Highly Selective C-H Functionalization/Halogenation of Acetanilide

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Experimental Section

General. All the reactions were carried out under dry nitrogen atmosphere. DCE was freshly distilled over P_2O_5 . Anhydrous $Cu(OAc)_2$ and $CuCl_2$ were purchased from Acros Chemical and used without further purification. $Pd(OAc)_2$ was purchased from Strem Chemical. 1H NMR (200 MHz) and ^{13}C NMR (50 MHz) were registered on Varian 200M spectrometers with $CDCl_3$ as solvent and tetramethylsilane (TMS) as internal standard. Chemical shifts were reported in units (ppm) by assigning TMS resonance in the 1H spectrum as 0.00 ppm and $CDCl_3$ resonance in the ^{13}C spectrum as 77.0 ppm. All coupling constants (J values) were reported in Hertz (Hz). Column chromatography was performed on silica gel 200-300 mesh. IR, X-ray, GC, MS, and HRMS were performed by the State-authorized Analytical Center in Peking University.

General procedures for halogenation of acetanilide:

Acetanilide **1** (0.5 mmol), $Pd(OAc)_2$ (0.05 mmol), anhydrous $Cu(OAc)_2$ (1.0 mmol) and anhydrous $CuCl_2$ (1.0 mmol) were added to an oven-dried Schlenk tube. The septumsealed tube was evacuated and refilled with N_2 three times. DCE (4.0 mL) was added via syringe. The reaction mixture was heated at 90 °C in an oil bath for 48 h. After the reaction was complete, the product **2** was obtained by silica gel flash chromatography with petroleum ethers:EtOAc mixtures as eluent.

N-(2-chlorophenyl)acetamide (2a).¹ Starting from 0.0675g **1a** to afford **2a** 0.0679g. yield 80 %, mp 90-91 °C. ¹H NMR (CDCl₃, 200 MHz): δ 8.25 (d, 1 H, *J* = 8.2 Hz), 7.60 (bs, 1 H), 7.28 (d, 1 H, *J* = 7.8 Hz), 7.22-7.14 (m, 1 H), 6.99-6.92 (m, 1 H), 2.15 (s, 3 H). ¹³C NMR (CDCl₃, 50 MHz): δ 168.4, 134.3, 128.7, 127.2, 124.6, 123.1, 122.1, 24.3. MS (C₈H₈ClNO): 169 (M⁺, ³⁵Cl), 171 (M⁺, ³⁷Cl). IR (KBr, cm⁻¹): ν 3244, 1661, 1531, 1439, 1302, 1060.

N-(2-chlorophenyl)benzamide (2c).² Starting from 0.0985g **1c** to afford **2c** 0.0301g. yield 26 %, mp 104-105 °C. ¹H NMR (CDCl₃, 200 MHz): δ 8.59-8.56 (m, 1 H), 8.46 (bs, 1 H), 7.94-7.91 (m, 2 H), 7.61-7.26 (m, 5 H), 7.11-7.06 (m, 1 H). ¹³C NMR (CDCl₃, 50 MHz): δ 165.2, 134.7, 134.5, 132.2, 129.0, 128.9, 127.8, 127.1, 124.8, 123.1, 121.6. MS (C₁₃H₁₀ClNO): 231 (M⁺, ³⁵Cl), 233 (M⁺, ³⁷Cl). IR (KBr, cm⁻¹): ν 3285, 1652, 1531, 1440, 1311.

N-(2-chlorophenyl)pivalamide (2h).³ Starting from 0.0885g **1h** to afford **2h** 0.0708g. yield 67 %, mp 75-76 °C. ¹H NMR (CDCl₃, 200 MHz): δ 8.43-8.39 (m, 1 H), 8.02 (bs, 1 H), 7.38-7.23 (m, 2 H), 7.06-6.98 (m, 1 H), 1.34 (s, 9 H). ¹³C NMR (CDCl₃, 50 MHz): δ 176.6, 134.7, 128.8, 127.7, 124.3, 122.8, 121.3, 40.1, 27.5. MS (C₁₁H₁₄ClNO): 211 (M⁺, ³⁵Cl), 213 (M⁺, ³⁷Cl). IR (KBr, cm⁻¹): ν 3435, 1692, 1593, 1513, 1436, 1305, 1156, 1053.

