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Carbonyl[hydrotris(3,5-dimethylpyrazol-1-yl)-borato]copper(I) acetonitrile solvate

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.005 Å
R factor = 0.042
wR factor = 0.125
Data-to-parameter ratio = 19.0

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

The title compound, $[Cu(C_{15}H_{22}BN_6)(CO)]\cdot C_2H_3N$, crystallizes as neutral $[Tp^*Cu(CO)]$ {$[Tp^*]^-$ = hydrotris(3,5-dimethylpyrazol-1-yl)borate} molecular units and non-coordinated acetonitrile molecules. The distorted tetrahedral coordination geometry of the copper(I) centre comprises the three N atoms of the $[Tp^*]^-$ anion [Cu—N 2.033 (2)–2.054 (2) Å] and the C atom of the carbon monoxide molecule [Cu—C 1.785 (4) Å].

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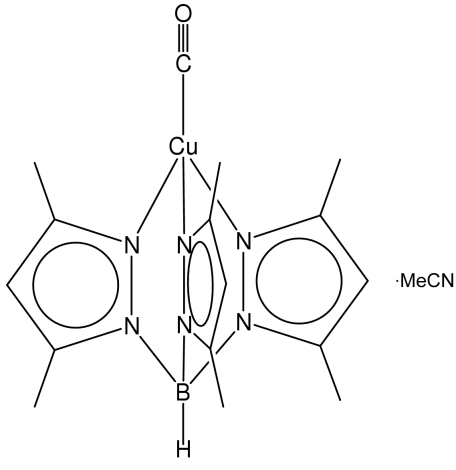
Comment

The structure of the title compound $[Tp^*Cu(CO)]\cdot MeCN$ {$[Tp^*]^-$ = hydrotris(3,5-dimethylpyrazol-1-yl)borate}, (I), comprises neutral $[Tp^*Cu(CO)]$ molecular units and non-coordinated acetonitrile molecules. The $[Tp^*Cu(CO)]$ molecular unit is similar to those of previously structurally characterized analogues, which differ solely in the identities of the 3,5-substituents on the pyrazole rings (Churchill *et al.*, 1975; Conry *et al.*, 1999; Dias & Kim, 1996; Dias *et al.*, 1996; Imai *et al.*, 1998; Kitajima *et al.*, 1992).



(I)

The copper(I) centre has a distorted tetrahedral geometry comprising the three N atoms of the $[Tp^*]^-$ anion and the C atom of the carbon monoxide molecule. The Cu—N and Cu—C interatomic distances [Cu—N 2.033 (2)–2.054 (2) and Cu—C 1.785 (4) Å] and N—Cu—C and Cu—C—O interatomic angles [N—Cu—C 124.27 (14)–124.52 (14) and Cu—C—O 179.3 (4)°] fall within the range of values reported previously [Cu—N 2.014–2.086, Cu—C 1.752–1.808 Å, N—Cu—C 119.4–128.5 and Cu—C—O 176.6–180.0° (Churchill *et al.*, 1975; Conry *et al.*, 1999; Dias & Kim, 1996; Dias *et al.*, 1996; Imai *et al.*, 1998; Kitajima *et al.*, 1992)].

Experimental

The title compound was prepared following an adaptation of a literature method (Abu Salah *et al.*, 1982). $Cu(MeCN)_4BF_4$ (1.10 g, 3.50 mmol) and KTp* (1.18 g, 3.51 mmol) were dissolved in acetonitrile (200 ml), previously saturated with CO gas. The white solid, formed after stirring for 2 h under a stream of CO gas, was isolated by filtration (1.16 g, 2.69 mmol, 77% yield). A small crop of crystals was obtained from the mother liquor after a further 24 h under CO gas.

