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1,5-Bis(2,3,4,5-tetrafluorobenzoyl)-1,5-diazacyclooctane

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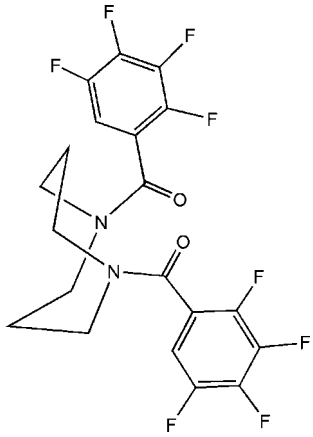
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.049; wR factor = 0.146; data-to-parameter ratio = 13.2.

In the title compound, $C_{20}H_{14}F_8N_2O_2$, the eight-membered 1,5-diazacyclooctane ring adopts a boat–chair conformation. The dihedral angle between the benzene ring planes is 88.81 (11)°.

Related literature

For related literature, see: Bu *et al.* (2001); Du & Bu (2004); Du *et al.* (2000, 2001); Grapperhaus & Darensbourg (1998); Halfen *et al.* (2002); Musker (1992); Watson *et al.* (2006); Zhang & Lu (2007).



Experimental

Crystal data

$C_{20}H_{14}F_8N_2O_2$
M_r = 466.33
Orthorhombic, *Pbcn*
a = 14.8085 (11) Å
b = 20.5518 (16) Å
c = 12.7062 (10) Å
V = 3867.0 (5) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.16 mm^{-1}
T = 295 (2) K
0.36 × 0.30 × 0.24 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.942, T_{max} = 0.962
27117 measured reflections
3805 independent reflections
2837 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.146
S = 1.03
3805 reflections
289 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); 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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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2666).

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supplementary materials

Acta Cryst. (2007). E**63**, o4850 [**doi:10.1107/S1600536807060242**]

1,5-Bis(2,3,4,5-tetrafluorobenzoyl)-1,5-diazacyclooctane

J. Dong, L.-J. Tian and Y. Qu

Comment

1,5-Diazacyclooctane (DACO), the most typical example of diazamesocycles, offers unique conformational requirements and potential for further functionalization (Musker 1992). A number of derivatives of DACO have been prepared by substituting the hydrogen atom on the amine groups with functional pendant arms such as pyridine, imidazole, phenol, carboxylic acid and thioalcohol (Bu *et al.*, 2001; Du & Bu, 2004; Grapperhaus & Darensbourg, 1998). Several strucures of the derivatives such as 1,5-bis(2-pyridylmethyl)-1,5-diazacyclooctane (Halfen *et al.*, 2002), 1,4,8,11-tetraazatricyclo(9.3.3.$3^{4,8}$)icosane (Watson *et al.*, 2006) and 1,5-bis(1-methyl-2-imidazolylmethyl)-1,5-diazoniacyclooctane (Du *et al.*, 2000) have been reported. We herein report the structure of title compound, (I), (Fig. 1).

The DACO ring in (I) adopts the normal boat/chair conformation, and the bond distances and angles are all in normal range (Du *et al.*, 2001; Halfen *et al.*, 2002) with the mean C–C and C–N distances being 1.507 (4) and 1.470 (3) Å, respectively, and the bond angles ranging from 114.27 (19) to 118.07 (18)°. The dihedral angles of two phenyl rings planes and two amide planes are 88.77 (7) and 37.86 (14)°, respectively. The C–O and C–N bond lengths of the amide are similar to those found in *N*,*N*'-bis(2,3,4,5-tetrafluorobenzoyl)piperazine [1.2275 (18)Å and 1.3409 (19) Å, respectively] (Zhang & Lu, 2007). The dihedral angle between the phenyl ring planes is 88.81 (11)°.

Experimental

The title compound was synthesized by the reaction of 2,3,4,5-tetrafluorobenzoyl chloride (2.12 g, 10 mmol) with 1,5-diazacyclooctane (0.57 g, 5 mmol) in the presence of triethylamine (1.01 g, 10 mmol) in ethanol solution (30 ml). Colourless blocks of (I) (yield 78%) were obtained by slow evaporation of an ethanol solution at room temperature.

