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3,6-Dimethyl-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) = 0.004 Å
R factor = 0.042
wR factor = 0.064
Data-to-parameter ratio = 16.0

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

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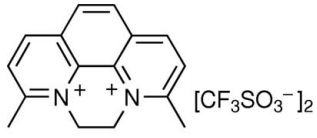
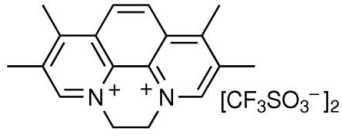
The crystal structure of the title compound, $C_{16}H_{16}N_2^{2+}\cdot 2CF_3O_3S^-$, is the first structure to be reported for a diquaternized derivative of 2,9-dimethyl-1,10-phenanthroline.

Comment

The compound 6,7-dihydrodipyrido[1,2-*a*:2′,1′-*c*]pyrazine-]pyrazinediium dibromide (diquat dibromide) is a potent herbicide (Brian *et al.*, 1958), and related salts derived from 2,2′-bipyridyl and other α-diimines have also generated considerable interest (Summers, 1981). In recent years, the attractive redox properties of diquats have led to other uses as electron acceptors in light-harvesting chromophore-quencher systems (Ryu *et al.*, 1992; Klumpp *et al.*, 1999; Kim *et al.*, 2003, 2005) and in ion-pair charge-transfer complexes (Nunn *et al.*, 1994; Hofbauer *et al.*, 1996; Unamuno *et al.*, 1998; Vitoria *et al.*, 2002). Our studies directed at using diquats in novel metal-based chromophore-quencher arrays have afforded an unusually facile method for the synthesis of such compounds, including salts (I) and (II) (Coe, Curati & Fitzgerald, 2006). The structure of salt (II), 1,2,7,8-tetramethyl-4,5-dihydro-3a,5a-diazapyrene ditriflate, is presented in the following paper (Coe, Fitzgerald & Raftery, 2006).



(I)



(II)

The molecular structures of the salts (I) (Fig. 1) and (II) are as indicated by ^{1}H NMR spectroscopy and, to our knowledge, the first to be reported containing these particular methyl-substituted cations. The geometrical parameters of the diquat units are as expected (Table 1), and largely identical for the two compounds. The C atoms of the ethylene bridge have normal tetrahedral geometries, with N1—C13—C14—N2 torsion angles of −58.2 (3)° for (I) and −58.83 (19)° for (II). Comparisons with previously published structures for other diquat compounds derived from 1,10-phenanthroline reveal generally similar bond lengths and angles, although the ethylene torsion angles are somewhat smaller at *ca* 53–55° (Hofbauer *et al.*, 1996; Unamuno *et al.*, 1998; Vitoria *et al.*,

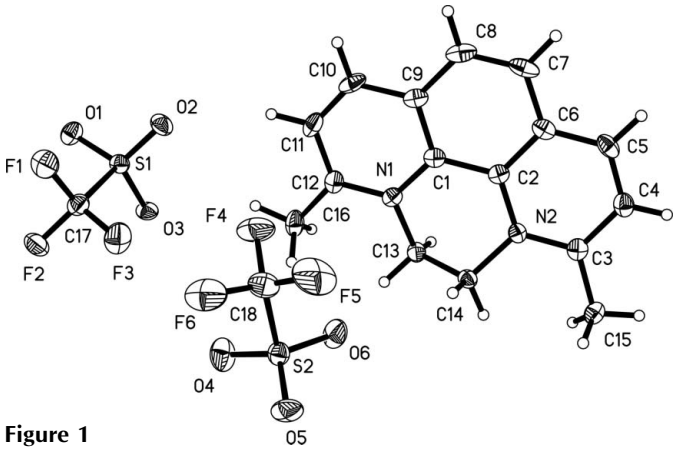


Figure 1
The asymmetric unit of salt (I), showing 50% probability displacement ellipsoids.

2002). In both compounds, the presence of the ethylene bridge imparts a small twist to the 3a,5a-diazapyrene unit, with dihedral angles between the two aromatic outer rings of 8.85 (7)° for (I) and 11.26 (5)° for (II). The crystal packing structures of both (I) and (II) reveal extensive C—H···O interactions between the diquat cations and the trifluoromethanesulfonate counter-anions.

