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Four-layered [3.3]metacyclophane with ethenetetracarbonitrile

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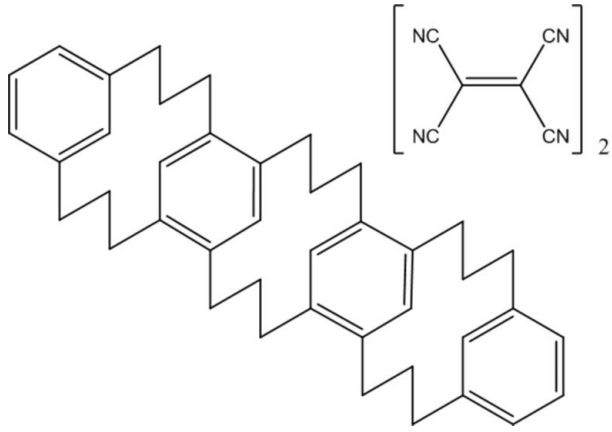
Key indicators: single-crystal X-ray study; T = 123 K; mean σ(C–C) = 0.002 Å; disorder in main residue; R factor = 0.060; wR factor = 0.178; data-to-parameter ratio = 12.1.

The title complex $C_{42}H_{48}\cdot 2C_6N_4$ {systematic name: heptacyclo-[21.13.1.1^{5,19}.1^{6,18}.1^{10,14}.1^{24,36}.1^{28,32}]dotetraconta-1(37),5(40),-6(41),10(42),11,13,18,23,28,30,32(39),36(38)-dodecaene–ethenetetracarbonitrile (1/2)}, consisting of four-layered [3.3]-metacyclophane (MCP) with two tetracyanoethylene (TCNE) molecules, was grown from a mixture of MCP and TCNE in chloroform solution. The four-layered [3.3]MCP has an S-shaped structure in which three [3.3]MCP moieties take *syn*-(chair-boat), *anti*-(chair-boat) and *syn*-(chair-boat) conformations. The two outer [3.3]MCP moieties with *syn* geometry contain benzene rings with a tilt of 32.95 (7)°. The central [3.3]MCP moiety has an *anti* geometry, in which the two benzene rings are oriented parallel to each other at a transannular distance of 2.31 Å. The TCNE molecules are stacked on either side of the outer [3.3]MCP units at a distance of 3.19 Å on one side and 3.24 Å on the other, and showed 0.80:0.20 and 0.44:0.56 disorder, respectively.

Related literature

For the previously reported $C_{42}H_{48}\cdot C_6N_4$ (1:1) complex, see: Shibahara *et al.* (2011*a*). For the free ligand $C_{42}H_{48}$, see: Shibahara *et al.* (2007). For multilayered [3.3]paracyclophanes, see: Shibahara *et al.* (2008, 2011*a*,*b*). For cyclophanes, see: Vögtle (1993).



Experimental

Crystal data

$C_{42}H_{48}\cdot 2C_6N_4$
M_r = 809.03
Triclinic, $P\overline{1}$
a = 9.563 (3) Å
b = 10.101 (4) Å
c = 11.679 (4) Å
α = 96.365 (14)°
β = 99.134 (13)°
γ = 107.683 (13)°
V = 1045.9 (6) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 123 K
0.35 × 0.16 × 0.09 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
17470 measured reflections
4775 independent reflections
4141 reflections with $F^2 > 2\sigma(F^2)$
R_{int} = 0.050

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.178
S = 1.00
4775 reflections
394 parameters
Only H-atom coordinates refined
$\Delta\rho_{max}$ = 0.80 e Å^{-3}
$\Delta\rho_{min}$ = −0.50 e Å^{-3}

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXD* (Schneider & Sheldrick, 2002); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *CrystalStructure* (Rigaku, 2010); software used to prepare material for publication: *CrystalStructure*.

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Supporting information for this paper is available from the IUCr electronic archives (Reference: GW2145).

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supporting information

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Four-layered [3.3]metacyclophane with ethenetetracarbonitrile

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S1. Comment

The title complex consists of four-layered [3.3]metacyclophane (MCP) with two tetracyanoethylene molecules (TCNE). The TCNE molecules are stacked on either side of the outer [3.3]MCP units at a distance of 3.19 Å on one side and 3.24 Å on the other, and showed 0.80:0.20 and 0.44:0.56 disorder, respectively.

S2. Experimental

The complex of single-crystal $C_{42}H_{48}.2C_6N_4$, consisting of four-layered [3.3]metacyclophane (MCP) with two tetracyanoethylene (TCNE) molecules, was synthesized. The black block crystals were obtained by slow diffusion from 2 m*M* of four-layered [3.3]MCP with 20 m*M* of TCNE in chloroform solution.

S3. Refinement

All the hydrogen atoms of the compound are fixed geometrically (C—H = 0.93–0.97 Å) and allowed to ride on their parent atoms. Structure was refined with unique reflections and with a cut-off sigma = 2.00.

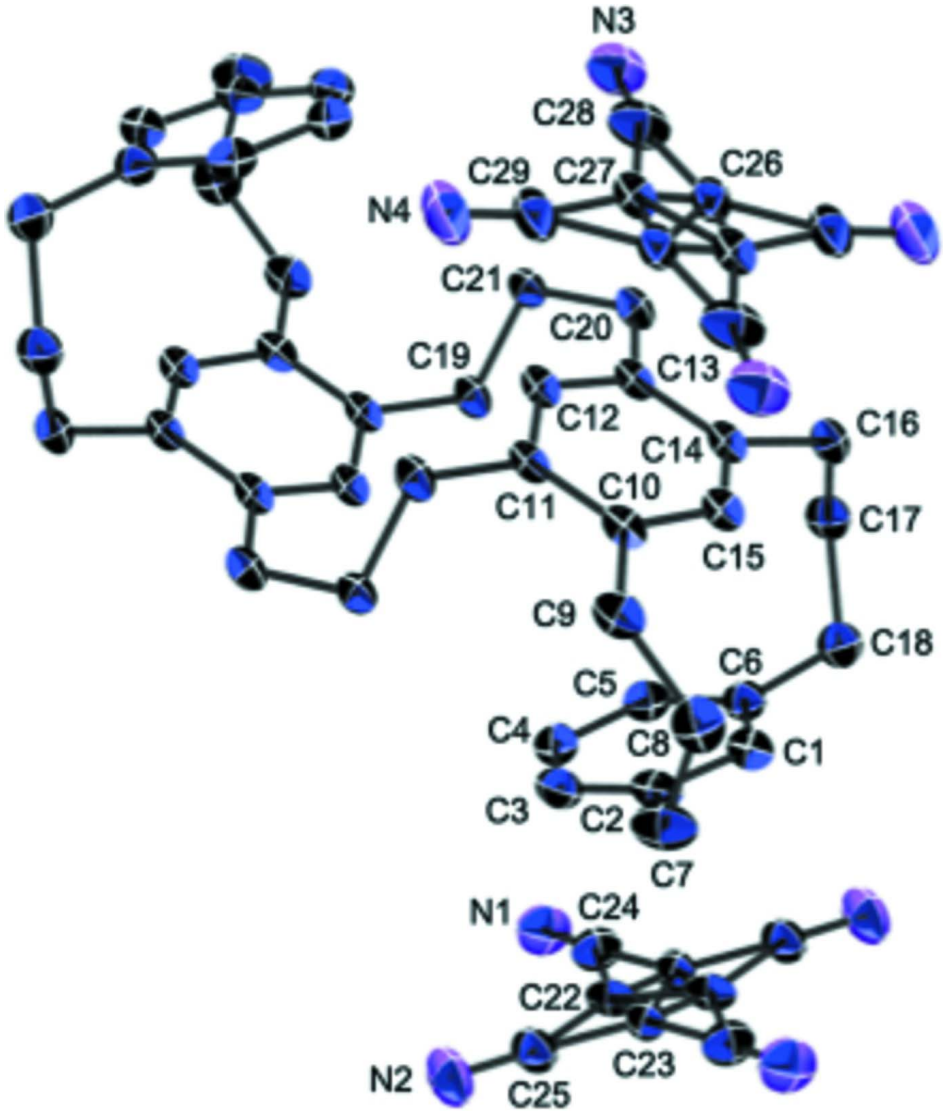

Figure 1

The molecular structure of $C_{42}H_{48}.2C_6N_4$ with the atom-labelling scheme and displacement ellipsoids are drawn at the 50% probability level. H atoms are omitted for clarity.

