Supporting Information

Polymeric, Molecular and Ionic Organotin Complexes Containing Hypoxanthine, Adenine and 2-Aminopurine. Synthesis and Supramolecular Structures

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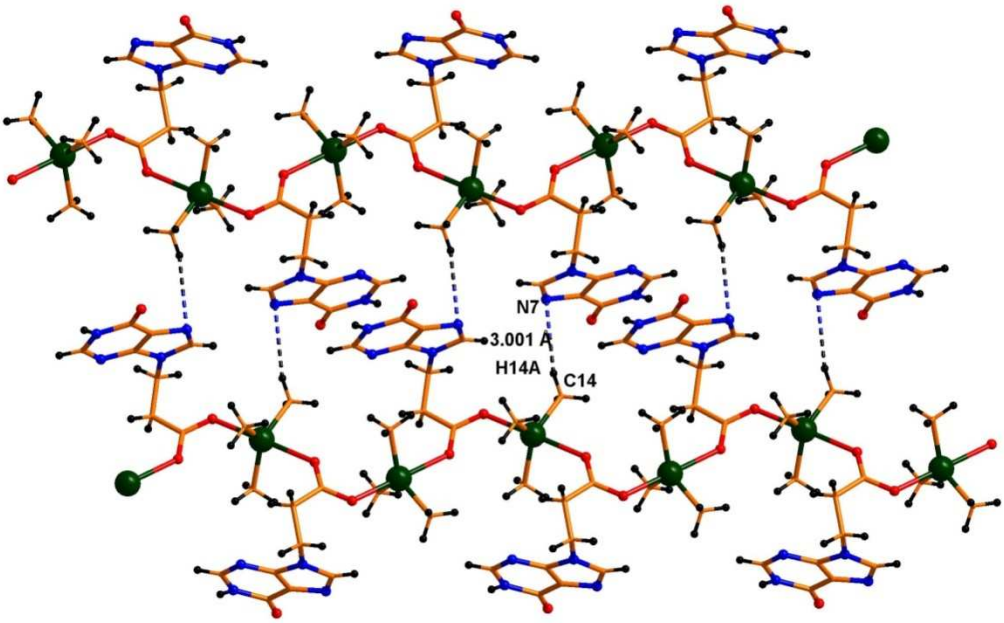


Figure S1.C-H···N hydrogen bonding interaction in **1**.

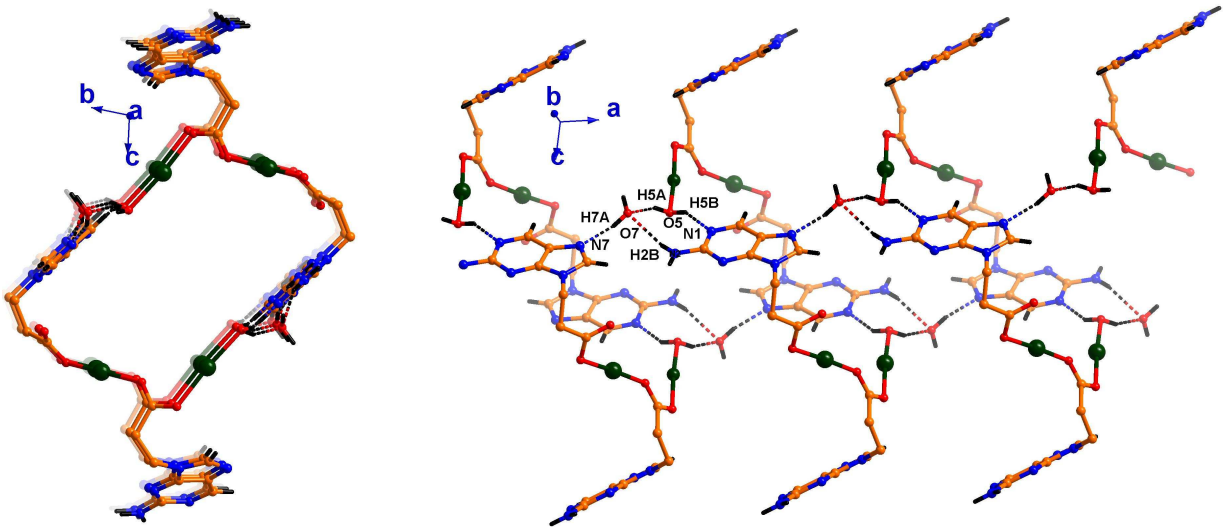


Figure S2. 1D supramolecular network of **3** via lattice water molecule has shown in different directions. Distances (Å):O7-H7A···N7, 1.968; N2-H2B···O7, 2.273; O5-H5B···N1, 1.945; O5-H5A···O7, 1.835. Angles (°):O7-H7A-N7, 160.36(4); N2-H2B-O7, 157.95(2); O5-H5B-N1,

145.181(4); O5-H5A-O7, 155.93(3).

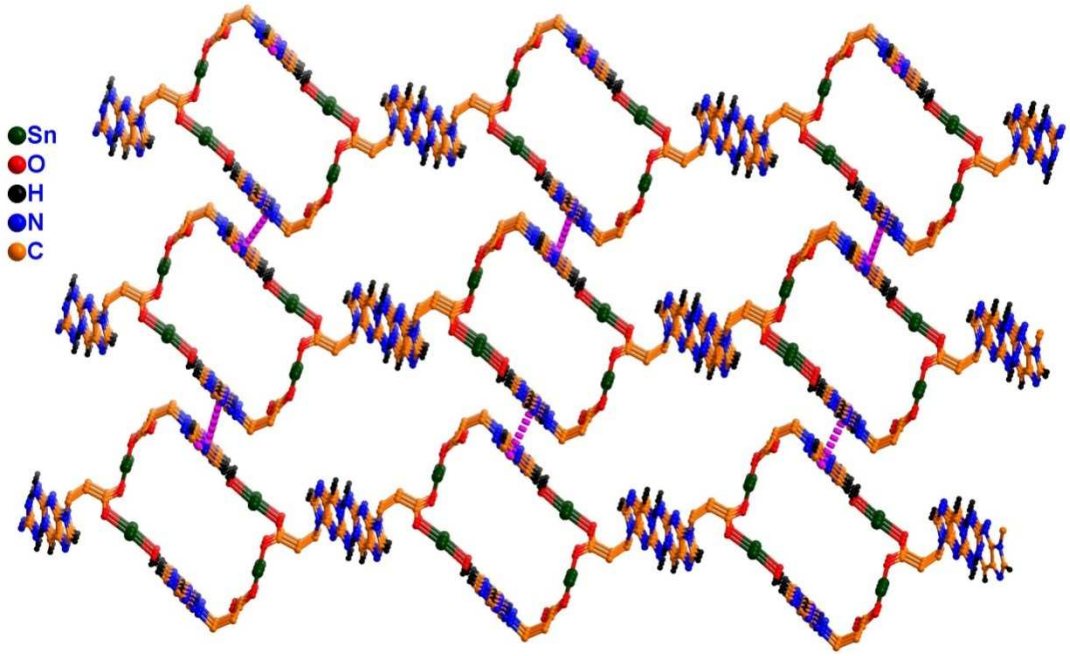


Figure S3: 3D supramolecular framework of **3**.

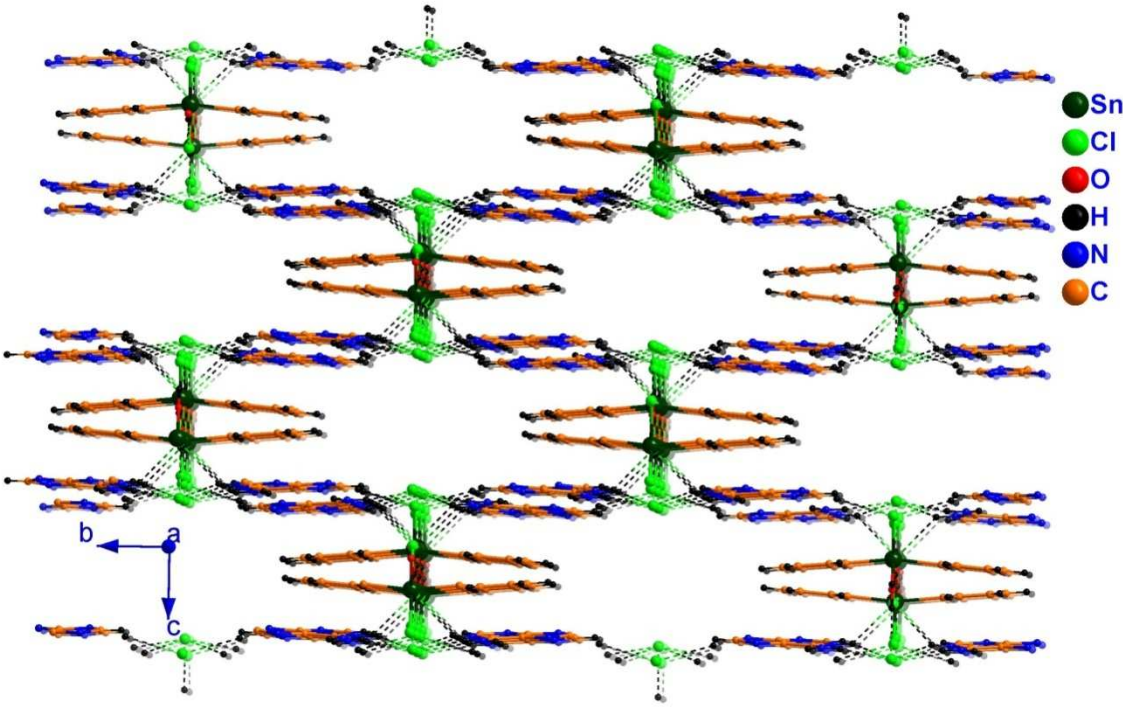


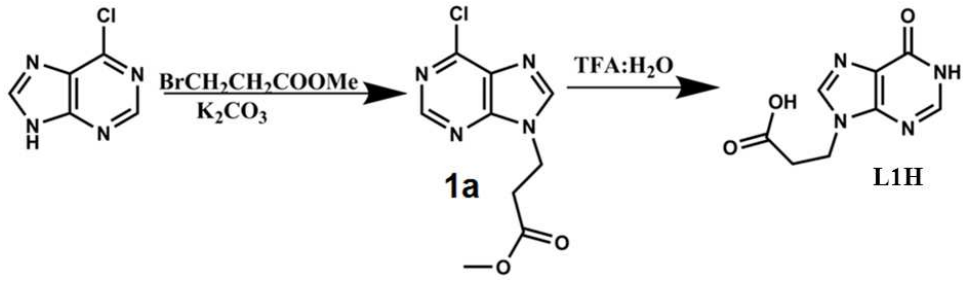
Figure S4: 3D supramolecular structure of **4**.

