Supporting Information 1

Rh(I)-Catalyzed Carbonylative Arylation of Alkynes with Arylboronic Acids using Formaldehyde as a Carbonyl Source

Chuang Wang, a Tsumoru Morimoto, *,a Hiroyuki Kanashiro, a Hiroki Tanimoto, a Yasuhiro Nishiyama, a Kiyomi Kakiuchi, a and Levent Artok b

a Graduate School of Materials Science, Nara Institute of Science and Technology (NAIST)
Ikoma, Nara 630-0101, Japan

b Department of Chemistry, Faculty of Science, Izmir Institute of Technology,
Urla 35430, Izmir, Turkey

E-mail: morimoto@ms.naist.jp
General Information.

$^1$H NMR and $^{13}$C NMR were recorded on a JEOL JNM-ECP500 spectrometer in CDCl$_3$ using tetramethylsilane (0 ppm) as an internal standard. Data are reported as follows: chemical shift in ppm (δ), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, and m = multiplet), coupling constant (Hz), integration, and interpretation. Infrared spectra (IR) were obtained on a JASCO FT/IR-420 spectrometer; Mass spectra were obtained on a JEOL JMS-700. Column chromatography was performed using a SiO$_2$ (MERCK Silica gel 60).

Materials.

[RhCl(cod)]$_2$ was prepared using the reported method. $^{1}$ 2,2'-Bis(diphenylphosphino)biphenyl (BIPHEP) was purchased by STREM CHEMICALS, INC. and used directly without further purification. 1,2-diphenylethyne (1a) was purchased by Tokyo Chemical Industry Co., Ltd. and used directly without further purification. Oct-4-yne (1d), Prop-1-yn-1-ylbenzene (1e) and aryloboronic acids (2) were purchased by Wako Pure Chemical Industries, Ltd. and used directly without further purification. Paraformaldehyde was purchased by Wako Pure Chemical Industries, Ltd. and dried with P$_2$O$_5$ under vacuum prior to use. 1, 4-dioxane dehydrated was purchased by Wako Pure Chemical Industries, Ltd. and dried with 4A molecular sieve, which was degassed using freeze-pump-thaw method for 3 times and stored in glove box.

Synthesis of starting materials: (1b) and (1c).

\[
\begin{align*}
\text{MeC-} & \equiv \circlearrowleft \equiv \text{OMe} & \text{F}_3\text{C-} & \equiv \circlearrowleft \equiv \text{CF}_3 \\
1b & & 1c
\end{align*}
\]

1,2-Bis(4-methoxyphenyl)ethyne (1b), 1,2-bis(4-(trifluoromethyl)phenyl)ethyne (1c) were synthesized from the commercially available starting materials according to a general procedure.$^2$
PPh₃ (3.0 equiv.) was added to a solution of CBr₄ (1.5 equiv.) in CH₂Cl₂ at 0°C, and subsequently stirred for 15 min. A solution of the aldehyde (0.1 mol) in CH₂Cl₂ was added dropwise over 3 min and the mixture was stirred for an additional 30 min. The solvent was then removed under reduced pressure and a mixture of hexane/AcOEt (1:1) was added. The resulting mixture was filtered through a plug of silica. After the filtration, the silica plug was washed several times with hexane/AcOEt (1:1). The solvent of the combined filtrate was evaporated. A mixture of hexane/AcOEt (5:1) was added to the solid residue. The resulting solution was filtered again through a plug of silica to remove triphenylphosphine oxide and the solvent was removed under reduced pressure to yield dibromo-olefins.

Dibromo-olefin (0.1 mol) was then dissolved in dry THF and cooled to -78°C under N₂. n-BuLi (4.0 equiv.) was added dropwise over 30 min and the solution was stirred at -78°C for 2h, followed by the addition of 100 mL saturated NH₄Cl solution, and warmed to room temperature. The two layers were separated and the aqueous phase was extracted with ether. The combined organic phase was washed with brine, dried over MgSO₄, filtered and concentrated. The residue was purified by flash chromatography (hexane/AcOEt).

Sonogashira coupling reaction: desired terminal alkyne and 1-iodo-4-methoxybenzene or 1-iodo-4-(trifluoromethyl)benzene (mole ratio: 1.2:1) were dissolved in pre-dried Et₂NH at r.t. under N₂. Subsequently, Pd(PPh₃)₄ (5 mol%)
and CuI (10 mol%) were then added in the mixture under N₂ which was stirred under reflux. The resulting precipitate was filtered over silica. The solvent was removed and the residue was purified by column chromatography on silica to give relevant internal alkyne in 85% yield as white solid (hexane/AcOEt as the eluent).

