Organogold(I)-Uracil Conjugates: Synthesis and Structural Characterization

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Abstract.

The conjugation of the gold(I) complex having planar phenyl isocyanide or bulky triphenylphosphine with 6-ethynyl-1-octyluracil afforded the corresponding gold(I) complexes **U6AuCNPh** and **U6AuPPh₃**, respectively, as bioorganometallic conjugates. The crystal structure of **U6AuCNPh** revealed the formation of a head-to-tail dimer through the Au(I)-Au(I) and π - π interactions between the uracil and benzene moieties of phenyl isocyanide. Furthermore, each head-to-tail dimer was connected not only through the intermolecular hydrogen bonds of N-H $\cdots$ O pattern between the uracil moieties but the weak hydrogen bonds of C-H $\cdots$ O pattern between the uracil and benzene moieties of phenyl isocyanide. In contrast, the Au(I)-Au(I) interaction was not observed in a crystal structure of **U6AuPPh₃** probably due to the steric hindrance of the bulky triphenylphosphine ligand although a dimeric structure through the intermolecular hydrogen bonds of N-H $\cdots$ O pattern between the uracil moieties was formed.

Keywords: Nucleobases; Gold(I) complex; Hydrogen bond; Crystal structure; Self-assembly; Auophilic interaction

1. Introduction.

The control of molecular assemblies is important for development of functional materials. The design of supramolecular self-organized systems with specific properties and functions has been actively investigated in recent years [1]. Nucleobases play an important role to form the highly-organized double helical structures of DNA. The complementary hydrogen bond of nucleobases is a powerful tool for construction of self-assembly systems because of its directionality and specificity [2]. Recently, the research field of bioorganometallic chemistry, which is a hybrid area between organometallic chemistry and biology, has drawn much attention [3]. We reported the tuning of emission properties of the organoplatinum(II) complexes bearing the uracil moiety by regulation of the aggregated structures based on the hydrogen bonds of the uracil moiety [4]. On the other hand, organogold(I) complex has attracted increasing attention because of their aggregation properties through an attractive aurophilic interaction [5]. This aurophilic interaction is comparable to the strength of a hydrogen bonding and useful for construction of supramolecular architectures in a solid state. Conjugation of organogold(I) complexes with nucleobases is envisioned to provide highly-organized assembly bioorganometallic systems depending on both properties. The control of aurophilic interaction of the organogold(I) complexes bearing the guanosine moiety was demonstrated through the formation of the guanine-octamer [6]. In this paper, we report the structural characterization of organogold(I)-uracil conjugates to reveal the steric effects of ancillary ligands on assembly properties of the uracil and the gold(I) moieties in a solid state.

2. Results and Discussion.

The organogold(I) complexes bearing the uracil moiety were designed by introduction of planar phenyl isocyanide and bulky triphenylphosphine as an ancillary ligand to elucidate the

effect of ancillary ligands on the assembly properties. The synthesis of organogold(I)-uracil conjugates **U6AuCNPh** and **U6AuPPh₃** is outlined in Scheme 1. The coupling reaction of 6-ethynyl-1-octyluracil (**1**) with chloro(phenyl isocyanide)gold(I) [(PhNC)AuCl], which was obtained by the reaction of chloro(tetrahydrothiophene)gold(I) [(tht)AuCl] with phenyl isocyanide, in the presence of CuI as a catalyst produced the organogold(I)-uracil conjugate bearing planar phenyl isocyanide **U6AuCNPh**. The organogold(I)-uracil conjugate bearing bulky triphenylphosphine **U6AuPPh₃** could be obtained by the treatment of **1** with chloro(triphenylphosphine)gold(I), which was prepared by the reaction of chloro(tetrahydrothiophene)gold(I) with triphenylphosphine *in situ*, in the presence of sodium bis(trimethylsilyl)amide. The formation of thus-obtained organogold(I)-uracil conjugates was supported by ¹H NMR, ¹³C NMR, ³¹P NMR, IR, HRMS, and elemental analysis. For example, the upfield shift was observed for the uracil proton in the ¹H NMR spectra after the introduction of the gold(I) center.