Table S1. Hydrogen Bonding Parameters Found in **1**−**5**.

D−H···A	symmetry of A	D−H	H···A	D−A	∠D−H···A
Complex **1**					
N1-H1···N7	[-x+2, y-1/2, -z+1/2]	0.732	2.124	2.852	173.50
C2-H2···O6	[-x, -2-y, 1-Z]	0.930	2.395	3.189	143.24
C14-H14A···N7	[-x+2, y-1/2, -z+1/2]	0.920	3.001	3.985	165.02
Complex **2**					
N1-H1···N7A	[x, y+1, z]	0.859	2.046	2.900	172.35
C2-H2···O6A	[x, y+1, z]	0.929	2.324	3.319	136.45
Complex **3**					
O5-H5B··· N1	[-x+2, -y+1, -z+1]	0.851	1.946	2.711	149.16
N2A-H2AB···N1A	[-x+2, -y+1, -z]	0.860	2.188	3.018	162.12
N2-H2A···O6	[x+1, y-1, z]	0.860	2.122	2.980	175.12
N2-H2B···O7	[-x+2, -y+1, -z+1]	0.860	2.273	3.087	157.86
O7-H7A···N7	[-x+1, -y+1, -z+1]	0.850	1.966	2.781	160.34
Complex **4**					
N6-H6A ··· Cl4	[-x+1/2, -y+2, z-1/2]	0.860	2.421	3.187	148.70
N6-H6B··· N7	[-x+1, -y+2, -z+1]	0.860	2.081	2.897	157.99
N1-H1··· Cl4	[-x+1/2, -y+2, z-1/2]	0.864	2.370	3.160	152.36
N1-H1··· Cl2	[-x+1/2, -y+2, z+1/2]	0.864	2.903	3.376	116.28
O4-H5W··· Cl2	[x-1/2, y, -z+1/2]	0.867	2.367	3.223	169.59
O4-H4W··· Cl4	[x, y, z-1]	0.964	2.261	3.164	155.78
Complex **5**					

N6-H6A···Cl2	[-x+2, -y+2, -z+2]	0.860	2.630	3.347	141.68
N6-H6A···Cl1		0.860	2.631	3.243	129.13
N6-H6B···N7	[-x+2, -y+1, -z+2]	0.860	2.125	2.914	152.14
N1-H1···Cl1	[-x+2, -y+2, -z+2]	0.758	2.583	3.176	136.52
N1-H1·· Cl1		0.758	2.877	3.410	129.58

Scheme S1. Synthetic Procedure for the complexes L1H.

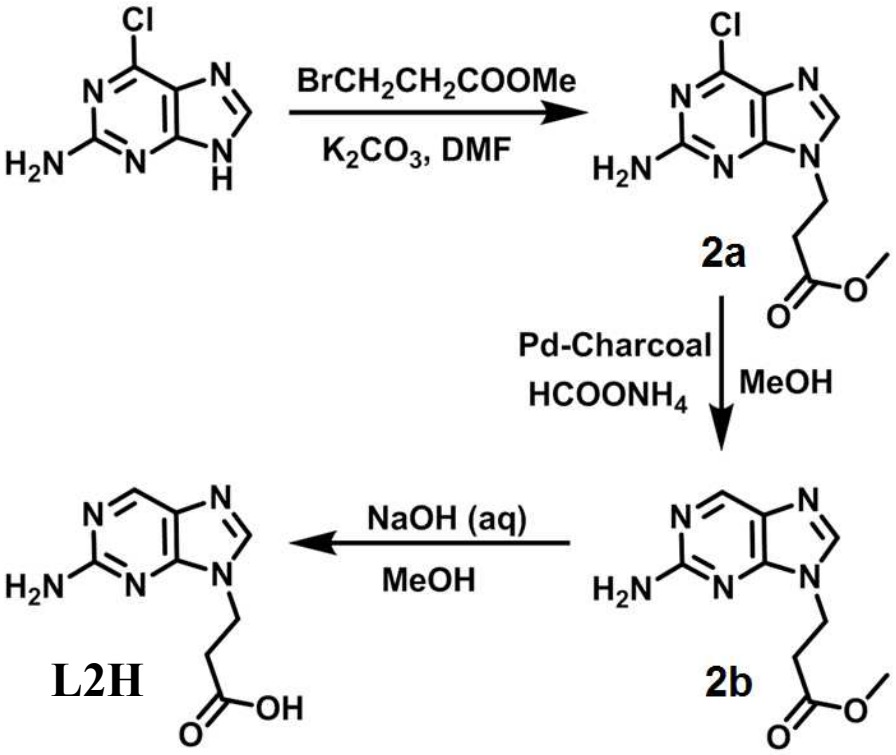


Synthesis of methyl 3-(6-chloro-9H-purin-9-yl) propionate (1a): 6-chloropurine (2.00 g, 12.94 mmol) was dissolved in dry DMF followed by addition of anhydrous potassium carbonate(2.14 gm,15.53 mmol) the reaction mixture was allowed to stir at 0°C under N_2 atm for 1 hours. Methyl 3-bromopropionate (1.72 mL, 15.53 mmol) was added drop wise into the reaction mixture. The reaction was continued for 48 hours at room temperature. Then the reaction mixture was concentrated under reduced pressure and further purified by column chromatography using DCM:MeOH (99.5:0.5) and the yield obtained was 84%.

The HRMS: $(L+H)^+$ calculated: 241.0492, observed: 241.0490. ^{1}H NMR: (500 MHz, DMSO-d^6, 25 °C, TMS) δ (ppm) = 2.98-3.00 (t, 2H, C*H*$_2$), 3.53 (s, 3H, O-*CH*$_3$), 4.48-4.51 (t, 2H. -N-C*H*$_2$-), 8.64(s, 1H, C8-*H*), 8.74(s, 1H, C2-*H*),

3-(N9-hypoxanthyl)propanoic acid (L1H): L1H was synthesized based on slightly modified literature procedure.[1] Compound **1a** was dissolved in 3:1 mixture of TFA-H_2O (12ml) and then stirred for 48 hrs at room temperature. The reaction mixture was evaporated and washed with diethyl ether to afford compound L1H as a white solid (71% Yield). The HRMS: $(L+H)^+$ calculated: 209.0675, observed: 209.0673. ^{1}H NMR: (500 MHz, DMSO-d^6, 25 °C, TMS) δ (ppm) = 2.68-2.81 (t, 2H, C*H*$_2$), 4.29-4.31 (t, 2H. -N-C*H*$_2$-), 8.01(s, 1H, C8-H), 8.03(s, 1H, C2-*H*), 12.28 (s, 1H, O-*H*).

Scheme S2. Synthetic Procedure for the complexes L2H.



Synthesis of methyl 3-(2-amino-6-chloro-9H-purin-9-yl)propionate (2a): 6-chloroguanine (3 g, 17.7498 mmol) was dissolved in dry DMF followed by addition of anhydrous potassium carbonate (2.93 gm, 21.2997 mmol) the reaction mixture was

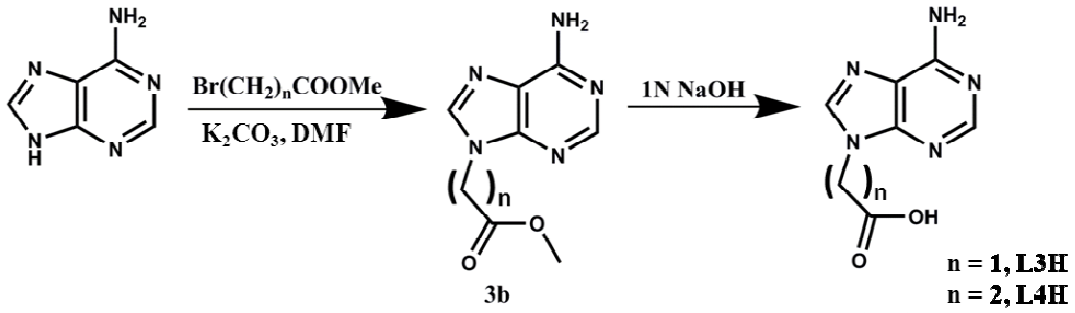
allowed to stir at 0°C under N_2 atm for 2 hours. Methyl 3-bromopropionate (2.37 mL, 21.2997 mmol) was added drop wise into the reaction mixture. The reaction was continued for 24 hours at room temperature. Then the reaction mixture was concentrated under reduced pressure and further purified by column chromatography using DCM: MeOH (98:2) and the yield obtained was (70% Yield). HRMS: $(M+H)^+$ calculated: 255.0523, observed: 255.0523. ^{1}H NMR: (500 MHz, DMSO-d^6, 25 °C, TMS) δ (ppm) 2.88-2.91 (t, 2H, -CH_2-), 3.54 (s, 3H, O-CH_3), 4.23-4.26 (t, 2H, -CH_2-), 6.90 (s, 2H, N2-*H*), 8.05 (s, 1H, C8-*H*).

