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3,4-Dichloro-1-nitrobenzene–aniline (2/1)

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Key indicators

Single-crystal X-ray study
T = 123 K
Mean σ(C–C) = 0.003 Å
R factor = 0.038
wR factor = 0.080
Data-to-parameter ratio = 14.7

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

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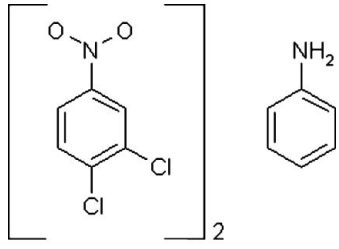
The solvate structure of 3,4-dichloro-1-nitrobenzene with aniline, $2C_6H_3Cl_2NO_2\cdot C_6H_7N$, is reported. Ribbons of 3,4-dichloronitrobenzene, formed by Cl···Cl and N—O···Cl interactions, are linked together *via* N—H···O hydrogen bonds with aniline into an undulating two-dimensional sheet.

Comment

The title compound, (I), was produced during an automated parallel crystallization polymorph screen on 3,4-dichloronitrobenzene (3,4-DCNB). The sample was identified as a novel form using multi-sample X-ray powder diffraction analysis of all recrystallized samples (Florence *et al.*, 2003). Subsequent manual recrystallization from a saturated aniline solution by slow evaporation at 298 K yielded samples suitable for single-crystal X-ray analysis. The title solvate, (I), crystallizes in the space group $P2_1/n$ with two molecules of 3,4-DCNB and one molecule of aniline in the asymmetric unit (Fig. 1).



(I)

The crystal structure of (I) is characterized by ribbons of 3,4-DCNB, which are linked by aniline molecules to form a

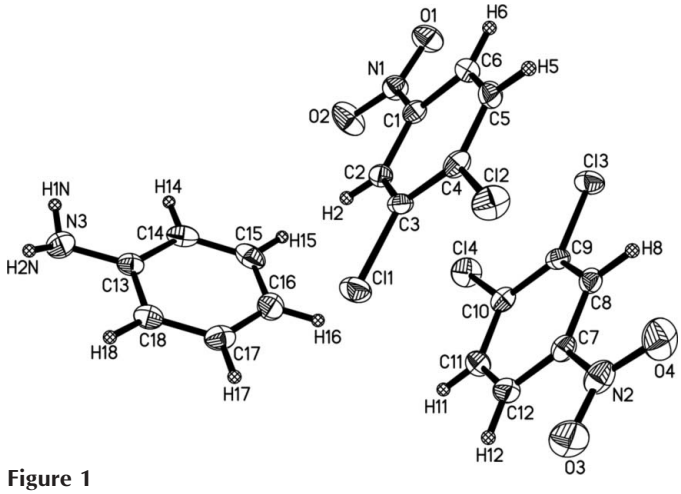


Figure 1
The asymmetric unit of (I), showing the numbering scheme used. Displacement ellipsoids are drawn at the 50% probability level.

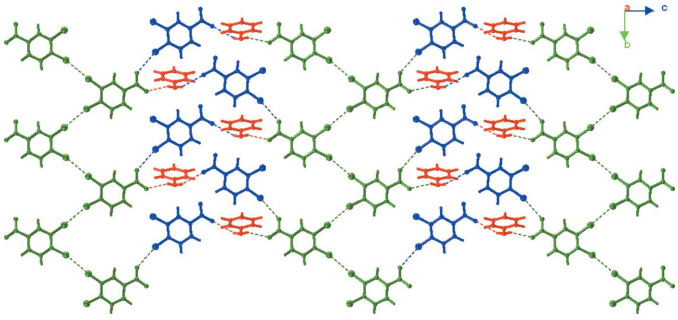


Figure 2
The two-dimensional network formed by (I), showing the intermolecular interactions involved as dashed lines (3,4-DCNB molecule 1: green; 3,4-DCNB molecule 2: blue; aniline: red).