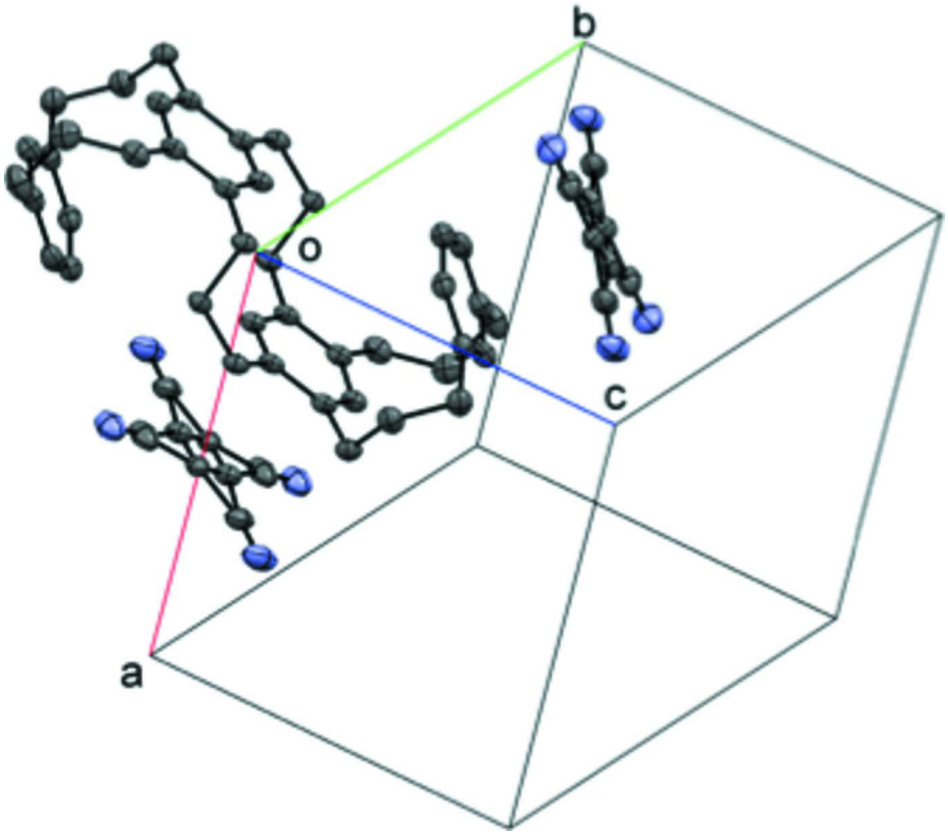

Figure 2

A packing diagram of $C_{42}H_{48}.2C_6N_4$.

Heptacyclo[21.13.1.1^{5,19}.1^{6,18}.1^{10,14}.1^{24,36}.1^{28,32}]dotetraconta-1(37),5(40),6(41),10 (42),11,13,18,23,28,30,32 (39), 36 (38)-dodecaene–ethenetetracarbonitrile (1/2)

Crystal data

$C_{42}H_{48}·2C_6N_4$
M_r = 809.03
Triclinic, $P\overline{1}$
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c = 11.679 (4) Å
α = 96.365 (14)°
β = 99.134 (13)°
γ = 107.683 (13)°
V = 1045.9 (6) Å^3
Z = 1
$F(000)$ = 428.00
D_x = 1.284 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71075 Å
Cell parameters from 13845 reflections
θ = 3.0–27.5°
μ = 0.08 mm^{-1}
T = 123 K
Block, black
0.35 × 0.16 × 0.09 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
$\omega/2\theta$ scans
17470 measured reflections
4775 independent reflections
4141 reflections with $F^2 > 2\sigma(F^2)$
R_{int} = 0.050
θ_{max} = 27.5°
h = −12→11
k = −13→13
l = −15→15

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.060$
$wR(F^2) = 0.178$
$S = 1.00$
4775 reflections
394 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
Only H-atom coordinates refined
$w = 1/[\sigma^2(F_o^2) + (0.1296P)^2 + 0.1947P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.80$ e Å^{-3}
$\Delta\rho_{min} = -0.50$ e Å^{-3}

Special details

Geometry. ENTER SPECIAL DETAILS OF THE MOLECULAR GEOMETRY

Refinement. Refinement was performed using all reflections. The weighted *R*-factor (*wR*) and goodness of fit (*S*) are based on F^2. *R*-factor (gt) are based on *F*. The threshold expression of $F^2 > 2.0\ \sigma(F^2)$ is used only for calculating *R*-factor (gt).

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
N1	0.30526 (16)	0.71021 (14)	0.53324 (14)	0.0447 (4)	
N2	−0.13890 (17)	0.62272 (16)	0.31010 (12)	0.0437 (4)	
N3	0.70465 (15)	0.29951 (14)	0.04664 (13)	0.0426 (4)	
N4	0.63339 (18)	−0.04481 (19)	0.23634 (12)	0.0507 (4)	
C1	0.27496 (16)	0.35932 (14)	0.38821 (12)	0.0292 (3)	
C2	0.17966 (15)	0.23727 (14)	0.41376 (11)	0.0271 (3)	
C3	0.02899 (16)	0.18988 (15)	0.35613 (12)	0.0308 (3)	
C4	−0.02123 (17)	0.26252 (16)	0.27325 (13)	0.0344 (4)	
C5	0.07747 (18)	0.38055 (16)	0.24516 (12)	0.0344 (4)	
C6	0.22797 (17)	0.42945 (14)	0.30050 (13)	0.0314 (4)	
C7	0.3425 (3)	0.54751 (16)	0.26353 (17)	0.0421 (4)	
C8	0.46096 (18)	0.50271 (16)	0.21084 (14)	0.0379 (4)	
C9	0.40369 (16)	0.39146 (14)	0.10058 (13)	0.0306 (3)	
C10	0.33220 (14)	0.23804 (13)	0.11189 (12)	0.0247 (3)	
C11	0.22263 (14)	0.14374 (13)	0.01981 (11)	0.0232 (3)	
C12	0.16183 (14)	0.00361 (13)	0.03416 (11)	0.0237 (3)	
C13	0.19319 (14)	−0.04508 (13)	0.13956 (11)	0.0232 (3)	
C14	0.30253 (14)	0.04905 (13)	0.23209 (11)	0.0235 (3)	
C15	0.37473 (14)	0.18541 (13)	0.21330 (12)	0.0251 (3)	
C16	0.34394 (15)	0.00796 (14)	0.35098 (12)	0.0271 (3)	
C17	0.23470 (17)	0.00835 (14)	0.43550 (12)	0.0309 (3)	
C18	0.23976 (18)	0.15347 (15)	0.49632 (12)	0.0332 (4)	
C19	0.15916 (14)	0.18891 (14)	−0.09117 (11)	0.0248 (3)	
C20	0.11033 (14)	−0.19487 (13)	0.15283 (12)	0.0253 (3)	
C21	−0.04379 (14)	−0.26541 (13)	0.07162 (11)	0.0240 (3)	
C22	0.0677 (9)	0.5125 (7)	0.5331 (7)	0.0274 (14)	0.2000
C23	0.0276 (2)	0.55598 (17)	0.47359 (15)	0.0251 (4)	0.8000
C24	0.18542 (17)	0.63929 (15)	0.51109 (13)	0.0343 (4)	
C25	−0.07150 (17)	0.58885 (15)	0.38230 (12)	0.0332 (4)	