Synthesis of methyl 3-(2-amino-9H-purin-9-yl) propionate (2b): 2a (2 g, 7.8228 mmol) was dissolved in dry methanol followed by the addition of ammonium formate (1.97 g, 31.2914 mmol) and catalytic amount palladium-charcoal (0.020 g) was added. The reaction was continued for 4 hours, after which the reaction mixture was filtered through cellite for the decolorisation of charcoal. The solvent was evaporated under reduced pressure. White crystalline powder of **2b** was separated through column chromatography (85% Yield). HRMS: $(M+H)^+$ calculated: 222.0991, observed: 222.0994. ^{1}H NMR: (500 MHz, DMSO-d^6, 25 °C, TMS) δ (ppm) 2.88-2.91 (t, 2H, CH_2), 3.54 (s, 3H, -OCH_3), 4.24-4.26 (t, 2H.-CH_2-), 6.49 (s, 2H, N2-*H*), 7.98 (s, 1H, C8-*H*), 8.52 (s, 1H, C6-*H*).

Synthesis of 3-(2-amino-9H-purin-9-yl) propanoic acid (L2H): Ligand L2H was synthesized through the base hydrolysis of **2b**; the methyl ester (0.500 g, 2.2602 mmol) was suspended in 30 mL methanol and 1N NaOH solution (3 mL) was added drop wise, and stirred for one hour. Then it was neutralized using 1N HCl until neutralized, wherein, the white precipitate obtained was filtered and dried (Yield 91%). The HRMS: $(L+H)^+$ calculated: 255.0523, observed: 255.0523. ^{1}H NMR: (500 MHz, DMSO-d^6, 25 °C, TMS) δ (ppm) 2.79-2.81 (t, 2H, CH_2), 3.54 (s, 3H, O-CH_3), 4.19-4.22 (t, 2H. -N-CH_2-), 6.50 (s, 2H, N2-H), 7.97 (s, 1H, C8-H), 8.51(s, 1H, C8-

H), ^{13}C NMR: (125 MHz, $CDCl_3$, 25°C, TMS); δ (ppm) 33.84, 39.08, 127.36, 143.36, 149.49, 153.42, 160.99, 172.68.

Scheme S3. Synthetic Procedure for the complexes **L3H-L4H**.



Synthesis of methyl 2-(6-amino-9H-purin-9-yl)acetate (3b): The ester terminated adenine derivative was synthesized by modified reported procedure.[2] Adenine (3 g, 22.2132 mmol) was dissolved in dry DMF followed by addition of anhydrous potassium carbonate (3.68 gm, 26.6559 mmol) the reaction mixture was allowed to stir at 0°C under N_2 atm for 2 hours. Methyl 2-bromoacetate (2.54 mL, 26.6559 mmol) was added drop wise into the reaction mixture. The reaction was continued for 24 hours at room temperature. Then the reaction mixture was concentrated under reduced pressure and further purified by column chromatography using DCM: MeOH (98:2) and the yield obtained was (50% Yield). HRMS: $(M+H)^+$ calculated: 208.0835, observed: 208.0835. ^1H NMR: (500 MHz, DMSO-d^6, 25 °C, TMS) δ (ppm) 3.76 (s, 3H, O-CH_3), 4.94 (s, 2H, CH_2), 6.90 (s, 2H, N6-*H*), 7.84 (s, 1H, C2-*H*) 8.05 (s, 1H, C8-*H*).

Synthesis of 2-(N9-adeninyl)acetic acid (L3H): Ligand L3H was synthesized through the base hydrolysis of **3b**; the methyl ester (1g, 4.8291 mmol) was suspended in 30 mL methanol and 1N NaOH solution (5 mL) was added drop wise, and stirred for one hour. Then it was neutralized using 1N HCl until neutralized, wherein, the white precipitate obtained was filtered and dried (yield 89%). The HRMS: $(L+H)^+$ calculated: 194.0678, observed: 194.0675. ^1H NMR: (500

MHz, DMSO-d^6, 25 °C, TMS) δ (ppm) 4.82 (t, 2H, *CH₂*), 6.52 (s, 2H, N2-*H*), 7.99 (s, 1H, C8-*H*), 8.54 (s, 1H, C8-*H*).

3-(N9-adeninyl)propanoic acid (L4H): L4H was prepared using the same procedure of L3H, instead of using methyl-2-bromoacetate, methyl-3-bromopropionate was used (yield 91%). HRMS: $(M-1H)^-$ calculated: 206.0683, found: 206.0674; ^{1}H NMR (400 MHz, DMSO-d_6, 25°C, TMS): δ (ppm) 2.85 (t, 2H, CH_2), 4.32 (t, 2H, CH_2), 7.22 (s, 2H, NH_2), 8.07 (s, 1H, C8-*H*), 8.12 (s, 1H, C2-*H*).

Referencess :

1. Fletcher. S.; Shahani, V. M.; Gunning, P. T. *Tetrahedron Lett.* **2009**, *50*, 4258.

2. Mishra, A. K.; Kumar, A.; Khanna, S.; Verma, S. *Cryst.Growth Des.* **2011**, *11*, 1623.

3. Weisser M.; Kashammer J.; Menges B.; Matsumoto J.; Nakamura F.; Ijiro K.; Shimomura M.; Mittler S. *J. Am. Chem. Soc.* **2000**, *122*, 87.

Table S2: Bond distances and bond angles of complexes **1-5**.

Bond lengths [Å] of **1**	Bond angles [deg] of **1**
Sn1-O22.3378(18)	O1-Sn1-O2176.91(6)
Sn1-O12.2225(18)	C14-Sn1-O289.35(9)
Sn1-C142.116(3)	C14-Sn1-O189.25(9)
Sn1-C122.115(3)	C14-Sn1-C12117.95(12)
Sn1-C132.119(3)	C14-Sn1-C13117.90(11)
O2-C11^{1}1.253(3)	C12-Sn1-O291.40(9)
O1-C111.268(3)	C12-Sn1-O191.69(9)
O6-C61.230(3)	C12-Sn1-C13124.13(11)
N7-C81.308(3)	C13-Sn1-O287.66(8)
N7-C51.378(3)	C13-Sn1-O190.56(9)
N9-C81.366(3)	C11^1-O2-Sn1132.04(15)
N9-C91.455(3)	C11-O1-Sn1123.25(15)
N9-C41.374(3)	C8-N7-C5104.2(2)
C5-C41.368(3)	C8-N9-C9127.5(2)

N3-C41.359(3) N3-C21.302(3) N1-C61.396(3) N1-C21.357(3) C10-C91.525(3) C10-C111.510(3) C6-C51.429(4) C11-O2[2]1.253(3) [1]1-X,1/2+Y,1/2-Z; [2]1-X,-1/2+Y,1/2-Z	C8-N9-C4105.8(2) C4-N9-C9126.5(2) C2-N3-C4110.9(2)C2-N1-C6125.7(2) C11-C10-C9113.7(2) N7-C8-N9113.3(2) N9-C9-C10110.6(2) O6-C6-N1121.5(2) O6-C6-C5128.6(2) N1-C6-C5109.9(2) O2[2]-C11-O1123.3(2) O2[2]-C11-C10120.6(2) O1-C11-C10116.1(2) N7-C5-C6129.9(2) C4-C5-N7110.8(2) C4-C5-C6119.3(2) N3-C4-N9125.3(2) N3-C4-C5128.9(2) C5-C4-N9105.9(2) N3-C2-N1125.3(2)

Bond lengths [Å] of **2**		Bond lengths [Å] of **2**	
C(11)-O(2)#1	1.25(4)	C(19)-H(19B)	0.9600
C(11)-O(1A)	1.27(4)	C(19)-H(19C)	0.9600
C(11)-C(10)	1.51(4)	C(10)-C(9)	1.52(5)
Sn(1)-C(28)	2.15(3)	C(31)-H(31B)	0.9600
Sn(1)-C(24)	2.15(4)	C(31)-H(31C)	0.9600
Sn(1)-O(3A)	2.22(2)	C(24)-C(25)	1.51(5)
Sn(1)-C(32)	2.25(9)	C(24)-H(24A)	0.9700
Sn(1)-O(2)	2.38(2)	C(24)-H(24B)	0.9700
Sn(2)-C(20)	2.14(4)	O(6)-C(6)	1.22(4)
Sn(2)-C(12)	2.18(5)	O(6A)-C(6A)	1.22(4)
Sn(2)-O(1A)	2.21(2)	C(11A)-C(10A)	1.52(4)
Sn(2)-C(16)	2.241(6)	C(12)-C(13)	1.50(6)
Sn(2)-O(2A)	2.41(2)	C(12)-H(12A)	0.9700
O(3A)-C(11A)	1.27(4)	C(12)-H(12B)	0.9700
O(2A)-C(11A)	1.24(4)	C(10)-H(10A)	0.9700
N(1)-C(2)	1.36(5)	C(10)-H(10B)	0.9700
N(1)-C(6)	1.41(4)	C(9)-N(9)	1.47(5)
N(1)-H(1)	0.8600	C(9)-H(9A)	0.9700
C(2)-N(3)	1.32(5)	C(9)-H(9B)	0.9700
C(2)-H(2)	0.9300	N(9)-C(4)	1.38(4)
N(3)-C(4)	1.36(4)	C(4)-C(5)	1.38(5)
N(7)-C(8)	1.33(5)	C(5)-C(6)	1.43(5)