Crystal data

$[Cu(C_{15}H_{22}BN_6)(CO)]\cdot C_2H_3N$	D_x = 1.344 Mg m^{-3}
M_r = 429.80	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 2631 reflections
a = 14.915 (2) Å	θ = 2.5–25.4°
b = 7.6811 (10) Å	μ = 1.05 mm^{-1}
c = 18.688 (2) Å	T = 150 (2) K
β = 97.360 (2)°	Plate, colourless
V = 2123.3 (5) Å^3	0.30 × 0.14 × 0.03 mm
Z = 4	

Data collection

Bruker SMART1000 CCD area-detector diffractometer	4937 independent reflections
	3300 reflections with $I > 2\sigma(I)$
ω scans	R_{int} = 0.050
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)	θ_{max} = 28.7°
	$h = -19 \rightarrow 19$
T_{min} = 0.854, T_{max} = 1.000	$k = -10 \rightarrow 10$
14745 measured reflections	$l = -24 \rightarrow 24$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.061P)^2 + 0.255P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.042	
$wR(F^2)$ = 0.125	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.07	$\Delta\rho_{max}$ = 0.50 e Å^{-3}
4937 reflections	$\Delta\rho_{min}$ = −0.49 e Å^{-3}
260 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Cu1—C1	1.785 (4)	Cu1—N2*B*	2.033 (2)
Cu1—N2*A*	2.033 (3)	Cu1—N2*C*	2.054 (2)
		C1—O1	1.125 (4)
C1—Cu1—N2*A*	124.52 (14)	N2*A*—Cu1—N2*C*	91.46 (10)
C1—Cu1—N2*B*	124.27 (14)	N2*B*—Cu1—N2*C*	91.05 (10)
N2*A*—Cu1—N2*B*	91.18 (10)	O1—C1—Cu1	179.3 (4)
C1—Cu1—N2*C*	124.38 (14)		

Methyl H atoms were located from ΔF syntheses and refined as part of a rigid rotating group with C—H = 0.96 Å and with U_{iso}(H) = 1.5U_{eq}(C). After location from ΔF syntheses, other H atoms were placed geometrically and refined using a riding model; B—H and C—H distances were constrained to 0.98 and 0.93 Å, respectively, with U_{iso}(H) = 1.2U_{eq}(B or C).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT* and *SHELXTL* (Bruker, 1997); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* and *CAMERON* (Watkin *et al.*, 1996); software used to prepare material for publication: *SHELXL*97 and *PLATON* (Spek, 2001).

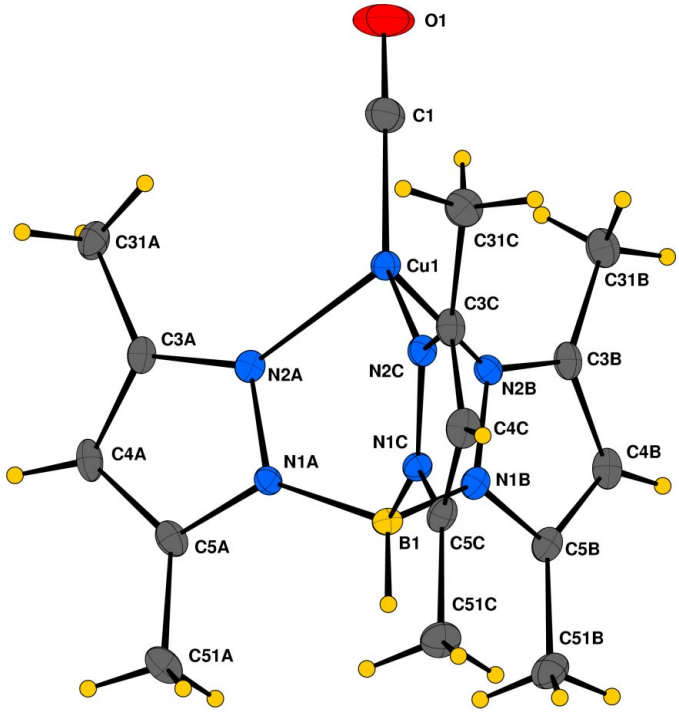


Figure 1
A view of the title compound showing the atom-numbering scheme, but with the non-coordinated acetonitrile solvent molecule omitted for clarity. Displacement ellipsoids are drawn at the 30% probability level.