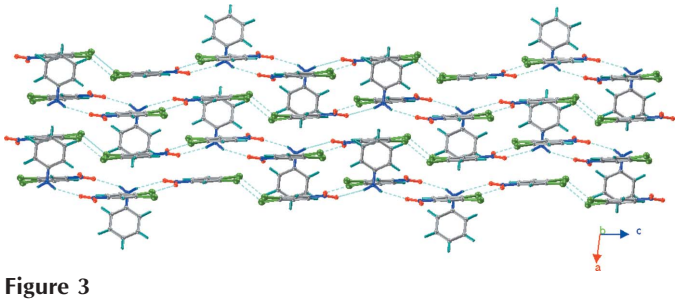


Figure 3
Packing diagram viewed perpendicular to the sheets, illustrating the out-of-plane aniline molecules and the stacking arrangement of the sheets. Intermolecular interactions are shown as dashed lines.

continuous sheet (Fig. 2). Molecules of type 1 (C1–C6) form a zigzag chain *via* Cl···Cl interactions [Cl1···Cl2^{i} = 3.399 (1) Å and C3—Cl1···Cl2^{i} = 149.4 (1)°; symmetry code: (i) $\frac{3}{2} - x, \frac{1}{2} + y, \frac{3}{2} - z$]. These molecules are then involved in a second contact with molecules of type 2 (C7–C12) *via* N—O···Cl interactions [O2···Cl4^{ii} = 3.056 (2) Å and N1—O2···Cl4^{ii} = 140.1 (1)°; symmetry code: (ii) $1 - x, 1 - y, 1 - z$], thus forming 3,4-DCNB ribbons running parallel to the *b* axis. The aniline solvent molecules, which lie in a perpendicular plane, link these ribbons into an undulating sheet through two N—H···O interactions [N3···O1^{iii} = 2.52 (2) Å and N3—H1N···O1^{iii} = 157 (2)°, and N3···O3^{i} = 2.64 (2) Å and N3—H2N···O3^{i} = 147 (2)°; symmetry code: (iii) $2 - x, 1 - y, 1 - z$]. These sheets form an interdigitated *ABAB* stack parallel to the *a* axis (Fig. 3).

Experimental

A single-crystal sample of the title compound was recrystallized from aniline solution by slow evaporation at *ca* 293 K.

Crystal data

$2C_6H_3Cl_2NO_2\cdot C_6H_7N$	D_x = 1.625 Mg m^{-3}
M_r = 477.11	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 4734 reflections
a = 6.9774 (2) Å	θ = 1.0–27.9°
b = 10.1668 (3) Å	μ = 0.64 mm^{-1}
c = 27.6762 (7) Å	T = 123 (2) K
β = 96.495 (2)°	Triangle, orange
V = 1950.69 (9) Å^3	0.45 × 0.30 × 0.15 mm
Z = 4	

Data collection

Nonius KappaCCD diffractometer	R_{int} = 0.058
ω and φ scans	θ_{max} = 27.9°
Absorption correction: none	$h = -9 \rightarrow 9$
22354 measured reflections	$k = -13 \rightarrow 13$
4629 independent reflections	$l = -36 \rightarrow 36$
3314 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0275P)^2 + 0.7246P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.038	$(\Delta/\sigma)_{max}$ = 0.002
$wR(F^2)$ = 0.081	$\Delta\rho_{max}$ = 0.28 e Å^{-3}
S = 1.04	$\Delta\rho_{min}$ = −0.32 e Å^{-3}
4629 reflections	
314 parameters	
All H-atom parameters refined	

C—H distances are in the range 0.09 (2)–1.00 (2) Å, and N—H distances are 0.86 (2) and 0.87 (2) Å.