N(7)-C(5)	1.38(4)	C(20)-C(21)	1.49(6)
C(8)-N(9)	1.36(4)	C(20)-H(20A)	0.9700
C(8)-H(8)	0.9300	C(20)-H(20B)	0.9700
O(2)-C(11)#2	1.25(4)	C(21)-C(22)	1.61(7)
C(9A)-N(9A)	1.48(5)	C(21)-H(21A)	0.9700
C(9A)-C(10A)	1.51(6)	C(21)-H(21B)	0.9700
C(9A)-H(9A1)	0.9700	C(22)-C(23)	1.46(7)
C(9A)-H(9A2)	0.9700	C(22)-H(22A)	0.9700
C(8A)-N(7A)	1.31(5)	C(22)-H(22B)	0.9700
C(8A)-N(9A)	1.36(5)	C(23)-H(23A)	0.9600
C(8A)-H(8A)	0.9300	C(23)-H(23B)	0.9600
N(7A)-C(5A)	1.38(4)	C(23)-H(23C)	0.9600
N(3A)-C(2A)	1.31(5)	C(10A)-H(10C)	0.9700
N(3A)-C(4A)	1.36(5)	C(10A)-H(10D)	0.9700
N(1A)-C(2A)	1.36(5)	N(9A)-C(4A)	1.37(4)
N(1A)-C(6A)	1.40(4)	C(5A)-C(4A)	1.36(5)
N(1A)-H(1A)	0.8600	C(5A)-C(6A)	1.44(5)
C(28)-C(29)	1.52(5)	C(2A)-H(2A)	0.9300
C(28)-H(28A)	0.9700	C(32)-C(33)	1.34(11)
C(28)-H(28B)	0.9700	C(32)-H(32A)	0.9700
C(29)-C(30)	1.53(4)	C(32)-H(32B)	0.9700
C(29)-H(29A)	0.9700	C(33)-C(34)	1.77(12)
C(29)-H(29B)	0.9700	C(33)-H(33A)	0.9700
C(30)-C(31)	1.52(5)	C(33)-H(33B)	0.9700
C(30)-H(30A)	0.9700	C(34)-C(35)	1.44(10)
C(30)-H(30B)	0.9700	C(34)-H(34A)	0.9700
C(31)-H(31A)	0.9600	C(34)-H(34B)	0.9700
C(13)-C(14)	1.50(7)	C(35)-H(35A)	0.9600
C(13)-H(13A)	0.9700	C(35)-H(35B)	0.9600
C(13)-H(13B)	0.9700	C(35)-H(35C)	0.9600
C(14)-C(15)	1.47(7)	C(25)-C(26)	1.52(7)
C(14)-H(14A)	0.9700	C(25)-H(25A)	0.9700
C(14)-H(14B)	0.9700	C(25)-H(25B)	0.9700
C(15)-H(15A)	0.9600	C(26)-C(27)	1.47(6)
C(15)-H(15B)	0.9600	C(26)-H(26A)	0.9700

C(15)-H(15C)	0.9600	C(26)-H(26B)	0.9700
C(17)-C(16)	1.47(8)	C(27)-H(27A)	0.9600
C(17)-C(18)	1.50(9)	C(27)-H(27B)	0.9600
C(17)-H(17A)	0.9700	C(27)-H(27C)	0.9600
C(17)-H(17B)	0.9700	C(18)-H(18A)	0.9700
C(19)-C(18)	1.540(4)	C(18)-H(18B)	0.9700
C(19)-H(19A)	0.9600	C(16)-H(16A)	0.9700
		C(16)-H(16B)	0.9700

Bond angles [deg] of **2**		Bond angles [deg] of **2**	
O(2)#1-C(11)-O(1A)	123(3)	C(9)-C(10)-H(10A)	108.7
O(2)#1-C(11)-C(10)	120(3)	C(11)-C(10)-H(10B)	108.7
O(1A)-C(11)-C(10)	117(3)	C(9)-C(10)-H(10B)	108.7
C(28)-Sn(1)-C(24)	121.1(14)	H(10A)-C(10)-H(10B)	107.6
C(28)-Sn(1)-O(3A)	95.9(11)	N(9)-C(9)-C(10)	111(3)
C(24)-Sn(1)-O(3A)	94.0(11)	N(9)-C(9)-H(9A)	109.4
C(28)-Sn(1)-C(32)	112(3)	C(10)-C(9)-H(9A)	109.4
C(24)-Sn(1)-C(32)	126(3)	N(9)-C(9)-H(9B)	109.4
O(3A)-Sn(1)-C(32)	85(3)	C(10)-C(9)-H(9B)	109.4
C(28)-Sn(1)-O(2)	89.6(11)	H(9A)-C(9)-H(9B)	108.0
C(24)-Sn(1)-O(2)	87.5(11)	C(8)-N(9)-C(4)	106(3)
O(3A)-Sn(1)-O(2)	172.5(8)	C(8)-N(9)-C(9)	128(3)
C(32)-Sn(1)-O(2)	89(3)	C(4)-N(9)-C(9)	126(3)
C(20)-Sn(2)-C(12)	120.5(19)	N(3)-C(4)-C(5)	128(3)
C(20)-Sn(2)-O(1A)	95.6(15)	N(3)-C(4)-N(9)	125(3)
C(12)-Sn(2)-O(1A)	95.7(15)	C(5)-C(4)-N(9)	106(3)
C(20)-Sn(2)-C(16)	104.6(17)	N(7)-C(5)-C(4)	110(3)
C(12)-Sn(2)-C(16)	133.8(19)	N(7)-C(5)-C(6)	130(3)
O(1A)-Sn(2)-C(16)	88.4(13)	C(4)-C(5)-C(6)	120(3)
C(20)-Sn(2)-O(2A)	90.2(15)	O(6)-C(6)-N(1)	121(3)
C(12)-Sn(2)-O(2A)	85.1(16)	O(6)-C(6)-C(5)	129(3)
O(1A)-Sn(2)-O(2A)	172.8(8)	N(1)-C(6)-C(5)	110(3)
C(16)-Sn(2)-O(2A)	85.9(13)	C(21)-C(20)-Sn(2)	117(3)
C(11A)-O(3A)-Sn(1)	121(2)	C(21)-C(20)-H(20A)	108.0
C(11A)-O(2A)-Sn(2)	136(2)	Sn(2)-C(20)-H(20A)	108.0
C(2)-N(1)-C(6)	125(3)	C(21)-C(20)-H(20B)	108.0

C(2)-N(1)-H(1)	117.7	Sn(2)-C(20)-H(20B)	108.0
C(6)-N(1)-H(1)	117.7	H(20A)-C(20)-H(20B)	107.2
N(3)-C(2)-N(1)	126(3)	C(20)-C(21)-C(22)	121(4)
N(3)-C(2)-H(2)	117.0	C(20)-C(21)-H(21A)	107.1
N(1)-C(2)-H(2)	117.0	C(22)-C(21)-H(21A)	107.1
C(2)-N(3)-C(4)	111(3)	C(20)-C(21)-H(21B)	107.1
C(8)-N(7)-C(5)	104(3)	C(22)-C(21)-H(21B)	107.1
N(7)-C(8)-N(9)	114(3)	H(21A)-C(21)-H(21B)	106.8
N(7)-C(8)-H(8)	123.2	C(23)-C(22)-C(21)	110(4)
N(9)-C(8)-H(8)	123.2	C(23)-C(22)-H(22A)	109.6
C(11)#2-O(2)-Sn(1)	135(2)	C(21)-C(22)-H(22A)	109.6
N(9A)-C(9A)-C(10A)	111(3)	C(23)-C(22)-H(22B)	109.6
N(9A)-C(9A)-H(9A1)	109.3	C(21)-C(22)-H(22B)	109.6
C(10A)-C(9A)-H(9A1)	109.3	H(22A)-C(22)-H(22B)	108.1
N(9A)-C(9A)-H(9A2)	109.3	C(22)-C(23)-H(23A)	109.5
C(10A)-C(9A)-H(9A2)	109.3	C(22)-C(23)-H(23B)	109.5
H(9A1)-C(9A)-H(9A2)	108.0	H(23A)-C(23)-H(23B)	109.5
N(7A)-C(8A)-N(9A)	114(3)	C(22)-C(23)-H(23C)	109.5
N(7A)-C(8A)-H(8A)	122.9	H(23A)-C(23)-H(23C)	109.5
N(9A)-C(8A)-H(8A)	122.9	H(23B)-C(23)-H(23C)	109.5
C(8A)-N(7A)-C(5A)	104(3)	C(9A)-C(10A)-C(11A)	114(3)
C(2A)-N(3A)-C(4A)	110(3)	C(9A)-C(10A)-H(10C)	108.6
C(2A)-N(1A)-C(6A)	126(3)	C(11A)-C(10A)-H(10C)	108.6
C(2A)-N(1A)-H(1A)	117.2	C(9A)-C(10A)-H(10D)	108.6
C(6A)-N(1A)-H(1A)	117.2	C(11A)-C(10A)-H(10D)	108.6
C(29)-C(28)-Sn(1)	114(2)	H(10C)-C(10A)-H(10D)	107.6
C(29)-C(28)-H(28A)	108.7	C(8A)-N(9A)-C(4A)	105(3)
Sn(1)-C(28)-H(28A)	108.7	C(8A)-N(9A)-C(9A)	128(3)
C(29)-C(28)-H(28B)	108.7	C(4A)-N(9A)-C(9A)	127(3)
Sn(1)-C(28)-H(28B)	108.7	C(4A)-C(5A)-N(7A)	110(3)
H(28A)-C(28)-H(28B)	107.6	C(4A)-C(5A)-C(6A)	120(3)
C(28)-C(29)-C(30)	114(3)	N(7A)-C(5A)-C(6A)	130(3)
C(28)-C(29)-H(29A)	108.7	C(5A)-C(4A)-N(3A)	129(3)
C(30)-C(29)-H(29A)	108.7	C(5A)-C(4A)-N(9A)	107(3)
C(28)-C(29)-H(29B)	108.7	N(3A)-C(4A)-N(9A)	124(3)