N-(2-chlorophenyl)-3-phenylpropanamide (2i).⁴ Starting from 0.1125g **1i** to afford **2i** 0.0714g. yield 55 %, mp 118-119 °C. ¹H NMR (CDCl₃, 200 MHz): δ 8.37 (d, 1 H, *J* = 8.0 Hz), 7.55 (bs, 1 H), 7.36-7.18 (m, 7 H), 7.07-6.98 (m, 1 H), 3.08 (t, 2 H, *J* = 7.6 Hz), 2.75 (t, 2 H, *J* = 7.6 Hz). ¹³C NMR (CDCl₃, 50 MHz): δ 170.3, 140.2, 134.3, 128.8, 128.5, 128.2, 127.5, 126.2, 124.5, 122.7, 121.8, 39.2, 31.2. MS (C₁₅H₁₄ClNO): 259 (M⁺, ³⁵Cl), 261 (M⁺, ³⁷Cl). IR (KBr, cm⁻¹): ν 3278, 1660, 1529, 1443, 1301, 1063.

N-(2-chloro-4-methylphenyl)acetamide (2j).⁵ Starting from 0.0745g **1j** to afford **2j**

0.0725g, yield 79 %, mp 115-116 °C. ¹H NMR (CDCl₃, 200 MHz): δ 8.16 (d, 1 H, *J* = 8.2 Hz), 7.61 (bs, 1 H), 7.17 (s, 1 H), 7.05 (d, 1 H, *J* = 8.2 Hz), 2.29 (s, 3 H), 2.21 (s, 3 H). ¹³C NMR (CDCl₃, 50 MHz): δ 168.3, 134.7, 132.0, 129.2, 128.2, 122.6, 121.8, 24.6, 20.5. MS (C₉H₁₀ClNO): 183 (M⁺, ³⁵Cl), 185 (M⁺, ³⁷Cl). IR (KBr, cm⁻¹): ν 3279, 1661, 1532, 1297

N-(2-chloro-5-methylphenyl)acetamide (2ka).¹ 5% Pd(OAc)₂. Starting from 0.0745g **1k** to afford **2ka** 0.0881g, yield 96 %, mp 91-92 °C. ¹H NMR (CDCl₃, 200 MHz): δ 8.17 (s, 1 H), 7.56 (bs, 1 H), 7.21 (d, 1 H, *J* = 8.2 Hz), 6.83 (d, 1 H, *J* = 8.2 Hz), 2.32 (s, 3 H), 2.22 (s, 3 H). ¹³C NMR (CDCl₃, 50 MHz): δ 168.3, 137.7, 134.1, 128.4, 125.4, 122.3, 119.7, 24.6, 21.1. MS (C₉H₁₀ClNO): 183 (M⁺, ³⁵Cl), 185 (M⁺, ³⁷Cl). IR (KBr, cm⁻¹): ν 3273, 1665, 1584, 1534, 1293, 1057.

N-(2-bromo-5-methylphenyl)acetamide (2kb).⁶ Starting from 0.0745g **1k** to afford **2kb** 0.0980g, yield 86 %, mp 120-121 °C. ¹H NMR (CDCl₃, 200 MHz): δ 7.45-7.16 (m, 4 H), 2.35 (s, 3 H), 2.15 (s, 3 H). ¹³C NMR (CDCl₃, 50 MHz): δ 169.2, 138.3, 137.1, 132.3, 122.3, 119.4, 119.1, 24.3, 22.9. MS (C₉H₁₀BrNO): 227 (M⁺, ⁷⁹Br), 229 (M⁺, ⁸¹Br). IR (KBr, cm⁻¹): ν 3300, 1666, 1608, 1541, 1478, 1401, 1315, 1027.

N-(2-chloro-4-methoxyphenyl)acetamide (2l).⁷ Starting from 0.0825g **1l** to afford **2l** 0.0778g, yield 78 %, mp 114-115 °C. ¹H NMR (CDCl₃, 200 MHz): δ 8.13 (d, 1 H, *J* = 9.0 Hz), 7.41 (bs, 1 H), 6.91 (d, 1 H, *J* = 2.8 Hz), 6.81 (dd, 1 H, *J* = 9.0 Hz, *J* = 2.8 Hz), 3.77 (s, 3 H), 2.21 (s, 3 H). ¹³C NMR (CDCl₃, 50 MHz): δ 168.1, 156.2, 127.8, 124.1, 123.4, 114.4, 113.1, 55.6, 24.5. MS (C₉H₁₀ClNO₂): 199 (M⁺, ³⁵Cl), 201 (M⁺, ³⁷Cl). IR (KBr, cm⁻¹): ν 3274, 1657, 1532, 1284, 1053.