Data collection: *COLLECT* (Hooft, 1998) and *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; cell refinement: *DENZO*; data reduction: *DENZO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000) and *OLEX* (Dolomanov *et al.*, 2003); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

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supporting information

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$2C_6H_3Cl_2NO_2{\cdot}C_6H_7N$
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Monoclinic, $P2_1/n$
$a = 6.9774$ (2) Å
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$c = 27.6762$ (7) Å
$\beta = 96.495$ (2)°
$V = 1950.69$ (9) Å^3
$Z = 4$
$F(000) = 968$
$D_x = 1.625$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4734 reflections
$\theta = 1.0$–$27.9°$
$\mu = 0.64$ mm^{-1}
$T = 123$ K
Triangle, orange
0.45 × 0.30 × 0.15 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
22354 measured reflections
4629 independent reflections
3314 reflections with $I > 2\sigma(I)$
$R_{int} = 0.058$
$\theta_{max} = 27.9°$, $\theta_{min} = 1.5°$
$h = -9 \rightarrow 9$
$k = -13 \rightarrow 13$
$l = -36 \rightarrow 36$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.081$
$S = 1.04$
4629 reflections
314 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
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0275P)^2 + 0.7246P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.28$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ 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}
Cl1	0.65101 (8)	0.29879 (5)	0.704181 (17)	0.02699 (13)
Cl2	0.59533 (8)	−0.00859 (5)	0.710847 (18)	0.02975 (14)
O1	0.6570 (2)	0.17232 (14)	0.48418 (5)	0.0305 (4)
O2	0.7091 (3)	0.36004 (14)	0.51992 (5)	0.0384 (4)
N1	0.6761 (2)	0.24168 (17)	0.52060 (6)	0.0232 (4)
C1	0.6599 (3)	0.17966 (19)	0.56799 (7)	0.0180 (4)
C2	0.6634 (3)	0.2596 (2)	0.60845 (7)	0.0190 (4)
C3	0.6455 (3)	0.20088 (19)	0.65295 (7)	0.0179 (4)
C4	0.6246 (3)	0.0651 (2)	0.65591 (7)	0.0200 (4)
C5	0.6249 (3)	−0.0128 (2)	0.61466 (7)	0.0213 (4)
C6	0.6426 (3)	0.0441 (2)	0.57025 (7)	0.0210 (4)
H2	0.679 (3)	0.350 (2)	0.6043 (7)	0.021 (5)*
H5	0.611 (3)	−0.100 (2)	0.6179 (7)	0.026 (6)*
H6	0.640 (3)	−0.0082 (19)	0.5428 (7)	0.023 (6)*
Cl3	0.13987 (8)	0.11529 (5)	0.541764 (17)	0.02701 (13)
Cl4	0.19771 (8)	0.42446 (5)	0.550794 (19)	0.03159 (14)
O3	0.1424 (2)	0.15949 (17)	0.76614 (5)	0.0396 (4)
O4	0.0924 (2)	−0.01482 (16)	0.72154 (6)	0.0385 (4)
N2	0.1219 (2)	0.10362 (19)	0.72661 (6)	0.0276 (4)
C7	0.1347 (3)	0.1830 (2)	0.68264 (7)	0.0199 (4)
C8	0.1309 (3)	0.1183 (2)	0.63845 (7)	0.0197 (4)
C9	0.1471 (3)	0.19368 (19)	0.59743 (7)	0.0190 (4)
C10	0.1676 (3)	0.3298 (2)	0.60112 (7)	0.0217 (4)
C11	0.1690 (3)	0.3914 (2)	0.64595 (8)	0.0246 (5)
C12	0.1527 (3)	0.3178 (2)	0.68721 (7)	0.0250 (5)
H8	0.116 (3)	0.025 (2)	0.6355 (7)	0.024 (6)*
H11	0.181 (3)	0.481 (2)	0.6486 (8)	0.039 (7)*
H12	0.155 (3)	0.359 (2)	0.7179 (8)	0.036 (6)*
N3	1.1864 (3)	0.79026 (19)	0.62461 (8)	0.0298 (4)
C13	1.0052 (3)	0.73193 (19)	0.62348 (7)	0.0217 (4)
C14	0.8979 (3)	0.7006 (2)	0.57924 (7)	0.0263 (5)
C15	0.7159 (3)	0.6460 (2)	0.57829 (8)	0.0304 (5)
C16	0.6376 (3)	0.6211 (2)	0.62136 (8)	0.0297 (5)
C17	0.7429 (3)	0.6525 (2)	0.66525 (8)	0.0269 (5)
C18	0.9240 (3)	0.7080 (2)	0.66656 (7)	0.0241 (5)
H1N	1.246 (3)	0.778 (2)	0.5990 (8)	0.035 (7)*
H2N	1.265 (3)	0.783 (2)	0.6505 (8)	0.035 (7)*
H14	0.959 (3)	0.716 (2)	0.5499 (7)	0.027 (6)*
H15	0.646 (3)	0.625 (2)	0.5480 (8)	0.030 (6)*
H16	0.514 (3)	0.584 (2)	0.6203 (7)	0.021 (5)*

