.424 (4) and 1.421 (4) Å, respectively. These values are close to the N—C_{aryl} bond length for *p*-nitrophenylmaleimide (Moreno-Fuquen *et al.*, 2003) and are slightly smaller than the average value reported for nine *N*-arylmaleimide derivatives (Miller *et al.*, 2000). The benzene ring mean plane is rotated 56.2 (1) and 52.9 (1)° with respect to the imide ring mean plane. These values are dictated probably by the weak hydrogen bond between an O atom of

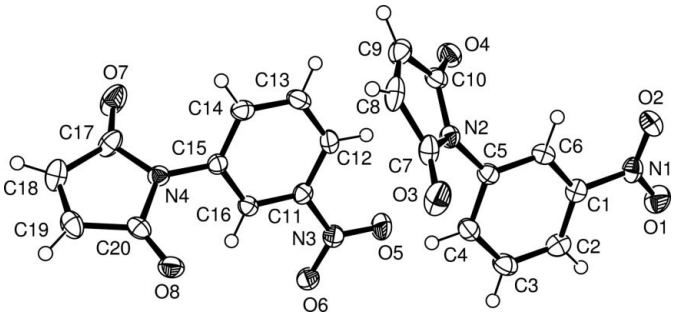


Figure 1
The asymmetric unit of the title compound with the atomic labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radii.

the maleimide group and a C atom of the benzene ring. The rotation is smaller in the case of *p*-NPM, which has an angle of 42.98 (5)°. This is consistent with the literature values, where other maleimides with bulky *ortho* substituents show angles of rotation greater than 80°. Other bond lengths and internal geometrical parameters of the title compound (Table 1) are similar to those in *p*-NPM. There are no significant intermolecular hydrogen bonds in the structure.

Experimental

Reagents and solvents for the synthesis were obtained from Aldrich Chemical Co., and were used without additional purification. The title compound was prepared by taking equimolar quantities of *m*-nitroaniline and maleic anhydride in nitrobenzene and refluxing at 513 K for 3 h. The reaction product was filtered and washed with hexane and then it was dissolved in a mixture of ethyl acetate–hexane (15% hexane) in order to purify it by column chromatography. The solid was crystallized from chloroform, giving pale-yellow prisms with a melting point of 395 (1) K.

Crystal data

$C_{10}H_6N_2O_4$
M_r = 218.17
Orthorhombic, $Pna2_1$
a = 18.9815 (6) Å
b = 6.6643 (2) Å
c = 14.8702 (4) Å
V = 1881.06 (10) Å^3
Z = 8
D_x = 1.541 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 123 (2) K
Prism, pale yellow
0.40 × 0.25 × 0.07 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
4072 measured reflections
2238 independent reflections
1693 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 27.5°
2 standard reflections
frequency: 150 min
intensity decay: 0.1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.119
S = 1.05
2238 reflections
289 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0754P)^2 + 0.0433P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N2—C10	1.393 (4)	C4—C5	1.394 (5)
N2—C7	1.404 (4)	C5—C6	1.392 (4)
N2—C5	1.424 (4)	C8—C9	1.318 (6)
N4—C17	1.400 (5)	C14—C15	1.383 (4)
N4—C20	1.403 (4)	C15—C16	1.386 (5)
N4—C15	1.421 (4)	C18—C19	1.329 (6)
C10—N2—C5	124.8 (3)	C20—N4—C15	124.8 (3)
C7—N2—C5	124.2 (3)	C2—C1—N1	118.8 (3)
C17—N4—C15	124.8 (3)	C16—C11—N3	118.4 (3)
O1—N1—C1—C2	−6.9 (5)	O5—N3—C11—C16	175.7 (3)
C7—N2—C5—C6	116.7 (4)	C20—N4—C15—C16	−47.8 (5)

In the absence of significant anomalous scattering, Friedel pairs were merged. H atoms were located in electron-density difference maps and subsequently treated as riding atoms, with C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *CAD-4 SDP* (Frenz, 1978); program(s) used to solve structure: *SHELXS86* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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m-Nitrophenylmaleimide