[Insert Scheme 1.]

The structural features of **U6AuCNPh** and **U6AuPPh₃** were elucidated by single-crystal X-ray structure determination, disclosing the self-assembly properties of the gold(I) and uracil moieties (Table 1). Selected bond distances and angles are shown in Table 2. The crystal structure of **U6AuCNPh** revealed a propeller twist conformation with a dihedral angle of 45.9(4)° between the planes of the uracil and benzene moieties of phenyl isocyanide (Fig. 1a). It is noteworthy that a head-to-tail dimer through the Au(I)-Au(I) and π - π interactions between the uracil and benzene moieties of phenyl isocyanide was formed in a crystal packing as shown in Fig. 1b. Furthermore, each head-to-tail dimer was connected not only through the intermolecular hydrogen bonds of N-H $\cdots$ O pattern between the uracil moieties but the weak hydrogen bonds of

C-H...O pattern between the uracil and benzene moieties of phenyl isocyanide (Fig. 1c and Table 3).

[Insert Table 1.]

[Insert Table 2.]

[Insert Table 3.]

[Insert Fig. 1.]

The organogold(I)-uracil conjugate **U6AuPPh₃** crystallized in the space group *C2/c* (*Z* = 16) two independent molecules exist in an asymmetric unit (Tables 1-3). The molecular structure of **U6AuPPh₃** is characterized by the formation of the dimeric structure through intermolecular hydrogen bonds of N-H...O pattern between the uracil moieties of two independent molecules as depicted in Fig. 2. Self-assembly properties of the organogold(I)-uracil conjugates were found to depend on the ancillary ligands. In comparison with the self-assembly properties of **U6AuCNPh**, the Au(I)-Au(I) interaction was not observed in a crystal structure of **U6AuPPh₃** probably due to the sterically bulky triphenylphosphine ligand (Fig. 2b).

[Insert Fig. 2.]

3. Conclusions

The bioorganometallic compounds composed of the organogold(I) complexes and uracil moiety as a nucleobase were designed and synthesized. The structural characterization of organogold(I)-uracil conjugates was demonstrated to reveal the assembly properties of the gold(I)

and the uracil moieties in a solid state. Interesting feature of organogold(I)-uracil conjugates is their strong tendency to self-assemble through intermolecular hydrogen bonds, wherein hydrogen bonding patterns were found to depend on the ancillary ligands. Furthermore, the introduction of planar phenyl isocyanide as an ancillary ligand induced the formation of a head-to-tail dimer through the Au(I)-Au(I) and π - π interactions between the uracil and the benzene moieties of phenyl isocyanide. On the contrary, the Au(I)-Au(I) interaction was not observed in the case of bulky triphenylphosphine ancillary ligand probably due to the steric hindrance. It is worth mentioning that the gold alkynyl complexes show the cytotoxicity, but the studies for biological activity have scarcely been investigated [7]. Application of the bioorganometallic compounds to metallodrug research is envisioned to develop new chemotherapeutics. Studies on the application of the bioorganometallic compounds to material and medicinal chemistry are now in progress.

4. Experimental

4.1. General materials and experimental procedures

All reagents and solvents were purchased from commercial sources and were further purified by the standard methods, if necessary. 6-ethynyl-1-octyluracil (**1**) [8], chloro(tetrahydrothiophene)gold(I) [(tth)AuCl] [9] and chloro(phenyl isocyanide)gold(I) [(PhNC)AuCl] [10] were prepared by the literature methods. Infrared spectra were obtained with a JASCO FT/IR-6200 spectrometer. ^1H , ^{13}C , and ^{31}P NMR spectra were recorded on a JNM-ECS 400 (400, 100, and 160 MHz, respectively) spectrometer. For ^1H and ^{31}P NMR spectra, chemical shifts were determined by using of tetramethylsilane and 85% H_3PO_4 aq. as standard samples, respectively. Chemical shifts of ^{13}C NMR spectra were determined relative to the solvent residual peaks. Mass spectra were run on a JEOL JMS-700 mass spectrometer.