C26	0.5541 (3)	0.0410 (3)	0.0464 (3)	0.0283 (5)	0.5600
C27	0.4895 (4)	−0.0541 (4)	0.0308 (3)	0.0263 (6)	0.4400
C28	0.62892 (17)	0.18694 (17)	0.03210 (17)	0.0426 (4)	
C29	0.58456 (17)	−0.02573 (17)	0.14916 (13)	0.0354 (4)	
H1	0.383 (2)	0.3942 (18)	0.4314 (15)	0.033 (5)*	
H2	−0.045 (3)	0.101 (3)	0.3716 (17)	0.049 (6)*	
H3	−0.131 (3)	0.228 (2)	0.2321 (16)	0.041 (5)*	
H4	0.041 (3)	0.428 (3)	0.1855 (19)	0.050 (6)*	
H5	0.297 (3)	0.587 (3)	0.205 (3)	0.081 (8)*	
H6	0.390 (3)	0.626 (3)	0.327 (2)	0.058 (6)*	
H7	0.534 (3)	0.588 (3)	0.1889 (17)	0.051 (6)*	
H8	0.530 (3)	0.469 (2)	0.2774 (17)	0.042 (5)*	
H9	0.322 (3)	0.419 (3)	0.0470 (18)	0.051 (6)*	
H10	0.488 (2)	0.3976 (19)	0.0554 (16)	0.043 (5)*	
H11	0.0882 (17)	−0.0620 (16)	−0.0336 (14)	0.021 (4)*	
H12	0.4578 (18)	0.2534 (17)	0.2809 (14)	0.027 (4)*	
H13	0.452 (2)	0.0727 (18)	0.3944 (15)	0.033 (5)*	
H14	0.3556 (17)	−0.0871 (17)	0.3366 (13)	0.024 (4)*	
H15	0.260 (2)	−0.0488 (19)	0.4963 (16)	0.038 (5)*	
H16	0.125 (2)	−0.0487 (19)	0.3960 (16)	0.037 (5)*	
H17	0.179 (3)	0.138 (2)	0.5597 (18)	0.048 (5)*	
H18	0.352 (3)	0.212 (3)	0.5384 (18)	0.050 (6)*	
H19	0.1086 (18)	0.0987 (18)	−0.1549 (14)	0.029 (4)*	
H20	0.242 (2)	0.2516 (18)	−0.1231 (15)	0.034 (5)*	
H21	0.0979 (19)	−0.1933 (17)	0.2372 (14)	0.029 (4)*	
H22	0.1777 (19)	−0.2508 (18)	0.1392 (15)	0.035 (5)*	
H23	−0.0359 (18)	−0.2743 (17)	−0.0123 (15)	0.029 (4)*	
H24	−0.0813 (19)	−0.3631 (18)	0.0886 (14)	0.028 (4)*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0341 (8)	0.0348 (7)	0.0587 (9)	0.0038 (6)	0.0098 (6)	0.0017 (6)
N2	0.0523 (9)	0.0596 (9)	0.0346 (7)	0.0334 (7)	0.0143 (6)	0.0209 (7)
N3	0.0335 (7)	0.0360 (7)	0.0599 (9)	0.0112 (6)	0.0152 (6)	0.0066 (6)
N4	0.0539 (9)	0.0834 (12)	0.0354 (8)	0.0470 (9)	0.0129 (7)	0.0190 (7)
C1	0.0316 (8)	0.0267 (7)	0.0322 (7)	0.0119 (6)	0.0093 (6)	0.0056 (6)
C2	0.0324 (7)	0.0262 (7)	0.0252 (7)	0.0116 (6)	0.0086 (5)	0.0048 (5)
C3	0.0321 (8)	0.0283 (7)	0.0326 (7)	0.0101 (6)	0.0100 (6)	0.0023 (6)
C4	0.0354 (8)	0.0381 (8)	0.0310 (7)	0.0181 (6)	0.0033 (6)	−0.0021 (6)
C5	0.0500 (9)	0.0357 (8)	0.0272 (7)	0.0266 (7)	0.0097 (6)	0.0064 (6)
C6	0.0422 (8)	0.0266 (7)	0.0336 (7)	0.0178 (6)	0.0160 (6)	0.0077 (6)
C7	0.0601 (11)	0.0261 (7)	0.0492 (10)	0.0170 (7)	0.0262 (8)	0.0138 (7)
C8	0.0360 (8)	0.0302 (7)	0.0450 (9)	0.0051 (6)	0.0083 (7)	0.0134 (7)
C9	0.0333 (8)	0.0256 (7)	0.0385 (8)	0.0108 (6)	0.0145 (6)	0.0144 (6)
C10	0.0235 (7)	0.0250 (6)	0.0318 (7)	0.0118 (5)	0.0111 (5)	0.0119 (5)
C11	0.0222 (6)	0.0262 (6)	0.0288 (7)	0.0136 (5)	0.0102 (5)	0.0121 (5)
C12	0.0211 (6)	0.0263 (7)	0.0285 (7)	0.0113 (5)	0.0080 (5)	0.0104 (5)

C13	0.0214 (6)	0.0251 (6)	0.0294 (7)	0.0124 (5)	0.0087 (5)	0.0111 (5)
C14	0.0219 (6)	0.0265 (6)	0.0279 (7)	0.0130 (5)	0.0081 (5)	0.0104 (5)
C15	0.0235 (7)	0.0260 (7)	0.0296 (7)	0.0110 (5)	0.0079 (5)	0.0088 (5)
C16	0.0282 (7)	0.0271 (7)	0.0285 (7)	0.0115 (5)	0.0043 (5)	0.0104 (5)
C17	0.0395 (8)	0.0282 (7)	0.0295 (7)	0.0137 (6)	0.0098 (6)	0.0119 (6)
C18	0.0447 (9)	0.0305 (7)	0.0274 (7)	0.0153 (6)	0.0073 (6)	0.0088 (6)
C19	0.0249 (7)	0.0279 (7)	0.0275 (7)	0.0125 (5)	0.0087 (5)	0.0126 (5)
C20	0.0249 (7)	0.0249 (6)	0.0308 (7)	0.0115 (5)	0.0073 (5)	0.0126 (5)
C21	0.0266 (7)	0.0223 (6)	0.0268 (7)	0.0113 (5)	0.0065 (5)	0.0086 (5)
C22	0.040 (5)	0.017 (3)	0.031 (4)	0.010 (4)	0.019 (3)	0.012 (3)
C23	0.0266 (10)	0.0231 (8)	0.0266 (9)	0.0084 (8)	0.0064 (7)	0.0061 (7)
C24	0.0343 (8)	0.0280 (7)	0.0386 (8)	0.0063 (6)	0.0121 (6)	0.0022 (6)
C25	0.0437 (9)	0.0334 (7)	0.0293 (7)	0.0195 (6)	0.0101 (6)	0.0101 (6)
C26	0.0248 (12)	0.0312 (16)	0.0336 (16)	0.0135 (12)	0.0075 (11)	0.0101 (11)
C27	0.0206 (14)	0.0318 (19)	0.0283 (17)	0.0114 (14)	0.0046 (12)	0.0046 (14)
C28	0.0300 (8)	0.0343 (8)	0.0663 (11)	0.0112 (7)	0.0186 (7)	0.0048 (8)
C29	0.0316 (8)	0.0508 (9)	0.0325 (8)	0.0241 (7)	0.0081 (6)	0.0110 (7)