**Synthesis of starting material: hex-1-yn-1-ylbenzene (1f).**

![1f](image)

Sonogashira coupling reaction: hex-1-yne and iodobenzene (mole ratio: 1.2:1) were dissolved in pre-dried Et₂NH at r.t. under N₂. Subsequently, Pd(PPh₃)₄ (5 mol%) and CuI (10 mol%) were then added in the mixture under N₂ which was stirred under reflux. The resulting reaction mixture was filtered over silica. The solvent was removed and the residue was purified by column chromatography on silica to give relevant internal alkyne in 92% yield as colorless liquid (hexane as the eluent).

**Typical Procedure for the Rh(I)-Catalyzed Carbonylative Arylation of Alkyne 1a with phenylboronic acid 2a in the presence of formaldehyde (Table 1, entry 2).**

In a 10mL screw-capped vial were placed [RhCl(cod)]₂ (24.6 mg, 0.05 mmol), BIPHEP (5.3 mg, 0.01 mmol), diphenylacetylene (1a) (178.2 mg, 1 mmol), phenylboronic acid (2a) (243.9 mg, 2 mmol), paraformaldehyde (150.2 mg, 5 mmol) and 1,4-dioxane (1 mL). The mixture was degassed by three freeze-pump-thaw cycles and sealed under N₂. The mixture was stirred at 80 °C for 20 h, cooled to room temperature and then concentrated in vacuo. The residue was purified by flash chromatography on silica gel to give the mixture of (E) and (Z)-3aa (176.0 mg, 0.62 mmol, R₇ 0.14 and 0.20, hexane/AcOEt = 30/1) in 62% yield as white solid.
**E/Z-Isomerization Attempts under the Catalytic Conditions.**

Each of \((E)-\) and \((Z)-3\text{aa}\) isolated in pure form was introduced into the reactions of \(p\)-methoxyphenylboronic acid \((2b)\) and alkyne \(1a\) under the standard conditions (Scheme 2). Each reaction gave the product \(3\text{ab}\) in almost the same yields and ratios. \(3\text{aa}\) was obtained in the same \(E/Z\)-ratio \((E/Z = 32/68)\) in each case and that they are also same as that of the reaction in the entry 2 of Table 1.

\[
1a + 2b \quad (2 \text{ equiv}) \quad \text{Ph} \quad \text{O} \quad \text{Ph} \\
(\text{E})-3\text{aa} \quad (0.3 \text{ equiv}) \quad (E/Z = \geq 99/1) \quad \rightarrow \quad 3\text{ab} \quad 78\% \quad (E/Z = 24/76) \quad \text{Ph} \quad \text{O} \quad \text{Ph} \\
+ \quad \text{Ph} \quad \text{O} \quad \text{Ph} \\
(\text{Z})-3\text{aa} \quad (0.3 \text{ equiv}) \quad (E/Z = 1/\geq 99) \quad \rightarrow \quad 3\text{ab} \quad 79\% \quad (E/Z = 24/76) \quad \text{Ph} \quad \text{O} \quad \text{Ph} \\
3\text{aa} \quad \geq 99\% \quad (E/Z = 32/68) \\
\]

**Scheme S1-1**   \(E/Z\)-Isomerization under Reaction Conditions

**E/Z-Isomerization Attempts Using RhH(CO)(PPh₃)₃ as a Catalyst.**

The reaction of \((E)-\) and \((Z)-3\text{aa}\) isolated in pure form in the presence of a catalytic amount of RhH(CO)(PPh₃)₃ in dioxane at 80 °C for 20 h gave a \(E/Z\)-mixture of \(3\text{aa}\) quantitative yield in a similar ratio, \(E/Z = 36/64\) and 34/66, respectively.

\[
\text{(E)-3aa} \quad (0.3 \text{ equiv}) \quad (E/Z = \geq 99/1) \quad \rightarrow \quad 3\text{aa} \quad \geq 99\% \quad (E/Z = 30/64) \\
\text{(Z)-3aa} \quad (0.3 \text{ equiv}) \quad (E/Z = 1/\geq 99) \quad \rightarrow \quad 3\text{aa} \quad \geq 99\% \quad (E/Z = 34/66) \\
\]