4.1.1 Synthesis of (1-octyluracil-6-ethynyl(phenyl isocyanide)gold(I) **U6AuCNPh**

To a mixture of chloro(phenyl isocyanide)gold(I) (67 mg, 0.20 mmol), 6-ethynyl-1-octyluracil (**1**) (50 mg, 0.20 mmol), CuI (1.9 mg, 10 μ mol), and NaOAc (33 mg, 0.40 mmol) were added dichloromethane (16 mL) and methanol (4.0 mL). The resulting mixture was stirred at room temperature for 9 h under Ar in the dark. The solvent was evaporated and the residue was extracted with dichloromethane, insoluble impurities were filtered out. The solvent was evaporated and purification of the crude product by recrystallization from dichloromethane, diethyl ether, and hexane gave the desired gold(I) complex **U6AuCNPh** (53 mg, 0.096 mmol) as a pale yellow crystal.

U6AuCNPh: yield 48%; IR (KBr) 3150, 2924, 2855, 2228, 2124, 1712, 1656, 1574, 1465, 1416, 1364 cm^{-1} ; ^1H NMR (400 MHz, CD_2Cl_2 , 4.0×10^{-2} M): δ 8.97 (br, 1H), 7.64-7.52 (m, 5H), 5.73 (s, 1H), 4.03 (t, 1H, $J = 7.6$ Hz), 1.38-1.29 (m, 10H), 1.50-1.11 (m, 20H), 0.89 (t, 3H, $J = 6.8$ Hz); ^{13}C NMR (100 MHz, CD_2Cl_2 , 4.0×10^{-2} M): 163.4, 155.0 (t, $J = 24.9$ Hz), 151.4, 140.2, 140.0, 132.3, 130.5, 127.4, 124.6 (t, $J = 14.4$ Hz), 105.7, 93.7, 46.7, 32.4, 29.7, 29.6, 28.9, 27, 23.2, 14.4 ppm; HRMS (FAB) m/z calcd for $\text{C}_{21}\text{H}_{25}\text{N}_3\text{O}_2\text{Au}$ ($\text{M} + \text{H}^+$), 548.1607; found, 548.1612; Anal. Calcd. for $\text{C}_{21}\text{H}_{24}\text{N}_3\text{O}_2\text{Au}$: C, 46.08; H, 4.42; N, 7.68. found: C, 45.78; H, 4.37; N, 7.68.

4.1.3 Synthesis of (1-octyluracil-6-ethynyl(triphenylphosphine)gold(I) **U6AuPPh₃**

A mixture of triphenylphosphine (53 mg, 0.20 mmol), chloro(tetrahydrothiophene)gold(I) (64 mg, 0.20 mmol), and 6-ethynyl-1-octyluracil (**1**) (50 mg, 0.20 mmol) was stirred in THF (10 mL) at room temperature for 15 minutes under Ar. To the solution was added sodium bis(trimethylsilyl)amide (40 mg, 0.22 mmol) and the resulting solution was stirred at room

temperature under Ar for 21 h. The mixture was diluted with dichloromethane, washed with water, brine, and then dried over Na₂SO₄. The solvent was evaporated and purification of the crude product by recrystallization from dichloromethane, diethyl ether, and hexane gave the desired gold(I) complex **U6AuPPh₃** (68 mg, 0.096 mmol) as a colorless crystal.

