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Poly[chlorido[μ_4-2,2′-(2-methyl-1*H*-benzimidazol-3-ium-1,3-diyl)diacetato]-zinc]

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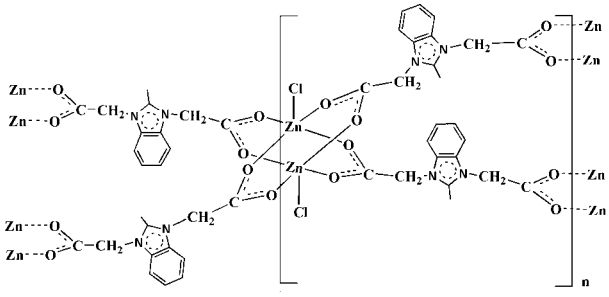
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.027; wR factor = 0.078; data-to-parameter ratio = 14.6.

The title compound, $[Zn(C_{12}H_{11}N_2O_4)Cl]_n$, contains a centrosymmetric dimetal tetracarboxylate paddle-wheel moiety in which the Zn^{II} atom is square-pyramidally coordinated by four carboxylate O atoms at the basal positions and one Cl^- anion at the apical position. Each paddle-wheel unit is joined to four such neighbours through bridging dicarboxylate ligands, producing a two-dimensional undulating layer parallel to $(\bar{1}01)$. Adjacent sheets are stacked in a parallel fashion to form a three-dimensional supramolecular structure which is stabilized by interlayer π–π interactions between benzene rings, with a centroid–centroid distance of 3.722 Å. The range of Zn—O bond lengths is 2.0440 (17)–2.1256 (15) Å and the Zn—Cl bond length is 2.2622 (6) Å.

Related literature

For background to and potential applications of carboxylate-containing coordination polymers, see Bourne *et al.* (2001); Chen *et al.* (2005); Kitagawa *et al.* (2004); Li *et al.* (2012); Xuan *et al.* (2012).



Experimental

Crystal data

$[Zn(C_{12}H_{11}N_2O_4)Cl]$
M_r = 348.05
Monoclinic, $P2_1/n$
a = 7.1285 (17) Å
b = 13.301 (3) Å
c = 12.804 (3) Å
β = 90.540 (4)°
V = 1214.0 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.26 mm^{-1}
T = 173 K
0.48 × 0.32 × 0.30 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.424, T_{max} = 0.508
6072 measured reflections
2640 independent reflections
2327 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.078
S = 1.07
2640 reflections
181 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2452).

References

Bourne, S. A., Lu, J., Mondal, A., Moulton, B. & Zaworotko, M. J. (2001). *Angew. Chem. Int. Ed.* **40**, 2111–2113.
Bruker (1998). *SMART*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chen, B., Ockwig, N. W., Fronczek, F. R., Contreras, D. S. & Yaghi, O. M. (2005). *Inorg. Chem.* **44**, 181–183.
Kitagawa, S., Kitaura, R. & Noro, S. (2004). *Angew. Chem. Int. Ed.* **43**, 2334–2375.
Li, J.-R., Sculley, J. & Zhou, H.-C. (2012). *Chem. Rev.* **112**, 869–932.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Xuan, W., Zhu, C., Liu, Y. & Cui, Y. (2012). *Chem. Soc. Rev.* **42**, 1677–1695.

supporting information

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Poly[chlorido[μ_4-2,2′-(2-methyl-1*H*-benzimidazol-3-ium-1,3-diyl)diacetato]-zinc]

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S1. Comment

Carboxylate-containing ligands have been intensively investigated to construct metal-organic frameworks with an intriguing variety of topologies and potential applications in gas sorption, separation and/or catalysis (Bourne *et al.*, 2001; Chen *et al.*, 2005; Kitagawa *et al.*, 2004; Li *et al.*, 2012; Xuan *et al.*, 2012). Polycarboxylate ligands with suitable spacers are good choices for such architectures because the topological structures can be adjusted not only by carboxylate groups but also by the organic spacers. Here we use a flexible zwitterionic ligand, 1-acetoxy-2-methylbenzimidazole-3-acetate acid [HL], to prepare the title compound $[Zn(L)Cl]_n$ (I).