Geometric parameters (Å, º)

N1—C24	1.1223 (19)	C23—C25	1.447 (3)
N2—C25	1.126 (3)	C26—C26^{iii}	1.362 (4)
N3—C28	1.124 (2)	C26—C27^{iii}	0.972 (5)
N4—C29	1.113 (3)	C26—C28	1.472 (4)
C1—C2	1.3873 (19)	C26—C29	1.472 (4)
C1—C6	1.400 (3)	C27—C27^{iii}	1.356 (6)
C2—C3	1.4000 (19)	C27—C28^{iii}	1.488 (4)
C2—C18	1.509 (3)	C27—C29	1.475 (4)
C3—C4	1.389 (3)	C1—H1	1.007 (17)
C4—C5	1.386 (3)	C3—H2	1.01 (2)
C5—C6	1.391 (3)	C4—H3	1.015 (19)
C6—C7	1.510 (3)	C5—H4	0.97 (3)
C7—C8	1.529 (3)	C7—H5	0.95 (3)
C8—C9	1.517 (2)	C7—H6	0.96 (2)
C9—C10	1.5221 (19)	C8—H7	1.02 (2)
C10—C11	1.4037 (16)	C8—H8	1.09 (2)
C10—C15	1.403 (2)	C9—H9	1.05 (3)
C11—C12	1.3975 (19)	C9—H10	1.02 (2)
C11—C19	1.519 (2)	C12—H11	0.992 (13)
C12—C13	1.398 (2)	C15—H12	1.037 (14)
C13—C14	1.4052 (16)	C16—H13	1.047 (15)
C13—C20	1.5178 (18)	C16—H14	0.999 (18)
C14—C15	1.3997 (18)	C17—H15	1.01 (2)
C14—C16	1.520 (2)	C17—H16	1.029 (17)
C16—C17	1.547 (3)	C18—H17	1.01 (3)
C17—C18	1.540 (3)	C18—H18	1.060 (19)
C19—C21^{i}	1.557 (3)	C19—H19	1.042 (15)
C20—C21	1.5323 (17)	C19—H20	1.006 (18)

C22—C22^{ii}	1.333 (11)	C20—H21	1.010 (18)
C22—C24	1.504 (7)	C20—H22	1.00 (2)
C22—C25^{ii}	1.504 (8)	C21—H23	0.991 (18)
C23—C23^{ii}	1.354 (3)	C21—H24	0.996 (18)
C23—C24	1.454 (3)		
N1···C22^{ii}	3.499 (8)	C20···H14	2.762 (14)
N1···C23^{ii}	3.470 (3)	C20···H16	3.013 (18)
N1···C25	3.523 (3)	C20···H19^{i}	2.56 (2)
N1···C25^{ii}	3.515 (3)	C20···H20^{i}	3.198 (19)
N2···C22	3.503 (8)	C21···H4^{i}	3.27 (3)
N2···C23^{ii}	3.478 (3)	C21···H9^{i}	2.697 (19)
N2···C24	3.528 (3)	C21···H11	2.608 (16)
N2···C24^{ii}	3.517 (3)	C21···H11^{i}	3.526 (18)
N3···C26^{iii}	3.504 (3)	H1···H5	3.59 (4)
N3···C27	3.506 (4)	H1···H6	2.74 (4)
N3···C29	3.544 (3)	H1···H8	2.50 (3)
N3···C29^{iii}	3.531 (2)	H1···H12	2.47 (3)
N4···C26^{iii}	3.509 (4)	H1···H13	3.50 (3)
N4···C27^{iii}	3.514 (4)	H1···H17	3.39 (3)
N4···C28	3.527 (3)	H1···H18	2.31 (3)
N4···C28^{iii}	3.535 (3)	H2···H3	2.38 (3)
C1···C4	2.757 (2)	H2···H16	2.54 (4)
C1···C8	3.134 (3)	H2···H17	2.72 (3)
C1···C10	3.508 (3)	H2···H19^{i}	2.91 (3)
C1···C14	3.550 (3)	H3···H4	2.36 (3)
C1···C15	3.002 (3)	H3···H11^{i}	2.86 (3)
C1···C17	3.563 (3)	H3···H19^{i}	3.40 (3)
C2···C5	2.794 (3)	H3···H23^{i}	3.23 (3)
C2···C14	3.279 (3)	H4···H5	2.44 (3)
C2···C15	3.308 (3)	H4···H6	3.37 (3)
C2···C16	3.251 (3)	H4···H9	3.37 (4)
C3···C6	2.800 (2)	H4···H23^{i}	2.39 (3)
C3···C17	3.175 (3)	H4···H24^{i}	3.30 (3)
C5···C8	3.600 (3)	H5···H7	2.30 (4)
C6···C9	3.140 (3)	H5···H8	2.89 (4)
C6···C10	3.241 (3)	H5···H9	2.45 (4)
C6···C15	3.329 (3)	H5···H10	3.53 (4)
C7···C10	3.383 (3)	H6···H7	2.35 (4)
C8···C15	3.062 (3)	H6···H8	2.44 (4)
C9···C19	3.0140 (18)	H6···H9	3.53 (3)
C9···C21^{i}	3.476 (2)	H7···H9	2.44 (3)
C10···C13	2.843 (2)	H7···H10	2.22 (3)
C10···C21^{i}	3.316 (2)	H7···H12	3.56 (3)
C11···C12^{i}	3.444 (2)	H8···H9	2.97 (3)
C11···C14	2.831 (2)	H8···H10	2.55 (3)
C12···C12^{i}	3.048 (2)	H8···H12	2.09 (3)
C12···C15	2.7237 (17)	H9···H20	2.32 (3)