Experimental

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

Crystal data

$C_{16}H_{16}N_2^{2+}\cdot 2CF_3O_3S^-$
M_r = 534.45
Monoclinic, $P2_1/c$
a = 9.976 (1) Å
b = 12.653 (1) Å
c = 16.559 (2) Å
β = 97.426 (2)°
V = 2072.7 (3) Å^3
Z = 4
D_x = 1.713 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.35 mm^{-1}
T = 100 (2) K
Block, white
0.10 × 0.10 × 0.05 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: none
17755 measured reflections
4947 independent reflections
2354 reflections with $I > 2\sigma(I)$
R_{int} = 0.083
θ_{max} = 28.3°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.064
S = 0.72
4947 reflections
309 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0121P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—N1	1.379 (3)	C5—C6	1.402 (3)
C1—C9	1.397 (3)	C6—C7	1.416 (3)
C1—C2	1.427 (3)	C7—C8	1.348 (3)
C3—N2	1.344 (3)	C10—C11	1.352 (3)
C3—C4	1.397 (3)	C11—C12	1.403 (3)
C3—C15	1.486 (3)	C13—N1	1.481 (3)
C4—C5	1.360 (3)	C13—C14	1.498 (3)
N1—C1—C2	121.3 (2)	N2—C14—C13	110.2 (2)
N2—C2—C1	120.8 (2)	C1—N1—C13	116.6 (2)
N1—C13—C14	109.9 (2)	C2—N2—C14	115.4 (2)
N1—C13—C14—N2	−58.2 (3)		

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, 1997); cell refinement: *SAINT* (Bruker, 1997); 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, 1997); software used to prepare material for publication: *SHELXTL*.

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supporting information

Acta Cryst. (2006). E**62**, o4333–o4334 [https://doi.org/10.1107/S1600536806034945]