**Scheme S1-2**   \(E/Z\)-Isomerization Reactions Catalyzed by RhH(CO)(PPh₃)₃
1,2-Bis(4-methoxyphenyl)ethyne (1b).

![Image](image1.png)

Colorless solid; 140.8-142.2 °C; \( R_f \) 0.15; (hexane/AcOEt = 10/1); \(^1\)H NMR (500 MHz, CDCl\(_3\)) \( \delta \): 3.83 (s, 6H), 6.86-6.89 (m, 4H), 7.44-7.47 (m, 4H); \(^{13}\)C NMR (125 MHz, CDCl\(_3\)) \( \delta \): 55.3, 87.9, 113.9, 115.6, 132.8, 159.3; IR (neat, cm\(^{-1}\)) 2965, 2837, 1606, 1566, 1518, 1457, 1440, 1302, 1285, 1171, 1024, 834; MS (EI): \( m/z \) (%): 238 (99) \([M^+\]), 223 (65), 195 (25), 180 (8), 152 (15), 119 (5), 83 (5); HRMS: \( m/z \) calcd \([M^+\]): 238.0994, found 238.0994.

1,2-Bis(4-(trifluoromethyl)phenyl)ethyne (1c).

![Image](image2.png)

Colorless solid; 106.2-107.0 °C; \( R_f \) 0.44; (hexane); \(^1\)H NMR (500 MHz, CDCl\(_3\)) \( \delta \): 7.63-7.67 (m, 8H); \(^{13}\)C NMR (125 MHz, CDCl\(_3\)) \( \delta \): 90.1, 123.8 (q, \( J_{C-F} = 270.6 \) Hz), 125.4 (q, \( J_{C-F} = 3.6 \) Hz), 126.3, 130.4 (q, \( J_{C-F} = 32.3 \) Hz), 132.0; IR (neat, cm\(^{-1}\)) 2918, 2850, 1614, 1406, 1332, 1173, 1135, 1067, 1018, 840; MS (EI): \( m/z \) (%): 314 (99) \([M^+\]), 295 (25), 264 (15), 245 (6), 225 (8), 194 (5), 176 (5), 107 (5), 75 (2); HRMS: \( m/z \) calcd \([M^+\]): 314.0530, found 314.0529.

Hex-1-yn-1-ylbenzene (1f).

![Image](image3.png)

Colorless liquid; \( R_f \) 0.38 (hexane); \(^1\)H NMR (500 MHz, CDCl\(_3\)) \( \delta \): 0.95 (t, \( J = 7.5 \) Hz 3H), 1.44-1.52 (m, 2H), 1.55-1.62 (m, 2H), 2.41 (t, \( J = 7.0 \) Hz 2H), 7.25-7.29 (m, 3H), 7.38-7.40 (m, 2H); \(^{13}\)C NMR (125 MHz, CDCl\(_3\)) \( \delta \): 13.6, 19.1, 22.0, 30.8, 80.5,
90.3, 124.0, 127.4, 128.1, 131.5; IR (neat, cm\(^{-1}\)) 2957, 2932, 2871, 2231, 1598, 1489, 1441, 1069, 912, 754, 691; MS (EI): \(m/z\) (%) = 159 (M\(^{+}\), 12), 158 (M\(^{+}\), 99), 143 (92), 115 (63), 102 (10), 89 (9), 63 (7), 51 (3); HRMS: \(m/z\) calcd [M\(^{+}\)]: 158.1096, found 158.1095.

*(Z)-1,2,3-Triphenyl-2-propen-1-one ((Z)-3aa).*

![Chemical Structure](image)

Colorless solid; mp 85.0-86.7 °C; \(R_f\) 0.20 (hexane/AcOEt = 30/1); \(^1\)H NMR (500 MHz, CDCl\(_3\)) \(\delta\): 7.14-7.21 (m, 4H), 7.29-7.32 (m, 3H), 7.34-7.38 (m, 4H), 7.46-7.50 (m, 3H), 7.99 (d, \(J = 7.5\) Hz, 2H); \(^{13}\)C NMR (125 MHz, CDCl\(_3\)) \(\delta\): 126.3, 128.0, 128.1, 128.4, 128.7, 128.7, 128.8, 129.6, 130.0, 133.6, 135.3, 136.2, 137.9, 140.7, 199.3; IR (neat, cm\(^{-1}\)) 3057, 3025, 2924, 2359, 1666 (C=O), 1596, 1579, 1448, 1224; MS (EI): \(m/z\) (%) = 284 (100) [M\(^{+}\)], 283 (21), 206 (12), 179 (35), 178 (53), 167 (18), 105 (82), 77 (42), 60 (11), 57 (15), 55 (11); HRMS: \(m/z\) calcd [M\(^{+}\)]: 284.1201, found 284.1201.