Refinement

The H atoms were placed at calculated positions (C—H = 0.93–0.97 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C).

Figures

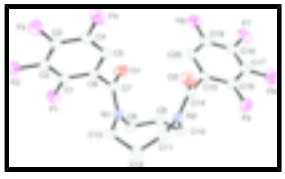


Fig. 1. The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level. H atoms are omitted for clarity.

1,5-Bis(2,3,4,5-tetrafluorobenzoyl)-1,5-diazacyclooctane

Crystal data

$C_{20}H_{14}F_8N_2O_2$	F_{000} = 1888
M_r = 466.33	D_x = 1.602 Mg m^{-3}
Orthorhombic, *Pbcn*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2n 2ab	Cell parameters from 7221 reflections
a = 14.8085 (11) Å	θ = 2.3–21.6º
b = 20.5518 (16) Å	μ = 0.16 mm^{-1}
c = 12.7062 (10) Å	*T* = 295 (2) K
V = 3867.0 (5) Å^3	Block, colourless
Z = 8	0.36 × 0.30 × 0.24 mm

Data collection

Bruker SMART APEX CCD diffractometer	3805 independent reflections
Radiation source: fine-focus sealed tube	2837 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.026
T = 295(2) K	θ_{max} = 26.0º
φ and ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (SADABS; Bruker, 2002)	*h* = −18→18
T_{min} = 0.942, T_{max} = 0.962	*k* = −25→25
27117 measured reflections	*l* = −15→15

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.049	H-atom parameters constrained
$wR(F^2)$ = 0.146	$w = 1/[\sigma^2(F_o^2) + (0.0719P)^2 + 1.346P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.04	$(\Delta/\sigma)_{max} < 0.001$
3805 reflections	$\Delta\rho_{max}$ = 0.50 e Å^{-3}
289 parameters	$\Delta\rho_{min}$ = −0.17 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}
F1	1.03822 (13)	0.40699 (9)	−0.15578 (13)	0.1034 (6)
F2	1.12461 (12)	0.50629 (8)	−0.06219 (14)	0.0970 (5)
F3	1.16418 (12)	0.49973 (7)	0.14554 (15)	0.0955 (5)
F4	1.11569 (13)	0.39500 (7)	0.25721 (11)	0.0916 (5)
F5	0.74987 (11)	0.08897 (8)	0.18853 (14)	0.0910 (5)
F6	0.81750 (14)	−0.03319 (8)	0.18206 (17)	0.1094 (6)
F7	0.99332 (15)	−0.05255 (8)	0.13222 (13)	0.1056 (6)
F8	1.10061 (12)	0.04879 (10)	0.08864 (14)	0.1003 (6)
N1	0.90720 (12)	0.29461 (9)	−0.09016 (14)	0.0599 (5)
N2	0.80349 (12)	0.22324 (9)	0.06928 (14)	0.0579 (5)
O1	1.03989 (12)	0.24206 (10)	−0.06866 (16)	0.0849 (6)
O2	0.87133 (16)	0.23209 (9)	0.22774 (15)	0.0912 (6)
C1	1.05645 (15)	0.40272 (13)	−0.05361 (18)	0.0650 (6)
C2	1.10072 (16)	0.45372 (12)	−0.0062 (2)	0.0663 (6)
C3	1.12042 (16)	0.45057 (11)	0.0988 (2)	0.0641 (6)
C4	1.09579 (16)	0.39645 (12)	0.15442 (18)	0.0619 (6)
C5	1.05293 (15)	0.34503 (11)	0.10727 (17)	0.0586 (5)
H5	1.0381	0.3083	0.1463	0.070*
C6	1.03189 (13)	0.34806 (11)	0.00162 (17)	0.0560 (5)
C7	0.99237 (15)	0.29038 (12)	−0.05516 (17)	0.0593 (5)
C8	0.87319 (18)	0.24394 (13)	−0.16115 (18)	0.0717 (7)
H8A	0.9187	0.2352	−0.2142	0.086*
H8B	0.8200	0.2604	−0.1970	0.086*
C9	0.84910 (18)	0.18079 (13)	−0.10705 (19)	0.0713 (7)
H9A	0.8286	0.1504	−0.1604	0.086*
H9B	0.9038	0.1629	−0.0766	0.086*
C10	0.77848 (16)	0.18371 (12)	−0.02210 (18)	0.0662 (6)
H10A	0.7233	0.2011	−0.0520	0.079*
H10B	0.7658	0.1398	0.0016	0.079*
C11	0.76174 (17)	0.28843 (13)	0.0803 (2)	0.0717 (6)
H11A	0.7957	0.3128	0.1324	0.086*
H11B	0.7009	0.2829	0.1072	0.086*
C12	0.75687 (16)	0.32815 (13)	−0.0184 (2)	0.0761 (7)
H12A	0.7219	0.3670	−0.0037	0.091*
H12B	0.7241	0.3033	−0.0709	0.091*
C13	0.84638 (16)	0.34870 (12)	−0.0655 (2)	0.0716 (7)
H13A	0.8348	0.3731	−0.1294	0.086*
H13B	0.8765	0.3777	−0.0165	0.086*