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$M_r = 534.45$
Monoclinic, $P2_1/c$
$a = 9.9760\ (9)$ Å
$b = 12.6530\ (12)$ Å
$c = 16.5590\ (15)$ Å
$\beta = 97.426\ (2)°$
$V = 2072.7\ (3)$ Å^3
$Z = 4$
$F(000) = 1088$
$D_x = 1.713$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1610 reflections
$\theta = 2.5–21.7°$
$\mu = 0.35$ mm^{-1}
$T = 100$ K
Block, white
0.10 × 0.10 × 0.05 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
17755 measured reflections
4947 independent reflections
2354 reflections with $I > 2\sigma(I)$
$R_{int} = 0.083$
$\theta_{max} = 28.3°$, $\theta_{min} = 2.0°$
$h = -13\rightarrow13$
$k = -16\rightarrow16$
$l = -21\rightarrow21$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.064$
$S = 0.72$
4947 reflections
309 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
$w = 1/[\sigma^2(F_o^2) + (0.0121P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.39$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ 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	0.1567 (3)	0.1077 (2)	0.15172 (14)	0.0174 (6)
C2	0.0181 (3)	0.1359 (2)	0.13050 (15)	0.0167 (6)
C3	−0.1544 (3)	0.2676 (2)	0.12110 (15)	0.0190 (6)
C4	−0.2452 (3)	0.1945 (2)	0.08142 (15)	0.0230 (7)
H4	−0.3342	0.2164	0.0609	0.028*
C5	−0.2075 (3)	0.0925 (2)	0.07179 (14)	0.0222 (7)
H5	−0.2721	0.0428	0.0478	0.027*
C6	−0.0743 (3)	0.0598 (2)	0.09695 (15)	0.0188 (7)
C7	−0.0315 (3)	−0.0463 (2)	0.09105 (15)	0.0248 (7)
H7	−0.0949	−0.0983	0.0695	0.030*
C8	0.0976 (3)	−0.0747 (2)	0.11544 (15)	0.0251 (7)
H8	0.1233	−0.1468	0.1131	0.030*
C9	0.1952 (3)	0.0023 (2)	0.14464 (15)	0.0193 (6)
C10	0.3325 (3)	−0.0229 (2)	0.16485 (15)	0.0252 (7)
H10	0.3610	−0.0942	0.1614	0.030*
C11	0.4247 (3)	0.0527 (2)	0.18913 (15)	0.0248 (7)
H11	0.5170	0.0340	0.2033	0.030*
C12	0.3847 (3)	0.1586 (2)	0.19352 (15)	0.0203 (7)
C13	0.2087 (2)	0.29466 (19)	0.17123 (15)	0.0188 (6)
H13A	0.2072	0.3208	0.1148	0.023*
H13B	0.2730	0.3387	0.2073	0.023*
C14	0.0704 (2)	0.30377 (19)	0.19652 (15)	0.0180 (6)
H14A	0.0731	0.2815	0.2540	0.022*
H14B	0.0402	0.3783	0.1922	0.022*
C15	−0.1984 (2)	0.37606 (18)	0.13973 (15)	0.0228 (7)
H15A	−0.1960	0.3841	0.1988	0.034*
H15B	−0.2907	0.3879	0.1131	0.034*
H15C	−0.1375	0.4278	0.1196	0.034*
C16	0.4851 (2)	0.2445 (2)	0.21452 (15)	0.0268 (7)
H16A	0.4811	0.2946	0.1691	0.040*
H16B	0.5760	0.2140	0.2248	0.040*
H16C	0.4644	0.2814	0.2634	0.040*
C17	0.8492 (3)	0.0991 (2)	0.41836 (16)	0.0226 (7)
C18	0.3750 (3)	0.1503 (2)	0.44510 (19)	0.0326 (8)
F1	0.87856 (15)	0.00203 (12)	0.44659 (9)	0.0344 (4)
F2	0.94339 (16)	0.16427 (11)	0.45590 (9)	0.0313 (4)
F3	0.73160 (15)	0.12689 (13)	0.44114 (9)	0.0394 (5)
F4	0.43119 (17)	0.10610 (13)	0.38467 (9)	0.0454 (5)
F5	0.25290 (18)	0.11155 (14)	0.44460 (11)	0.0623 (6)
F6	0.44811 (18)	0.11972 (12)	0.51482 (10)	0.0517 (6)
N1	0.2535 (2)	0.18299 (16)	0.17606 (12)	0.0176 (5)
N2	−0.0262 (2)	0.23661 (16)	0.14401 (12)	0.0164 (5)
O1	0.97977 (17)	0.06831 (13)	0.29701 (10)	0.0249 (5)
O2	0.73879 (17)	0.02953 (13)	0.28035 (10)	0.0259 (5)
O3	0.81677 (17)	0.21236 (13)	0.28858 (10)	0.0224 (5)