Crystallographic data for (Z)-3aa is as follows: \(C_{21}H_{16}O\), \(Mr = 284.36\), colorless, block, \(0.180 \times 0.090 \times 0.080\) mm, monoclinic, Primitive, \(a = 9.4396(2)\) Å, \(b = 11.0396(2)\) Å, \(c = 14.6225(3)\) Å, \(\beta = 91.1326(7)\) °, \(V = 1523.50(5)\) Å\(^3\), \(Z = 4\), \(\rho_c = 1.240\) g/cm\(^3\), \(\mu = 0.745\) cm\(^{-1}\), \(T = 123\) K, \(\lambda = 0.71075\) Å, 25829 reflections, 3490 unique \([R(int) = 0.0271]\), Final \(GoF = 1.084\), \(R_1 = 0.0725\) ([\(I > 2.00\sigma(I)\)], w\(R_2 = 0.1876\) (all data). CCDC No.: 982719.
**Figure 1.** ORTEP representation of (Z)-3aa (50% thermal ellipsoids)

$(E)$-1,2,3-Triphenyl-2-propen-1-one ($(E)$-3aa).

Colorless solid; mp 100.1–101.2 °C; $R_f$ 0.14 (hexane/AcOEt = 30/1); $^1$H NMR (500 MHz, CDCl$_3$) δ: 7.09 (d, $J = 7.5$ Hz, 2H), 7.16–7.23 (m, 4H), 7.27–7.29 (m, 2H), 7.33–7.36 (m, 3H) 7.45 (t, $J = 8.0$ Hz, 2H), 7.54 (t, $J = 7.0$, 1H), 7.86 (d, $J = 7.0$ Hz, 2H); $^{13}$C NMR (125 MHz, CDCl$_3$) δ: 127.9, 128.2, 128.3, 128.8, 128.9, 129.6, 129.8, 130.3, 132.1, 134.7, 136.5, 138.1, 140.2, 140.7, 197.6; IR (neat, cm$^{-1}$) 3047, 3021, 1644 (C=O), 1595, 1576, 1444, 1250; MS (EI): $m/z$ (%) = 284 (87) [M$^+$], 283 (33), 207 (13), 206 (20), 180 (10), 179 (60), 178 (82), 167 (32), 152 (15), 105 (100), 77 (60), 51 (14); HRMS: $m/z$ calcd [M$^+$]: 284.1201, found 284.1200.

Crystallographic data for $(E)$-3aa is as follows: C$_{21}$H$_{16}$O, $Mr = 284.36$, colorless, block, 0.210 × 0.110 × 0.100 mm, monoclinic, Primitive, $a = 13.5721(3)$ Å, $b = 5.7294(1)$ Å, $c = 18.9083(4)$ Å, $\beta = 93.4163(7)$ °, $V = 1467.68(5)$ Å$^3$, $Z = 4$, $\rho_c = 1.287$ g/cm$^3$, $\mu = 0.773$ cm$^{-1}$, $T = 123$ K, $\lambda = 0.71075$ Å, 13939 reflections, 3367 unique [$R$(int) = 0.0187], Final $GoF = 1.134$, $R_1 = 0.0449$ ([I > 2.00σ(I)], w$R_2 = 0.1174$ (all data). CCDC No.: 982715.
Figure 2. ORTEP representation of \((E)-3aa\) (50% thermal ellipsoids)

Triphenylethylene ((\(E\))-4aa).

\[
\text{Ph} = \text{Ph} = \text{Ph}
\]

((\(E\))-4aa)

Colorless oil; \(R_f\) 0.31 (hexane); \(^1\)H NMR (500 MHz, CDCl\(_3\)) \(\delta\): 6.99 (s, 2H), 7.04–7.07 (m, 2H), 7.11–7.17 (m, 3H), 7.20–7.25 (m, 2H), 7.26–7.38 (m, 8H); \(^1\)C NMR (125 MHz, CDCl\(_3\)) \(\delta\): 126.7, 127.4, 127.5, 127.6, 127.9, 128.1, 128.2, 128.6, 129.5, 130.4, 137.4, 140.3, 142.6, 143.4; IR (neat, cm\(^{-1}\)) 3021, 1716, 1540, 1507, 1489, 1445, 1075, 1029, 760, 694, 588; MS (El): \(m/z\) (\%) = 257 (23) [M+1\(^+\)], 256 (100) [M\(^+\)], 255 (25), 241(11), 215 (5), 178 (26), 165 (9), 135 (12), 83(4), 69 (7), 57(10); HRMS: \(m/z\) calcd [M\(^+\)]: 256.1252, found 256.1252.

