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1,2,7,8-Tetramethyl-4,5-dihydro-3a,5a-diazapyrene ditriflate

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Key indicators

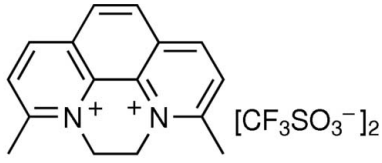
Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.003 Å
R factor = 0.047
wR factor = 0.131
Data-to-parameter ratio = 16.6

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

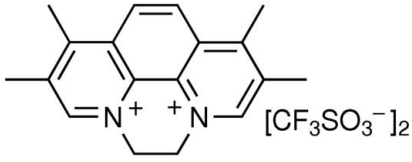
The title structure, $C_{18}H_{20}N_2^{2+}\cdot 2CF_3O_3S^-$, is the first to be reported for a diquaternized derivative of 3,4,7,8-tetramethyl-1,10-phenanthroline.

Comment

Relevant background information on this work and comments on the title structure, (II), together with that of the closely related salt 3,6-dimethyl-4,5-dihydro-3a,5a-diazapyrene ditriflate, (I), can be found in the preceding paper (Coe, Fitzgerald & Raftery, 2006). The molecular structure of (II) is shown in Fig. 1 and selected geometric parameters are given in Table 1.



(I)



(II)

Experimental

Salt (II) was synthesized as reported previously (Coe, Curati & Fitzgerald, 2006). Crystals suitable for single-crystal X-ray diffraction were obtained by slow diffusion of diethyl ether vapour into an acetone solution of (II) at 295 K.

Crystal data

$C_{18}H_{20}N_2^{2+}\cdot 2CF_3O_3S^-$
M_r = 562.50
Monoclinic, $P2_1/c$
a = 12.882 (1) Å
b = 8.152 (1) Å
c = 22.585 (1) Å
β = 104.284 (1)°
V = 2298.4 (2) Å^3
Z = 4
D_x = 1.626 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.32 mm^{-1}
T = 100 (2) K
Block, white
0.45 × 0.30 × 0.20 mm

Data collection

Bruker SMART APEX CCD diffractometer
φ and ω scans
Absorption correction: none
19382 measured reflections
5467 independent reflections
4426 reflections with $I > 2\sigma(I)$
R_{int} = 0.058
θ_{max} = 28.3°

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0667P)^2 + 1.2422P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.047$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.131$	$\Delta\rho_{max} = 0.81$ e Å^{-3}
$S = 1.08$	$\Delta\rho_{min} = -0.67$ e Å^{-3}
5467 reflections	
329 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

C1—N1	1.364 (2)	C7—C8	1.355 (3)
C1—C9	1.404 (3)	C8—C9	1.434 (3)
C1—C2	1.433 (3)	C9—C10	1.427 (3)
C2—N2	1.369 (2)	C10—C11	1.388 (3)
C2—C6	1.399 (3)	C10—C17	1.501 (3)
C3—N2	1.330 (2)	C11—C12	1.395 (3)
C3—C4	1.393 (3)	C11—C18	1.503 (3)
C4—C5	1.385 (3)	C12—N1	1.329 (2)
C4—C15	1.505 (3)	C13—N1	1.483 (2)
C5—C6	1.430 (3)	C13—C14	1.504 (3)
C5—C16	1.501 (3)	C14—N2	1.479 (2)
C6—C7	1.435 (3)		
N1—C1—C2	119.87 (17)	N2—C14—C13	108.35 (15)
N2—C2—C1	119.65 (17)	C1—N1—C13	118.55 (15)
N1—C13—C14	108.40 (15)	C2—N2—C14	117.71 (15)
N1—C13—C14—N2	−58.83 (19)		

All H atoms were included in calculated positions, with C—H = 0.95 (CH), 0.99 (CH_2) and 0.98 Å (CH_3); U_{iso}(H) values were fixed at $1.2U_{eq}$(C) or $1.5U_{eq}$(methyl C).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

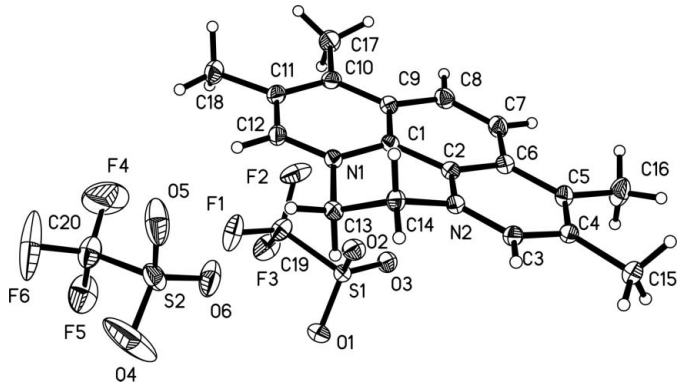


Figure 1
The asymmetric unit of (II), showing 50% probability displacement ellipsoids.