O4	0.51139 (18)	0.32162 (14)	0.44150 (12)	0.0380 (6)
O5	0.30593 (19)	0.32464 (14)	0.50635 (10)	0.0333 (5)
O6	0.29322 (18)	0.31170 (15)	0.35924 (10)	0.0367 (6)
S1	0.84551 (7)	0.10272 (5)	0.30835 (4)	0.01910 (17)
S2	0.37134 (7)	0.29347 (6)	0.43738 (4)	0.02275 (18)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0226 (16)	0.0185 (15)	0.0118 (14)	−0.0006 (14)	0.0055 (12)	0.0023 (12)
C2	0.0208 (16)	0.0182 (16)	0.0119 (14)	0.0005 (13)	0.0052 (12)	0.0022 (12)
C3	0.0205 (16)	0.0247 (17)	0.0127 (15)	−0.0008 (13)	0.0059 (13)	0.0033 (12)
C4	0.0207 (17)	0.0312 (18)	0.0168 (15)	−0.0008 (14)	0.0017 (13)	0.0008 (14)
C5	0.0228 (18)	0.0275 (18)	0.0167 (15)	−0.0107 (14)	0.0042 (13)	−0.0017 (13)
C6	0.0247 (17)	0.0205 (16)	0.0124 (15)	−0.0051 (13)	0.0067 (13)	0.0003 (12)
C7	0.043 (2)	0.0167 (17)	0.0164 (16)	−0.0101 (14)	0.0088 (15)	−0.0025 (12)
C8	0.045 (2)	0.0155 (16)	0.0171 (16)	0.0054 (15)	0.0112 (14)	0.0024 (13)
C9	0.0302 (18)	0.0161 (16)	0.0125 (15)	0.0027 (14)	0.0067 (13)	0.0028 (12)
C10	0.039 (2)	0.0168 (16)	0.0214 (17)	0.0129 (15)	0.0075 (15)	0.0052 (13)
C11	0.0231 (18)	0.0328 (19)	0.0186 (17)	0.0127 (15)	0.0030 (14)	0.0035 (14)
C12	0.0181 (16)	0.0319 (18)	0.0115 (15)	0.0032 (14)	0.0046 (12)	0.0010 (12)
C13	0.0182 (16)	0.0151 (15)	0.0225 (16)	−0.0010 (13)	0.0002 (12)	0.0030 (13)
C14	0.0202 (16)	0.0156 (15)	0.0175 (15)	−0.0001 (13)	−0.0003 (12)	0.0001 (12)
C15	0.0207 (16)	0.0218 (17)	0.0263 (17)	0.0032 (13)	0.0042 (13)	0.0027 (13)
C16	0.0164 (17)	0.0395 (19)	0.0247 (17)	0.0012 (14)	0.0035 (13)	0.0040 (14)
C17	0.0247 (17)	0.0223 (17)	0.0209 (16)	0.0038 (15)	0.0038 (14)	0.0012 (14)
C18	0.040 (2)	0.0323 (19)	0.0269 (19)	−0.0026 (17)	0.0094 (17)	−0.0039 (16)
F1	0.0492 (11)	0.0270 (10)	0.0253 (10)	−0.0003 (9)	−0.0012 (8)	0.0095 (8)
F2	0.0393 (10)	0.0283 (10)	0.0241 (9)	−0.0024 (8)	−0.0042 (8)	−0.0051 (8)
F3	0.0307 (10)	0.0633 (14)	0.0262 (10)	0.0108 (9)	0.0114 (8)	−0.0019 (9)
F4	0.0667 (13)	0.0380 (11)	0.0339 (11)	0.0090 (10)	0.0154 (10)	−0.0086 (9)
F5	0.0548 (13)	0.0509 (13)	0.0855 (16)	−0.0332 (11)	0.0257 (12)	−0.0145 (11)
F6	0.0901 (16)	0.0326 (12)	0.0324 (11)	0.0127 (10)	0.0079 (11)	0.0117 (9)
N1	0.0201 (14)	0.0191 (14)	0.0142 (12)	0.0022 (11)	0.0047 (10)	0.0016 (10)
N2	0.0155 (13)	0.0183 (13)	0.0155 (12)	−0.0021 (10)	0.0031 (10)	0.0013 (10)
O1	0.0234 (11)	0.0304 (12)	0.0226 (11)	0.0059 (9)	0.0089 (9)	0.0030 (9)
O2	0.0290 (12)	0.0187 (11)	0.0279 (12)	−0.0062 (9)	−0.0039 (10)	−0.0006 (9)
O3	0.0327 (12)	0.0128 (10)	0.0211 (11)	0.0003 (9)	0.0012 (9)	0.0017 (8)
O4	0.0237 (12)	0.0378 (14)	0.0516 (15)	−0.0110 (10)	0.0019 (11)	0.0070 (11)
O5	0.0487 (14)	0.0353 (13)	0.0175 (11)	0.0102 (11)	0.0099 (10)	−0.0025 (9)
O6	0.0357 (13)	0.0559 (15)	0.0176 (11)	0.0171 (11)	−0.0006 (10)	0.0024 (10)
S1	0.0236 (4)	0.0181 (4)	0.0154 (4)	0.0003 (4)	0.0019 (3)	0.0009 (3)
S2	0.0232 (4)	0.0237 (4)	0.0209 (4)	0.0011 (4)	0.0012 (3)	0.0021 (3)

Geometric parameters (Å, º)