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Carbonyl(hydrotris(3,5-dimethylpyrazol-1-yl)borato)copper(I) acetonitrile solvate (1/1)

Crystal data

$[Cu(C_{15}H_{22}BN_6)(CO)]\cdot C_2H_3N$
$M_r = 429.80$
Monoclinic, $P2_1/c$
$a = 14.915$ (2) Å
$b = 7.6811$ (10) Å
$c = 18.688$ (2) Å
$\beta = 97.360$ (2)°
$V = 2123.3$ (5) Å^3
$Z = 4$
$F(000) = 896$
$D_x = 1.344$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2631 reflections
$\theta = 2.5$–25.4°
$\mu = 1.05$ mm^{-1}
$T = 150$ K
Plate, colourless
0.30 × 0.14 × 0.03 mm

Data collection

Bruker SMART1000 CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2001)
$T_{min} = 0.854$, $T_{max} = 1.000$
14745 measured reflections
4937 independent reflections
3300 reflections with $I > 2\sigma(I)$
$R_{int} = 0.050$
$\theta_{max} = 28.7°$, $\theta_{min} = 1.4°$
$h = -19\rightarrow19$
$k = -10\rightarrow10$
$l = -24\rightarrow24$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.125$
$S = 1.07$
4937 reflections
260 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier
Hydrogen site location: see text
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.061P)^2 + 0.255P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.50$ e Å^{-3}
$\Delta\rho_{min} = -0.49$ 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.

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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.68232 (2)	0.10663 (5)	0.88437 (2)	0.01992 (13)
C1	0.6343 (2)	0.1052 (5)	0.9671 (2)	0.0346 (8)
O1	0.6033 (2)	0.1036 (5)	1.01886 (18)	0.0762 (11)
B1	0.7640 (2)	0.1106 (4)	0.74339 (19)	0.0195 (7)
H1	0.7904	0.1123	0.6980	0.023*
N1A	0.67236 (16)	0.0124 (3)	0.73298 (13)	0.0186 (5)
N2A	0.62374 (16)	−0.0025 (3)	0.79079 (14)	0.0208 (6)
C3A	0.54820 (19)	−0.0904 (4)	0.76696 (18)	0.0224 (7)
C31A	0.4787 (2)	−0.1273 (4)	0.81625 (19)	0.0289 (8)
H31A	0.5038	−0.1034	0.8652	0.043*
H31B	0.4611	−0.2475	0.8119	0.043*
H31C	0.4268	−0.0548	0.8032	0.043*
C4A	0.5475 (2)	−0.1329 (4)	0.69454 (19)	0.0271 (8)
H4A	0.5028	−0.1939	0.6656	0.033*
C5A	0.6267 (2)	−0.0663 (4)	0.67418 (18)	0.0244 (7)
C51A	0.6613 (3)	−0.0711 (5)	0.60224 (19)	0.0366 (9)
H51A	0.6668	0.0456	0.5849	0.055*
H51B	0.6197	−0.1351	0.5686	0.055*
H51C	0.7193	−0.1269	0.6072	0.055*
N1B	0.74858 (15)	0.2991 (3)	0.76854 (14)	0.0202 (5)
N2B	0.71211 (16)	0.3263 (3)	0.83149 (14)	0.0192 (5)
C3B	0.70537 (19)	0.4987 (4)	0.83980 (18)	0.0228 (7)
C31B	0.6683 (2)	0.5733 (4)	0.9036 (2)	0.0299 (8)
H31D	0.6052	0.5458	0.9008	0.045*
H31E	0.6760	0.6974	0.9041	0.045*
H31F	0.7000	0.5247	0.9470	0.045*
C4B	0.7378 (2)	0.5842 (4)	0.78203 (19)	0.0257 (7)
H4B	0.7409	0.7038	0.7750	0.031*
C5B	0.76420 (19)	0.4554 (4)	0.73758 (18)	0.0222 (7)
C51B	0.7996 (2)	0.4708 (4)	0.66653 (19)	0.0316 (8)
H51D	0.8541	0.4039	0.6676	0.047*
H51E	0.8123	0.5908	0.6574	0.047*
H51F	0.7553	0.4278	0.6289	0.047*
N1C	0.82865 (15)	0.0165 (3)	0.80260 (14)	0.0192 (5)
N2C	0.80546 (16)	0.0001 (3)	0.87128 (14)	0.0204 (5)