C(30)-C(29)-H(29B)	108.7	N(3A)-C(2A)-N(1A)	126(3)
H(29A)-C(29)-H(29B)	107.6	N(3A)-C(2A)-H(2A)	117.0
C(31)-C(30)-C(29)	114(3)	N(1A)-C(2A)-H(2A)	117.0
C(31)-C(30)-H(30A)	108.7	O(6A)-C(6A)-N(1A)	122(3)
C(29)-C(30)-H(30A)	108.7	O(6A)-C(6A)-C(5A)	129(3)
C(31)-C(30)-H(30B)	108.7	N(1A)-C(6A)-C(5A)	109(3)
C(29)-C(30)-H(30B)	108.7	C(33)-C(32)-Sn(1)	109(7)
H(30A)-C(30)-H(30B)	107.6	C(33)-C(32)-H(32A)	109.8
C(30)-C(31)-H(31A)	109.5	Sn(1)-C(32)-H(32A)	109.8
C(30)-C(31)-H(31B)	109.5	C(33)-C(32)-H(32B)	109.8
H(31A)-C(31)-H(31B)	109.5	Sn(1)-C(32)-H(32B)	109.8
C(30)-C(31)-H(31C)	109.5	H(32A)-C(32)-H(32B)	108.3
H(31A)-C(31)-H(31C)	109.5	C(32)-C(33)-C(34)	94(7)
H(31B)-C(31)-H(31C)	109.5	C(32)-C(33)-H(33A)	113.0
C(25)-C(24)-Sn(1)	117(3)	C(34)-C(33)-H(33A)	113.0
C(25)-C(24)-H(24A)	108.1	C(32)-C(33)-H(33B)	113.0
Sn(1)-C(24)-H(24A)	108.1	C(34)-C(33)-H(33B)	113.0
C(25)-C(24)-H(24B)	108.1	H(33A)-C(33)-H(33B)	110.4
Sn(1)-C(24)-H(24B)	108.1	C(35)-C(34)-C(33)	103(7)
H(24A)-C(24)-H(24B)	107.3	C(35)-C(34)-H(34A)	111.2
C(11)-O(1A)-Sn(2)	121(2)	C(33)-C(34)-H(34A)	111.2
O(2A)-C(11A)-O(3A)	123(3)	C(35)-C(34)-H(34B)	111.2
O(2A)-C(11A)-C(10A)	120(3)	C(33)-C(34)-H(34B)	111.2
O(3A)-C(11A)-C(10A)	116(3)	H(34A)-C(34)-H(34B)	109.1
C(13)-C(12)-Sn(2)	118(3)	C(34)-C(35)-H(35A)	109.5
C(13)-C(12)-H(12A)	107.7	C(34)-C(35)-H(35B)	109.5
Sn(2)-C(12)-H(12A)	107.7	H(35A)-C(35)-H(35B)	109.5
C(13)-C(12)-H(12B)	107.7	C(34)-C(35)-H(35C)	109.5
Sn(2)-C(12)-H(12B)	107.7	H(35A)-C(35)-H(35C)	109.5
H(12A)-C(12)-H(12B)	107.1	H(35B)-C(35)-H(35C)	109.5
C(14)-C(13)-C(12)	117(4)	C(24)-C(25)-C(26)	114(4)
C(14)-C(13)-H(13A)	108.0	C(24)-C(25)-H(25A)	108.8
C(12)-C(13)-H(13A)	108.0	C(26)-C(25)-H(25A)	108.8
C(14)-C(13)-H(13B)	108.0	C(24)-C(25)-H(25B)	108.8
C(12)-C(13)-H(13B)	108.0	C(26)-C(25)-H(25B)	108.8

H(13A)-C(13)-H(13B)	107.3	H(25A)-C(25)-H(25B)	107.7
C(15)-C(14)-C(13)	116(4)	C(27)-C(26)-C(25)	119(5)
C(15)-C(14)-H(14A)	108.2	C(27)-C(26)-H(26A)	107.6
C(13)-C(14)-H(14A)	108.2	C(25)-C(26)-H(26A)	107.6
C(15)-C(14)-H(14B)	108.2	C(27)-C(26)-H(26B)	107.6
C(13)-C(14)-H(14B)	108.2	C(25)-C(26)-H(26B)	107.6
H(14A)-C(14)-H(14B)	107.4	H(26A)-C(26)-H(26B)	107.1
C(14)-C(15)-H(15A)	109.5	C(26)-C(27)-H(27A)	109.5
C(14)-C(15)-H(15B)	109.5	C(26)-C(27)-H(27B)	109.5
H(15A)-C(15)-H(15B)	109.5	H(27A)-C(27)-H(27B)	109.5
C(14)-C(15)-H(15C)	109.5	C(26)-C(27)-H(27C)	109.5
H(15A)-C(15)-H(15C)	109.5	H(27A)-C(27)-H(27C)	109.5
H(15B)-C(15)-H(15C)	109.5	H(27B)-C(27)-H(27C)	109.5
C(16)-C(17)-C(18)	117(6)	C(17)-C(18)-C(19)	106(6)
C(16)-C(17)-H(17A)	108.2	C(17)-C(18)-H(18A)	110.5
C(18)-C(17)-H(17A)	108.2	C(19)-C(18)-H(18A)	110.5
C(16)-C(17)-H(17B)	108.2	C(17)-C(18)-H(18B)	110.5
C(18)-C(17)-H(17B)	108.2	C(19)-C(18)-H(18B)	110.5
H(17A)-C(17)-H(17B)	107.3	H(18A)-C(18)-H(18B)	108.7
C(18)-C(19)-H(19A)	109.5	C(17)-C(16)-Sn(2)	114(4)
C(18)-C(19)-H(19B)	109.5	C(17)-C(16)-H(16A)	108.7
H(19A)-C(19)-H(19B)	109.5	Sn(2)-C(16)-H(16A)	108.7
C(18)-C(19)-H(19C)	109.5	C(17)-C(16)-H(16B)	108.7
H(19A)-C(19)-H(19C)	109.5	Sn(2)-C(16)-H(16B)	108.7
H(19B)-C(19)-H(19C)	109.5	H(16A)-C(16)-H(16B)	107.6
C(11)-C(10)-C(9)	114(3)	#1 x-1,y,z #2 x+1,y,z	
C(11)-C(10)-H(10A)	108.7		

Bond lengths [Å] of **3**		Bond lengths [Å] of **3**	
Sn(2)-C(37)	2.117(6)	C(35)-C(36)	1.389(9)
Sn(2)-C(31)	2.127(6)	C(35)-H(35)	0.9300
Sn(2)-C(43)	2.129(6)	C(6)-H(6)	0.9300
Sn(2)-O(4)	2.209(4)	N(2A)-C(2A)	1.311(10)

Sn(2)-O(5)	2.268(4)	N(2A)-H(2AA)	0.8600
Sn(1)-C(13)	2.110(6)	N(2A)-H(2AB)	0.8600
Sn(1)-C(25)	2.113(6)	C(21)-C(20)	1.379(10)
Sn(1)-C(19)	2.135(6)	C(21)-H(21)	0.9300
Sn(1)-O(1)	2.175(4)	C(13)-C(14)	1.394(9)
Sn(1)-O(3)	2.324(4)	C(13)-C(18)	1.405(9)
O(4)-C(12A)	1.271(7)	C(36)-C(31)	1.391(9)
O(5)-H(5A)	0.8513	C(36)-H(36)	0.9300
O(5)-H(5B)	0.8513	C(47)-C(46)	1.376(10)
O(3)-C(12A)	1.254(7)	C(47)-C(48)	1.390(9)
C(22)-C(23)	1.364(10)	C(47)-H(47)	0.9300
C(22)-C(21)	1.381(10)	C(30)-C(25)	1.383(8)
C(22)-H(22)	0.9300	C(30)-H(30)	0.9300
C(24)-C(23)	1.379(9)	C(32)-C(31)	1.387(8)
C(24)-C(19)	1.383(9)	C(32)-H(32)	0.9300
C(24)-H(24)	0.9300	C(39)-C(40)	1.364(10)
O(1)-C(12)	1.282(7)	C(39)-C(38)	1.388(8)
N(9A)-C(8A)	1.358(9)	C(39)-H(39)	0.9300
N(9A)-C(4A)	1.374(8)	C(10)-H(10C)	0.9700
N(9A)-C(10A)	1.450(8)	C(10)-H(10D)	0.9700
N(3)-C(4)	1.322(7)	C(48)-C(43)	1.379(8)
N(3)-C(2)	1.350(8)	C(48)-H(48)	0.9300
N(2)-C(2)	1.339(8)	C(25)-C(26)	1.395(9)
N(2)-H(2A)	0.8600	C(41)-C(40)	1.369(10)
N(2)-H(2B)	0.8600	C(41)-C(42)	1.394(9)
N(1)-C(6)	1.344(8)	C(41)-H(41)	0.9300
N(1)-C(2)	1.361(8)	C(23)-H(23)	0.9300
N(7)-C(8)	1.294(8)	C(46)-H(46)	0.9300
N(7)-C(5)	1.400(8)	C(20)-H(20)	0.9300
O(2)-C(12)	1.233(7)	C(37)-C(42)	1.387(9)
N(3A)-C(4A)	1.343(9)	C(37)-C(38)	1.389(9)
N(3A)-C(2A)	1.356(9)	C(4A)-C(5A)	1.374(10)
N(9)-C(4)	1.374(8)	C(5A)-C(6A)	1.397(10)
N(9)-C(8)	1.390(8)	C(42)-H(42)	0.9300
N(9)-C(10)	1.452(8)	C(43)-C(44)	1.399(8)