N-(2-chloro-5-methoxyphenyl)acetamide (2m).⁸ 5% Pd(OAc)₂. Starting from 0.0825g **1m** to afford **2m** 0.0780g, yield 78 %, mp 100-101 °C. ¹H NMR (CDCl₃, 200 MHz): δ 8.07 (d, 1 H, *J* = 2.8 Hz), 7.61 (bs, 1 H), 7.22 (d, 1 H, *J* = 9.0 Hz), 6.51 (dd, 1 H, *J* = 9.0 Hz, *J* = 2.8 Hz), 3.79 (s, 3 H), 2.23 (s, 3 H). ¹³C NMR (CDCl₃, 50

MHz): δ 168.4, 158.8, 135.2, 129.1, 113.6, 110.8, 106.6, 55.4, 24.8. MS ($\text{C}_9\text{H}_9\text{ClNO}_2$): 199 (M^+ , ^{35}Cl), 201 (M^+ , ^{37}Cl). IR (KBr, cm^{-1}): ν 2923, 1678, 1593, 1528, 1463, 1308, 1260, 1028.

N-(2, 4-dichlorophenyl)acetamide (2n).⁹ Starting from 0.0848g **1n** to afford **2n** 0.0275g. yield 27 %, mp 144-145 °C. ^1H NMR (CDCl_3 , 200 MHz): δ 8.34 (d, 1 H, J = 8.8 Hz), 7.56 (bs, 1 H), 7.38 (d, 1 H, J = 2.4 Hz), 7.24 (dd, 1 H, J = 8.8 Hz, J = 2.4 Hz), 2.24 (s, 3 H). ^{13}C NMR (CDCl_3 , 50 MHz): δ 168.2, 133.3, 129.0, 128.6, 127.8, 123.0, 122.3, 24.8. MS ($\text{C}_8\text{H}_7\text{Cl}_2\text{NO}$): 203 (M^+ , ^{35}Cl), 205 (M^+ , ^{37}Cl). IR (KBr, cm^{-1}): ν 3278, 1664, 1525, 1302, 1059.

N-(2-chloro-5-methoxy-4-methylphenyl)acetamide (2oa). 5% $\text{Pd}(\text{OAc})_2$. Starting from 0.0895g **1o** to afford **2oa** 0.0993g. yield 93 %, mp 119-120 °C. ^1H NMR (CDCl_3 , 200 MHz): δ 7.99 (s, 1 H), 7.55 (bs, 1 H), 7.08 (s, 1 H), 3.82 (s, 3 H), 2.22 (s, 3 H), 2.14 (s, 3 H). ^{13}C NMR (CDCl_3 , 50 MHz): δ 168.4, 156.6, 132.9, 129.7, 123.3, 112.8, 103.8, 55.5, 24.7, 15.4. MS ($\text{C}_{10}\text{H}_{12}\text{ClNO}_2$): 213 (M^+ , ^{35}Cl), 215 (M^+ , ^{37}Cl). HRMS: Anal. Calcd. for $\text{C}_{10}\text{H}_{12}^{35}\text{ClNO}_2$ 213.05566. Found: 213.05526. EA (%): Anal. Calcd. for $\text{C}_{10}\text{H}_{12}\text{ClNO}_2$ C, 56.21; H, 5.66; N, 6.56. Found: C, 56.10; H, 5.76; N, 6.41. IR (KBr, cm^{-1}): ν 3275, 1667, 1592, 1523, 1395, 1291, 1168, 1019.