U6AuPPh₃: yield 48%; IR (KBr) 3170, 3074, 2923, 2852, 2116, 1698, 1661, 1574, 1456, 1402, 1366 cm⁻¹; ¹H NMR (400 MHz, CD₂Cl₂, 1.0 x 10⁻² M): δ 8.30 (br, 1H), 7.59-7.48 (m, 15H), 5.74 (s, 1H), 4.06 (t, 2H, J = 7.6 Hz), 1.77-1.69 (m, 2H), 1.41-1.21 (m, 10H), 0.80 (t, 3H, J = 6.8 Hz); ¹³C NMR (100 MHz, CD₂Cl₂, 1.0 x 10⁻² M): 163, 151.4 (d, $^2J_{C-P}$ = 142.3 Hz), 151.2, 140.3 (d, $^4J_{C-P}$ = 3.1 Hz), 134.6 (d, $^2J_{C-P}$ = 13.7 Hz), 132.2 (d, $^4J_{C-P}$ = 2.2 Hz), 129.6 (d, $^3J_{C-P}$ = 11.3 Hz), 129.6 (d, $^1J_{C-P}$ = 57 Hz), 105.2, 93.8 (d, $^3J_{C-P}$ = 26.6 Hz), 46.7, 32.2, 29.6, 29.5, 28.9, 27, 23, 14.2 ppm; ³¹P NMR (160 MHz, CD₂Cl₂, 1.0 x 10⁻² M): 41.8 ppm; HRMS (FAB) m/z calcd for C₃₂H₃₅N₂O₂PAu (M + H⁺), 707.2096; found, 707.2096; Anal. Calcd. for C₃₂H₃₄N₂O₂PAu: C, 54.40; H, 4.85; N, 3.96. Found: C, 54.37; H, 4.95; N, 4.02.

4.2. X-ray structure analysis

All measurements for **U6AuCNPh** were performed with a Rigaku R-Axis RAPID diffractometer by using graphite-monochromated Mo-K α radiation. All measurements for **U6AuPPh₃** were performed with a Rigaku R-Axis RAPID diffractometer by using filtered Mo-K α radiation. The structures of **U6AuCNPh** and **U6AuPPh₃** were solved by direct methods and expanded using Fourier techniques. The non-hydrogen atoms were refined anisotropically. The H atoms involved in hydrogen bonding were located in electron density maps. The remainder of the H atoms were placed in idealized positions and allowed to ride with the C atoms to which each was bonded. Crystallographic details are given in Table 1. Crystallographic data (excluding structure factors) for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC-1026761 for **U6AuCNPh**

and CCDC-1026762 for **U6AuPPh₃**. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK [Fax: (internat.) +44-1223/336-033; E-mail: deposit@ccdc.cam.ac.uk].

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Figure Captions

Fig. 1. (a) Molecular structure, (b) a head-to-tail dimer, and (c) a part of the intermolecular hydrogen bonds of N-H $\cdots$ O pattern between the uracil moieties and the weak hydrogen bonds of C-H $\cdots$ O pattern between the uracil and benzene moieties of phenyl isocyanide of **U6AuCNPh** (octyl moieties are omitted for clarity).

Fig. 2. (a) Molecular structure and (b) a hydrogen-bonded dimer through intermolecular hydrogen bonds between the uracil moieties of **U6AuPPh₃**.

Scheme 1.

Table 1.Crystallographic data for **U6AuCNPh** and **U6AuPPh₃**

	U6AuCNPh	U6AuPPh₃
Empirical formula	C ₂₁ H ₂₄ N ₃ O ₂ Au ₁	C ₃₂ H ₃₄ N ₂ O ₂ P ₁ Au ₁
Formula weight	541.41	706.57
Crystal system	Tetragonal	Monoclinic
Space group	<i>I</i> 4 ₁ /a (No. 88)	<i>C</i> 2/ <i>c</i> (No. 15)
<i>a</i> (Å)	35.091(3)	38.4526(14)
<i>b</i> (Å)		16.5099(4)
<i>c</i> (Å)	6.7679(6)	20.2551(7)
β (°)		114.7260(11)
<i>V</i> (Å ³)	8334.0(12)	11680.0(7)
<i>Z</i>	16	16
<i>D</i> _{calcd} (g cm ⁻³)	1.745	1.607
μ (Mo K α) (cm ⁻¹)	71.052	51.414
<i>T</i> (°C)	-150	-170
λ (Mo K α) (Å)	0.71075	0.71075
<i>R</i> 1 ^a	0.062	0.060
<i>wR</i> 2 ^b	0.156	0.152

^a $R1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$.^b $wR2 = [\Sigma w(F_o^2 - F_c^2)^2 / \Sigma w(F_o^2)^2]^{1/2}$.