C12···C19^{i}	3.310 (2)	H9···H23^{i}	2.63 (3)
C12···C21	2.9550 (19)	H9···H24^{i}	2.45 (3)
C12···C21^{i}	3.448 (3)	H10···H12	3.16 (3)
C13···C17	3.379 (3)	H10···H20	2.78 (3)
C13···C19^{i}	3.1660 (19)	H11···H11^{i}	2.55 (3)
C14···C18	3.354 (3)	H11···H19	2.26 (3)
C15···C17	3.522 (3)	H11···H19^{i}	3.10 (3)
C16···C20	3.0117 (18)	H11···H20	3.42 (3)
C17···C20	3.506 (2)	H11···H21	3.56 (3)
N1···C6	3.515 (3)	H11···H22	3.12 (3)
N1···C7	3.509 (3)	H11···H23	2.18 (3)
N1···C17^{iv}	3.547 (3)	H11···H23^{i}	3.58 (3)
N2···C2^{ii}	3.504 (3)	H11···H24	3.55 (3)
N2···C8^{v}	3.594 (3)	H12···H13	2.36 (3)
N2···C18^{ii}	3.469 (3)	H12···H14	3.44 (3)
N2···C19^{vi}	3.368 (3)	H12···H18	3.35 (3)
N2···C20^{iv}	3.453 (3)	H13···H15	2.43 (3)
N2···C21^{iv}	3.277 (3)	H13···H16	2.99 (3)
N3···C4^{vii}	3.553 (3)	H13···H18	2.55 (3)
N3···C9	3.408 (3)	H14···H15	2.25 (3)
N3···C20^{iii}	3.402 (3)	H14···H16	2.53 (3)
N4···C14	3.563 (3)	H14···H21	2.40 (2)
N4···C16	3.414 (3)	H14···H22	2.67 (2)
N4···C18^{viii}	3.576 (3)	H15···H17	2.33 (4)
N4···C19^{iii}	3.347 (3)	H15···H18	2.48 (3)
C1···C22	3.396 (9)	H15···H21	3.14 (3)
C1···C24	3.428 (3)	H16···H17	2.40 (3)
C2···N2^{ii}	3.504 (3)	H16···H18	2.97 (3)
C2···C22	3.499 (9)	H16···H19^{i}	3.19 (3)
C2···C23^{ii}	3.571 (3)	H16···H21	2.16 (3)
C2···C25^{ii}	3.284 (3)	H19···H21^{i}	2.55 (3)
C3···C22	3.544 (8)	H19···H22^{i}	3.54 (3)
C3···C22^{ii}	3.573 (9)	H19···H23^{i}	2.80 (3)
C3···C23^{ii}	3.300 (3)	H19···H24^{i}	2.80 (3)
C3···C24^{ii}	3.486 (3)	H20···H21^{i}	3.16 (3)
C3···C25^{ii}	3.469 (3)	H20···H23^{i}	2.76 (3)
C4···N3^{v}	3.553 (3)	H20···H24^{i}	2.22 (3)
C4···C22	3.534 (7)	H21···H23	2.91 (3)
C4···C22^{ii}	3.204 (8)	H21···H24	2.346 (19)
C4···C23	3.428 (3)	H22···H23	2.41 (3)
C4···C23^{ii}	3.321 (3)	H22···H24	2.33 (3)
C4···C24^{ii}	3.382 (3)	N1···H1^{x}	3.44 (2)
C4···C25	3.598 (3)	N1···H3^{ii}	3.52 (3)
C5···C22	3.504 (8)	N1···H6	2.79 (3)
C5···C22^{ii}	3.351 (9)	N1···H8^{x}	3.49 (3)
C5···C23	3.218 (3)	N1···H12^{x}	2.781 (16)
C5···C25	3.289 (3)	N1···H13^{x}	2.607 (15)
C6···N1	3.515 (3)	N1···H14^{iv}	3.239 (17)

C6···C22	3.468 (9)	N1···H15^{iv}	2.67 (2)
C6···C23	3.397 (3)	N1···H18^{x}	3.39 (3)
C6···C24	3.224 (3)	N2···H4	3.34 (3)
C7···N1	3.509 (3)	N2···H7^{v}	3.12 (2)
C8···N2^{vii}	3.594 (3)	N2···H8^{v}	3.010 (19)
C9···N3	3.408 (3)	N2···H16^{iv}	3.431 (16)
C9···C28	3.526 (3)	N2···H17^{ii}	2.87 (3)
C10···C26	3.434 (4)	N2···H18^{ii}	3.55 (3)
C10···C27^{iii}	3.358 (5)	N2···H19^{vi}	3.477 (18)
C10···C28	3.288 (3)	N2···H20^{vi}	2.838 (19)
C11···C26^{iii}	3.356 (4)	N2···H21^{iv}	2.777 (17)
C11···C27^{iii}	3.265 (5)	N2···H24^{iv}	2.740 (17)
C11···C29^{iii}	3.269 (3)	N3···H3^{vii}	2.76 (2)
C12···C26^{iii}	3.151 (4)	N3···H4^{vii}	3.16 (2)
C12···C27	3.362 (5)	N3···H5^{xi}	3.27 (3)
C12···C27^{iii}	3.436 (4)	N3···H9^{xi}	3.22 (3)
C12···C28^{iii}	3.288 (3)	N3···H10	2.56 (3)
C12···C29^{iii}	3.456 (3)	N3···H11^{iii}	3.550 (19)
C13···C26^{iii}	3.491 (4)	N3···H22^{iii}	2.663 (19)
C13···C27	3.305 (4)	N3···H23^{iii}	3.336 (19)
C13···C28^{iii}	3.300 (3)	N3···H24^{xii}	3.334 (16)
C14···N4	3.563 (3)	N4···H2^{vii}	3.055 (19)
C14···C26	3.497 (4)	N4···H3^{vii}	2.996 (18)
C14···C27	3.426 (5)	N4···H7^{ix}	3.49 (2)
C14···C29	3.269 (3)	N4···H13	3.10 (2)
C15···C26	3.289 (4)	N4···H14	3.003 (17)
C15···C27	3.580 (5)	N4···H15^{viii}	3.071 (17)
C15···C27^{iii}	3.599 (4)	N4···H17^{viii}	3.15 (3)
C15···C28	3.465 (3)	N4···H18^{viii}	3.29 (3)
C15···C29	3.444 (3)	N4···H19^{iii}	2.955 (19)
C16···N4	3.414 (3)	N4···H20^{iii}	2.99 (2)
C17···N1^{ix}	3.547 (3)	C3···H15^{xiii}	3.508 (19)
C18···N2^{ii}	3.469 (3)	C7···H18^{x}	3.476 (17)
C18···N4^{viii}	3.576 (3)	C7···H22^{iv}	3.26 (2)
C19···N2^{vi}	3.368 (3)	C8···H10^{xi}	3.435 (19)
C19···N4^{iii}	3.347 (3)	C8···H20^{xi}	3.532 (18)
C19···C29^{iii}	3.452 (3)	C9···H7^{xi}	3.54 (2)
C20···N2^{ix}	3.453 (3)	C9···H9^{xi}	3.55 (3)
C20···N3^{iii}	3.402 (3)	C9···H10^{xi}	3.008 (19)
C20···C28^{iii}	3.538 (3)	C17···H2^{xiii}	3.20 (3)
C21···N2^{ix}	3.277 (3)	C18···H2^{xiii}	3.37 (2)
C22···C1	3.396 (9)	C19···H7^{xi}	3.55 (2)
C22···C2	3.499 (9)	C20···H5^{ix}	3.28 (4)
C22···C3	3.544 (8)	C22···H3^{ii}	3.42 (2)
C22···C3^{ii}	3.573 (9)	C23···H4	3.50 (3)
C22···C4	3.534 (7)	C24···H2^{ii}	3.53 (3)
C22···C4^{ii}	3.204 (8)	C24···H3^{ii}	3.33 (2)
C22···C5	3.504 (8)	C24···H6	3.15 (3)