H17	0.689 (3)	0.633 (2)	0.6965 (8)	0.031 (6)*
H18	1.001 (3)	0.727 (2)	0.6966 (8)	0.035 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0332 (3)	0.0285 (3)	0.0199 (3)	−0.0004 (2)	0.0058 (2)	−0.0069 (2)
Cl2	0.0355 (3)	0.0310 (3)	0.0238 (3)	0.0033 (2)	0.0078 (2)	0.0099 (2)
O1	0.0421 (10)	0.0314 (9)	0.0180 (7)	0.0002 (7)	0.0040 (7)	−0.0039 (7)
O2	0.0666 (12)	0.0208 (8)	0.0293 (9)	−0.0109 (8)	0.0119 (8)	0.0038 (7)
N1	0.0258 (10)	0.0241 (10)	0.0201 (9)	−0.0004 (8)	0.0039 (7)	0.0001 (7)
C1	0.0174 (10)	0.0205 (10)	0.0165 (9)	0.0006 (8)	0.0042 (8)	0.0030 (8)
C2	0.0180 (10)	0.0164 (10)	0.0229 (10)	0.0016 (8)	0.0032 (8)	−0.0006 (8)
C3	0.0157 (10)	0.0215 (10)	0.0166 (9)	0.0033 (8)	0.0020 (8)	−0.0041 (8)
C4	0.0162 (10)	0.0243 (10)	0.0198 (10)	0.0020 (8)	0.0028 (8)	0.0053 (8)
C5	0.0213 (11)	0.0156 (10)	0.0272 (11)	−0.0018 (9)	0.0038 (8)	0.0012 (9)
C6	0.0217 (11)	0.0190 (10)	0.0225 (10)	−0.0003 (9)	0.0035 (9)	−0.0032 (9)
Cl3	0.0311 (3)	0.0305 (3)	0.0197 (2)	0.0026 (2)	0.0040 (2)	−0.0058 (2)
Cl4	0.0413 (3)	0.0272 (3)	0.0272 (3)	0.0012 (2)	0.0080 (2)	0.0093 (2)
O3	0.0443 (10)	0.0575 (11)	0.0172 (8)	−0.0067 (8)	0.0046 (7)	−0.0009 (8)
O4	0.0489 (11)	0.0328 (10)	0.0343 (9)	−0.0068 (8)	0.0070 (8)	0.0118 (7)
N2	0.0236 (10)	0.0384 (11)	0.0207 (9)	−0.0025 (9)	0.0030 (7)	0.0063 (8)
C7	0.0178 (10)	0.0239 (11)	0.0183 (10)	−0.0008 (8)	0.0031 (8)	0.0040 (8)
C8	0.0157 (10)	0.0191 (10)	0.0242 (10)	0.0000 (8)	0.0020 (8)	0.0006 (9)
C9	0.0167 (10)	0.0228 (10)	0.0177 (10)	0.0020 (8)	0.0030 (8)	−0.0022 (8)
C10	0.0187 (10)	0.0242 (11)	0.0226 (10)	0.0011 (9)	0.0048 (8)	0.0046 (9)
C11	0.0260 (12)	0.0189 (11)	0.0295 (11)	−0.0007 (9)	0.0050 (9)	−0.0025 (9)
C12	0.0237 (11)	0.0296 (12)	0.0220 (11)	−0.0019 (9)	0.0043 (9)	−0.0055 (9)
N3	0.0291 (11)	0.0332 (11)	0.0284 (11)	−0.0003 (9)	0.0089 (9)	0.0016 (9)
C13	0.0269 (11)	0.0156 (10)	0.0231 (11)	0.0035 (9)	0.0050 (9)	0.0013 (8)
C14	0.0380 (13)	0.0217 (11)	0.0202 (11)	0.0090 (10)	0.0078 (10)	0.0020 (9)
C15	0.0379 (14)	0.0217 (11)	0.0297 (12)	0.0077 (10)	−0.0046 (11)	−0.0065 (10)
C16	0.0288 (13)	0.0178 (11)	0.0431 (14)	0.0009 (10)	0.0061 (11)	−0.0013 (10)
C17	0.0329 (13)	0.0190 (11)	0.0305 (12)	0.0043 (9)	0.0115 (10)	0.0037 (9)
C18	0.0306 (12)	0.0208 (11)	0.0210 (11)	0.0047 (9)	0.0031 (9)	0.0009 (9)