Products of Deuterium-Labelling Experiments.

((\(Z\))-1,2,3-Triphenyl-2-propen-1-one ((\(Z\))-3aa). (See S2-14 in the Supporting Information 2)
(E)-1,2,3-Triphenyl-2-propen-1-one ((E)-3aa). (See S2-15 in the Supporting Information 2)

(E)-1,2,3-Triphenyl-2-propen-1-one ((E)-3aa).

(See S2-16 in the Supporting Information 2)

(E)-1,2,3-Triphenyl-2-propen-1-one ((E)-3aa). (See S2-17 in the Supporting Information 2)
$^1$H NMR (500 MHz, CDCl$_3$) $\delta$: 7.09 (d, $J = 7.5$ Hz, 2H), 7.16–7.23 (m, 4H), 7.27–7.29 (m, 2H), 7.33–7.36 (m, 3H) 7.45 (t, $J = 8.0$ Hz, 2H), 7.54 (t, $J = 7.0$, 1H), 7.86 (d, $J = 7.0$ Hz, 2H).

(Z)-1-(p-Methoxyphenyl)-2,3-diphenyl-2-propen-1-one ((Z)-3ab).

Colorless solid; 88.5-89.9 °C; $R_f$ 0.18 (hexane/AcOEt = 20/1). $^1$H NMR (500 MHz, CDCl$_3$) $\delta$: 3.80 (s, 3H), 6.83 (d, $J = 8.5$, 2H), 7.13–7.22 (m, 4H), 7.27–7.36 (m, 5H), 7.47 (d, $J = 8.0$, 2H), 7.97 (d, $J = 8.5$, 2H); $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$: 55.3, 114.0, 126.2, 127.9, 128.1, 128.4, 128.8, 129.4, 129.5, 132.0, 135.4, 138.1, 140.9, 163.9, 197.8; IR (neat, cm$^{-1}$) 3056, 3026, 2932, 2839, 1658 (C=O), 1652, 1595, 1575, 1508, 1258, 1235, 1164; MS (EI): $m/z$ (%) = 316 (27) [M+2$^+$], 315 (68) [M+1$^+$], 314 (100) [M$^-$], 286 (38), 236 (21), 198 (21), 197 (62), 179 (55), 178 (68), 177 (47), 176 (52), 152 (41), 136 (56), 135 (100), 107 (52), 92 (57), 85 (31), 83 (47), 77 (60), 64 (26), 51 (23); HRMS: $m/z$ calcd [M$^+$]: 314.1307, found 314.1308.

Crystallographic data for (Z)-3ab is as follows: C$_{22}$H$_{18}$O$_2$, $M_r$ = 314.38, colorless, block, 0.150 x 0.110 x 0.080 mm, monoclinic, Primitive, $a = 5.9337(3)$ Å, $b =$ 16.7259(8) Å, $c = 16.9156(7)$ Å, $\beta = 101.092(1)$ °, $V = 1647.5(2)$ Å$^3$, $Z = 4$, $\rho_c = 1.267$ g/cm$^3$, $\mu = 0.798$ cm$^{-1}$, $T = 123$ K, $\lambda = 0.71075$ Å, 16055 reflections, 3768 unique [$R$(int) = 0.0298), Final $GoF = 1.055$, $R_1 = 0.0584$ ([I > 2.00σ(I)]), $wR_2 = 0.1392$ (all data). CCDC No.: 982709.
Figure 3. ORTEP representation of (Z)-3ab (50% thermal ellipsoids).

$$(E)-1-(p\text{-Methoxyphenyl})\text{-2,3-diphenyl-2-propen-1-one (}(E)\text{-3ab}).$$