C3C	0.8732 (2)	−0.0840 (4)	0.91076 (18)	0.0229 (7)
C31C	0.8691 (2)	−0.1212 (4)	0.98875 (19)	0.0304 (8)
H31G	0.8192	−0.0596	1.0044	0.046*
H31H	0.9244	−0.0840	1.0166	0.046*
H31I	0.8613	−0.2440	0.9953	0.046*
C4C	0.9404 (2)	−0.1238 (4)	0.86767 (19)	0.0263 (7)
H4C	0.9944	−0.1821	0.8819	0.032*
C5C	0.91071 (19)	−0.0593 (4)	0.79994 (18)	0.0230 (7)
C51C	0.9538 (2)	−0.0682 (4)	0.73189 (19)	0.0313 (8)
H51G	0.9146	−0.1292	0.6956	0.047*
H51H	1.0104	−0.1287	0.7411	0.047*
H51I	0.9641	0.0476	0.7154	0.047*
N1S	0.8671 (2)	0.3607 (5)	1.0328 (2)	0.0518 (9)
C2S	0.8918 (2)	0.3687 (4)	0.9777 (2)	0.0336 (8)
C3S	0.9254 (2)	0.3816 (5)	0.9080 (2)	0.0344 (8)
H3S1	0.9880	0.4143	0.9152	0.052*
H3S2	0.8913	0.4680	0.8790	0.052*
H3S3	0.9190	0.2710	0.8840	0.052*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.01721 (19)	0.02267 (19)	0.0197 (2)	0.00006 (15)	0.00168 (14)	0.00044 (17)
C1	0.0290 (18)	0.047 (2)	0.029 (2)	−0.0015 (16)	0.0047 (15)	−0.0046 (18)
O1	0.072 (2)	0.124 (3)	0.039 (2)	−0.015 (2)	0.0303 (18)	−0.008 (2)
B1	0.0193 (16)	0.0214 (16)	0.0185 (18)	0.0003 (13)	0.0046 (14)	0.0007 (15)
N1A	0.0183 (12)	0.0204 (12)	0.0164 (14)	−0.0006 (10)	−0.0005 (10)	0.0000 (10)
N2A	0.0184 (13)	0.0203 (12)	0.0231 (15)	0.0014 (10)	0.0006 (11)	0.0020 (11)
C3A	0.0185 (14)	0.0190 (15)	0.0282 (18)	0.0009 (11)	−0.0028 (13)	0.0013 (13)
C31A	0.0200 (15)	0.0324 (18)	0.033 (2)	−0.0049 (13)	−0.0003 (14)	0.0016 (15)
C4A	0.0235 (16)	0.0227 (16)	0.032 (2)	−0.0030 (12)	−0.0094 (14)	−0.0018 (14)
C5A	0.0265 (16)	0.0231 (16)	0.0213 (18)	0.0032 (12)	−0.0053 (13)	−0.0002 (13)
C51A	0.043 (2)	0.043 (2)	0.023 (2)	−0.0058 (16)	−0.0017 (16)	−0.0057 (16)
N1B	0.0154 (12)	0.0216 (13)	0.0228 (15)	0.0002 (10)	−0.0011 (10)	0.0034 (11)
N2B	0.0177 (12)	0.0211 (12)	0.0179 (14)	0.0002 (10)	−0.0007 (10)	−0.0001 (11)
C3B	0.0174 (15)	0.0220 (15)	0.0267 (19)	0.0001 (12)	−0.0057 (13)	−0.0002 (13)
C31B	0.0311 (18)	0.0254 (17)	0.032 (2)	0.0010 (13)	0.0007 (15)	−0.0033 (14)
C4B	0.0233 (16)	0.0194 (16)	0.032 (2)	0.0001 (12)	−0.0061 (14)	0.0024 (14)
C5B	0.0170 (15)	0.0231 (15)	0.0252 (18)	0.0001 (11)	−0.0024 (13)	0.0059 (13)
C51B	0.0336 (19)	0.0304 (18)	0.031 (2)	−0.0039 (14)	0.0045 (16)	0.0092 (15)
N1C	0.0172 (12)	0.0204 (12)	0.0201 (14)	0.0004 (10)	0.0030 (11)	0.0006 (11)
N2C	0.0181 (13)	0.0218 (13)	0.0205 (15)	−0.0005 (10)	−0.0009 (11)	0.0015 (11)
C3C	0.0203 (15)	0.0198 (15)	0.0265 (18)	0.0006 (12)	−0.0048 (13)	0.0012 (13)
C31C	0.0264 (17)	0.0353 (19)	0.028 (2)	0.0024 (14)	−0.0042 (14)	0.0050 (15)
C4C	0.0172 (15)	0.0265 (16)	0.033 (2)	0.0059 (12)	−0.0040 (13)	0.0035 (14)
C5C	0.0147 (14)	0.0228 (15)	0.031 (2)	0.0000 (11)	0.0035 (13)	0.0006 (13)
C51C	0.0228 (17)	0.038 (2)	0.035 (2)	0.0053 (13)	0.0082 (15)	0.0001 (15)
N1S	0.051 (2)	0.064 (2)	0.041 (2)	0.0064 (17)	0.0058 (18)	0.0069 (18)