C1—N1	1.379 (3)	C13—H13A	0.9900
C1—C9	1.397 (3)	C13—H13B	0.9900

C1—C2	1.427 (3)	C14—N2	1.480 (3)
C2—N2	1.377 (3)	C14—H14A	0.9900
C2—C6	1.398 (3)	C14—H14B	0.9900
C3—N2	1.344 (3)	C15—H15A	0.9800
C3—C4	1.397 (3)	C15—H15B	0.9800
C3—C15	1.486 (3)	C15—H15C	0.9800
C4—C5	1.360 (3)	C16—H16A	0.9800
C4—H4	0.9500	C16—H16B	0.9800
C5—C6	1.402 (3)	C16—H16C	0.9800
C5—H5	0.9500	C17—F3	1.325 (3)
C6—C7	1.416 (3)	C17—F1	1.333 (3)
C7—C8	1.348 (3)	C17—F2	1.342 (3)
C7—H7	0.9500	C17—S1	1.818 (3)
C8—C9	1.419 (3)	C18—F5	1.312 (3)
C8—H8	0.9500	C18—F4	1.332 (3)
C9—C10	1.403 (3)	C18—F6	1.341 (3)
C10—C11	1.352 (3)	C18—S2	1.816 (3)
C10—H10	0.9500	O1—S1	1.4435 (17)
C11—C12	1.403 (3)	O2—S1	1.4418 (17)
C11—H11	0.9500	O3—S1	1.4456 (17)
C12—N1	1.340 (3)	O4—S2	1.4349 (18)
C12—C16	1.488 (3)	O5—S2	1.4417 (18)
C13—N1	1.481 (3)	O6—S2	1.4402 (17)
C13—C14	1.498 (3)		

N1—C1—C9	119.6 (2)	N2—C14—H14B	109.6
N1—C1—C2	121.3 (2)	C13—C14—H14B	109.6
C9—C1—C2	119.1 (2)	H14A—C14—H14B	108.1
N2—C2—C6	119.5 (2)	C3—C15—H15A	109.5
N2—C2—C1	120.8 (2)	C3—C15—H15B	109.5
C6—C2—C1	119.6 (2)	H15A—C15—H15B	109.5
N2—C3—C4	118.4 (2)	C3—C15—H15C	109.5
N2—C3—C15	120.4 (2)	H15A—C15—H15C	109.5
C4—C3—C15	121.2 (2)	H15B—C15—H15C	109.5
C5—C4—C3	120.7 (3)	C12—C16—H16A	109.5
C5—C4—H4	119.6	C12—C16—H16B	109.5
C3—C4—H4	119.6	H16A—C16—H16B	109.5
C4—C5—C6	120.7 (3)	C12—C16—H16C	109.5
C4—C5—H5	119.7	H16A—C16—H16C	109.5
C6—C5—H5	119.7	H16B—C16—H16C	109.5
C2—C6—C5	117.8 (2)	F3—C17—F1	107.9 (2)
C2—C6—C7	119.4 (2)	F3—C17—F2	107.3 (2)
C5—C6—C7	122.8 (3)	F1—C17—F2	107.2 (2)
C8—C7—C6	121.2 (3)	F3—C17—S1	111.99 (18)
C8—C7—H7	119.4	F1—C17—S1	110.49 (18)
C6—C7—H7	119.4	F2—C17—S1	111.77 (19)
C7—C8—C9	120.4 (3)	F5—C18—F4	108.6 (2)
C7—C8—H8	119.8	F5—C18—F6	107.4 (3)

C9—C8—H8	119.8	F4—C18—F6	106.9 (2)
C1—C9—C10	117.9 (2)	F5—C18—S2	111.2 (2)
C1—C9—C8	120.0 (3)	F4—C18—S2	111.9 (2)
C10—C9—C8	122.1 (3)	F6—C18—S2	110.6 (2)
C11—C10—C9	121.0 (3)	C12—N1—C1	122.2 (2)
C11—C10—H10	119.5	C12—N1—C13	120.7 (2)
C9—C10—H10	119.5	C1—N1—C13	116.6 (2)
C10—C11—C12	120.3 (3)	C3—N2—C2	122.5 (2)
C10—C11—H11	119.9	C3—N2—C14	121.5 (2)
C12—C11—H11	119.9	C2—N2—C14	115.4 (2)
N1—C12—C11	119.0 (3)	O2—S1—O1	115.05 (11)
N1—C12—C16	119.5 (2)	O2—S1—O3	115.28 (11)
C11—C12—C16	121.5 (2)	O1—S1—O3	114.85 (11)
N1—C13—C14	109.9 (2)	O2—S1—C17	102.96 (12)
N1—C13—H13A	109.7	O1—S1—C17	102.93 (11)
C14—C13—H13A	109.7	O3—S1—C17	103.25 (12)
N1—C13—H13B	109.7	O4—S2—O6	114.42 (12)
C14—C13—H13B	109.7	O4—S2—O5	115.60 (12)
H13A—C13—H13B	108.2	O6—S2—O5	114.84 (11)
N2—C14—C13	110.2 (2)	O4—S2—C18	103.52 (13)
N2—C14—H14A	109.6	O6—S2—C18	103.10 (13)
C13—C14—H14A	109.6	O5—S2—C18	102.95 (13)