N-(2-bromo-5-methoxy-4-methylphenyl)acetamide (2ob). Starting from 0.0895g **1o** to afford **2ob** 0.1161g. yield 90 %, mp 115-116 °C. ^1H NMR (CDCl_3 , 200 MHz): δ 7.91 (s, 1 H), 7.57 (bs, 1 H), 7.20 (s, 1 H), 3.79 (s, 3 H), 2.20 (s, 3 H), 2.11 (s, 3 H). ^{13}C NMR (CDCl_3 , 50 MHz): δ 168.2, 157.1, 134.0, 132.6, 123.9, 104.1, 102.5, 55.4, 24.8, 15.5. MS ($\text{C}_{10}\text{H}_{12}\text{BrNO}_2$): 257 (M^+ , ^{79}Br), 259 (M^+ , ^{81}Br). HRMS: Anal. Calcd. for $\text{C}_{10}\text{H}_{12}\text{BrNO}_2$ 257.00514 Found. 257.00560. EA (%): Anal. Calcd. for $\text{C}_{10}\text{H}_{12}\text{BrNO}_2$ C, 46.53; H, 4.69; N, 5.43. Found: C, 46.55; H, 4.65; N, 5.26. IR (KBr, cm^{-1}): ν 3274, 1670, 1519, 1392, 1166

N-(2-chloro-3,4,5-trimethoxyphenyl)acetamide (2pa). Starting from 0.1125g **1p** to afford **2pa** 0.0856g. yield 66 %, mp 104-105 °C. ¹H NMR (CDCl₃, 200 MHz): δ 7.90 (s, 1 H), 7.55 (bs, 1 H), 3.91 (s, 3 H), 3.87 (s, 3 H), 3.85 (s, 3 H), 2.23 (s, 3 H). ¹³C NMR (CDCl₃, 50 MHz): δ 168.4, 152.1, 149.5, 139.2, 130.8, 108.6, 100.9, 61.1, 55.9, 24.6. MS (C₁₁H₁₄ClNO₄): 259 (M⁺, ³⁵Cl), 261 (M⁺, ³⁷Cl). HRMS: Anal. Calcd. for C₁₁H₁₄³⁵ClNO₄ 259.06114 Found. 259.06070. EA (%):Anal. Calcd. for C₁₁H₁₄ClNO₄ C, 50.88; H, 5.43; N, 5.39. Found: C, 50.90; H, 5.29; N, 5.26. IR (KBr, cm⁻¹): ν 3281, 1671, 1590, 1520, 1398, 1238, 1112, 1016

N-(2-bromo-3,4,5-trimethoxyphenyl)acetamide (2pb).¹⁰ Starting from 0.1125g **1p** to afford **2pb** 0.1383g. yield 91 %, mp 92-93 °C. ¹H NMR (CDCl₃, 200 MHz): δ 7.86 (s, 1 H), 7.60 (bs, 1 H), 3.87 (s, 3 H), 3.84 (s, 3 H), 3.82 (s, 3 H), 2.20 (s, 3 H). ¹³C NMR (CDCl₃, 50 MHz): δ 168.3, 152.7, 150.3, 139.2, 131.8, 101.4, 99.7, 61.0, 60.9, 55.9, 24.7. MS (C₁₁H₁₄BrNO₄): 303 (M⁺, ⁷⁹Br), 305 (M⁺, ⁸¹Br). IR (KBr, cm⁻¹): ν 3271, 1669, 1584, 1393, 1108

Methyl 4-acetamido-5-chloro-2-methoxybenzoate (2qa).¹¹ Starting from 0.1115g **1q** to afford **2qa** 0.0386g. yield 30 %, mp 152-153 °C. ¹H NMR (CDCl₃, 200 MHz): δ 8.23 (s, 1 H), 7.80 (s, 2 H), 3.86 (s, 3 H), 3.82 (s, 3 H), 2.23 (s, 3 H). ¹³C NMR (CDCl₃, 50 MHz): δ 168.6, 164.7, 159.0, 138.9, 131.8, 114.7, 112.3, 104.1, 56.2, 51.9, 25.0. MS (C₁₁H₁₂ClNO₄): 257 (M⁺, ³⁵Cl), 259 (M⁺, ³⁷Cl). IR (KBr, cm⁻¹): ν 3416, 1726, 1703, 1580, 1400, 1233, 1100.