Geometric parameters (Å, º)

Cl1—C3	1.7293 (19)	C8—C9	1.385 (3)
Cl2—C4	1.7278 (19)	C8—H8	0.96 (2)
O1—N1	1.225 (2)	C9—C10	1.394 (3)
O2—N1	1.226 (2)	C10—C11	1.389 (3)
N1—C1	1.471 (2)	C11—C12	1.380 (3)
C1—C2	1.381 (3)	C11—H11	0.91 (2)
C1—C6	1.385 (3)	C12—H12	0.95 (2)
C2—C3	1.387 (3)	N3—C13	1.393 (3)
C2—H2	0.94 (2)	N3—H1N	0.87 (2)
C3—C4	1.391 (3)	N3—H2N	0.86 (2)

C4—C5	1.390 (3)	C13—C14	1.398 (3)
C5—C6	1.376 (3)	C13—C18	1.398 (3)
C5—H5	0.90 (2)	C14—C15	1.383 (3)
C6—H6	0.93 (2)	C14—H14	0.97 (2)
Cl3—C9	1.7301 (19)	C15—C16	1.389 (3)
Cl4—C10	1.725 (2)	C15—H15	0.95 (2)
O3—N2	1.227 (2)	C16—C17	1.384 (3)
O4—N2	1.227 (2)	C16—H16	0.94 (2)
N2—C7	1.471 (2)	C17—C18	1.381 (3)
C7—C12	1.381 (3)	C17—H17	1.00 (2)
C7—C8	1.386 (3)	C18—H18	0.96 (2)