C14	0.85343 (15)	0.20073 (11)	0.14872 (17)	0.0603 (6)
C15	0.89052 (15)	0.13281 (11)	0.13940 (16)	0.0578 (5)
C16	0.83737 (17)	0.07971 (12)	0.16267 (18)	0.0659 (6)
C17	0.8707 (2)	0.01773 (13)	0.1597 (2)	0.0746 (7)
C18	0.9594 (2)	0.00780 (13)	0.13399 (18)	0.0746 (7)
C19	1.01321 (18)	0.06046 (14)	0.11227 (18)	0.0710 (7)
C20	0.98093 (16)	0.12265 (13)	0.11452 (17)	0.0642 (6)
H20	1.0187	0.1576	0.0997	0.077*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.1175 (14)	0.1279 (14)	0.0649 (10)	−0.0298 (11)	−0.0231 (9)	0.0331 (9)
F2	0.1127 (12)	0.0797 (10)	0.0986 (12)	−0.0191 (9)	−0.0009 (10)	0.0303 (9)
F3	0.1125 (13)	0.0683 (9)	0.1057 (13)	−0.0139 (9)	−0.0222 (10)	−0.0067 (8)
F4	0.1335 (14)	0.0847 (10)	0.0566 (8)	−0.0044 (9)	−0.0140 (8)	−0.0050 (7)
F5	0.0745 (10)	0.0937 (11)	0.1049 (12)	−0.0148 (8)	0.0144 (9)	0.0077 (9)
F6	0.1366 (16)	0.0754 (10)	0.1161 (15)	−0.0261 (10)	0.0034 (12)	0.0104 (10)
F7	0.1576 (17)	0.0815 (11)	0.0776 (11)	0.0311 (11)	−0.0003 (11)	−0.0045 (8)
F8	0.0860 (11)	0.1299 (14)	0.0850 (11)	0.0268 (10)	0.0088 (9)	−0.0015 (10)
N1	0.0538 (10)	0.0715 (12)	0.0543 (10)	−0.0045 (9)	−0.0046 (8)	0.0054 (9)
N2	0.0504 (10)	0.0667 (11)	0.0565 (10)	−0.0085 (8)	−0.0036 (8)	−0.0016 (8)
O1	0.0597 (10)	0.0946 (13)	0.1006 (14)	0.0095 (9)	0.0001 (9)	−0.0280 (11)
O2	0.1234 (16)	0.0831 (12)	0.0671 (11)	0.0120 (11)	−0.0308 (11)	−0.0211 (9)
C1	0.0562 (13)	0.0834 (16)	0.0553 (13)	−0.0008 (12)	−0.0063 (10)	0.0120 (11)
C2	0.0580 (13)	0.0664 (14)	0.0745 (15)	−0.0007 (11)	0.0015 (11)	0.0173 (12)
C3	0.0620 (13)	0.0569 (13)	0.0734 (15)	0.0024 (11)	−0.0034 (11)	−0.0029 (11)
C4	0.0662 (14)	0.0673 (14)	0.0521 (12)	0.0100 (11)	−0.0016 (10)	−0.0026 (10)
C5	0.0603 (13)	0.0609 (13)	0.0545 (12)	0.0051 (10)	0.0076 (10)	0.0038 (10)
C6	0.0434 (10)	0.0687 (13)	0.0559 (12)	0.0029 (10)	0.0032 (9)	0.0040 (10)
C7	0.0500 (12)	0.0741 (14)	0.0537 (12)	0.0008 (11)	0.0052 (9)	−0.0008 (10)
C8	0.0716 (15)	0.0956 (18)	0.0480 (12)	−0.0049 (13)	−0.0106 (11)	−0.0005 (12)
C9	0.0801 (16)	0.0776 (16)	0.0562 (13)	−0.0080 (13)	−0.0150 (12)	−0.0166 (12)
C10	0.0620 (13)	0.0731 (14)	0.0636 (14)	−0.0156 (11)	−0.0180 (11)	−0.0012 (11)
C11	0.0558 (13)	0.0807 (16)	0.0784 (16)	0.0056 (12)	0.0011 (12)	−0.0039 (13)
C12	0.0549 (13)	0.0829 (16)	0.0905 (18)	0.0100 (12)	−0.0161 (13)	−0.0035 (14)
C13	0.0603 (14)	0.0677 (14)	0.0867 (17)	0.0053 (11)	−0.0142 (12)	0.0147 (13)
C14	0.0600 (13)	0.0688 (14)	0.0522 (12)	−0.0085 (11)	−0.0024 (10)	−0.0037 (10)
C15	0.0639 (13)	0.0669 (14)	0.0427 (10)	−0.0081 (11)	−0.0042 (9)	−0.0017 (9)
C16	0.0687 (15)	0.0749 (16)	0.0541 (13)	−0.0068 (12)	0.0009 (11)	−0.0015 (11)
C17	0.099 (2)	0.0675 (16)	0.0574 (14)	−0.0140 (14)	−0.0018 (14)	0.0004 (11)
C18	0.107 (2)	0.0706 (16)	0.0464 (13)	0.0142 (15)	−0.0052 (13)	−0.0056 (11)
C19	0.0711 (16)	0.0952 (19)	0.0466 (12)	0.0102 (14)	0.0014 (11)	−0.0032 (12)
C20	0.0678 (15)	0.0777 (15)	0.0472 (12)	−0.0041 (12)	−0.0031 (10)	0.0008 (10)