Colorless oil; $R_f$ 0.18 (hexane/AcOEt = 20/1); $^1$H NMR (500 MHz, CDCl$_3$) $\delta$: 3.87 (s, 3H), 6.92 (d, $J = 8.5$, 2H), 7.11 (d, $J = 7.5$ Hz, 2H), 7.14 (s, 1H), 7.15–7.24 (m, 3H), 7.27–7.37 (m, 5H), 7.90 (d, $J = 8.5$, 2H); $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$: 55.5, 113.6, 127.9, 128.2, 128.6, 128.8, 129.5, 130.2, 130.4, 132.3, 135.0, 136.8, 137.8, 141.0, 163.1, 196.3; IR (neat, cm$^{-1}$) 3056, 2931, 2838, 1646 (C=O), 1599, 1574, 1312, 1508, 1253, 1166, 1027; MS (EI): $m/z$ (%) = 316 (21) [M+2$^+$], 315 (70) [M+1$^+$], 314 (96) [M$^+$], 286 (25), 236 (22), 221 (17), 198 (18), 197 (63), 179 (57), 178 (76), 177 (37), 176 (48), 152 (33), 151 (22), 149 (34), 136 (56), 135 (100), 107 (50), 92 (53), 86 (60), 84 (71), 77 (65), 57 (52); HRMS: $m/z$ calcd [M$^+$]: 314.1307, found 314.1305.

$$(Z)-1-(p\text{-Methylphenyl})\text{-2,3-diphenyl-2-propen-1-one ((}(Z)\text{-3ac}).$$
Colorless oil; \( R_f \) 0.18 (hexane/AcOEt = 30/1); \(^1\)H NMR (500 MHz, CDCl\(_3\)) \( \delta \): 2.33 (s, 3H), 7.12–7.21 (m, 6H), 7.26–7.36 (m, 5H), 7.46 (d, \( J = 7.5 \), 2H), 7.89 (d, \( J = 8.5 \), 2H); \(^1^3\)C NMR (125 MHz, CDCl\(_3\)) \( \delta \): 21.7, 126.3, 127.9, 128.1, 128.4, 128.8, 129.5, 129.7, 129.9, 133.9, 135.4, 138.1, 140.9, 144.6, 199.0; IR (neat, cm\(^{-1}\)) 3056, 3025, 1663 (C=O), 1605, 1492, 1448, 1227, 1174; MS (EI): \( m/z \) (%) = 299 (12) [M+1\(^+\)], 298 (52) [M\(^+\)], 179 (12), 178 (28), 119 (100), 91 (39), 65 (13); HRMS: \( m/z \) calcd [M\(^+\)]: 298.1358, found 298.1357.

\( (E)-1-(p\text{-Methylphenyl})-2,3\text{-diphenyl-2-propen-1-one ((E)-3ac).} \)

Colorless solid; mp 88.1–89.3 °C; \( R_f \) 0.14 (hexane/AcOEt = 30/1); \(^1\)H NMR (500 MHz, CDCl\(_3\)) \( \delta \): 2.41 (s, 3H), 7.09 (d, \( J = 6.5 \), 2H), 7.15–7.37 (m, 11H), 7.79 (d, \( J = 8.5 \), 2H); \(^1^3\)C NMR (125 MHz, CDCl\(_3\)) \( \delta \): 21.6, 127.8 128.2, 128.7, 128.7, 129.0, 129.6, 130.0, 130.2, 134.9, 135.3, 136.6, 139.1, 140.9, 143.0, 197.3; IR (neat, cm\(^{-1}\)) 3044, 1644 (C=O), 1605, 1494, 1448, 1381, 1318, 1264, 1181, 1064; MS (EI): \( m/z \) (%) = 299 (53) [M+1\(^+\)], 298 (71) [M\(^+\)], 297 (25), 236 (35), 221 (43), 220 (40), 182 (27), 181 (61), 180 (26), 179 (63), 178 (87), 177 (52), 176 (51), 152 (62), 151 (53), 119 (100); HRMS: \( m/z \) calcd [M\(^+\)]: 298.1358, found 298.1357.

Crystallographic data for \( (E)-3ac \) is as follows: \( C_{22}H_{18}O \), \( Mr = 298.38 \), colorless, block, 0.180 \( \times \) 0.140 \( \times \) 0.120 mm, orthorhombic, Primitive, \( a = 5.5301(2) \) Å, \( b = 8.0317(2) \) Å, \( c = 37.0417(7) \) Å, \( V = 1645.25(7) \) Å\(^3\), \( Z = 4 \), \( \rho_c = 1.205 \) g/cm\(^3\), \( \mu = 0.721 \)
cm⁻¹, $T = 123$ K, $\lambda = 0.71075$ Å, 28474 reflections, 3773 unique [$R$(int) = 0.0286), Final $GoF = 1.112$, $R_1 = 0.0609 ([I > 2.00\sigma(I)])$, $wR_2 = 0.1478$ (all data). CCDC No.: 982708.