The motive consists of a centrosymmetric paddle-wheel dimetal tetracarboxylate moiety $[Zn_2(CO_2)_4]$ (Fig. 1) in which each Zn^{II} is square-pyramidally coordinated by four carboxylate oxygen atoms at the basal position and one Cl^- anion at the apical position. Each paddle-wheel unit is bridged by four such neighbors through bridging dicarboxylate ligands, producing a two-dimensional undulate layer in which π-π interactions between phenyl rings of benzimidazole moieties (ring-centroid distance: 3.579 (2) Å) cooperate in the 2-D sheet formation (Fig. 2). Adjacent sheets are stacked in a parallel fashion to form a 3-D supramolecular structure stabilized by interlayer π-π interactions between phenyl rings with a ring-centroid distance of 3.722 (2) Å. The Zn—O span is 2.0440 (17)-2.1256 (15) Å and the Zn—Cl distance is 2.2622 (6) Å.

S2. Experimental

After the pH of an ethanol/water mixture solution (10 ml with ratio of 4:1) containing $ZnCl_2.2H_2O$ (0.0408 g, 0.3 mmol) and the HL ligand (0.0498 g,0.2 mmol) was adjusted to 7 by addition of triethylamine, the resulting solution was sealed in a Teflon-lined steel bomb (25 ml) and then heated at 140°C for 2 days. Colorless block crystals were collected. Yield: 16%. Elemental analysis (%) calcd for the title compound: C 41.38, H 3.16, N 8.04; found: C 41.24, H 3.23, N 8.47. IR: 1672(*s*), 1472(*m*), 1436(*m*), 1389(*s*), 1310(*m*), 764(*s*), 721(*m*), 619(*m*), 574(*m*).

S3. Refinement

All hydrogen atoms were generated geometrically and refined with a riding model, U_{iso}(H)= x×U_{eq}(Host) (aromatic: C—H: 0.95Å, x=1.2; methyl, C—H: 0.98Å, x=1.5; methylene, C—H: 0.99Å, x=1.2)