C(29)-C(30)	1.371(9)	C(44)-H(44)	0.9300
C(29)-C(28)	1.380(8)	C(40)-H(40)	0.9300
C(29)-H(29)	0.9300	C(38)-H(38)	0.9300
N(7A)-C(8A)	1.319(9)	C(26)-H(26)	0.9300
N(7A)-C(5A)	1.389(9)	C(18)-C(17)	1.384(10)
N(1A)-C(6A)	1.328(11)	C(18)-H(18)	0.9300
N(1A)-C(2A)	1.362(11)	C(17)-C(16)	1.358(12)
C(34)-C(33)	1.370(9)	C(17)-H(17)	0.9300
C(34)-C(35)	1.381(9)	C(16)-C(15)	1.365(12)
C(34)-H(34)	0.9300	C(16)-H(16)	0.9300
C(28)-C(27)	1.372(9)	C(14)-C(15)	1.386(11)
C(28)-H(28)	0.9300	C(14)-H(14)	0.9300
C(5)-C(6)	1.376(8)	C(15)-H(15)	0.9300
C(5)-C(4)	1.395(8)	C(8A)-H(8A)	0.9300
C(27)-C(26)	1.379(9)	C(6A)-H(6A)	0.9300
C(27)-H(27)	0.9300	O(7)-H(7A)	0.8500
C(8)-H(8)	0.9300	O(7)-H(7B)	0.8500
C(11A)-C(12A)	1.499(8)	O(6)-C(49)	1.423(8)
C(11A)-C(10A)	1.521(8)	O(6)-H(6B)	0.8200
C(11A)-H(11A)	0.9700	C(49)-H(49A)	0.9600
C(11A)-H(11B)	0.9700	C(49)-H(49B)	0.9600
C(11)-C(12)	1.511(8)	C(49)-H(49C)	0.9600
C(11)-C(10)	1.514(8)	O(10)-H(10E)	0.8501
C(11)-H(11C)	0.9700	O(10)-H(10F)	0.8500
C(11)-H(11D)	0.9700	O(11)-C(51)	1.480(19)
C(33)-C(32)	1.392(9)	O(11)-H(11)	0.8200
C(33)-H(33)	0.9300	C(51)-H(51A)	0.9600
C(45)-C(44)	1.387(10)	C(51)-H(51B)	0.9600
C(45)-C(46)	1.388(10)	C(51)-H(51C)	0.9600
C(45)-H(45)	0.9300	O(12)-C(53)	1.70(6)
C(19)-C(20)	1.396(9)	O(12)-H(12)	0.8200
C(10A)-H(10A)	0.9700	C(53)-H(53A)	0.9600
C(10A)-H(10B)	0.9700	C(53)-H(53B)	0.9600
		C(53)-H(53C)	0.9600

Bond angles [deg] of **3**		Bond angles [deg] of **3**	
C(37)-Sn(2)-C(31)	121.5(2)	C(29)-C(30)-C(25)	120.7(6)
C(37)-Sn(2)-C(43)	116.2(2)	C(29)-C(30)-H(30)	119.7
C(31)-Sn(2)-C(43)	122.3(2)	C(25)-C(30)-H(30)	119.7
C(37)-Sn(2)-O(4)	83.49(19)	N(2A)-C(2A)-N(3A)	118.4(8)
C(31)-Sn(2)-O(4)	92.39(19)	N(2A)-C(2A)-N(1A)	115.4(7)
C(43)-Sn(2)-O(4)	95.13(18)	N(3A)-C(2A)-N(1A)	126.2(8)
C(37)-Sn(2)-O(5)	90.8(2)	C(26)-C(25)-Sn(1)	118.3(4)
C(31)-Sn(2)-O(5)	90.07(19)	C(40)-C(41)-C(42)	118.8(7)
C(43)-Sn(2)-O(5)	87.97(18)	C(40)-C(41)-H(41)	120.6
O(4)-Sn(2)-O(5)	174.22(14)	C(42)-C(41)-H(41)	120.6
C(13)-Sn(1)-C(25)	122.3(2)	O(3)-C(12A)-O(4)	122.9(5)
C(13)-Sn(1)-C(19)	119.6(2)	O(3)-C(12A)-C(11A)	121.4(5)
C(25)-Sn(1)-C(19)	117.1(2)	O(4)-C(12A)-C(11A)	115.7(5)
C(13)-Sn(1)-O(1)	96.4(2)	C(22)-C(23)-C(24)	120.9(6)
C(25)-Sn(1)-O(1)	95.52(19)	C(22)-C(23)-H(23)	119.5
C(19)-Sn(1)-O(1)	87.74(19)	C(24)-C(23)-H(23)	119.5
C(13)-Sn(1)-O(3)	87.2(2)	C(47)-C(46)-C(45)	119.2(6)
C(25)-Sn(1)-O(3)	84.47(19)	C(47)-C(46)-H(46)	120.4
C(19)-Sn(1)-O(3)	88.45(19)	C(45)-C(46)-H(46)	120.4
O(1)-Sn(1)-O(3)	175.71(15)	C(21)-C(20)-C(19)	121.4(7)
C(12A)-O(4)-Sn(2)	123.0(4)	C(21)-C(20)-H(20)	119.3
Sn(2)-O(5)-H(5A)	109.6	C(19)-C(20)-H(20)	119.3
Sn(2)-O(5)-H(5B)	109.2	C(42)-C(37)-C(38)	117.1(6)
H(5A)-O(5)-H(5B)	109.4	C(42)-C(37)-Sn(2)	123.7(5)
C(12A)-O(3)-Sn(1)	134.0(4)	C(38)-C(37)-Sn(2)	118.8(5)
C(23)-C(22)-C(21)	118.9(6)	N(3A)-C(4A)-C(5A)	127.5(7)
C(23)-C(22)-H(22)	120.6	N(3A)-C(4A)-N(9A)	126.5(7)
C(21)-C(22)-H(22)	120.6	C(5A)-C(4A)-N(9A)	106.1(6)
C(23)-C(24)-C(19)	121.6(6)	C(4A)-C(5A)-N(7A)	110.5(6)
C(23)-C(24)-H(24)	119.2	C(4A)-C(5A)-C(6A)	115.4(7)
C(19)-C(24)-H(24)	119.2	N(7A)-C(5A)-C(6A)	134.0(8)
C(12)-O(1)-Sn(1)	116.4(4)	C(37)-C(42)-C(41)	122.5(6)
C(8A)-N(9A)-C(4A)	106.1(6)	C(37)-C(42)-H(42)	118.7
C(8A)-N(9A)-C(10A)	127.1(6)	C(41)-C(42)-H(42)	118.7

C(4A)-N(9A)-C(10A)	126.8(6)	C(48)-C(43)-C(44)	118.4(6)
C(4)-N(3)-C(2)	112.7(5)	C(48)-C(43)-Sn(2)	121.5(4)
C(2)-N(2)-H(2A)	120.0	C(44)-C(43)-Sn(2)	120.0(5)
C(2)-N(2)-H(2B)	120.0	C(45)-C(44)-C(43)	120.4(6)
H(2A)-N(2)-H(2B)	120.0	C(45)-C(44)-H(44)	119.8
C(6)-N(1)-C(2)	118.9(5)	C(43)-C(44)-H(44)	119.8
C(8)-N(7)-C(5)	104.2(5)	C(32)-C(31)-C(36)	118.6(6)
C(4A)-N(3A)-C(2A)	111.8(7)	C(32)-C(31)-Sn(2)	121.2(4)
C(4)-N(9)-C(8)	105.2(5)	C(36)-C(31)-Sn(2)	120.1(4)
C(4)-N(9)-C(10)	126.6(5)	C(39)-C(40)-C(41)	119.9(6)
C(8)-N(9)-C(10)	128.2(5)	C(39)-C(40)-H(40)	120.1
C(30)-C(29)-C(28)	120.9(6)	C(41)-C(40)-H(40)	120.1
C(30)-C(29)-H(29)	119.6	C(39)-C(38)-C(37)	120.2(6)
C(28)-C(29)-H(29)	119.6	C(39)-C(38)-H(38)	119.9
C(8A)-N(7A)-C(5A)	103.7(6)	C(37)-C(38)-H(38)	119.9
C(6A)-N(1A)-C(2A)	118.5(7)	C(27)-C(26)-C(25)	121.3(6)
C(33)-C(34)-C(35)	120.9(6)	C(27)-C(26)-H(26)	119.3
C(33)-C(34)-H(34)	119.5	C(25)-C(26)-H(26)	119.3
C(35)-C(34)-H(34)	119.5	C(17)-C(18)-C(13)	120.5(7)
C(27)-C(28)-C(29)	119.5(6)	C(17)-C(18)-H(18)	119.7
C(27)-C(28)-H(28)	120.2	C(13)-C(18)-H(18)	119.7
C(29)-C(28)-H(28)	120.2	C(16)-C(17)-C(18)	120.3(8)
C(6)-C(5)-C(4)	115.8(6)	C(16)-C(17)-H(17)	119.8
C(6)-C(5)-N(7)	134.1(6)	C(18)-C(17)-H(17)	119.8
C(4)-C(5)-N(7)	110.0(5)	C(17)-C(16)-C(15)	120.8(8)
C(28)-C(27)-C(26)	119.7(6)	C(17)-C(16)-H(16)	119.6
C(28)-C(27)-H(27)	120.1	C(15)-C(16)-H(16)	119.6
C(26)-C(27)-H(27)	120.1	C(15)-C(14)-C(13)	120.8(8)
N(2)-C(2)-N(3)	116.5(5)	C(15)-C(14)-H(14)	119.6
N(2)-C(2)-N(1)	117.9(6)	C(13)-C(14)-H(14)	119.6
N(3)-C(2)-N(1)	125.6(5)	C(16)-C(15)-C(14)	120.0(8)
N(7)-C(8)-N(9)	114.4(5)	C(16)-C(15)-H(15)	120.0
N(7)-C(8)-H(8)	122.8	C(14)-C(15)-H(15)	120.0
N(9)-C(8)-H(8)	122.8	N(7A)-C(8A)-N(9A)	113.7(6)
C(12A)-C(11A)-C(10A)	114.6(5)	N(7A)-C(8A)-H(8A)	123.2