Methyl 4-acetamido-5-bromo-2-methoxybenzoate (2qb).¹² Starting from 0.1115g **1q** to afford **2qb** 0.1314g. yield 87 %, mp 170-172 °C. ¹H NMR (CDCl₃, 200 MHz): δ 8.29 (s, 1 H), 8.01 (s, 1 H), 7.75 (bs, 1H), 3.91 (s, 3 H), 3.86 (s, 3 H), 2.26 (s, 3 H). ¹³C NMR (CDCl₃, 50 MHz): δ 168.6, 164.6, 159.6, 140.0, 134.9, 115.3, 104.2, 101.7, 56.1, 51.9, 25.0. MS (C₁₁H₁₂BrNO₄): 301 (M⁺, ⁷⁹Br), 303 (M⁺, ⁸¹Br). IR (KBr, cm⁻¹): ν 3400, 1685, 1457, 1404, 1237.

1-(8-chloro-3,4-dihydroquinolin-1(2H)-yl)ethanone (2r).¹³ 5% Pd(OAc)₂. Starting from 0.0875g **1r** to afford **2r** 0.0995g. yield 95 %, mp 56-57 °C. ¹H NMR (CDCl₃, 200 MHz): δ 7.30-7.12 (m, 3 H), 4.78-4.64 (m, 1 H), 2.95-2.65 (m, 2 H), 2.56-2.26 (m, 2 H), 2.03 (s, 3 H), 1.68-1.63 (m, 1 H). ¹³C NMR (CDCl₃, 50 MHz): δ 170.9, 139.0, 137.8, 129.9, 128.0, 127.2, 126.2, 41.2, 26.6, 23.9, 21.6. MS (C₁₁H₁₂ClNO): 209 (M⁺, ³⁵Cl), 211 (M⁺, ³⁷Cl). IR (KBr, cm⁻¹): ν 1672, 1464, 1375, 1267.

2i

21

2n

2a

2ob

2pa

2pb

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2a

2m

Table S1. Crystallographic data and refinement details for compounds **2a**, **2m**

	2a	2m
Formula	C ₈ H ₈ ClNO	C ₉ H ₉ ClNO ₂
M/g mol ⁻¹	169.60	198.62
Color	colourless	colourless
Crystal size/mm	0.40 x 0.12 x 0.12 mm	0.50 x 0.15 x 0.15 mm
Crystal system,	Orthorhombic	Monoclinic
Space group	Pbca	P2(1)/c
a/ Å	10.516(2)	9.3602(19)
b/ Å	9.5540(19)	12.290(3)
c/ Å	16.670(3)	8.5900(17)
α/ °	90	90.00
β/ °	90	105.34(3)
γ/ °	90	90.00
V/Å ³	1674.9(6)	953.0(3)
ρ calc/g cm ⁻³	1.345	1.384
Z	8	4
F(000)	704	412
Radiation used	Mo-Kα	Mo-Kα

μ/mm^{-1}	0.395	0.366
T / K	293(2) K	293(2) K
hkl range	-12 $\leq$ h $\leq$ 12, -11 $\leq$ k $\leq$ 11,	-11 $\leq$ h $\leq$ 11, -15 $\leq$ k $\leq$ 15,
	-19 $\leq$ l $\leq$ 19	-10 $\leq$ l $\leq$ 10
θ range/ $^{\circ}$	2.44 - 25.01	2.26 - 26.49
Reflections measured	5828	4131
Unique reflections (R_{int})	1465 (0.0337)	1840 (0.0603)
Reflections, n [$I \geq 2\sigma(I)$]	776	984
Refinement method	Full-matrix least-squares	Full-matrix least-squares
	on F^2	on F^2
Refined parameters/restraints	105 / 0	123 / 0
R1 [$I > 2\sigma$]		
R1 (all data)	0.0323, wR2 = 0.0634	0.0551, wR2 = 0.1391
Goodness-of-fit on F2	0.0670, wR2 = 0.0663	0.0977, wR2 = 0.1548
Largest diff. peak and hole/e. $\text{\AA}$	0.936	1.004
$^{-3}$	0.212 and -0.153	0.263 and -0.280

Table S2. Selected bond distances ($\text{\AA}$) and angles ($^{\circ}$) for compounds **2a**, **2m**

Compound 2a	
Cl(1)-C(1)	1.740(2)
O(1)-C(7)	1.229(3)
N(1)-C(7)	1.345(3)
N(1)-C(6)	1.409(3)
N(1)-HN	0.852(18)
C(1)-C(2)	1.374(3)
C(1)-C(6)	1.387(3)
C(2)-C(3)	1.370(3)

