

Supplementary Materials

Synthesis of Alkenylgold(I) Complexes Relevant to Catalytic Carboxylative Cyclization of Unsaturated Amines and Alcohols

Shun Hase, Kyohei Yamashita, and Yoshihito Kayaki*

Department of Chemical Science and Engineering, School of Materials and Chemical Technology,
Tokyo Institute of Technology, 2-12-1-E4-1 O-okayama, Meguro-ku Tokyo 152-8552, Japan

*E-mail: ykayaki@o.cc.titech.ac.jp

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X-ray Crystallographic Data

Table S1. Crystallographic data for **7**, **9**, and **11**

	7	9	11
Empirical Formula	C ₄₅ H ₅₂ AuN ₃ O ₂	C ₃₂ H ₄₁ AuN ₂ O ₃	C ₃₂ H ₄₁ AuN ₂ O ₃
Formula Weight	863.89	698.65	698.65
Crystal Color, Habit	colorless, prism	colorless, prism	colorless, prism
Crystal System	monoclinic	orthorhombic	monoclinic
Space Group	<i>P</i> 2 ₁ / <i>n</i> (#14)	<i>Pbca</i> (#61)	<i>P</i> 2 ₁ / <i>n</i> (#14)
Lattice Parameters	<i>a</i> = 12.504(2) Å <i>b</i> = 19.815(4) Å <i>c</i> = 16.172(3) Å <i>β</i> = 97.681(2) ° <i>V</i> = 3970.8(12) Å ³	<i>a</i> = 15.729(2) Å <i>b</i> = 17.415 (2) Å <i>c</i> = 22.599(3) Å <i>V</i> = 6190.7(10) Å ³	<i>a</i> = 10.153(3) Å <i>b</i> = 16.657(4) Å <i>c</i> = 18.566(4) Å <i>β</i> = 95.620(4) ° <i>V</i> = 3165.0(13) Å ³
Z value	4	8	4
<i>D</i> _{calc}	1.445 g/cm ³	1.499 g/cm ³	1.485 g/cm ³
<i>F</i> ₀₀₀	1752.00	2800.00	1400.00
μ(MoKα)	37.576 cm ⁻¹	48.019 cm ⁻¹	47.563 cm ⁻¹
Exposure Rate	10.0 sec./°	16.0 sec./°	16.0 sec./°
No. of Reflections Measured	32619	48693	25391
No. of Unique Reflections	8978	7068	7030
No. Variables	512	384	343
<i>R</i> 1 (<i>I</i> > 2.00σ(<i>I</i>))	0.0581	0.0310	0.0484
w <i>R</i> 2 (All Reflections)	0.1345	0.0897	0.1322
Max Shift/Error in Final Cycle	0.000	0.000	0.002
GOF on <i>F</i> ²	1.000	1.000	0.894