C(12A)-C(11A)-H(11A)	108.6	N(9A)-C(8A)-H(8A)	123.2
C(10A)-C(11A)-H(11A)	108.6	O(2)-C(12)-O(1)	124.1(6)
C(12A)-C(11A)-H(11B)	108.6	O(2)-C(12)-C(11)	121.0(6)
C(10A)-C(11A)-H(11B)	108.6	O(1)-C(12)-C(11)	114.9(5)
H(11A)-C(11A)-H(11B)	107.6	N(1A)-C(6A)-C(5A)	120.6(8)
C(12)-C(11)-C(10)	112.3(5)	N(1A)-C(6A)-H(6A)	119.7
C(12)-C(11)-H(11C)	109.1	C(5A)-C(6A)-H(6A)	119.7
C(10)-C(11)-H(11C)	109.1	H(7A)-O(7)-H(7B)	109.5
C(12)-C(11)-H(11D)	109.1	C(49)-O(6)-H(6B)	109.5
C(10)-C(11)-H(11D)	109.1	O(6)-C(49)-H(49A)	109.5
H(11C)-C(11)-H(11D)	107.9	O(6)-C(49)-H(49B)	109.5
C(34)-C(33)-C(32)	119.4(6)	H(49A)-C(49)-H(49B)	109.5
C(34)-C(33)-H(33)	120.3	O(6)-C(49)-H(49C)	109.5
C(32)-C(33)-H(33)	120.3	H(49A)-C(49)-H(49C)	109.5
C(44)-C(45)-C(46)	120.5(7)	H(49B)-C(49)-H(49C)	109.5
C(44)-C(45)-H(45)	119.8	H(10E)-O(10)-H(10F)	109.5
C(46)-C(45)-H(45)	119.8	C(51)-O(11)-H(11)	109.5
C(24)-C(19)-C(20)	116.8(6)	O(11)-C(51)-H(51A)	109.5
C(24)-C(19)-Sn(1)	121.3(4)	O(11)-C(51)-H(51B)	109.5
C(20)-C(19)-Sn(1)	121.8(5)	H(51A)-C(51)-H(51B)	109.5
N(9A)-C(10A)-C(11A)	112.8(5)	O(11)-C(51)-H(51C)	109.5
N(9A)-C(10A)-H(10A)	109.0	H(51A)-C(51)-H(51C)	109.5
C(11A)-C(10A)-H(10A)	109.0	H(51B)-C(51)-H(51C)	109.5
N(9A)-C(10A)-H(10B)	109.0	C(53)-O(12)-H(12)	109.5
C(11A)-C(10A)-H(10B)	109.0	O(12)-C(53)-H(53A)	109.5
H(10A)-C(10A)-H(10B)	107.8	O(12)-C(53)-H(53B)	109.5
C(34)-C(35)-C(36)	119.5(6)	H(53A)-C(53)-H(53B)	109.5
C(34)-C(35)-H(35)	120.3	O(12)-C(53)-H(53C)	109.5
C(36)-C(35)-H(35)	120.3	H(53A)-C(53)-H(53C)	109.5
N(1)-C(6)-C(5)	119.9(6)	H(53B)-C(53)-H(53C)	109.5
N(1)-C(6)-H(6)	120.0	C(31)-C(32)-C(33)	121.0(6)
C(5)-C(6)-H(6)	120.0	C(31)-C(32)-H(32)	119.5
N(3)-C(4)-N(9)	126.8(6)	C(33)-C(32)-H(32)	119.5
N(3)-C(4)-C(5)	127.1(6)	C(40)-C(39)-C(38)	121.4(6)
N(9)-C(4)-C(5)	106.1(5)	C(40)-C(39)-H(39)	119.3

C(2A)-N(2A)-H(2AA)	120.0	C(38)-C(39)-H(39)	119.3
C(2A)-N(2A)-H(2AB)	120.0	N(9)-C(10)-C(11)	112.8(5)
H(2AA)-N(2A)-H(2AB)	120.0	N(9)-C(10)-H(10C)	109.0
C(20)-C(21)-C(22)	120.4(7)	C(11)-C(10)-H(10C)	109.0
C(20)-C(21)-H(21)	119.8	N(9)-C(10)-H(10D)	109.0
C(22)-C(21)-H(21)	119.8	C(11)-C(10)-H(10D)	109.0
C(14)-C(13)-C(18)	117.5(6)	H(10C)-C(10)-H(10D)	107.8
C(14)-C(13)-Sn(1)	121.1(5)	C(43)-C(48)-C(47)	121.1(6)
C(18)-C(13)-Sn(1)	121.3(5)	C(43)-C(48)-H(48)	119.5
C(35)-C(36)-C(31)	120.6(6)	C(47)-C(48)-H(48)	119.5
C(35)-C(36)-H(36)	119.7	C(30)-C(25)-C(26)	117.9(5)
C(31)-C(36)-H(36)	119.7	C(30)-C(25)-Sn(1)	123.8(4)
C(46)-C(47)-C(48)	120.5(7)		
C(46)-C(47)-H(47)	119.8		
C(48)-C(47)-H(47)	119.8		

Bond lengths [Å] of **4**		Bond lengths [Å] of **4**	
Sn(1)-C(12)	2.1397	C(6)-C(5)	1.4004
Sn(1)-C(12)#1	2.1397	O(2)-C(10)	1.1915
Sn(1)-O(4)	2.3511	C(9)-C(10)	1.4897
Sn(1)-Cl(1)	2.4809	C(9)-H(9A)	0.9700
Sn(1)-Cl(3)	2.5206	C(9)-H(9B)	0.9700
Sn(1)-Cl(2)	2.6080	C(5)-C(4)	1.3844
O(4)-H(4A)	0.8128	N(3)-C(2)	1.2948
O(4)-H(4B)	0.8128	N(3)-C(4)	1.3489
N(9)-C(4)	1.3649	C(14)-C(15)	1.3768
N(9)-C(8)	1.3657	C(14)-C(13)	1.3907
N(9)-C(9)	1.4501	C(14)-H(14)	0.9300
O(3)-C(10)	1.3273	C(17)-C(16)	1.3875
O(3)-C(11)	1.4704	C(17)-C(12)	1.3948
N(7)-C(8)	1.3149	C(17)-H(17)	0.9300
N(7)-C(5)	1.3793	C(12)-C(13)	1.3860
N(6)-C(6)	1.3103	C(8)-H(8)	0.9300
N(6)-H(6A)	0.8600	C(16)-C(15)	1.3726
N(6)-H(6B)	0.8600	C(16)-H(16)	0.9300