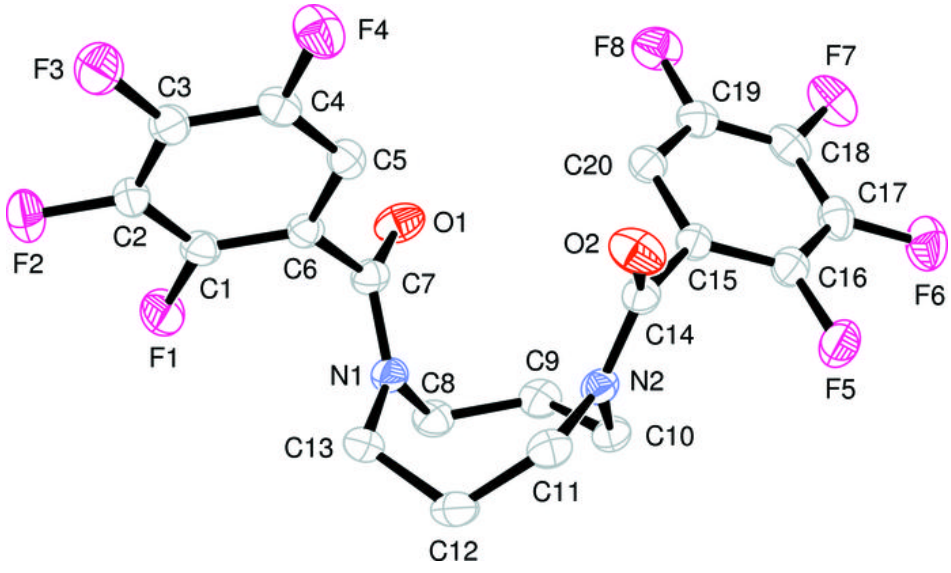
Geometric parameters (Å, °)