Figure 4. ORTEP representation of ($E$)-3ac (50% thermal ellipsoids)

(1-(p-Tolyl)-ethene-1,2-diyldibenzene ((E)-4ac).

Colorless oil; $Rf$: 0.32 (Hexane); $^1$H NMR (500 MHz, CDCl₃) $\delta$: 2.35 (s, 3H), 6.94 (s, 1H), 7.01 (d, $J = 8$ Hz, 2H), 7.10-7.12 (m, 5H), 7.19-7.22 (m, 4H), 7.31-7.33 (m, 3H); $^{13}$C NMR (125 MHz, CDCl₃) $\delta$: 21.12, 126.6, 127.5, 127.9, 128.9, 129.5, 130.3, 137.4, 137.5, 140.5, 142.4; IR (neat, cm⁻¹) 3020, 1707, 1596, 1509, 1444, 1217, 1028, 862, 811, 755, 695, 632, 586, 511; MS (EI): $m/z$ (%): 271 (22) [M+1⁺], 270 (100) [M⁺], 269 (12), 255 (25), 178 (40), 126 (16), 83 (20), 51 (13); HRMS: $m/z$ calcd [M⁺]: 270.1409, found 270.1407.

(Z)-1-(p-Chlorophenyl)-2,3-diphenyl-2-propen-1-one ((Z)-3ad).
Colorless solid; mp 104.3-105.6 °C; $R_f$ 0.31 (hexane/AcOEt = 20/1); $^1$H NMR (500 MHz, CDCl$_3$) $\delta$: 7.14–7.21 (m, 4H), 7.24–7.37 (m, 7H), 7.44 (d, $J = 8.0$ Hz, 2H), 7.91 (d, $J = 7.5$ Hz, 2H); $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$: 126.3, 128.2, 128.3, 128.5, 128.8, 128.9, 129.1, 130.4, 131.0, 134.7, 135.2, 137.7, 140.1, 140.3, 198.1; IR (neat, cm$^{-1}$) 3082, 3057, 3023, 1663 (C=O), 1596, 1584, 1494, 1450, 1401, 1223, 1176, 1090, 1011; MS (EI): $m/z$ (%) = 321 (10) [M+3$^+$], 320 (44) [M+2$^+$], 319 (42) [M+1$^+$], 318 (100) [M$^+$], 317 (32), 283 (47), 206 (12), 179 (38), 178 (48), 139 (50), 111 (16). HRMS: $m/z$ calcd [M$^+$]: 318.0811, found 318.0810.

Crystallographic data for (Z)-3ad is as follows: C$_{21}$H$_{15}$ClO, Mr = 318.80, colorless, block, 0.180 × 0.080 × 0.070 mm, monoclinic, Primitive; $a = 5.8633(2)$ Å, $b = 16.0703(4)$ Å, $c = 17.1381(4)$ Å, $\beta = 101.1664(7)$ $^\circ$, $V = 1584.27(6)$ Å$^3$, $Z = 4$, $\rho_c = 1.336$ g/cm$^3$, $\mu = 2.424$ cm$^{-1}$, $T = 123$ K, $\lambda = 0.71075$ Å, 15557 reflections, 3631 unique [$R$(int) = 0.0244), Final $GoF = 1.137$, $R_1 = 0.0524$ ([I > 2.00$\sigma$(I)], $wR_2 = 0.1284$ (all data). CCDC No.: 982713.

Figure 5. ORTEP representation of (Z)-3ad (50% thermal ellipsoids)
(E)-1-(p-Chlorophenyl)-2,3-diphenyl-2-propen-1-one ((E)-3ad).

![Chemical Structure](image)

Colorless solid; mp 89.3-90.1 °C; Rf 0.26 (hexane/AcOEt = 20/1); $^1$H NMR (500 MHz, CDCl$_3$) δ: 7.09 (d, J = 7.0 Hz, 2H), 7.19 (t, J = 7.5 Hz, 2H), 7.20–7.27 (m, 4H), 7.31–7.37 (m, 3H), 7.40 (d, J = 7.5 Hz, 2H), 7.78 (d, J = 8.0 Hz, 2H); $^{13}$C NMR (125 MHz, CDCl$_3$) δ: 128.0, 128.3, 128.6, 128.8, 129.1, 129.6, 130.4, 131.1, 134.6, 136.2, 136.4, 138.5, 140.2, 140.4, 196.3; IR (neat, cm$^{-1}$) 3054, 3025, 1647 (C=O), 1592, 1443, 1257, 1087, 1013; MS (EI): m/z (%) = 321 (10) [M+3$^+$], 320 (48) [M+2$^+$], 319 (44) [M+1$^+$], 318 (M$^+$, 100), 317 (37), 283 (57), 201 (12), 180 (12), 179 (72), 178 (79), 177 (13), 176 (16), 152 (14), 141 (24), 139 (77), 111 (19). HRMS: m/z calcd [M$^+$]: 318.0811, found 318.0810.