C2S	0.0276 (18)	0.034 (2)	0.036 (2)	0.0003 (14)	−0.0070 (16)	0.0020 (16)
C3S	0.0290 (18)	0.039 (2)	0.034 (2)	−0.0060 (15)	−0.0027 (15)	0.0023 (17)

Geometric parameters (Å, º)

Cu1—C1	1.785 (4)	N1C—N2C	1.377 (3)
Cu1—N2A	2.033 (3)	N2C—C3C	1.338 (4)
Cu1—N2B	2.033 (2)	C3C—C4C	1.398 (5)
Cu1—N2C	2.054 (2)	C3C—C31C	1.494 (5)
C1—O1	1.125 (4)	C4C—C5C	1.378 (5)
B1—N1B	1.548 (4)	C5C—C51C	1.498 (5)
B1—N1C	1.550 (4)	N1S—C2S	1.139 (5)
B1—N1A	1.552 (4)	C2S—C3S	1.457 (5)
N1A—C5A	1.358 (4)	C4B—H4B	0.93
N1A—N2A	1.381 (3)	C51B—H51D	0.96
N2A—C3A	1.340 (4)	C51B—H51E	0.96
C3A—C4A	1.391 (5)	C51B—H51F	0.96
C3A—C31A	1.499 (4)	C31C—H31G	0.96
C4A—C5A	1.385 (5)	C31C—H31H	0.96
C5A—C51A	1.500 (5)	C31C—H31I	0.96
N1B—C5B	1.365 (4)	C4C—H4C	0.93
N1B—N2B	1.374 (3)	C51C—H51G	0.96
N2B—C3B	1.339 (4)	C51C—H51H	0.96
C3B—C4B	1.402 (5)	C51C—H51I	0.96
C3B—C31B	1.491 (5)	C3S—H3S1	0.96
C4B—C5B	1.382 (4)	C3S—H3S2	0.96
C5B—C51B	1.495 (5)	C3S—H3S3	0.96
N1C—C5C	1.362 (4)		