O1—N1—O2	123.75 (17)	C10—C9—Cl3	121.00 (15)
O1—N1—C1	118.34 (16)	C11—C10—C9	120.24 (18)
O2—N1—C1	117.91 (16)	C11—C10—Cl4	118.70 (16)
C2—C1—C6	122.82 (18)	C9—C10—Cl4	121.04 (15)
C2—C1—N1	118.33 (17)	C12—C11—C10	120.1 (2)
C6—C1—N1	118.85 (17)	C12—C11—H11	119.2 (14)
C1—C2—C3	118.14 (18)	C10—C11—H11	120.7 (14)
C1—C2—H2	118.1 (12)	C11—C12—C7	118.52 (19)
C3—C2—H2	123.8 (12)	C11—C12—H12	120.4 (14)
C2—C3—C4	119.98 (17)	C7—C12—H12	121.0 (14)
C2—C3—Cl1	118.99 (15)	C13—N3—H1N	115.9 (15)
C4—C3—Cl1	121.03 (15)	C13—N3—H2N	118.6 (16)
C5—C4—C3	120.46 (18)	H1N—N3—H2N	111 (2)
C5—C4—Cl2	119.15 (16)	N3—C13—C14	120.76 (19)
C3—C4—Cl2	120.39 (15)	N3—C13—C18	120.62 (19)
C6—C5—C4	120.18 (19)	C14—C13—C18	118.6 (2)
C6—C5—H5	121.7 (13)	C15—C14—C13	120.5 (2)
C4—C5—H5	118.1 (13)	C15—C14—H14	122.4 (12)
C5—C6—C1	118.39 (19)	C13—C14—H14	117.0 (12)
C5—C6—H6	119.7 (12)	C14—C15—C16	120.4 (2)
C1—C6—H6	121.9 (12)	C14—C15—H15	119.2 (13)
O3—N2—O4	123.89 (18)	C16—C15—H15	120.4 (13)
O3—N2—C7	118.15 (18)	C17—C16—C15	119.3 (2)
O4—N2—C7	117.95 (18)	C17—C16—H16	121.0 (12)
C12—C7—C8	122.97 (18)	C15—C16—H16	119.7 (12)
C12—C7—N2	118.83 (18)	C18—C17—C16	120.7 (2)
C8—C7—N2	118.20 (18)	C18—C17—H17	119.4 (12)
C9—C8—C7	117.72 (19)	C16—C17—H17	119.9 (13)
C9—C8—H8	119.8 (12)	C17—C18—C13	120.5 (2)
C7—C8—H8	122.4 (12)	C17—C18—H18	121.8 (13)
C8—C9—C10	120.45 (18)	C13—C18—H18	117.7 (13)
C8—C9—Cl3	118.55 (16)		

O1—N1—C1—C2	−174.07 (18)	C12—C7—C8—C9	0.3 (3)
O2—N1—C1—C2	6.3 (3)	N2—C7—C8—C9	−178.68 (17)
O1—N1—C1—C6	6.2 (3)	C7—C8—C9—C10	0.4 (3)

O2—N1—C1—C6	−173.42 (19)	C7—C8—C9—Cl3	−179.25 (15)
C6—C1—C2—C3	−1.2 (3)	C8—C9—C10—C11	−1.1 (3)
N1—C1—C2—C3	179.14 (17)	Cl3—C9—C10—C11	178.60 (15)
C1—C2—C3—C4	0.0 (3)	C8—C9—C10—Cl4	177.36 (15)
C1—C2—C3—Cl1	179.61 (14)	Cl3—C9—C10—Cl4	−3.0 (2)
C2—C3—C4—C5	1.1 (3)	C9—C10—C11—C12	1.0 (3)
Cl1—C3—C4—C5	−178.47 (15)	Cl4—C10—C11—C12	−177.50 (16)
C2—C3—C4—Cl2	−178.18 (14)	C10—C11—C12—C7	−0.2 (3)
Cl1—C3—C4—Cl2	2.2 (2)	C8—C7—C12—C11	−0.4 (3)
C3—C4—C5—C6	−1.1 (3)	N2—C7—C12—C11	178.58 (18)
Cl2—C4—C5—C6	178.16 (16)	N3—C13—C14—C15	−178.26 (19)
C4—C5—C6—C1	0.0 (3)	C18—C13—C14—C15	−0.6 (3)
C2—C1—C6—C5	1.1 (3)	C13—C14—C15—C16	−0.1 (3)
N1—C1—C6—C5	−179.17 (17)	C14—C15—C16—C17	0.4 (3)
O3—N2—C7—C12	−5.4 (3)	C15—C16—C17—C18	0.1 (3)
O4—N2—C7—C12	175.02 (19)	C16—C17—C18—C13	−0.9 (3)
O3—N2—C7—C8	173.64 (18)	N3—C13—C18—C17	178.78 (19)
O4—N2—C7—C8	−5.9 (3)	C14—C13—C18—C17	1.1 (3)