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

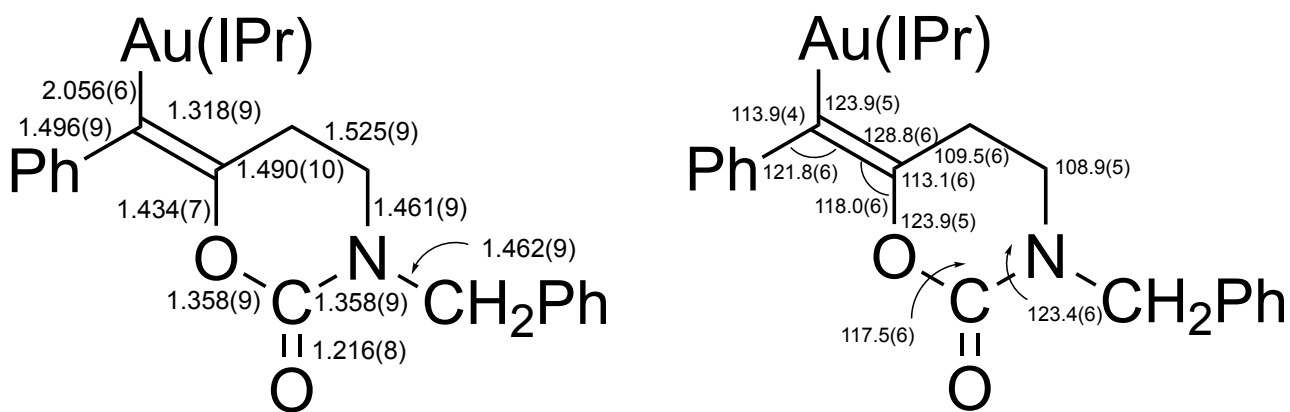


Figure S1. Selected bond lengths (Å; left) and angles (°; right) for 7.

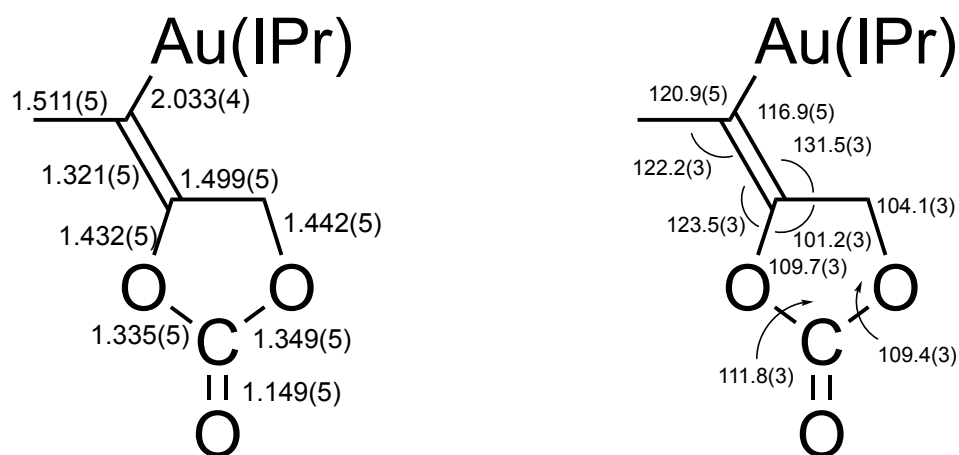


Figure S2. Selected bond lengths (Å; left) and angles (°; right) for 9.

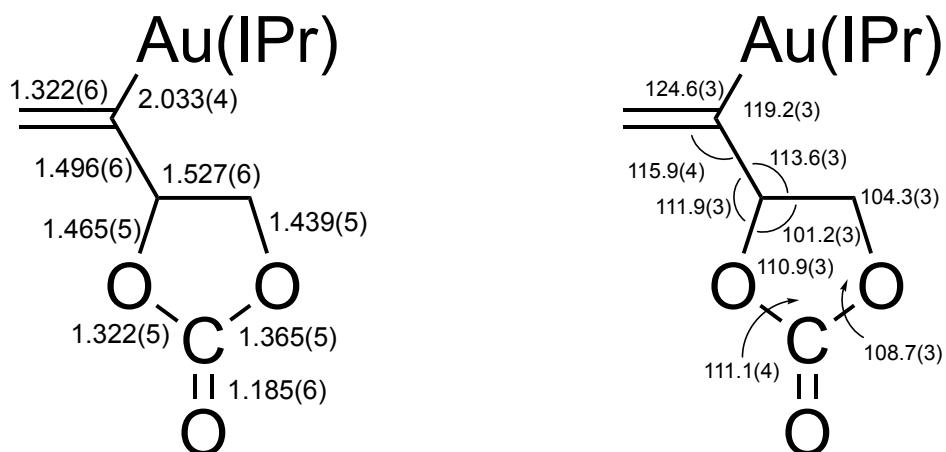


Figure S3. Selected bond lengths (Å) and angles (°) for **11**.