Crystal data

$C_{10}H_6N_2O_4$
$M_r = 218.17$
Orthorhombic, $Pna2_1$
Hall symbol: P 2c -2n
$a = 18.9815$ (6) Å
$b = 6.6643$ (2) Å
$c = 14.8702$ (4) Å
$V = 1881.06$ (10) Å^3
$Z = 8$
$F(000) = 896$
$D_x = 1.541$ Mg m^{-3}
Melting point: 395(1) K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 2.6$–$27.5°$
$\mu = 0.12$ mm^{-1}
$T = 123$ K
Prism, pale yellow
0.40 × 0.25 × 0.07 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
4072 measured reflections
2238 independent reflections
1693 reflections with $I > 2\sigma(I)$
$R_{int} = 0.032$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.6°$
$h = -24 \rightarrow 24$
$k = -8 \rightarrow 8$
$l = -19 \rightarrow 19$
2 standard reflections every 150 min
intensity decay: 0.1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.119$
$S = 1.05$
2238 reflections
289 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0754P)^2 + 0.0433P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.39$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.55002 (13)	0.9037 (4)	0.9815 (2)	0.0418 (7)
O2	0.61359 (13)	1.1499 (4)	1.0305 (2)	0.0336 (6)
O3	0.91013 (14)	0.7232 (5)	1.0915 (2)	0.0443 (7)
O4	0.84956 (12)	1.2131 (4)	0.8924 (2)	0.0330 (6)
O5	0.81692 (13)	0.5768 (4)	0.7350 (2)	0.0373 (6)
O6	0.88410 (13)	0.3317 (3)	0.6919 (2)	0.0324 (6)
O7	1.17689 (15)	0.7919 (5)	0.6292 (2)	0.0474 (8)
O8	1.11689 (14)	0.2920 (3)	0.82382 (19)	0.0310 (6)
N1	0.60690 (15)	0.9805 (4)	0.9992 (2)	0.0288 (7)
N2	0.86358 (14)	0.9338 (4)	0.98297 (19)	0.0237 (6)
N3	0.87500 (15)	0.5040 (4)	0.7210 (2)	0.0281 (7)
N4	1.13008 (15)	0.5751 (4)	0.73457 (19)	0.0237 (6)
C1	0.67096 (18)	0.8626 (5)	0.9812 (2)	0.0254 (8)
C2	0.6639 (2)	0.6636 (5)	0.9546 (2)	0.0282 (8)
H2	0.6188	0.6041	0.9476	0.034*
C3	0.7248 (2)	0.5549 (5)	0.9387 (3)	0.0320 (8)
H3	0.7216	0.4178	0.9217	0.038*
C4	0.7910 (2)	0.6447 (5)	0.9473 (3)	0.0279 (8)
H4	0.8326	0.5699	0.9350	0.033*
C5	0.79573 (18)	0.8449 (5)	0.9739 (2)	0.0239 (8)
C6	0.73525 (17)	0.9557 (5)	0.9921 (2)	0.0240 (7)
H6	0.7382	1.0913	1.0114	0.029*
C7	0.91483 (18)	0.8697 (6)	1.0447 (3)	0.0303 (8)
C8	0.97290 (19)	1.0196 (6)	1.0392 (3)	0.0360 (9)
H8	1.0162	1.0124	1.0712	0.043*
C9	0.95494 (19)	1.1638 (5)	0.9830 (3)	0.0323 (8)
H9	0.9827	1.2780	0.9686	0.039*
C10	0.88335 (19)	1.1171 (5)	0.9458 (3)	0.0258 (7)
C11	0.93765 (18)	0.6284 (5)	0.7381 (2)	0.0232 (7)
C12	0.92815 (18)	0.8288 (5)	0.7621 (2)	0.0272 (8)
H12	0.8824	0.8839	0.7696	0.033*
C13	0.9875 (2)	0.9439 (5)	0.7746 (3)	0.0295 (8)
H13	0.9828	1.0820	0.7893	0.035*
C14	1.05406 (19)	0.8610 (5)	0.7661 (2)	0.0266 (8)
H14	1.0945	0.9420	0.7757	0.032*
C15	1.06188 (17)	0.6608 (4)	0.7437 (2)	0.0229 (7)
C16	1.00312 (17)	0.5423 (5)	0.7282 (2)	0.0225 (7)
H16	1.0079	0.4055	0.7111	0.027*