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supporting information

Acta Cryst. (2006). E**62**, o4335–o4336 [https://doi.org/10.1107/S1600536806035379]

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$M_r = 562.50$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 12.8820\ (7)$ Å
$b = 8.1520\ (4)$ Å
$c = 22.5850\ (12)$ Å
$\beta = 104.284\ (1)°$
$V = 2298.4\ (2)$ Å^3
$Z = 4$
$F(000) = 1152$
$D_x = 1.626$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7763 reflections
$\theta = 2.8–28.2°$
$\mu = 0.32$ mm^{-1}
$T = 100$ K
Plate, white
0.45 × 0.30 × 0.20 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
19382 measured reflections
5467 independent reflections
4426 reflections with $I > 2\sigma(I)$
$R_{int} = 0.058$
$\theta_{max} = 28.3°$, $\theta_{min} = 1.6°$
$h = -17\rightarrow17$
$k = -10\rightarrow10$
$l = -29\rightarrow28$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.131$
$S = 1.08$
5467 reflections
329 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
$w = 1/[\sigma^2(F_o^2) + (0.0667P)^2 + 1.2422P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.81$ e Å^{-3}
$\Delta\rho_{min} = -0.67$ 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}
C1	0.08483 (15)	0.0957 (2)	0.11781 (9)	0.0156 (4)
C2	−0.02962 (15)	0.1074 (2)	0.09903 (9)	0.0156 (4)
C3	−0.19641 (15)	0.0541 (2)	0.12015 (9)	0.0176 (4)
H3	−0.2360	0.0051	0.1458	0.021*
C4	−0.25087 (15)	0.1421 (2)	0.06899 (9)	0.0177 (4)
C5	−0.19378 (16)	0.2071 (2)	0.03000 (9)	0.0196 (4)
C6	−0.07995 (15)	0.1883 (2)	0.04492 (9)	0.0175 (4)
C7	−0.01382 (16)	0.2462 (3)	0.00665 (9)	0.0214 (4)
H7	−0.0461	0.3025	−0.0301	0.026*
C8	0.09358 (16)	0.2223 (3)	0.02173 (9)	0.0211 (4)
H8	0.1342	0.2561	−0.0060	0.025*
C9	0.14745 (15)	0.1474 (2)	0.07845 (9)	0.0172 (4)
C10	0.26105 (15)	0.1317 (2)	0.09824 (9)	0.0190 (4)
C11	0.30618 (15)	0.0739 (2)	0.15676 (9)	0.0195 (4)
C12	0.23917 (15)	0.0322 (2)	0.19440 (9)	0.0184 (4)
H12	0.2701	−0.0045	0.2348	0.022*
C13	0.06579 (15)	0.0115 (2)	0.21866 (9)	0.0168 (4)
H13A	0.0487	0.1164	0.2362	0.020*
H13B	0.1047	−0.0594	0.2525	0.020*
C14	−0.03566 (15)	−0.0715 (2)	0.18461 (9)	0.0165 (4)
H14A	−0.0187	−0.1781	0.1682	0.020*
H14B	−0.0827	−0.0921	0.2125	0.020*
C15	−0.37036 (15)	0.1594 (3)	0.05822 (10)	0.0217 (4)
H15A	−0.3905	0.2748	0.0504	0.032*
H15B	−0.3926	0.1216	0.0944	0.032*
H15C	−0.4059	0.0930	0.0228	0.032*
C16	−0.25076 (18)	0.2982 (3)	−0.02644 (10)	0.0299 (5)
H16A	−0.3246	0.2584	−0.0399	0.045*
H16B	−0.2137	0.2798	−0.0589	0.045*
H16C	−0.2511	0.4157	−0.0174	0.045*
C17	0.33141 (17)	0.1812 (3)	0.05728 (10)	0.0259 (5)
H17A	0.3547	0.2951	0.0659	0.039*
H17B	0.2912	0.1716	0.0145	0.039*
H17C	0.3943	0.1093	0.0647	0.039*
C18	0.42501 (16)	0.0582 (3)	0.18268 (10)	0.0256 (5)
H18A	0.4543	−0.0210	0.1584	0.038*
H18B	0.4391	0.0201	0.2251	0.038*
H18C	0.4591	0.1652	0.1814	0.038*
C19	0.29745 (17)	0.5445 (3)	0.19959 (11)	0.0245 (4)
C20	0.41878 (19)	0.1440 (3)	0.39136 (12)	0.0326 (5)
F1	0.33941 (11)	0.45210 (19)	0.24792 (8)	0.0426 (4)
F2	0.32142 (11)	0.47396 (18)	0.15109 (7)	0.0379 (4)
F3	0.34766 (11)	0.68971 (17)	0.20785 (7)	0.0354 (3)
F4	0.46066 (15)	0.1354 (3)	0.34373 (11)	0.0848 (8)
F5	0.43790 (12)	0.29605 (19)	0.41287 (8)	0.0491 (4)