Table 2.Selected bond distances (Å) and angles (°) for **U6AuCNPPh** and **U6AuPPh₃**

	U6AuCNPPh	U6AuPPh₃^a	U6AuCNPPh	U6AuPPh₃^a
<i>Bond distances (Å)</i>				
Au(1)–C(15)	1.982(11)		N(1)–C(4)	1.391(10) 1.356(12)
Au(1)–P(1)		2.2783(18)	N(2)–C(1)	1.381(9) 1.333(12)
Au(1)–C(14)	1.990(11)	1.998(8)	N(2)–C(2)	1.393(9) 1.360(10)
P(1)–C(15)		1.818(10)	N(3)–C(15)	
P(1)–C(21)		1.811(8)	N(3)–C(16)	1.134(14)
P(1)–C(27)		1.812(7)	C(2)–C(3)	1.404(13)
O(1)–C(1)	1.242(14)	1.220(9)	C(3)–C(4)	1.425(15) 1.433(11)
O(2)–C(2)	1.215(15)	1.230(8)	C(4)–C(13)	1.364(10) 1.356(11)
N(1)–C(1)	1.361(14)	1.392(10)	C(13)–C(14)	1.421(14) 1.410(10)
				1.205(12) 1.214(11)
<i>Bond angles (°)</i>				
C(14)–Au(1)–C(15)	176.0(4)		N(1)–C(1)–N(2)	116.1(10) 116.7(9)
P(1)–Au(1)–C(14)		176.3(3)	N(1)–C(4)–C(3)	121.2(7) 118.5(7)
Au(1)–C(15)–N(3)	176.4(9)		N(1)–C(4)–C(13)	117.9(9) 119.4(7)
Au(1)–P(1)–C(15)		111.5(2)	N(2)–C(2)–C(3)	125.9(7) 115.1(7)
Au(1)–P(1)–C(21)		116.2(3)	C(1)–N(1)–C(4)	121.6(6) 123.0(9)
Au(1)–P(1)–C(27)		110.8(2)	C(1)–N(2)–C(2)	126.7(6) 125.5(7)
Au(1)–C(14)–C(13)	173.6(9)	177.6(8)	C(2)–C(3)–C(4)	121.0(7) 120.7(7)
O(1)–C(1)–N(1)	123.1(11)	122.9(7)	C(3)–C(4)–C(13)	122.2(10) 121.9(7)
O(1)–C(1)–N(2)	120.7(10)	122.3(7)	C(4)–C(13)–C(14)	172.7(11) 174.7(11)
O(2)–C(2)–N(2)	120.2(10)	119.5(6)	C(15)–N(3)–C(16)	
O(2)–C(2)–C(3)	126.0(11)	125.9(7)		

^a Two independent molecules exist in an asymmetric unit.

Table 3.Intermolecular hydrogen bonds for **U6AuCNPh** and **U6AuPPh₃**^a

Crystal	Donor	Acceptor	D...A (Å)	D–H...A (°)
U6AuCNPh	N(2)	O(2) ^b	2.827(12)	160(11)
	C(19)	O(1) ^c	3.159(14)	125.2(8)
	C(20)	O(1) ^c	3.210(13)	119.0(8)
	C(20)	O(2) ^d	3.468(15)	146.2(2)
U6AuPPh₃	N(2)	O(52) ^e	2.854(9)	168(5)
	N(52)	O(2) ^e	2.849(8)	168(3)

^a Two independent molecules exist in the asymmetric unit.^b -X, -Y, -Z-1.^c X, Y+1/2, -Z.^d -X, -Y+1/2, Z+1.^e -X+1/2, -Y+1/2, -Z+1

Figure 2.

Graphical Abstract: Pictogram

Organogold(I)–Uracil Conjugates: Synthesis and Structural Characterization

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Conjugates consisting of organogold(I) complexes and uracil as a nucleobase were synthesized. The single-crystal X-ray structure determination demonstrated the formation of assembling structures through hydrogen bonds of the uracil moieties, in which Au(I)–Au(I) interaction was observed in the case of phenyl isocyanide ligand.