Supporting Information (JO0357465)

Ruthenium-Catalyzed Cycloaddition between Propargylic Alcohols and Cyclic 1,3-Dicarbonyl Compounds via Allenylidene Intermediates

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X-ray Crystallographic Studies of 4a. Colorless crystals of **4a** suitable for X-ray analysis were obtained by recrystallization from CH₂Cl₂–*n*-hexane. The single crystal was sealed in a Pyrex glass capillary under N₂ atmosphere and used for data collection. All measurements were made on a Rigaku RAXIS imaging plate area detector with graphite monochromated Mo-K α radiation. Details of crystal and data collection parameters are summarized in Table S1. The positions of non-hydrogen atoms were determined by direct methods (SIR92) and subsequent Fourier syntheses (DIRDIF PATTY). An ORTEP drawing of **4a** is shown in Figure S1.

Table S1. Crystallographic Data for **4a**.

formula	C ₁₅ H ₁₄ O ₂
formula weigh	226.27
cryst size (mm ³)	0.40 x 0.30 x 0.10
cryst system	orthorhombic
space group	P2 ₁ 2 ₁ 2 ₁ (#19)
cryst color	colorless
<i>a</i> (Å)	8.2640(7)
<i>b</i> (Å)	11.829(1)
<i>c</i> (Å)	12.102(1)
<i>V</i> (Å ³)	1183.0(2)
<i>Z</i>	4
<i>d</i> _{calc} (g cm ⁻³)	1.270
<i>F</i> (000)	480.00
μ _{calc} (cm ⁻¹)	0.83
no. of unique data	1565
no. of data used (<i>I</i> > 3 σ (<i>I</i>))	875
no. of params refined	210
<i>R</i> ^a	0.042
<i>R</i> _w ^b	0.039
goodness of fit indicator	1.08
maximum residuals (e Å ⁻³)	0.16

$$^a R = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|.$$

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

Figure S1. Crystal structure of **4a**.

X-ray Crystallographic Studies of 4j. Colorless crystals of **4j** suitable for X-ray analysis were obtained by recrystallization from CH_2Cl_2 –*n*-hexane. The single crystal was sealed in a Pyrex glass capillary under N_2 atmosphere and used for data collection. All measurements were made on a Rigaku RAXIS imaging plate area detector with graphite monochromated Mo- $\text{K}\alpha$ radiation. Details of crystal and data collection parameters are summarized in Table S2. The positions of non-hydrogen atoms were determined by direct methods (SIR97) and subsequent Fourier syntheses (DIRDIF PATTY). An ORTEP drawing of **4j** is shown in Figure S2.

Table S2. Crystallographic Data for **4j**.

formula	C ₁₃ H ₁₀ O ₃
formula weigh	214.22
cryst size (mm ³)	1.20 x 0.60 x 0.10
cryst system	orthorhombic
space group	Iba2 (#45)
cryst color	colorless
<i>a</i> (Å)	16.5752(2)
<i>b</i> (Å)	17.3959(1)
<i>c</i> (Å)	7.3023(1)
<i>V</i> (Å ³)	2105.55(3)
<i>Z</i>	8
<i>d</i> _{calc} (g cm ⁻³)	1.351
<i>F</i> (000)	896.00
<i>μ</i> _{calc} (cm ⁻¹)	0.96
no. of unique data	1314
no. of data used (<i>I</i> > 3σ(<i>I</i>))	757
no. of params refined	120
<i>R</i> ^a	0.058
<i>R</i> _w ^b	0.055
goodness of fit indicator	0.20
maximum residuals (e Å ⁻³)	0.34

^a $R = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$.

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

Figure S2. Crystal structure of **4j**.