F6	0.47371 (16)	0.0461 (2)	0.43370 (12)	0.0923 (9)
N1	0.13323 (13)	0.0425 (2)	0.17525 (7)	0.0153 (3)
N2	−0.09044 (12)	0.0369 (2)	0.13402 (7)	0.0152 (3)
O1	0.14522 (12)	0.65279 (18)	0.24348 (6)	0.0224 (3)
O2	0.11371 (12)	0.40314 (18)	0.18258 (7)	0.0243 (3)
O3	0.12341 (12)	0.6681 (2)	0.13390 (7)	0.0257 (3)
O4	0.2466 (2)	0.1162 (5)	0.42530 (11)	0.1106 (14)
O5	0.27358 (16)	−0.0663 (2)	0.34630 (9)	0.0495 (6)
O6	0.23670 (15)	0.2165 (2)	0.32313 (9)	0.0448 (5)
S1	0.15330 (4)	0.56891 (6)	0.18837 (2)	0.01698 (13)
S2	0.27643 (4)	0.09789 (8)	0.36958 (2)	0.02868 (16)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0166 (9)	0.0146 (9)	0.0145 (9)	0.0008 (7)	0.0016 (7)	−0.0027 (7)
C2	0.0157 (9)	0.0156 (9)	0.0151 (9)	−0.0002 (7)	0.0034 (7)	−0.0022 (7)
C3	0.0153 (9)	0.0189 (9)	0.0186 (9)	−0.0006 (7)	0.0040 (7)	−0.0029 (7)
C4	0.0158 (9)	0.0171 (9)	0.0191 (9)	0.0015 (7)	0.0018 (7)	−0.0040 (7)
C5	0.0179 (9)	0.0213 (10)	0.0175 (9)	0.0030 (7)	0.0006 (7)	0.0000 (8)
C6	0.0171 (9)	0.0184 (9)	0.0164 (9)	0.0011 (7)	0.0028 (7)	−0.0008 (7)
C7	0.0223 (10)	0.0258 (11)	0.0151 (9)	0.0011 (8)	0.0030 (8)	0.0028 (8)
C8	0.0201 (10)	0.0266 (11)	0.0170 (9)	−0.0018 (8)	0.0055 (7)	−0.0002 (8)
C9	0.0157 (9)	0.0186 (9)	0.0168 (9)	−0.0004 (7)	0.0028 (7)	−0.0028 (7)
C10	0.0163 (9)	0.0196 (10)	0.0212 (10)	−0.0006 (7)	0.0049 (7)	−0.0051 (8)
C11	0.0152 (9)	0.0198 (10)	0.0222 (10)	0.0004 (7)	0.0020 (7)	−0.0048 (8)
C12	0.0166 (9)	0.0171 (9)	0.0191 (9)	0.0016 (7)	−0.0002 (7)	−0.0021 (7)
C13	0.0176 (9)	0.0193 (9)	0.0135 (9)	0.0005 (7)	0.0034 (7)	0.0000 (7)
C14	0.0164 (9)	0.0165 (9)	0.0154 (9)	0.0010 (7)	0.0019 (7)	0.0023 (7)
C15	0.0156 (9)	0.0247 (10)	0.0239 (10)	0.0016 (8)	0.0036 (8)	−0.0004 (8)
C16	0.0217 (11)	0.0397 (14)	0.0264 (11)	0.0060 (9)	0.0023 (9)	0.0119 (10)
C17	0.0186 (10)	0.0363 (13)	0.0240 (11)	−0.0016 (9)	0.0073 (8)	−0.0023 (9)
C18	0.0151 (10)	0.0341 (12)	0.0260 (11)	0.0015 (8)	0.0018 (8)	−0.0005 (9)
C19	0.0192 (10)	0.0205 (10)	0.0339 (12)	0.0005 (8)	0.0070 (9)	0.0026 (9)
C20	0.0246 (11)	0.0269 (12)	0.0411 (14)	−0.0015 (9)	−0.0016 (10)	0.0042 (10)
F1	0.0236 (7)	0.0438 (9)	0.0533 (10)	0.0043 (6)	−0.0037 (6)	0.0211 (7)
F2	0.0319 (7)	0.0327 (8)	0.0566 (10)	0.0036 (6)	0.0251 (7)	−0.0068 (7)
F3	0.0248 (7)	0.0250 (7)	0.0571 (9)	−0.0071 (5)	0.0116 (6)	−0.0029 (6)
F4	0.0396 (10)	0.127 (2)	0.0984 (17)	−0.0115 (12)	0.0374 (11)	−0.0415 (16)
F5	0.0384 (9)	0.0333 (8)	0.0651 (11)	−0.0111 (7)	−0.0075 (8)	−0.0052 (8)
F6	0.0620 (12)	0.0471 (11)	0.1228 (19)	−0.0214 (9)	−0.0630 (13)	0.0411 (12)
N1	0.0152 (8)	0.0154 (8)	0.0144 (8)	0.0002 (6)	0.0020 (6)	−0.0013 (6)
N2	0.0150 (8)	0.0155 (8)	0.0145 (8)	0.0006 (6)	0.0024 (6)	−0.0006 (6)
O1	0.0299 (8)	0.0199 (7)	0.0184 (7)	−0.0013 (6)	0.0078 (6)	−0.0024 (6)
O2	0.0233 (8)	0.0209 (8)	0.0288 (8)	−0.0034 (6)	0.0065 (6)	−0.0061 (6)
O3	0.0264 (8)	0.0315 (8)	0.0190 (7)	0.0069 (6)	0.0051 (6)	0.0044 (6)
O4	0.0672 (17)	0.236 (4)	0.0405 (13)	−0.080 (2)	0.0354 (12)	−0.0597 (19)
O5	0.0530 (12)	0.0271 (9)	0.0497 (12)	−0.0114 (8)	−0.0231 (9)	0.0104 (8)