N1—C1—C2—N2	−8.8 (4)	C2—C1—N1—C12	−177.6 (2)
C9—C1—C2—N2	173.7 (2)	C9—C1—N1—C13	171.7 (2)
N1—C1—C2—C6	172.4 (2)	C2—C1—N1—C13	−5.8 (3)
C9—C1—C2—C6	−5.1 (4)	C14—C13—N1—C12	−149.1 (2)
N2—C3—C4—C5	4.9 (4)	C14—C13—N1—C1	38.9 (3)
C15—C3—C4—C5	−173.5 (2)	C4—C3—N2—C2	−0.6 (4)
C3—C4—C5—C6	−4.0 (4)	C15—C3—N2—C2	177.8 (2)
N2—C2—C6—C5	5.5 (4)	C4—C3—N2—C14	−171.0 (2)
C1—C2—C6—C5	−175.7 (2)	C15—C3—N2—C14	7.4 (3)
N2—C2—C6—C7	−173.4 (2)	C6—C2—N2—C3	−4.6 (4)
C1—C2—C6—C7	5.4 (4)	C1—C2—N2—C3	176.6 (2)
C4—C5—C6—C2	−1.3 (4)	C6—C2—N2—C14	166.3 (2)
C4—C5—C6—C7	177.6 (2)	C1—C2—N2—C14	−12.5 (3)
C2—C6—C7—C8	−1.6 (4)	C13—C14—N2—C3	−143.2 (2)
C5—C6—C7—C8	179.6 (2)	C13—C14—N2—C2	45.8 (3)
C6—C7—C8—C9	−2.6 (4)	F3—C17—S1—O2	−59.0 (2)
N1—C1—C9—C10	1.6 (4)	F1—C17—S1—O2	61.3 (2)
C2—C1—C9—C10	179.1 (2)	F2—C17—S1—O2	−179.42 (17)
N1—C1—C9—C8	−176.6 (2)	F3—C17—S1—O1	−178.89 (19)
C2—C1—C9—C8	1.0 (4)	F1—C17—S1—O1	−58.6 (2)
C7—C8—C9—C1	2.9 (4)	F2—C17—S1—O1	60.7 (2)
C7—C8—C9—C10	−175.2 (2)	F3—C17—S1—O3	61.3 (2)
C1—C9—C10—C11	−1.1 (4)	F1—C17—S1—O3	−178.36 (17)
C8—C9—C10—C11	177.0 (3)	F2—C17—S1—O3	−59.1 (2)
C9—C10—C11—C12	−0.9 (4)	F5—C18—S2—O4	178.2 (2)

C10—C11—C12—N1	2.3 (4)	F4—C18—S2—O4	−60.2 (2)
C10—C11—C12—C16	−175.7 (2)	F6—C18—S2—O4	58.9 (2)
N1—C13—C14—N2	−58.2 (3)	F5—C18—S2—O6	−62.3 (2)
C11—C12—N1—C1	−1.8 (4)	F4—C18—S2—O6	59.3 (2)
C16—C12—N1—C1	176.3 (2)	F6—C18—S2—O6	178.4 (2)
C11—C12—N1—C13	−173.3 (2)	F5—C18—S2—O5	57.5 (2)
C16—C12—N1—C13	4.8 (4)	F4—C18—S2—O5	179.1 (2)
C9—C1—N1—C12	−0.1 (4)	F6—C18—S2—O5	−61.8 (2)