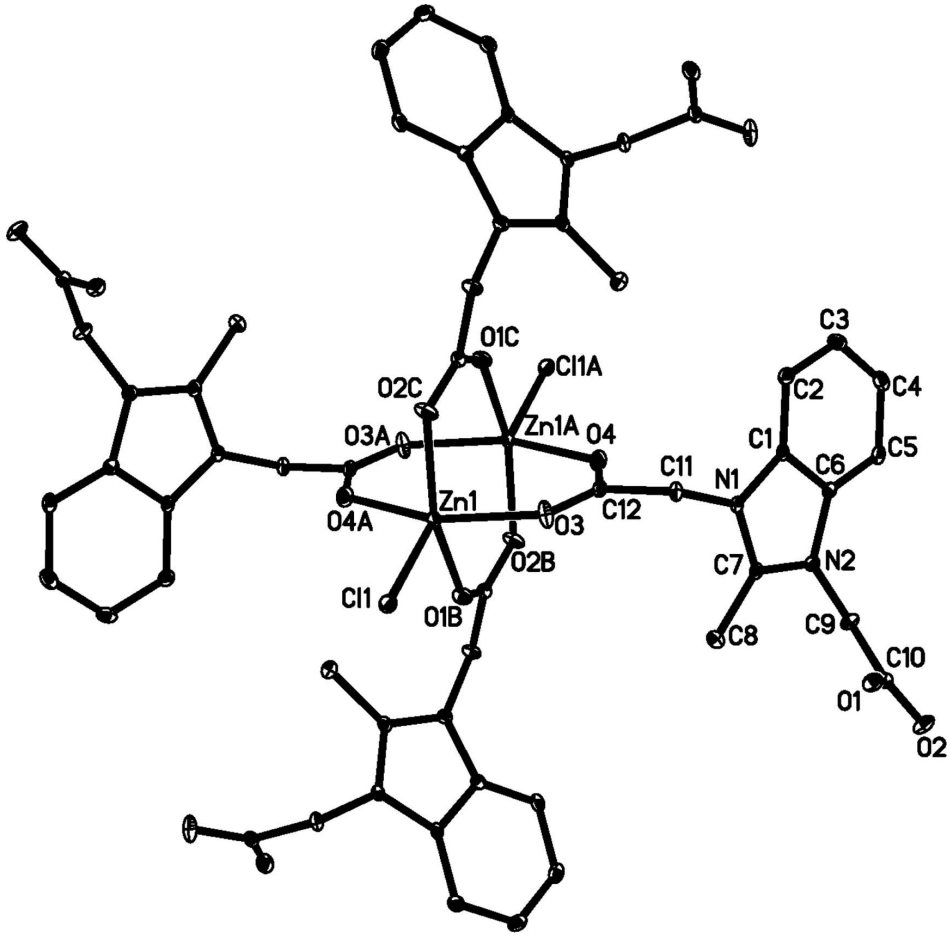

Figure 1

ORTEP drawing (at 30% probability) of a paddle-wheel unit in the title compound (symmetry codes: A, -*x*, -*y*, -*z*; B, -0.5 + *x*, 1.5 - *y*, -0.5 + *z*; C, 0.5 - *x*, -0.5 + *y*, 1.5 - *z*). Hydrogen atoms are omitted for clarity.