N(1)-C(6)	1.3644	C(13)-H(13)	0.9300
N(1)-C(2)	1.3703	C(2)-H(2)	0.9300
N(1)-H(1)	0.8599	C(15)-H(15)	0.9300
C(11)-H(11B)	0.9600	C(11)-H(11A)	0.9600
C(11)-H(11C)	0.9600		
Bond angles [deg] of **4**		Bond angles [deg] of **4**	
C(12)-Sn(1)-Cl(2)	87.2	C(4)-C(5)-C(6)	117.9
C(12)#1-Sn(1)-Cl(2)	87.2	C(2)-N(3)-C(4)	111.9
O(4)-Sn(1)-Cl(2)	95.4	N(3)-C(4)-N(9)	126.3
Cl(1)-Sn(1)-Cl(2)	89.0	N(3)-C(4)-C(5)	127.9
Cl(3)-Sn(1)-Cl(2)	179.5	N(9)-C(4)-C(5)	105.8
C(12)-Sn(1)-C(12)#1	167.8	C(15)-C(14)-C(13)	120.2
C(12)-Sn(1)-O(4)	84.9	C(15)-C(14)-H(14)	119.9
C(12)#1-Sn(1)-O(4)	84.9	C(13)-C(14)-H(14)	119.9
C(12)-Sn(1)-Cl(1)	95.3	C(16)-C(17)-C(12)	120.6
C(12)#1-Sn(1)-Cl(1)	95.3	C(16)-C(17)-H(17)	119.7
O(4)-Sn(1)-Cl(1)	175.7	C(12)-C(17)-H(17)	119.7
C(12)-Sn(1)-Cl(3)	92.8	C(13)-C(12)-C(17)	118.6
C(12)#1-Sn(1)-Cl(3)	92.8	C(13)-C(12)-Sn(1)	122.3
O(4)-Sn(1)-Cl(3)	85.1	C(17)-C(12)-Sn(1)	119.0
Cl(1)-Sn(1)-Cl(3)	90.6	O(2)-C(10)-O(3)	124.9
Sn(1)-O(4)-H(4A)	127.1	O(2)-C(10)-C(9)	125.6
Sn(1)-O(4)-H(4B)	127.1	O(3)-C(10)-C(9)	109.4
H(4A)-O(4)-H(4B)	105.7	N(7)-C(8)-N(9)	114.0
C(4)-N(9)-C(8)	105.9	N(7)-C(8)-H(8)	123.0
C(4)-N(9)-C(9)	126.4	N(9)-C(8)-H(8)	123.0
C(8)-N(9)-C(9)	127.7	C(15)-C(16)-C(17)	120.0
C(10)-O(3)-C(11)	116.1	C(15)-C(16)-H(16)	120.0
C(8)-N(7)-C(5)	103.4	C(17)-C(16)-H(16)	120.0
C(6)-N(6)-H(6A)	120.0	C(12)-C(13)-C(14)	120.4
C(6)-N(6)-H(6B)	120.0	C(12)-C(13)-H(13)	119.8
H(6A)-N(6)-H(6B)	120.0	C(14)-C(13)-H(13)	119.8
C(6)-N(1)-C(2)	123.6	N(3)-C(2)-N(1)	125.2
C(6)-N(1)-H(1)	118.1	N(3)-C(2)-H(2)	117.4
C(2)-N(1)-H(1)	118.0	N(1)-C(2)-H(2)	117.4

N(6)-C(6)-N(1)	120.8	C(16)-C(15)-C(14)	120.1
N(6)-C(6)-C(5)	125.7	C(16)-C(15)-H(15)	119.9
N(1)-C(6)-C(5)	113.5	C(14)-C(15)-H(15)	119.9
N(9)-C(9)-C(10)	112.9	O(3)-C(11)-H(11A)	109.5
N(9)-C(9)-H(9A)	109.0	O(3)-C(11)-H(11B)	109.5
C(10)-C(9)-H(9A)	109.0	H(11A)-C(11)-H(11B)	109.5
N(9)-C(9)-H(9B)	109.0	O(3)-C(11)-H(11C)	109.5
C(10)-C(9)-H(9B)	109.0	H(11A)-C(11)-H(11C)	109.5
H(9A)-C(9)-H(9B)	107.8	H(11B)-C(11)-H(11C)	109.5
N(7)-C(5)-C(4)	111.0	#1 x,-y+3/2,z	
N(7)-C(5)-C(6)	131.2		

Bond lengths [Å] of **5**		Bond lengths [Å] of **5**	
Sn(1)-C(13)#1	2.149(6)	C(4)-C(5)	1.388(9)
Sn(1)-C(13)	2.149(6)	C(8)-H(8)	0.9300
Sn(1)-Cl(1)	2.561(2)	C(9)-C(10)	1.516(9)
Sn(1)-Cl(1)#1	2.561(2)	C(9)-H(9A)	0.9700
Sn(1)-Cl(2)#1	2.5908(17)	C(9)-H(9B)	0.9700
Sn(1)-Cl(2)	2.5908(17)	C(10)-C(11)	1.503(10)
N(6)-C(6)	1.315(8)	C(10)-H(10A)	0.9700
N(6)-H(6A)	0.8600	C(10)-H(10B)	0.9700
N(6)-H(6B)	0.8600	C(12)-H(12A)	0.9600
N(1)-C(6)	1.362(8)	C(12)-H(12B)	0.9600
N(1)-C(2)	1.363(8)	C(12)-H(12C)	0.9600
N(1)-H(1)	0.76(8)	C(13)-C(18)	1.393(9)
N(3)-C(2)	1.308(8)	C(13)-C(14)	1.405(9)
N(3)-C(4)	1.361(8)	C(14)-C(15)	1.394(9)
N(9)-C(8)	1.365(8)	C(14)-H(14)	0.9300
N(9)-C(4)	1.369(8)	C(15)-C(16)	1.377(10)
N(9)-C(9)	1.466(8)	C(15)-H(15)	0.9300
N(7)-C(8)	1.313(8)	C(16)-C(17)	1.390(10)
N(7)-C(5)	1.390(8)	C(16)-H(16)	0.9300
O(1)-C(11)	1.334(8)	C(17)-C(18)	1.386(9)
O(1)-C(12)	1.78(2)	C(17)-H(17)	0.9300

O(2)-C(11) 1.208(9) C(6)-C(5) 1.393(9) C(2)-H(2) 0.9300	C(18)-H(18) 0.9300
Bond angles [deg] of **5**	Bond angles [deg] of **5**
C(13)#1-Sn(1)-C(13) 179.999(2) C(13)#1-Sn(1)-Cl(1) 89.40(16) C(13)-Sn(1)-Cl(1) 90.60(16) C(13)#1-Sn(1)-Cl(1)#1 90.60(16) C(13)-Sn(1)-Cl(1)#1 89.40(16) Cl(1)-Sn(1)-Cl(1)#1 180.0 C(13)#1-Sn(1)-Cl(2)#1 89.61(16) C(13)-Sn(1)-Cl(2)#1 90.39(16) Cl(1)-Sn(1)-Cl(2)#1 89.69(6) Cl(1)#1-Sn(1)-Cl(2)#1 90.31(6) C(13)#1-Sn(1)-Cl(2) 90.39(16) C(13)-Sn(1)-Cl(2) 89.61(16) Cl(1)-Sn(1)-Cl(2) 90.31(6) Cl(1)#1-Sn(1)-Cl(2) 89.69(6) Cl(2)#1-Sn(1)-Cl(2) 180.00(6) C(6)-N(6)-H(6A) 120.0 C(6)-N(6)-H(6B) 120.0 H(6A)-N(6)-H(6B) 120.0 C(6)-N(1)-C(2) 124.3(6) C(6)-N(1)-H(1) 124(6) C(2)-N(1)-H(1) 111(6) C(2)-N(3)-C(4) 111.8(5) C(8)-N(9)-C(4) 105.8(5) C(8)-N(9)-C(9) 127.8(5) C(4)-N(9)-C(9) 126.3(5) C(8)-N(7)-C(5) 103.4(5) C(11)-O(1)-C(12) 114.4(6) N(6)-C(6)-N(1) 121.2(6) N(6)-C(6)-C(5) 125.7(6) N(1)-C(6)-C(5) 113.1(5)	N(9)-C(8)-H(8) 122.8 N(9)-C(9)-C(10) 112.7(5) N(9)-C(9)-H(9A) 109.0 C(10)-C(9)-H(9A) 109.0 N(9)-C(9)-H(9B) 109.0 C(10)-C(9)-H(9B) 109.0 H(9A)-C(9)-H(9B) 107.8 C(11)-C(10)-C(9) 118.1(6) C(11)-C(10)-H(10A) 107.8 C(9)-C(10)-H(10A) 107.8 C(11)-C(10)-H(10B) 107.8 C(9)-C(10)-H(10B) 107.8 H(10A)-C(10)-H(10B) 107.1 O(2)-C(11)-O(1) 124.0(7) O(2)-C(11)-C(10) 123.3(6) O(1)-C(11)-C(10) 112.7(6) O(1)-C(12)-H(12A) 109.5 O(1)-C(12)-H(12B) 109.5 H(12A)-C(12)-H(12B) 109.5 O(1)-C(12)-H(12C) 109.5 H(12A)-C(12)-H(12C) 109.5 H(12B)-C(12)-H(12C) 109.5 C(18)-C(13)-C(14) 118.8(6) C(18)-C(13)-Sn(1) 120.0(4) C(14)-C(13)-Sn(1) 121.1(5) C(15)-C(14)-C(13) 119.5(6) C(15)-C(14)-H(14) 120.3 C(13)-C(14)-H(14) 120.3 C(16)-C(15)-C(14) 120.8(6) C(16)-C(15)-H(15) 119.6

N(3)-C(2)-N(1)	124.9(6)	C(14)-C(15)-H(15)	119.6
N(3)-C(2)-H(2)	117.5	C(15)-C(16)-C(17)	120.2(6)
N(1)-C(2)-H(2)	117.5	C(15)-C(16)-H(16)	119.9
N(3)-C(4)-N(9)	127.1(6)	C(17)-C(16)-H(16)	119.9
N(3)-C(4)-C(5)	127.0(6)	C(18)-C(17)-C(16)	119.4(6)
N(9)-C(4)-C(5)	105.9(5)	C(18)-C(17)-H(17)	120.3
C(4)-C(5)-N(7)	110.5(5)	C(16)-C(17)-H(17)	120.3
C(4)-C(5)-C(6)	118.8(6)	C(17)-C(18)-C(13)	121.3(6)
N(7)-C(5)-C(6)	130.6(6)	C(17)-C(18)-H(18)	119.3
N(7)-C(8)-N(9)	114.4(6)	C(13)-C(18)-H(18)	119.3
N(7)-C(8)-H(8)	122.8		
		#1 -x+1,-y+2,-z+2	