O6	0.0371 (10)	0.0260 (9)	0.0555 (12)	0.0093 (7)	−0.0188 (9)	−0.0055 (8)
S1	0.0166 (2)	0.0177 (2)	0.0162 (2)	0.00113 (17)	0.00335 (17)	−0.00091 (18)
S2	0.0228 (3)	0.0432 (4)	0.0186 (3)	−0.0093 (2)	0.0025 (2)	−0.0046 (2)

Geometric parameters (Å, º)

C1—N1	1.364 (2)	C14—H14A	0.9900
C1—C9	1.404 (3)	C14—H14B	0.9900
C1—C2	1.433 (3)	C15—H15A	0.9800
C2—N2	1.369 (2)	C15—H15B	0.9800
C2—C6	1.399 (3)	C15—H15C	0.9800
C3—N2	1.330 (2)	C16—H16A	0.9800
C3—C4	1.393 (3)	C16—H16B	0.9800
C3—H3	0.9500	C16—H16C	0.9800
C4—C5	1.385 (3)	C17—H17A	0.9800
C4—C15	1.505 (3)	C17—H17B	0.9800
C5—C6	1.430 (3)	C17—H17C	0.9800
C5—C16	1.501 (3)	C18—H18A	0.9800
C6—C7	1.435 (3)	C18—H18B	0.9800
C7—C8	1.355 (3)	C18—H18C	0.9800
C7—H7	0.9500	C19—F1	1.326 (3)
C8—C9	1.434 (3)	C19—F2	1.339 (3)
C8—H8	0.9500	C19—F3	1.340 (2)
C9—C10	1.427 (3)	C19—S1	1.822 (2)
C10—C11	1.388 (3)	C20—F6	1.311 (3)
C10—C17	1.501 (3)	C20—F4	1.319 (3)
C11—C12	1.395 (3)	C20—F5	1.332 (3)
C11—C18	1.503 (3)	C20—S2	1.817 (2)
C12—N1	1.329 (2)	O1—S1	1.4461 (15)
C12—H12	0.9500	O2—S1	1.4389 (15)
C13—N1	1.483 (2)	O3—S1	1.4430 (15)
C13—C14	1.504 (3)	O4—S2	1.411 (2)
C13—H13A	0.9900	O5—S2	1.435 (2)
C13—H13B	0.9900	O6—S2	1.4257 (19)
C14—N2	1.479 (2)		