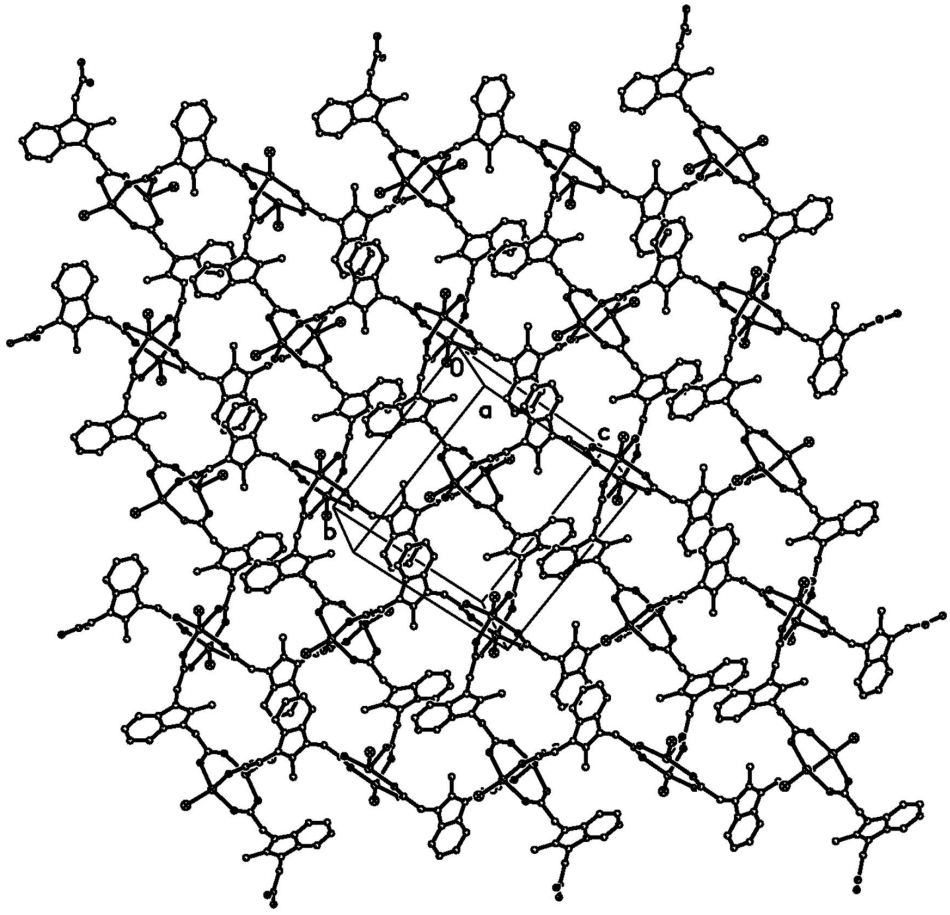

Figure 2

The 2-D sheet structure parallel to the (-101) plane, hydrogen atoms are omitted for clarity.

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c = 12.804 (3) Å
β = 90.540 (4)°
V = 1214.0 (5) Å^3
Z = 4
$F(000)$ = 704
D_x = 1.904 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
θ = 2.2–27.1°
μ = 2.26 mm^{-1}
T = 173 K
Block, colorless
0.48 × 0.32 × 0.30 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.424, T_{max} = 0.508
6072 measured reflections
2640 independent reflections
2327 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 27.1°, θ_{min} = 2.2°
h = −9→8
k = −11→17
l = −16→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.078$
$S = 1.07$
2640 reflections
181 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
$w = 1/[\sigma^2(F_o^2) + (0.0438P)^2 + 0.6356P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.45$ e Å^{-3}
$\Delta\rho_{min} = -0.45$ 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}
Zn1	0.13104 (3)	0.553340 (17)	0.417142 (17)	0.01203 (10)
Cl1	0.29440 (7)	0.65999 (4)	0.31470 (4)	0.01697 (13)
O1	0.4360 (2)	0.84000 (11)	0.97522 (12)	0.0181 (3)
O2	0.2502 (2)	0.91230 (12)	1.09352 (13)	0.0217 (4)
O3	0.2669 (2)	0.56544 (13)	0.55787 (12)	0.0241 (4)
O4	0.0830 (2)	0.49535 (12)	0.67900 (12)	0.0203 (3)
N1	0.3143 (2)	0.58092 (13)	0.83280 (13)	0.0122 (3)
N2	0.2081 (2)	0.67202 (13)	0.96116 (14)	0.0131 (4)
C1	0.2938 (3)	0.51606 (15)	0.91696 (16)	0.0123 (4)
C2	0.3314 (3)	0.41392 (16)	0.92770 (17)	0.0164 (4)
H2A	0.3829	0.3755	0.8724	0.020*
C3	0.2899 (3)	0.37134 (16)	1.02313 (18)	0.0190 (5)
H3A	0.3135	0.3018	1.0338	0.023*
C4	0.2140 (3)	0.42806 (17)	1.10429 (18)	0.0190 (5)
H4A	0.1854	0.3957	1.1683	0.023*
C5	0.1792 (3)	0.53041 (16)	1.09412 (16)	0.0157 (4)
H5A	0.1280	0.5689	1.1495	0.019*
C6	0.2235 (3)	0.57346 (15)	0.99858 (16)	0.0133 (4)
C7	0.2610 (3)	0.67345 (15)	0.86146 (16)	0.0128 (4)
C8	0.2578 (3)	0.75932 (16)	0.78819 (17)	0.0197 (5)
H8A	0.2142	0.8196	0.8246	0.030*
H8B	0.1726	0.7443	0.7297	0.030*
H8C	0.3844	0.7709	0.7617	0.030*
C9	0.1487 (3)	0.75902 (15)	1.02331 (17)	0.0159 (4)
H9A	0.1187	0.7357	1.0946	0.019*