C(2)-H(2)	0.9300
C(3)-C(4)	1.379(3)
C(3)-H(3)	0.9300
C(4)-C(5)	1.379(3)
C(4)-H(4)	0.9300
C(5)-C(6)	1.390(3)
C(5)-H(5)	0.9300
C(7)-C(8)	1.500(3)
C(8)-H(8A)	0.9600
C(8)-H(8B)	0.9600
C(8)-H(8C)	0.9600
C(7)-N(1)-C(6)	125.3(2)
C(7)-N(1)-HN	118.1(14)
C(6)-N(1)-HN	116.5(14)
C(2)-C(1)-C(6)	121.0(2)
C(2)-C(1)-Cl(1)	118.2(2)
C(6)-C(1)-Cl(1)	120.81(17)
C(3)-C(2)-C(1)	119.7(3)
C(3)-C(2)-H(2)	120.1
C(1)-C(2)-H(2)	120.1
C(2)-C(3)-C(4)	120.6(3)
C(2)-C(3)-H(3)	119.7
C(4)-C(3)-H(3)	119.7
C(5)-C(4)-C(3)	119.6(3)
C(5)-C(4)-H(4)	120.2
C(3)-C(4)-H(4)	120.2
C(4)-C(5)-C(6)	120.6(2)
C(4)-C(5)-H(5)	119.7

C(6)-C(5)-H(5)	119.7
C(1)-C(6)-C(5)	118.5(2)
C(1)-C(6)-N(1)	119.8(2)
C(5)-C(6)-N(1)	121.7(2)
O(1)-C(7)-N(1)	123.4(2)
O(1)-C(7)-C(8)	121.5(2)
N(1)-C(7)-C(8)	115.1(2)
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5

Compound **2m**

C(11)-C(1)	1.739(3)
O(1)-C(7)	1.224(3)
O(2)-C(4)	1.367(4)
O(2)-C(9)	1.420(4)
N(1)-C(7)	1.347(4)
N(1)-C(2)	1.408(4)
N(1)-HN(1)	0.79(3)
C(1)-C(6)	1.378(5)
C(1)-C(2)	1.391(4)
C(2)-C(3)	1.388(4)
C(3)-C(4)	1.376(4)
C(3)-H(3)	0.9300
C(4)-C(5)	1.383(4)
C(5)-C(6)	1.373(5)

C(5)-H(5)	0.9300
C(6)-H(6)	0.9300
C(7)-C(8)	1.498(4)
C(8)-H(8A)	0.9600
C(8)-H(8B)	0.9600
C(8)-H(8C)	0.9600
C(9)-H(9A)	0.9600
C(9)-H(9B)	0.9600
C(9)-H(9C)	0.9600
C(4)-O(2)-C(9)	118.6(3)
C(7)-N(1)-C2	124.8(3)
C(7)-N(1)-H(N1)	122(2)
C(2)-N(1)-H(N1)	113(2)
C(6)-C(1)-C(2)	120.6(3)
C(6)-C(1)-C(11)	120.0(2)
C(2)-C(1)-C(11)	119.3(2)
C(3)-C(2)-C(1)	118.0(3)
C(3)-C(2)-N(1)	120.7(3)
C(1)-C(2)-N(1)	121.3(3)
C(4)-C(3)-C(2)	121.4(3)
C(4)-C(3)-H(3)	119.3
C(2)-C(3)-H(3)	119.3
O(2)-C(4)-C(3)	115.0(3)
O(2)-C(4)-C(5)	125.3(3)
C(3)-C(4)-C(5)	119.7(3)
C(6)-C(5)-C(4)	119.7(3)
C(6)-C(5)-H(5)	120.1
C(4)-C(5)-H(5)	120.1

C(5)-C(6)-C(1)	120.5(3)
C(5)-C(6)-H(6)	119.7
C(1)-C(6)-H(6)	119.7
O(1)-C(7)-N(1)	122.0(3)
O(1)-C(7)-C(8)	122.9(3)
N(1)-C(7)-C(8)	115.1(3)
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
O(2)-C(9)-H(9A)	109.5
O(2)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
O(2)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5