N1—C1—C9	119.88 (17)	C4—C15—H15C	109.5
N1—C1—C2	119.87 (17)	H15A—C15—H15C	109.5
C9—C1—C2	120.15 (17)	H15B—C15—H15C	109.5
N2—C2—C6	119.61 (17)	C5—C16—H16A	109.5
N2—C2—C1	119.65 (17)	C5—C16—H16B	109.5
C6—C2—C1	120.73 (17)	H16A—C16—H16B	109.5
N2—C3—C4	121.80 (18)	C5—C16—H16C	109.5
N2—C3—H3	119.1	H16A—C16—H16C	109.5
C4—C3—H3	119.1	H16B—C16—H16C	109.5
C5—C4—C3	119.13 (17)	C10—C17—H17A	109.5
C5—C4—C15	122.96 (18)	C10—C17—H17B	109.5
C3—C4—C15	117.90 (18)	H17A—C17—H17B	109.5

C4—C5—C6	118.93 (17)	C10—C17—H17C	109.5
C4—C5—C16	120.29 (18)	H17A—C17—H17C	109.5
C6—C5—C16	120.77 (18)	H17B—C17—H17C	109.5
C2—C6—C5	118.95 (18)	C11—C18—H18A	109.5
C2—C6—C7	117.71 (17)	C11—C18—H18B	109.5
C5—C6—C7	123.34 (18)	H18A—C18—H18B	109.5
C8—C7—C6	121.52 (18)	C11—C18—H18C	109.5
C8—C7—H7	119.2	H18A—C18—H18C	109.5
C6—C7—H7	119.2	H18B—C18—H18C	109.5
C7—C8—C9	121.64 (18)	F1—C19—F2	107.46 (18)
C7—C8—H8	119.2	F1—C19—F3	107.60 (18)
C9—C8—H8	119.2	F2—C19—F3	107.00 (17)
C1—C9—C10	118.68 (17)	F1—C19—S1	111.77 (15)
C1—C9—C8	117.79 (17)	F2—C19—S1	111.47 (15)
C10—C9—C8	123.43 (18)	F3—C19—S1	111.30 (14)
C11—C10—C9	119.01 (18)	F6—C20—F4	107.9 (3)
C11—C10—C17	120.21 (18)	F6—C20—F5	106.4 (2)
C9—C10—C17	120.76 (18)	F4—C20—F5	105.7 (2)
C10—C11—C12	119.09 (18)	F6—C20—S2	113.50 (18)
C10—C11—C18	123.14 (19)	F4—C20—S2	110.91 (18)
C12—C11—C18	117.75 (18)	F5—C20—S2	112.01 (17)
N1—C12—C11	121.79 (18)	C12—N1—C1	121.42 (17)
N1—C12—H12	119.1	C12—N1—C13	119.76 (16)
C11—C12—H12	119.1	C1—N1—C13	118.55 (15)
N1—C13—C14	108.40 (15)	C3—N2—C2	121.33 (16)
N1—C13—H13A	110.0	C3—N2—C14	120.74 (16)
C14—C13—H13A	110.0	C2—N2—C14	117.71 (15)
N1—C13—H13B	110.0	O2—S1—O3	115.78 (9)
C14—C13—H13B	110.0	O2—S1—O1	115.03 (9)
H13A—C13—H13B	108.4	O3—S1—O1	114.08 (9)
N2—C14—C13	108.35 (15)	O2—S1—C19	103.66 (9)
N2—C14—H14A	110.0	O3—S1—C19	103.20 (10)
C13—C14—H14A	110.0	O1—S1—C19	102.66 (10)
N2—C14—H14B	110.0	O4—S2—O6	117.2 (2)
C13—C14—H14B	110.0	O4—S2—O5	115.9 (2)
H14A—C14—H14B	108.4	O6—S2—O5	113.02 (11)
C4—C15—H15A	109.5	O4—S2—C20	102.44 (13)
C4—C15—H15B	109.5	O6—S2—C20	102.36 (12)
H15A—C15—H15B	109.5	O5—S2—C20	103.00 (12)