F1—C1	1.329 (3)	C8—C9	1.511 (4)
F2—C2	1.341 (3)	C8—H8A	0.9700

F3—C3	1.339 (3)	C8—H8B	0.9700
F4—C4	1.339 (3)	C9—C10	1.504 (4)
F5—C16	1.350 (3)	C9—H9A	0.9700
F6—C17	1.341 (3)	C9—H9B	0.9700
F7—C18	1.339 (3)	C10—H10A	0.9700
F8—C19	1.350 (3)	C10—H10B	0.9700
N1—C7	1.340 (3)	C11—C12	1.498 (4)
N1—C13	1.465 (3)	C11—H11A	0.9700
N1—C8	1.467 (3)	C11—H11B	0.9700
N2—C14	1.334 (3)	C12—C13	1.514 (4)
N2—C10	1.465 (3)	C12—H12A	0.9700
N2—C11	1.482 (3)	C12—H12B	0.9700
O1—C7	1.229 (3)	C13—H13A	0.9700
O2—C14	1.222 (3)	C13—H13B	0.9700
C1—C6	1.374 (3)	C14—C15	1.505 (3)
C1—C2	1.375 (4)	C15—C16	1.378 (3)
C2—C3	1.367 (4)	C15—C20	1.391 (3)
C3—C4	1.367 (3)	C16—C17	1.367 (4)
C4—C5	1.371 (3)	C17—C18	1.368 (4)
C5—C6	1.380 (3)	C18—C19	1.372 (4)
C5—H5	0.9300	C19—C20	1.365 (4)
C6—C7	1.506 (3)	C20—H20	0.9300
C7—N1—C13	123.8 (2)	N2—C10—H10B	108.6
C7—N1—C8	118.8 (2)	C9—C10—H10B	108.6
C13—N1—C8	117.35 (19)	H10A—C10—H10B	107.6
C14—N2—C10	123.21 (19)	N2—C11—C12	115.7 (2)
C14—N2—C11	118.26 (19)	N2—C11—H11A	108.4
C10—N2—C11	118.07 (18)	C12—C11—H11A	108.4
F1—C1—C6	120.0 (2)	N2—C11—H11B	108.4
F1—C1—C2	118.3 (2)	C12—C11—H11B	108.4
C6—C1—C2	121.7 (2)	H11A—C11—H11B	107.4
F2—C2—C3	120.0 (2)	C11—C12—C13	116.1 (2)
F2—C2—C1	120.5 (2)	C11—C12—H12A	108.3
C3—C2—C1	119.6 (2)	C13—C12—H12A	108.3
F3—C3—C4	120.9 (2)	C11—C12—H12B	108.3
F3—C3—C2	120.0 (2)	C13—C12—H12B	108.3
C4—C3—C2	119.1 (2)	H12A—C12—H12B	107.4
F4—C4—C3	117.6 (2)	N1—C13—C12	114.3 (2)
F4—C4—C5	120.7 (2)	N1—C13—H13A	108.7
C3—C4—C5	121.7 (2)	C12—C13—H13A	108.7
C4—C5—C6	119.7 (2)	N1—C13—H13B	108.7
C4—C5—H5	120.2	C12—C13—H13B	108.7
C6—C5—H5	120.2	H13A—C13—H13B	107.6
C1—C6—C5	118.3 (2)	O2—C14—N2	124.0 (2)
C1—C6—C7	120.1 (2)	O2—C14—C15	118.3 (2)
C5—C6—C7	121.2 (2)	N2—C14—C15	117.67 (19)
O1—C7—N1	123.0 (2)	C16—C15—C20	118.7 (2)
O1—C7—C6	118.7 (2)	C16—C15—C14	120.6 (2)
N1—C7—C6	118.3 (2)	C20—C15—C14	120.5 (2)