C17	1.18201 (18)	0.6437 (6)	0.6752 (3)	0.0324 (8)
C18	1.24049 (19)	0.4970 (6)	0.6797 (3)	0.0361 (9)
H18	1.2836	0.5061	0.6475	0.043*
C19	1.22294 (19)	0.3507 (5)	0.7361 (3)	0.0332 (8)
H19	1.2515	0.2386	0.7511	0.040*
C20	1.15106 (18)	0.3915 (5)	0.7721 (2)	0.0255 (8)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0213 (14)	0.0482 (16)	0.0558 (18)	−0.0019 (11)	−0.0034 (12)	0.0033 (15)
O2	0.0333 (15)	0.0317 (13)	0.0357 (14)	0.0089 (11)	0.0003 (11)	−0.0034 (12)
O3	0.0297 (14)	0.0605 (18)	0.0427 (17)	0.0091 (13)	0.0019 (12)	0.0226 (16)
O4	0.0307 (13)	0.0293 (13)	0.0389 (14)	0.0035 (11)	−0.0014 (12)	−0.0011 (13)
O5	0.0227 (14)	0.0427 (14)	0.0465 (16)	0.0052 (11)	0.0025 (12)	0.0015 (14)
O6	0.0274 (14)	0.0299 (12)	0.0398 (15)	−0.0047 (10)	0.0007 (11)	−0.0053 (12)
O7	0.0312 (15)	0.0609 (19)	0.0501 (18)	−0.0012 (13)	0.0023 (13)	0.0282 (17)
O8	0.0369 (14)	0.0231 (11)	0.0331 (14)	0.0005 (10)	0.0011 (11)	0.0039 (12)
N1	0.0223 (16)	0.0373 (16)	0.0268 (17)	0.0027 (12)	0.0006 (12)	0.0024 (14)
N2	0.0192 (14)	0.0257 (14)	0.0262 (14)	0.0016 (11)	−0.0003 (12)	0.0003 (13)
N3	0.0265 (17)	0.0298 (15)	0.0281 (17)	0.0009 (13)	0.0011 (13)	0.0014 (14)
N4	0.0228 (14)	0.0224 (13)	0.0259 (15)	−0.0012 (11)	−0.0021 (12)	0.0011 (13)
C1	0.0230 (18)	0.0306 (18)	0.0226 (18)	0.0012 (14)	−0.0027 (14)	0.0028 (15)
C2	0.030 (2)	0.0311 (18)	0.0231 (18)	−0.0067 (15)	−0.0055 (15)	−0.0016 (15)
C3	0.039 (2)	0.0244 (17)	0.0324 (19)	0.0001 (16)	0.0005 (17)	−0.0061 (16)
C4	0.032 (2)	0.0256 (17)	0.0262 (18)	0.0048 (14)	0.0022 (15)	−0.0010 (14)
C5	0.0264 (19)	0.0228 (17)	0.0225 (17)	0.0014 (13)	−0.0010 (14)	0.0001 (14)
C6	0.0275 (19)	0.0218 (15)	0.0225 (17)	0.0007 (13)	−0.0039 (15)	−0.0006 (15)
C7	0.0221 (17)	0.044 (2)	0.0248 (19)	0.0082 (16)	0.0021 (15)	0.0038 (17)
C8	0.0180 (18)	0.060 (3)	0.030 (2)	0.0011 (17)	0.0026 (16)	−0.0065 (19)
C9	0.0289 (19)	0.036 (2)	0.0322 (19)	−0.0068 (14)	0.0047 (16)	−0.0083 (17)
C10	0.0305 (19)	0.0211 (16)	0.0259 (18)	0.0012 (13)	0.0013 (15)	−0.0025 (15)
C11	0.0243 (18)	0.0264 (16)	0.0191 (16)	−0.0019 (13)	0.0015 (14)	−0.0007 (14)
C12	0.0248 (19)	0.0300 (18)	0.027 (2)	0.0042 (14)	0.0049 (15)	−0.0019 (15)
C13	0.041 (2)	0.0191 (15)	0.0281 (19)	0.0035 (15)	0.0051 (17)	0.0000 (16)
C14	0.033 (2)	0.0227 (16)	0.0242 (18)	−0.0028 (14)	0.0021 (16)	0.0020 (14)
C15	0.0232 (18)	0.0231 (16)	0.0224 (16)	0.0009 (13)	0.0021 (14)	0.0033 (14)
C16	0.0257 (17)	0.0221 (16)	0.0197 (17)	0.0014 (13)	0.0011 (14)	−0.0003 (14)
C17	0.0232 (18)	0.046 (2)	0.0284 (19)	−0.0071 (16)	−0.0047 (16)	0.0102 (18)
C18	0.024 (2)	0.055 (2)	0.0290 (19)	0.0010 (17)	0.0001 (16)	0.0011 (17)
C19	0.0251 (18)	0.0362 (18)	0.038 (2)	0.0069 (15)	−0.0074 (17)	−0.0062 (18)
C20	0.0289 (19)	0.0225 (16)	0.0252 (17)	0.0029 (13)	−0.0061 (15)	−0.0062 (15)