H9B	0.0321	0.7867	0.9920	0.019*
C10	0.2944 (3)	0.84401 (15)	1.03157 (16)	0.0136 (4)
C11	0.3852 (3)	0.55606 (16)	0.72945 (16)	0.0142 (4)
H11A	0.4637	0.4948	0.7348	0.017*
H11B	0.4662	0.6116	0.7051	0.017*
C12	0.2295 (3)	0.53811 (15)	0.64823 (17)	0.0138 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.01287 (15)	0.01381 (14)	0.00939 (14)	−0.00070 (8)	−0.00114 (9)	0.00073 (8)
Cl1	0.0203 (3)	0.0164 (2)	0.0142 (2)	−0.00402 (19)	0.00246 (19)	−0.00035 (18)
O1	0.0171 (8)	0.0169 (7)	0.0205 (8)	−0.0037 (6)	0.0038 (6)	−0.0020 (6)
O2	0.0251 (9)	0.0166 (7)	0.0235 (8)	−0.0044 (6)	0.0047 (7)	−0.0089 (7)
O3	0.0191 (8)	0.0415 (10)	0.0114 (8)	−0.0005 (7)	−0.0032 (6)	0.0026 (7)
O4	0.0199 (8)	0.0227 (8)	0.0181 (8)	−0.0067 (7)	−0.0050 (6)	−0.0012 (6)
N1	0.0123 (8)	0.0143 (8)	0.0100 (8)	−0.0009 (7)	−0.0026 (6)	−0.0012 (7)
N2	0.0136 (9)	0.0126 (8)	0.0130 (8)	−0.0012 (7)	−0.0004 (7)	−0.0009 (7)
C1	0.0113 (10)	0.0153 (10)	0.0102 (9)	−0.0027 (8)	−0.0039 (7)	−0.0003 (8)
C2	0.0161 (10)	0.0153 (10)	0.0176 (10)	0.0004 (8)	−0.0048 (8)	−0.0025 (8)
C3	0.0172 (11)	0.0136 (10)	0.0261 (12)	−0.0031 (8)	−0.0065 (9)	0.0049 (9)
C4	0.0170 (11)	0.0222 (11)	0.0178 (11)	−0.0050 (9)	−0.0047 (8)	0.0066 (9)
C5	0.0153 (10)	0.0206 (10)	0.0112 (10)	−0.0045 (8)	−0.0019 (8)	−0.0014 (8)
C6	0.0117 (9)	0.0136 (9)	0.0145 (10)	−0.0035 (8)	−0.0032 (8)	−0.0012 (8)
C7	0.0110 (9)	0.0150 (10)	0.0121 (9)	−0.0027 (8)	−0.0038 (7)	−0.0015 (8)
C8	0.0264 (12)	0.0172 (10)	0.0154 (10)	0.0003 (9)	−0.0016 (9)	0.0030 (9)
C9	0.0154 (10)	0.0131 (10)	0.0191 (10)	−0.0007 (8)	0.0028 (8)	−0.0055 (8)
C10	0.0152 (10)	0.0131 (9)	0.0126 (9)	−0.0012 (8)	−0.0025 (8)	−0.0003 (8)
C11	0.0134 (10)	0.0198 (11)	0.0093 (9)	0.0010 (8)	−0.0014 (8)	−0.0014 (8)
C12	0.0142 (10)	0.0150 (10)	0.0121 (9)	0.0045 (8)	−0.0034 (8)	−0.0034 (8)

Geometric parameters (Å, º)

Zn1—O3	2.0440 (17)	C2—H2A	0.9500
Zn1—O4^{i}	2.0559 (16)	C3—C4	1.397 (3)
Zn1—O2^{ii}	2.0632 (16)	C3—H3A	0.9500
Zn1—O1^{iii}	2.1256 (15)	C4—C5	1.390 (3)
Zn1—Cl1	2.2622 (6)	C4—H4A	0.9500
O1—C10	1.247 (3)	C5—C6	1.390 (3)
O2—C10	1.248 (3)	C5—H5A	0.9500
O3—C12	1.244 (3)	C7—C8	1.478 (3)
O4—C12	1.256 (3)	C8—H8A	0.9800
N1—C7	1.340 (3)	C8—H8B	0.9800
N1—C1	1.389 (3)	C8—H8C	0.9800
N1—C11	1.459 (3)	C9—C10	1.538 (3)
N2—C7	1.335 (3)	C9—H9A	0.9900
N2—C6	1.400 (3)	C9—H9B	0.9900
N2—C9	1.469 (3)	C11—C12	1.532 (3)