C22···C5^{ii}	3.351 (9)	C24···H15^{iv}	3.043 (19)
C22···C6	3.468 (9)	C25···H4	3.18 (3)
C23···C2^{ii}	3.571 (3)	C25···H8^{v}	3.586 (19)
C23···C3^{ii}	3.300 (3)	C25···H16^{iv}	3.544 (18)
C23···C4	3.428 (3)	C25···H17^{ii}	3.27 (3)
C23···C4^{ii}	3.321 (3)	C25···H21^{iv}	3.142 (17)
C23···C5	3.218 (3)	C25···H24^{iv}	3.508 (17)
C23···C6	3.397 (3)	C26···H3^{vii}	3.304 (17)
C24···C1	3.428 (3)	C26···H11^{iii}	3.391 (18)
C24···C3^{ii}	3.486 (3)	C27···H10^{iii}	3.58 (2)
C24···C4^{ii}	3.382 (3)	C27···H22	3.549 (18)
C24···C6	3.224 (3)	C28···H3^{vii}	2.900 (19)
C25···C2^{ii}	3.284 (3)	C28···H10	2.85 (3)
C25···C3^{ii}	3.469 (3)	C28···H11^{iii}	3.313 (19)
C25···C4	3.598 (3)	C28···H22^{iii}	2.927 (19)
C25···C5	3.289 (3)	C29···H3^{vii}	3.049 (17)
C26···C10	3.434 (4)	C29···H11^{iii}	3.510 (17)
C26···C11^{iii}	3.356 (4)	C29···H13	3.479 (19)
C26···C12^{iii}	3.151 (4)	C29···H14	3.312 (17)
C26···C13^{iii}	3.491 (4)	C29···H19^{iii}	3.228 (19)
C26···C14	3.497 (4)	C29···H20^{iii}	3.22 (3)
C26···C15	3.289 (4)	H1···N1^{x}	3.44 (2)
C27···C10^{iii}	3.358 (5)	H1···H1^{x}	2.71 (2)
C27···C11^{iii}	3.265 (5)	H1···H6^{x}	3.34 (3)
C27···C12	3.362 (5)	H1···H8^{x}	3.39 (3)
C27···C12^{iii}	3.436 (4)	H2···N4^{v}	3.055 (19)
C27···C13	3.305 (4)	H2···C17^{xiii}	3.20 (3)
C27···C14	3.426 (5)	H2···C18^{xiii}	3.37 (2)
C27···C15	3.580 (5)	H2···C24^{ii}	3.53 (3)
C27···C15^{iii}	3.599 (4)	H2···H15^{xiii}	2.73 (3)
C28···C9	3.526 (3)	H2···H16^{xiii}	3.00 (3)
C28···C10	3.288 (3)	H2···H17^{xiii}	2.65 (3)
C28···C12^{iii}	3.288 (3)	H3···N1^{ii}	3.52 (3)
C28···C13^{iii}	3.300 (3)	H3···N3^{v}	2.76 (2)
C28···C15	3.465 (3)	H3···N4^{v}	2.996 (18)
C28···C20^{iii}	3.538 (3)	H3···C22^{ii}	3.42 (2)
C29···C11^{iii}	3.269 (3)	H3···C24^{ii}	3.33 (2)
C29···C12^{iii}	3.456 (3)	H3···C26^{v}	3.304 (17)
C29···C14	3.269 (3)	H3···C28^{v}	2.900 (19)
C29···C15	3.444 (3)	H3···C29^{v}	3.049 (17)
C29···C19^{iii}	3.452 (3)	H4···N2	3.34 (3)
C1···H2	3.321 (19)	H4···N3^{v}	3.16 (2)
C1···H4	3.27 (3)	H4···C23	3.50 (3)
C1···H5	3.30 (3)	H4···C25	3.18 (3)
C1···H6	2.80 (3)	H4···H22^{iv}	3.25 (3)
C1···H8	2.92 (2)	H4···H24^{iv}	2.95 (4)
C1···H12	2.70 (2)	H5···N3^{xi}	3.27 (3)
C1···H17	3.19 (3)	H5···C20^{iv}	3.28 (4)

C1···H18	2.58 (3)	H5···H14^{iv}	3.32 (4)
C2···H3	3.33 (2)	H5···H21^{iv}	3.36 (4)
C2···H12	3.257 (19)	H5···H22^{iv}	2.39 (4)
C2···H13	3.51 (2)	H6···N1	2.79 (3)
C2···H15	3.41 (2)	H6···C24	3.15 (3)
C2···H16	2.75 (2)	H6···H1^{x}	3.34 (3)
C3···H1	3.299 (16)	H6···H14^{iv}	3.01 (4)
C3···H4	3.28 (3)	H6···H18^{x}	2.64 (3)
C3···H16	2.89 (3)	H6···H22^{iv}	3.35 (4)
C3···H17	2.77 (2)	H7···N2^{vii}	3.12 (2)
C3···H18	3.39 (2)	H7···N4^{iv}	3.49 (2)
C3···H19^{i}	3.304 (15)	H7···C9^{xi}	3.54 (2)
C4···H11^{i}	3.119 (15)	H7···C19^{xi}	3.55 (2)
C4···H19^{i}	3.547 (17)	H7···H9^{xi}	3.27 (4)
C4···H23^{i}	3.189 (18)	H7···H10^{xi}	2.85 (3)
C5···H1	3.308 (18)	H7···H18^{x}	3.40 (3)
C5···H2	3.31 (2)	H7···H20^{xi}	2.55 (3)
C5···H5	2.62 (3)	H8···N1^{x}	3.49 (3)
C5···H6	3.17 (2)	H8···N2^{vii}	3.010 (19)
C5···H9	3.52 (3)	H8···C25^{vii}	3.586 (19)
C5···H11^{i}	3.587 (14)	H8···H1^{x}	3.39 (3)
C5···H23^{i}	2.731 (17)	H8···H18^{x}	3.42 (3)
C6···H3	3.327 (18)	H9···N3^{xi}	3.22 (3)
C6···H7	3.41 (2)	H9···C9^{xi}	3.55 (3)
C6···H8	2.86 (2)	H9···H7^{xi}	3.27 (4)
C6···H9	3.23 (3)	H9···H10^{xi}	2.70 (3)
C6···H12	3.24 (2)	H10···N3	2.56 (3)
C6···H23^{i}	3.504 (15)	H10···C8^{xi}	3.435 (19)
C7···H1	2.681 (19)	H10···C9^{xi}	3.008 (19)
C7···H4	2.72 (2)	H10···C27^{iii}	3.58 (2)
C7···H9	2.66 (2)	H10···C28	2.85 (3)
C7···H10	3.42 (2)	H10···H7^{xi}	2.85 (3)
C7···H12	3.484 (19)	H10···H9^{xi}	2.70 (3)
C8···H1	3.023 (19)	H10···H10^{xi}	2.53 (3)
C8···H12	2.726 (18)	H11···N3^{iii}	3.550 (19)
C9···H5	2.74 (3)	H11···C26^{iii}	3.391 (18)
C9···H6	3.39 (3)	H11···C28^{iii}	3.313 (19)
C9···H12	2.719 (18)	H11···C29^{iii}	3.510 (17)
C9···H20	2.789 (15)	H12···N1^{x}	2.781 (16)
C9···H23^{i}	3.299 (16)	H13···N1^{x}	2.607 (15)
C9···H24^{i}	3.410 (17)	H13···N4	3.10 (2)
C10···H7	3.411 (19)	H13···C29	3.479 (19)
C10···H8	2.817 (16)	H13···H13^{viii}	3.16 (3)
C10···H11	3.289 (13)	H13···H14^{viii}	3.34 (3)
C10···H19	3.368 (15)	H13···H15^{viii}	2.94 (3)
C10···H20	2.773 (18)	H14···N1^{ix}	3.239 (17)
C10···H23^{i}	3.033 (18)	H14···N4	3.003 (17)
C11···H9	2.62 (2)	H14···C29	3.312 (17)