Geometric parameters (Å, º)

O1—N1	1.223 (4)	C4—H4	0.950
O2—N1	1.228 (4)	C5—C6	1.392 (4)
O3—C7	1.202 (5)	C6—H6	0.950
O4—C10	1.204 (4)	C7—C8	1.490 (5)
O5—N3	1.222 (4)	C8—C9	1.318 (6)
O6—N3	1.239 (3)	C8—H8	0.950
O7—C17	1.205 (5)	C9—C10	1.500 (5)
O8—C20	1.205 (5)	C9—H9	0.950
N1—C1	1.473 (4)	C11—C16	1.377 (5)
N2—C10	1.393 (4)	C11—C12	1.394 (4)

N2—C7	1.404 (4)	C12—C13	1.375 (5)
N2—C5	1.424 (4)	C12—H12	0.950
N3—C11	1.472 (4)	C13—C14	1.385 (5)
N4—C17	1.400 (5)	C13—H13	0.950
N4—C20	1.403 (4)	C14—C15	1.383 (4)
N4—C15	1.421 (4)	C14—H14	0.950
C1—C6	1.379 (5)	C15—C16	1.386 (5)
C1—C2	1.390 (5)	C16—H16	0.950
C2—C3	1.385 (5)	C17—C18	1.481 (5)
C2—H2	0.950	C18—C19	1.329 (6)
C3—C4	1.398 (5)	C18—H18	0.950
C3—H3	0.950	C19—C20	1.490 (5)
C4—C5	1.394 (5)	C19—H19	0.950

O1—N1—O2	123.9 (3)	C8—C9—C10	108.5 (3)
O1—N1—C1	117.8 (3)	C8—C9—H9	125.7
O2—N1—C1	118.3 (3)	C10—C9—H9	125.7
C10—N2—C7	109.9 (3)	O4—C10—N2	125.7 (3)
C10—N2—C5	124.8 (3)	O4—C10—C9	128.0 (3)
C7—N2—C5	124.2 (3)	N2—C10—C9	106.2 (3)
O5—N3—O6	123.6 (3)	C16—C11—C12	122.9 (3)
O5—N3—C11	118.4 (3)	C16—C11—N3	118.4 (3)
O6—N3—C11	118.0 (3)	C12—C11—N3	118.6 (3)
C17—N4—C20	109.6 (3)	C13—C12—C11	117.6 (3)
C17—N4—C15	124.8 (3)	C13—C12—H12	121.2
C20—N4—C15	124.8 (3)	C11—C12—H12	121.2
C6—C1—C2	123.2 (3)	C12—C13—C14	120.8 (3)
C6—C1—N1	118.0 (3)	C12—C13—H13	119.6
C2—C1—N1	118.8 (3)	C14—C13—H13	119.6
C3—C2—C1	117.9 (3)	C15—C14—C13	120.3 (3)
C3—C2—H2	121.1	C15—C14—H14	119.8
C1—C2—H2	121.1	C13—C14—H14	119.8
C2—C3—C4	120.7 (3)	C14—C15—C16	120.2 (3)
C2—C3—H3	119.6	C14—C15—N4	120.5 (3)
C4—C3—H3	119.6	C16—C15—N4	119.2 (3)
C5—C4—C3	119.5 (3)	C11—C16—C15	118.1 (3)
C5—C4—H4	120.2	C11—C16—H16	121.0
C3—C4—H4	120.2	C15—C16—H16	121.0
C6—C5—C4	120.7 (3)	O7—C17—N4	124.7 (3)
C6—C5—N2	120.4 (3)	O7—C17—C18	128.9 (4)
C4—C5—N2	118.9 (3)	N4—C17—C18	106.5 (3)
C1—C6—C5	117.9 (3)	C19—C18—C17	109.0 (3)
C1—C6—H6	121.0	C19—C18—H18	125.5
C5—C6—H6	121.0	C17—C18—H18	125.5
O3—C7—N2	125.0 (3)	C18—C19—C20	108.8 (3)
O3—C7—C8	129.2 (3)	C18—C19—H19	125.6
N2—C7—C8	105.8 (3)	C20—C19—H19	125.6
C9—C8—C7	109.4 (3)	O8—C20—N4	125.5 (3)