N1—C1—C2—N2	−12.2 (3)	C18—C11—C12—N1	179.98 (18)
C9—C1—C2—N2	171.28 (17)	N1—C13—C14—N2	−58.83 (19)
N1—C1—C2—C6	168.58 (17)	C11—C12—N1—C1	−0.5 (3)
C9—C1—C2—C6	−7.9 (3)	C11—C12—N1—C13	−174.41 (17)
N2—C3—C4—C5	2.9 (3)	C9—C1—N1—C12	−2.6 (3)
N2—C3—C4—C15	−178.04 (18)	C2—C1—N1—C12	−179.12 (17)
C3—C4—C5—C6	−2.7 (3)	C9—C1—N1—C13	171.34 (17)
C15—C4—C5—C6	178.30 (18)	C2—C1—N1—C13	−5.2 (3)

C3—C4—C5—C16	178.20 (19)	C14—C13—N1—C12	−145.00 (17)
C15—C4—C5—C16	−0.8 (3)	C14—C13—N1—C1	40.9 (2)
N2—C2—C6—C5	5.1 (3)	C4—C3—N2—C2	1.1 (3)
C1—C2—C6—C5	−175.67 (17)	C4—C3—N2—C14	−173.38 (17)
N2—C2—C6—C7	−173.98 (18)	C6—C2—N2—C3	−5.1 (3)
C1—C2—C6—C7	5.2 (3)	C1—C2—N2—C3	175.66 (17)
C4—C5—C6—C2	−1.2 (3)	C6—C2—N2—C14	169.46 (17)
C16—C5—C6—C2	177.84 (19)	C1—C2—N2—C14	−9.7 (2)
C4—C5—C6—C7	177.84 (19)	C13—C14—N2—C3	−139.88 (18)
C16—C5—C6—C7	−3.1 (3)	C13—C14—N2—C2	45.5 (2)
C2—C6—C7—C8	0.7 (3)	F1—C19—S1—O2	−57.66 (18)
C5—C6—C7—C8	−178.4 (2)	F2—C19—S1—O2	62.62 (17)
C6—C7—C8—C9	−4.0 (3)	F3—C19—S1—O2	−178.00 (15)
N1—C1—C9—C10	4.4 (3)	F1—C19—S1—O3	−178.78 (16)
C2—C1—C9—C10	−179.06 (17)	F2—C19—S1—O3	−58.49 (17)
N1—C1—C9—C8	−171.96 (17)	F3—C19—S1—O3	60.88 (18)
C2—C1—C9—C8	4.5 (3)	F1—C19—S1—O1	62.40 (17)
C7—C8—C9—C1	1.3 (3)	F2—C19—S1—O1	−177.32 (14)
C7—C8—C9—C10	−174.9 (2)	F3—C19—S1—O1	−57.94 (18)
C1—C9—C10—C11	−3.3 (3)	F6—C20—S2—O4	59.4 (3)
C8—C9—C10—C11	172.95 (19)	F4—C20—S2—O4	−178.9 (3)
C1—C9—C10—C17	178.44 (18)	F5—C20—S2—O4	−61.1 (3)
C8—C9—C10—C17	−5.4 (3)	F6—C20—S2—O6	−178.7 (2)
C9—C10—C11—C12	0.3 (3)	F4—C20—S2—O6	−57.1 (2)
C17—C10—C11—C12	178.57 (19)	F5—C20—S2—O6	60.7 (2)
C9—C10—C11—C18	−177.92 (19)	F6—C20—S2—O5	−61.2 (2)
C17—C10—C11—C18	0.4 (3)	F4—C20—S2—O5	60.4 (2)
C10—C11—C12—N1	1.7 (3)	F5—C20—S2—O5	178.22 (18)