C11···H10	2.944 (17)	H14···H5^{ix}	3.32 (4)
C11···H11^{i}	2.870 (16)	H14···H6^{ix}	3.01 (4)
C11···H12	3.338 (15)	H14···H13^{viii}	3.34 (3)
C11···H23^{i}	2.52 (2)	H14···H18^{viii}	3.58 (3)
C11···H24^{i}	3.20 (2)	H15···N1^{ix}	2.67 (2)
C12···H3^{i}	3.592 (19)	H15···N4^{viii}	3.071 (17)
C12···H11^{i}	2.630 (18)	H15···C3^{xiii}	3.508 (19)
C12···H19	2.543 (18)	H15···C24^{ix}	3.043 (19)
C12···H19^{i}	3.099 (18)	H15···H2^{xiii}	2.73 (3)
C12···H20	3.245 (19)	H15···H13^{viii}	2.94 (3)
C12···H21	3.274 (18)	H16···N2^{ix}	3.431 (16)
C12···H22	3.00 (2)	H16···C25^{ix}	3.544 (18)
C12···H23	2.804 (15)	H16···H2^{xiii}	3.00 (3)
C12···H23^{i}	3.324 (19)	H16···H17^{xiii}	2.93 (3)
C13···H11^{i}	3.309 (18)	H17···N2^{ii}	2.87 (3)
C13···H12	3.339 (14)	H17···N4^{viii}	3.15 (3)
C13···H13	3.388 (16)	H17···C25^{ii}	3.27 (3)
C13···H14	2.715 (16)	H17···H2^{xiii}	2.65 (3)
C13···H16	3.165 (19)	H17···H16^{xiii}	2.93 (3)
C13···H19^{i}	2.809 (18)	H17···H19^{xiv}	3.54 (3)
C13···H23	2.842 (14)	H18···N1^{x}	3.39 (3)
C13···H24	3.394 (15)	H18···N2^{ii}	3.55 (3)
C14···H11	3.302 (14)	H18···N4^{viii}	3.29 (3)
C14···H15	3.390 (19)	H18···C7^{x}	3.476 (17)
C14···H16	2.82 (2)	H18···H6^{x}	2.64 (3)
C14···H21	2.643 (15)	H18···H7^{x}	3.40 (3)
C14···H22	2.905 (17)	H18···H8^{x}	3.42 (3)
C15···H1	3.098 (18)	H18···H14^{viii}	3.58 (3)
C15···H8	2.754 (18)	H19···N2^{vi}	3.477 (18)
C15···H9	3.32 (3)	H19···N4^{iii}	2.955 (19)
C15···H10	3.044 (19)	H19···C29^{iii}	3.228 (19)
C15···H13	2.620 (19)	H19···H17^{xv}	3.54 (3)
C15···H14	3.215 (17)	H20···N2^{vi}	2.838 (19)
C16···H12	2.663 (17)	H20···N4^{iii}	2.99 (2)
C16···H17	3.45 (3)	H20···C8^{xi}	3.532 (18)
C16···H18	2.81 (2)	H20···C29^{iii}	3.22 (3)
C16···H21	2.634 (14)	H20···H7^{xi}	2.55 (3)
C16···H22	3.205 (15)	H21···N2^{ix}	2.777 (17)
C17···H2	3.10 (3)	H21···C25^{ix}	3.142 (17)
C17···H12	3.597 (17)	H21···H5^{ix}	3.36 (4)
C17···H21	2.756 (15)	H22···N3^{iii}	2.663 (19)
C18···H1	2.659 (18)	H22···C7^{ix}	3.26 (2)
C18···H2	2.74 (2)	H22···C27	3.549 (18)
C18···H12	3.556 (18)	H22···C28^{iii}	2.927 (19)
C18···H13	2.78 (2)	H22···H4^{ix}	3.25 (3)
C18···H14	3.449 (18)	H22···H5^{ix}	2.39 (4)
C19···H9	2.574 (18)	H22···H6^{ix}	3.35 (4)
C19···H10	3.277 (16)	H23···N3^{iii}	3.336 (19)

C19···H11	2.610 (16)	H24···N2^{ix}	2.740 (17)
C19···H11^{i}	3.005 (17)	H24···N3^{xvi}	3.334 (16)
C19···H21^{i}	2.776 (17)	H24···C25^{ix}	3.508 (17)
C19···H22^{i}	3.44 (2)	H24···H4^{ix}	2.95 (4)
C20···H11	2.695 (17)		

C2—C1—C6	122.08 (13)	N4—C29—C26	162.91 (18)
C1—C2—C3	118.44 (14)	N4—C29—C27	159.5 (2)
C1—C2—C18	120.43 (13)	C26—C29—C27	37.62 (17)
C3—C2—C18	121.03 (13)	C2—C1—H1	118.1 (11)
C2—C3—C4	120.06 (13)	C6—C1—H1	119.8 (11)
C3—C4—C5	120.49 (14)	C2—C3—H2	121.3 (13)
C4—C5—C6	120.66 (15)	C4—C3—H2	118.6 (12)
C1—C6—C5	118.04 (13)	C3—C4—H3	119.8 (12)
C1—C6—C7	119.43 (14)	C5—C4—H3	119.7 (12)
C5—C6—C7	122.39 (15)	C4—C5—H4	119.3 (12)
C6—C7—C8	114.34 (15)	C6—C5—H4	120.1 (12)
C7—C8—C9	116.32 (13)	C6—C7—H5	111.3 (15)
C8—C9—C10	119.05 (14)	C6—C7—H6	111.8 (15)
C9—C10—C11	120.79 (13)	C8—C7—H5	105.0 (19)
C9—C10—C15	121.46 (11)	C8—C7—H6	109.9 (16)
C11—C10—C15	117.74 (12)	H5—C7—H6	104 (3)
C10—C11—C12	118.50 (13)	C7—C8—H7	109.4 (14)
C10—C11—C19	123.07 (12)	C7—C8—H8	110.1 (12)
C12—C11—C19	118.29 (10)	C9—C8—H7	106.1 (11)
C11—C12—C13	123.50 (11)	C9—C8—H8	110.0 (10)
C12—C13—C14	117.90 (12)	H7—C8—H8	104.2 (16)
C12—C13—C20	120.57 (10)	C8—C9—H9	106.3 (12)
C14—C13—C20	121.52 (12)	C8—C9—H10	109.4 (9)
C13—C14—C15	118.34 (13)	C10—C9—H9	106.8 (11)
C13—C14—C16	122.34 (12)	C10—C9—H10	108.3 (11)
C15—C14—C16	119.33 (10)	H9—C9—H10	106.2 (17)
C10—C15—C14	123.34 (11)	C11—C12—H11	117.0 (10)
C14—C16—C17	116.14 (13)	C13—C12—H11	119.5 (10)
C16—C17—C18	116.71 (12)	C10—C15—H12	118.4 (10)
C2—C18—C17	113.70 (12)	C14—C15—H12	118.0 (10)
C11—C19—C21^{i}	112.79 (12)	C14—C16—H13	110.5 (10)
C13—C20—C21	116.02 (12)	C14—C16—H14	107.8 (9)
C19^{i}—C21—C20	113.53 (11)	C17—C16—H13	108.5 (11)
C22^{ii}—C22—C24	113.7 (7)	C17—C16—H14	110.1 (10)
C22^{ii}—C22—C25^{ii}	113.6 (6)	H13—C16—H14	103.0 (14)
C24—C22—C25^{ii}	132.7 (6)	C16—C17—H15	105.0 (12)
C23^{ii}—C23—C24	118.44 (17)	C16—C17—H16	112.2 (11)
C23^{ii}—C23—C25	119.30 (15)	C18—C17—H15	110.0 (11)
C24—C23—C25	122.26 (15)	C18—C17—H16	108.7 (12)
N1—C24—C22	148.2 (4)	H15—C17—H16	103.3 (15)
N1—C24—C23	174.27 (19)	C2—C18—H17	109.3 (14)
C22—C24—C23	37.5 (4)	C2—C18—H18	109.4 (13)