C1—C2	1.391 (3)	C11—H11A	0.9900
C1—C6	1.392 (3)	C11—H11B	0.9900
C2—C3	1.381 (3)		

O3—Zn1—O4^{i}	153.56 (7)	C6—C5—H5A	121.8
O3—Zn1—O2^{ii}	86.48 (7)	C4—C5—H5A	121.8
O4^{i}—Zn1—O2^{ii}	88.65 (7)	C5—C6—C1	121.4 (2)
O3—Zn1—O1^{iii}	86.86 (7)	C5—C6—N2	132.0 (2)
O4^{i}—Zn1—O1^{iii}	86.31 (7)	C1—C6—N2	106.52 (18)
O2^{ii}—Zn1—O1^{iii}	154.17 (6)	N2—C7—N1	109.40 (18)
O3—Zn1—Cl1	102.68 (5)	N2—C7—C8	127.98 (19)
O4^{i}—Zn1—Cl1	103.50 (5)	N1—C7—C8	122.58 (19)
O2^{ii}—Zn1—Cl1	108.55 (5)	C7—C8—H8A	109.5
O1^{iii}—Zn1—Cl1	97.25 (5)	C7—C8—H8B	109.5
C10—O1—Zn1^{iv}	135.18 (14)	H8A—C8—H8B	109.5
C10—O2—Zn1^{v}	120.91 (14)	C7—C8—H8C	109.5
C12—O3—Zn1	133.86 (15)	H8A—C8—H8C	109.5
C12—O4—Zn1^{i}	124.71 (14)	H8B—C8—H8C	109.5
C7—N1—C1	109.00 (17)	N2—C9—C10	114.73 (17)
C7—N1—C11	123.92 (17)	N2—C9—H9A	108.6
C1—N1—C11	127.07 (18)	C10—C9—H9A	108.6
C7—N2—C6	108.60 (17)	N2—C9—H9B	108.6
C7—N2—C9	126.32 (18)	C10—C9—H9B	108.6
C6—N2—C9	125.06 (18)	H9A—C9—H9B	107.6
N1—C1—C2	131.4 (2)	O1—C10—O2	127.5 (2)
N1—C1—C6	106.45 (18)	O1—C10—C9	118.58 (18)
C2—C1—C6	122.14 (19)	O2—C10—C9	113.85 (18)
C3—C2—C1	116.4 (2)	N1—C11—C12	113.33 (17)
C3—C2—H2A	121.8	N1—C11—H11A	108.9
C1—C2—H2A	121.8	C12—C11—H11A	108.9
C2—C3—C4	121.6 (2)	N1—C11—H11B	108.9
C2—C3—H3A	119.2	C12—C11—H11B	108.9
C4—C3—H3A	119.2	H11A—C11—H11B	107.7
C5—C4—C3	122.0 (2)	O3—C12—O4	127.6 (2)
C5—C4—H4A	119.0	O3—C12—C11	115.17 (19)
C3—C4—H4A	119.0	O4—C12—C11	117.18 (19)
C6—C5—C4	116.4 (2)		

Symmetry codes: (i) −*x*, −*y*+1, −*z*+1; (ii) −*x*+1/2, *y*−1/2, −*z*+3/2; (iii) *x*−1/2, −*y*+3/2, *z*−1/2; (iv) *x*+1/2, −*y*+3/2, *z*+1/2; (v) −*x*+1/2, *y*+1/2, −*z*+3/2.