C1—Cu1—N2A	124.52 (14)	N1C—B1—H1	110.0
C1—Cu1—N2B	124.27 (14)	N1A—B1—H1	110.0
N2A—Cu1—N2B	91.18 (10)	C3A—C31A—H31A	109.5
C1—Cu1—N2C	124.38 (14)	C3A—C31A—H31B	109.5
N2A—Cu1—N2C	91.46 (10)	H31A—C31A—H31B	109.5
N2B—Cu1—N2C	91.05 (10)	C3A—C31A—H31C	109.5
O1—C1—Cu1	179.3 (4)	H31A—C31A—H31C	109.5
N1B—B1—N1C	108.8 (2)	H31B—C31A—H31C	109.5
N1B—B1—N1A	109.2 (2)	C5A—C4A—H4A	126.9
N1C—B1—N1A	108.7 (2)	C3A—C4A—H4A	126.9
C5A—N1A—N2A	109.7 (2)	C5A—C51A—H51A	109.5
C5A—N1A—B1	131.3 (3)	C5A—C51A—H51B	109.5
N2A—N1A—B1	119.0 (2)	H51A—C51A—H51B	109.5
C3A—N2A—N1A	106.6 (3)	C5A—C51A—H51C	109.5
C3A—N2A—Cu1	138.1 (2)	H51A—C51A—H51C	109.5
N1A—N2A—Cu1	115.34 (18)	H51B—C51A—H51C	109.5
N2A—C3A—C4A	110.0 (3)	C3B—C31B—H31D	109.5
N2A—C3A—C31A	120.6 (3)	C3B—C31B—H31E	109.5
C4A—C3A—C31A	129.4 (3)	H31D—C31B—H31E	109.5

C5A—C4A—C3A	106.3 (3)	C3B—C31B—H31F	109.5
N1A—C5A—C4A	107.4 (3)	H31D—C31B—H31F	109.5
N1A—C5A—C51A	122.8 (3)	H31E—C31B—H31F	109.5
C4A—C5A—C51A	129.8 (3)	C5B—C4B—H4B	126.9
C5B—N1B—N2B	109.7 (2)	C3B—C4B—H4B	126.9
C5B—N1B—B1	130.8 (3)	C5B—C51B—H51D	109.5
N2B—N1B—B1	119.5 (2)	C5B—C51B—H51E	109.5
C3B—N2B—N1B	107.1 (2)	H51D—C51B—H51E	109.5
C3B—N2B—Cu1	137.8 (2)	C5B—C51B—H51F	109.5
N1B—N2B—Cu1	115.16 (17)	H51D—C51B—H51F	109.5
N2B—C3B—C4B	109.6 (3)	H51E—C51B—H51F	109.5
N2B—C3B—C31B	120.9 (3)	C3C—C31C—H31G	109.5
C4B—C3B—C31B	129.5 (3)	C3C—C31C—H31H	109.5
C5B—C4B—C3B	106.3 (3)	H31G—C31C—H31H	109.5
N1B—C5B—C4B	107.3 (3)	C3C—C31C—H31I	109.5
N1B—C5B—C51B	123.0 (3)	H31G—C31C—H31I	109.5
C4B—C5B—C51B	129.6 (3)	H31H—C31C—H31I	109.5
C5C—N1C—N2C	109.2 (2)	C5C—C4C—H4C	126.9
C5C—N1C—B1	130.8 (3)	C3C—C4C—H4C	126.9
N2C—N1C—B1	120.0 (2)	C5C—C51C—H51G	109.5
C3C—N2C—N1C	107.2 (2)	C5C—C51C—H51H	109.5
C3C—N2C—Cu1	138.6 (2)	H51G—C51C—H51H	109.5
N1C—N2C—Cu1	114.19 (17)	C5C—C51C—H51I	109.5
N2C—C3C—C4C	109.5 (3)	H51G—C51C—H51I	109.5
N2C—C3C—C31C	120.6 (3)	H51H—C51C—H51I	109.5
C4C—C3C—C31C	129.9 (3)	C2S—C3S—H3S1	109.5
C5C—C4C—C3C	106.3 (3)	C2S—C3S—H3S2	109.5
N1C—C5C—C4C	107.7 (3)	H3S1—C3S—H3S2	109.5
N1C—C5C—C51C	122.4 (3)	C2S—C3S—H3S3	109.5
C4C—C5C—C51C	129.8 (3)	H3S1—C3S—H3S3	109.5
N1S—C2S—C3S	178.5 (4)	H3S2—C3S—H3S3	109.5
N1B—B1—H1	110.0		