N1—C8—C9	114.27 (19)	F5—C16—C17	119.0 (2)
N1—C8—H8A	108.7	F5—C16—C15	119.3 (2)
C9—C8—H8A	108.7	C17—C16—C15	121.7 (2)
N1—C8—H8B	108.7	F6—C17—C16	120.6 (3)
C9—C8—H8B	108.7	F6—C17—C18	119.9 (3)
H8A—C8—H8B	107.6	C16—C17—C18	119.5 (2)
C10—C9—C8	117.1 (2)	F7—C18—C17	120.2 (3)
C10—C9—H9A	108.0	F7—C18—C19	120.6 (3)
C8—C9—H9A	108.0	C17—C18—C19	119.2 (2)
C10—C9—H9B	108.0	F8—C19—C20	120.5 (3)
C8—C9—H9B	108.0	F8—C19—C18	117.5 (2)
H9A—C9—H9B	107.3	C20—C19—C18	122.1 (2)
N2—C10—C9	114.53 (18)	C19—C20—C15	118.8 (2)
N2—C10—H10A	108.6	C19—C20—H20	120.6
C9—C10—H10A	108.6	C15—C20—H20	120.6
F1—C1—C2—F2	0.0 (4)	C14—N2—C11—C12	144.2 (2)
C6—C1—C2—F2	179.4 (2)	C10—N2—C11—C12	−43.4 (3)
F1—C1—C2—C3	−179.9 (2)	N2—C11—C12—C13	−65.1 (3)
C6—C1—C2—C3	−0.5 (4)	C7—N1—C13—C12	−126.1 (2)
F2—C2—C3—F3	−0.5 (4)	C8—N1—C13—C12	56.7 (3)
C1—C2—C3—F3	179.4 (2)	C11—C12—C13—N1	57.1 (3)
F2—C2—C3—C4	−179.8 (2)	C10—N2—C14—O2	−176.4 (2)
C1—C2—C3—C4	0.2 (4)	C11—N2—C14—O2	−4.4 (3)
F3—C3—C4—F4	1.1 (3)	C10—N2—C14—C15	4.2 (3)
C2—C3—C4—F4	−179.7 (2)	C11—N2—C14—C15	176.21 (19)
F3—C3—C4—C5	−178.4 (2)	O2—C14—C15—C16	99.4 (3)
C2—C3—C4—C5	0.8 (4)	N2—C14—C15—C16	−81.2 (3)
F4—C4—C5—C6	179.0 (2)	O2—C14—C15—C20	−75.9 (3)
C3—C4—C5—C6	−1.5 (3)	N2—C14—C15—C20	103.5 (2)
F1—C1—C6—C5	179.2 (2)	C20—C15—C16—F5	179.0 (2)
C2—C1—C6—C5	−0.2 (3)	C14—C15—C16—F5	3.6 (3)
F1—C1—C6—C7	5.8 (3)	C20—C15—C16—C17	−1.4 (3)
C2—C1—C6—C7	−173.6 (2)	C14—C15—C16—C17	−176.8 (2)
C4—C5—C6—C1	1.2 (3)	F5—C16—C17—F6	0.0 (4)
C4—C5—C6—C7	174.5 (2)	C15—C16—C17—F6	−179.6 (2)
C13—N1—C7—O1	173.3 (2)	F5—C16—C17—C18	−179.7 (2)
C8—N1—C7—O1	−9.5 (3)	C15—C16—C17—C18	0.7 (4)
C13—N1—C7—C6	−7.8 (3)	F6—C17—C18—F7	−0.7 (4)
C8—N1—C7—C6	169.4 (2)	C16—C17—C18—F7	179.0 (2)
C1—C6—C7—O1	105.0 (3)	F6—C17—C18—C19	−179.4 (2)
C5—C6—C7—O1	−68.2 (3)	C16—C17—C18—C19	0.4 (4)
C1—C6—C7—N1	−73.9 (3)	F7—C18—C19—F8	0.4 (3)
C5—C6—C7—N1	112.9 (2)	C17—C18—C19—F8	179.1 (2)
C7—N1—C8—C9	76.8 (3)	F7—C18—C19—C20	−179.3 (2)
C13—N1—C8—C9	−105.8 (3)	C17—C18—C19—C20	−0.6 (4)
N1—C8—C9—C10	59.0 (3)	F8—C19—C20—C15	−179.9 (2)
C14—N2—C10—C9	−83.7 (3)	C18—C19—C20—C15	−0.2 (3)
C11—N2—C10—C9	104.3 (2)	C16—C15—C20—C19	1.1 (3)
C8—C9—C10—N2	−63.2 (3)	C14—C15—C20—C19	176.6 (2)

Fig. 1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