C9—C8—H8	125.3	O8—C20—C19	128.4 (3)
C7—C8—H8	125.3	N4—C20—C19	106.1 (3)
O1—N1—C1—C6	173.4 (3)	O5—N3—C11—C16	175.7 (3)
O2—N1—C1—C6	−6.3 (5)	O6—N3—C11—C16	−5.3 (5)
O1—N1—C1—C2	−6.9 (5)	O5—N3—C11—C12	−5.4 (5)
O2—N1—C1—C2	173.4 (3)	O6—N3—C11—C12	173.6 (3)
C6—C1—C2—C3	0.1 (5)	C16—C11—C12—C13	1.1 (5)
N1—C1—C2—C3	−179.5 (3)	N3—C11—C12—C13	−177.7 (3)
C1—C2—C3—C4	−1.4 (5)	C11—C12—C13—C14	−1.8 (5)
C2—C3—C4—C5	1.3 (6)	C12—C13—C14—C15	0.8 (6)
C3—C4—C5—C6	0.1 (5)	C13—C14—C15—C16	1.0 (5)
C3—C4—C5—N2	179.5 (3)	C13—C14—C15—N4	179.8 (3)
C10—N2—C5—C6	−50.0 (5)	C17—N4—C15—C14	−57.8 (5)
C7—N2—C5—C6	116.7 (4)	C20—N4—C15—C14	133.5 (4)
C10—N2—C5—C4	130.6 (4)	C17—N4—C15—C16	121.0 (4)
C7—N2—C5—C4	−62.7 (5)	C20—N4—C15—C16	−47.8 (5)
C2—C1—C6—C5	1.2 (5)	C12—C11—C16—C15	0.6 (5)
N1—C1—C6—C5	−179.2 (3)	N3—C11—C16—C15	179.5 (3)
C4—C5—C6—C1	−1.3 (5)	C14—C15—C16—C11	−1.7 (5)
N2—C5—C6—C1	179.3 (3)	N4—C15—C16—C11	179.5 (3)
C10—N2—C7—O3	175.1 (4)	C20—N4—C17—O7	175.6 (4)
C5—N2—C7—O3	6.7 (6)	C15—N4—C17—O7	5.4 (6)
C10—N2—C7—C8	−4.5 (4)	C20—N4—C17—C18	−2.9 (4)
C5—N2—C7—C8	−172.9 (3)	C15—N4—C17—C18	−173.1 (3)
O3—C7—C8—C9	−176.2 (4)	O7—C17—C18—C19	−176.9 (4)
N2—C7—C8—C9	3.3 (4)	N4—C17—C18—C19	1.5 (4)
C7—C8—C9—C10	−1.0 (4)	C17—C18—C19—C20	0.4 (4)
C7—N2—C10—O4	−178.0 (3)	C17—N4—C20—O8	−178.0 (3)
C5—N2—C10—O4	−9.7 (6)	C15—N4—C20—O8	−7.7 (6)
C7—N2—C10—C9	3.9 (4)	C17—N4—C20—C19	3.1 (4)
C5—N2—C10—C9	172.3 (3)	C15—N4—C20—C19	173.3 (3)
C8—C9—C10—O4	−179.8 (4)	C18—C19—C20—O8	178.9 (4)
C8—C9—C10—N2	−1.8 (4)	C18—C19—C20—N4	−2.1 (4)