N1B—B1—N1A—C5A	121.0 (3)	N2B—C3B—C4B—C5B	0.4 (3)
N1C—B1—N1A—C5A	−120.4 (3)	C31B—C3B—C4B—C5B	180.0 (3)
N1B—B1—N1A—N2A	−58.4 (3)	N2B—N1B—C5B—C4B	0.5 (3)
N1C—B1—N1A—N2A	60.2 (3)	B1—N1B—C5B—C4B	179.5 (3)
C5A—N1A—N2A—C3A	−0.1 (3)	N2B—N1B—C5B—C51B	−177.0 (3)
B1—N1A—N2A—C3A	179.4 (2)	B1—N1B—C5B—C51B	2.0 (5)
N1A—N2A—C3A—C4A	0.2 (3)	C3B—C4B—C5B—N1B	−0.5 (3)
N1A—N2A—C3A—C31A	−179.0 (3)	C3B—C4B—C5B—C51B	176.7 (3)
N2A—C3A—C4A—C5A	−0.2 (3)	N1B—B1—N1C—C5C	−121.0 (3)
C31A—C3A—C4A—C5A	178.9 (3)	N1A—B1—N1C—C5C	120.1 (3)
N2A—N1A—C5A—C4A	0.0 (3)	N1B—B1—N1C—N2C	58.9 (3)
B1—N1A—C5A—C4A	−179.5 (3)	N1A—B1—N1C—N2C	−60.0 (3)
N2A—N1A—C5A—C51A	179.3 (3)	C5C—N1C—N2C—C3C	0.5 (3)
B1—N1A—C5A—C51A	−0.1 (5)	B1—N1C—N2C—C3C	−179.4 (2)
C3A—C4A—C5A—N1A	0.1 (3)	N1C—N2C—C3C—C4C	−0.4 (3)

C3A—C4A—C5A—C51A	−179.2 (3)	N1C—N2C—C3C—C31C	179.4 (3)
N1C—B1—N1B—C5B	121.8 (3)	N2C—C3C—C4C—C5C	0.2 (4)
N1A—B1—N1B—C5B	−119.7 (3)	C31C—C3C—C4C—C5C	−179.6 (3)
N1C—B1—N1B—N2B	−59.2 (3)	N2C—N1C—C5C—C4C	−0.4 (3)
N1A—B1—N1B—N2B	59.2 (3)	B1—N1C—C5C—C4C	179.5 (3)
C5B—N1B—N2B—C3B	−0.2 (3)	N2C—N1C—C5C—C51C	178.1 (3)
B1—N1B—N2B—C3B	−179.4 (2)	B1—N1C—C5C—C51C	−2.0 (5)
N1B—N2B—C3B—C4B	−0.1 (3)	C3C—C4C—C5C—N1C	0.1 (3)
N1B—N2B—C3B—C31B	−179.7 (3)	C3C—C4C—C5C—C51C	−178.3 (3)