N2—C25—C22^{ii}	148.1 (3)	C17—C18—H17	107.9 (12)
N2—C25—C23	174.49 (16)	C17—C18—H18	109.1 (13)
C22^{ii}—C25—C23	37.4 (3)	H17—C18—H18	107.2 (16)
C26^{iii}—C26—C27^{iii}	44.2 (3)	C11—C19—H19	107.6 (10)
C26^{iii}—C26—C28	116.0 (3)	C11—C19—H20	110.4 (11)
C26^{iii}—C26—C29	116.9 (3)	C21^{i}—C19—H19	110.1 (11)
C27^{iii}—C26—C28	71.8 (3)	C21^{i}—C19—H20	109.6 (12)
C27^{iii}—C26—C29	161.1 (3)	H19—C19—H20	106.1 (14)
C28—C26—C29	127.10 (18)	C13—C20—H21	107.6 (9)
C26^{iii}—C27—C27^{iii}	44.5 (3)	C13—C20—H22	106.4 (10)
C26^{iii}—C27—C28^{iii}	69.9 (3)	C21—C20—H21	108.8 (9)
C26^{iii}—C27—C29	161.3 (4)	C21—C20—H22	110.0 (9)
C27^{iii}—C27—C28^{iii}	114.4 (3)	H21—C20—H22	107.8 (15)
C27^{iii}—C27—C29	116.8 (3)	C19^{i}—C21—H23	109.4 (12)
C28^{iii}—C27—C29	128.8 (3)	C19^{i}—C21—H24	109.3 (12)
N3—C28—C26	163.7 (2)	C20—C21—H23	111.4 (9)
N3—C28—C27^{iii}	157.9 (3)	C20—C21—H24	106.3 (9)
C26—C28—C27^{iii}	38.33 (18)	H23—C21—H24	106.6 (13)

C2—C1—C6—C5	5.5 (3)	C22^{ii}—C22—C24—N1	179.6 (5)
C2—C1—C6—C7	−170.23 (13)	C22^{ii}—C22—C24—C23	−0.7 (4)
C6—C1—C2—C3	−5.2 (3)	C24—C22—C22^{ii}—C25	1.8 (9)
C6—C1—C2—C18	171.25 (13)	C22^{ii}—C22—C25^{ii}—N2^{ii}	−178.7 (5)
C1—C2—C3—C4	1.7 (2)	C22^{ii}—C22—C25^{ii}—C23^{ii}	0.7 (4)
C1—C2—C18—C17	−111.99 (14)	C25^{ii}—C22—C22^{ii}—C24^{ii}	−1.8 (9)
C3—C2—C18—C17	64.33 (19)	C24—C22—C25^{ii}—N2^{ii}	−1.0 (13)
C18—C2—C3—C4	−174.72 (13)	C24—C22—C25^{ii}—C23^{ii}	178.4 (11)
C2—C3—C4—C5	1.3 (3)	C25^{ii}—C22—C24—N1	1.9 (13)
C3—C4—C5—C6	−0.9 (3)	C25^{ii}—C22—C24—C23	−178.4 (11)
C4—C5—C6—C1	−2.4 (3)	C23^{ii}—C23—C24—C22	0.71 (12)
C4—C5—C6—C7	173.19 (14)	C24—C23—C23^{ii}—C25^{ii}	0.0 (3)
C1—C6—C7—C8	61.87 (19)	C23^{ii}—C23—C25—C22^{ii}	0.72 (12)
C5—C6—C7—C8	−113.71 (18)	C25—C23—C23^{ii}—C24^{ii}	−0.0 (3)
C6—C7—C8—C9	60.3 (2)	C24—C23—C25—C22^{ii}	−179.3 (3)
C7—C8—C9—C10	−77.14 (19)	C25—C23—C24—C22	−179.3 (3)
C8—C9—C10—C11	151.51 (14)	C26^{iii}—C26—C27^{iii}—C27	0 (12936568)
C8—C9—C10—C15	−29.5 (2)	C26^{iii}—C26—C27^{iii}—C28	−179.6 (4)
C9—C10—C11—C12	179.26 (13)	C27^{iii}—C26—C26^{iii}—C28^{iii}	−179.6 (5)
C9—C10—C11—C19	−5.1 (3)	C27^{iii}—C26—C26^{iii}—C29^{iii}	−0.2 (4)
C9—C10—C15—C14	173.81 (13)	C26^{iii}—C26—C28—C27^{iii}	0.30 (17)
C11—C10—C15—C14	−7.2 (3)	C28—C26—C26^{iii}—C27	179.6 (4)
C15—C10—C11—C12	0.2 (2)	C28—C26—C26^{iii}—C29^{iii}	−0.6 (4)
C15—C10—C11—C19	175.82 (12)	C26^{iii}—C26—C29—C27	−0.16 (17)
C10—C11—C12—C13	6.5 (3)	C29—C26—C26^{iii}—C27	0.2 (3)
C10—C11—C19—C21^{i}	−76.48 (16)	C29—C26—C26^{iii}—C28^{iii}	0.6 (4)
C12—C11—C19—C21^{i}	99.13 (14)	C28—C26—C27^{iii}—C27	179.6 (3)
C19—C11—C12—C13	−169.30 (12)	C28—C26—C29—C27	−179.5 (4)
C11—C12—C13—C14	−6.3 (3)	C29—C26—C28—C27^{iii}	179.6 (4)

C11—C12—C13—C20	173.34 (13)	C26^{iii}—C27—C27^{iii}—C28	−179.6 (5)
C12—C13—C14—C15	−0.6 (2)	C26^{iii}—C27—C27^{iii}—C29^{iii}	0.2 (4)
C12—C13—C14—C16	179.13 (12)	C26^{iii}—C27—C28^{iii}—N3^{iii}	−178.8 (6)
C12—C13—C20—C21	−24.0 (2)	C27^{iii}—C27—C28^{iii}—N3^{iii}	−178.5 (5)
C14—C13—C20—C21	155.60 (13)	C27^{iii}—C27—C28^{iii}—C26^{iii}	0.3 (2)
C20—C13—C14—C15	179.77 (12)	C28^{iii}—C27—C27^{iii}—C26	179.6 (5)
C20—C13—C14—C16	−0.5 (3)	C28^{iii}—C27—C27^{iii}—C29^{iii}	−0.2 (5)
C13—C14—C15—C10	7.4 (3)	C27^{iii}—C27—C29—N4	−177.8 (5)
C13—C14—C16—C17	−78.71 (17)	C27^{iii}—C27—C29—C26	0.2 (2)
C15—C14—C16—C17	101.02 (14)	C29—C27—C27^{iii}—C26	−0.2 (3)
C16—C14—C15—C10	−172.37 (13)	C29—C27—C27^{iii}—C28	0.2 (5)
C14—C16—C17—C18	−75.03 (13)	C28^{iii}—C27—C29—N4	2.4 (9)
C16—C17—C18—C2	69.70 (16)	C28^{iii}—C27—C29—C26	−179.6 (6)
C11—C19—C21^{i}—C20^{i}	−122.71 (10)	C29—C27—C28^{iii}—N3^{iii}	1.3 (9)
C13—C20—C21—C19^{i}	−62.02 (16)	C29—C27—C28^{iii}—C26^{iii}	−179.9 (6)

Symmetry codes: (i) −*x*, −*y*, −*z*; (ii) −*x*, −*y*+1, −*z*+1; (iii) −*x*+1, −*y*, −*z*; (iv) *x*, *y*+1, *z*; (v) *x*−1, *y*, *z*; (vi) −*x*, −*y*+1, −*z*; (vii) *x*+1, *y*, *z*; (viii) −*x*+1, −*y*, −*z*+1; (ix) *x*, *y*−1, *z*; (x) −*x*+1, −*y*+1, −*z*+1; (xi) −*x*+1, −*y*+1, −*z*; (xii) *x*+1, *y*+1, *z*; (xiii) −*x*, −*y*, −*z*+1; (xiv) *x*, *y*, *z*+1; (xv) *x*, *y*, *z*−1; (xvi) *x*−1, *y*−1, *z*.