Crystallographic data for (E)-3ad is as follows: C$_{21}$H$_{15}$ClO, Mr = 318.80, colorless, block, 0.160 × 0.100 × 0.040 mm, monoclinic, Primitive, a = 13.9308(7) Å, b = 5.7298(3) Å, c = 20.307(1) Å, β = 102.919(1)°, V = 1579.9(2) Å$^3$, Z = 4, $\rho_c$ = 1.340 g/cm$^3$, $\mu$ = 2.430 cm$^{-1}$, $T$ = 123 K, $\lambda$ = 0.71075 Å, 14900 reflections, 3633 unique [R(int) = 0.0315], Final GoF = 1.139, $R_1$ = 0.0527 ([I > 2.00σ(I)]), wR$_2$ = 0.1562 (all data). CCDC No.: 982711.

**Figure 6.** ORTEP representation of (E)-3ad (50% thermal ellipsoids)
(1-(4-Chlorophenyl)ethene-1,2-diyl) dibenzene ((E)-4ad).

![Structure Image]

Colorless oil; \( R_f \) 0.36 (Hexane); \(^1\)H NMR (500 MHz, CDCl\(_3\)) \( \delta \): 6.94 (s, 1H), 7.01-7.02 (m, 2H), 7.11-7.12 (m, 3H), 7.17-7.18 (m, 2H), 7.25-7.28 (m, 4H), 7.32-7.34 (m, 3H); \(^{13}\)C NMR (125 MHz, CDCl\(_3\)) \( \delta \): 126.5, 126.9, 127.6, 128.0, 128.3, 130.0, 130.3, 133.3, 137.0, 139.9, 141.4, 141.9; IR (neat, cm\(^{-1}\)) 3021, 1490, 1444, 1420, 1091, 1012, 818, 775, 757, 695, 515; MS (EI): \( m/z \) (%) = 292 (32) \([\text{M}+2^+]\), 291 (25) \([\text{M}+1^+]\), 290 (99) \([\text{M}^-\]), 253 (21), 178 (29), 126 (11), 77 (6), 51 (8); HRMS: \( m/z \) calcd [\( \text{M}^-\)]: 290.0862, found 290.0860.

(Z)-2,3-Diphenyl-1-(p-trifluorophenylphenyl)-2-propen-1-one ((Z)-3ae).

![Structure Image]

Colorless solid; mp 105.3–107.2 °C; \( R_f \) 0.26 (hexane/AcOEt = 30/1); \(^1\)H NMR (500 MHz, CDCl\(_3\)) \( \delta \): 7.14–7.22 (m, 3H), 7.24–7.28 (m, 3H), 7.29–7.39 (m, 3H), 7.44 (d, \( J = 7.5 \), 2H), 7.61 (d, \( J = 8.5 \) Hz, 2H), 8.07 (d, \( J = 8.0 \), 2H); \(^{13}\)C NMR (125 MHz, CDCl\(_3\)) \( \delta \): 123.5 (q, \( 1J_{\text{C-F}}= 273 \) Hz), 125.8 (q, \( 3J_{\text{C-F}}= 3.8 \) Hz), 126.4, 128.4, 128.5, 128.6, 128.8, 129.0, 129.9, 131.0, 134.6 (q, \( 2J_{\text{C-F}} = 32.6 \) Hz), 135.1, 131.5, 138.9, 140.2, 198.3; IR (neat, cm\(^{-1}\)) 3069, 1672 (C=O), 1580, 1497, 1450, 1412, 1325, 1228, 1170, 1124, 1067, 1015; MS (EI): \( m/z \) (%) = 353 (15) \([\text{M}+1^+]\), 352 (57) \([\text{M}^-\]), 351 (21), 219 (10), 207 (12), 181 (12), 180 (16), 179 (95), 178 (100), 177 (43), 176 (35), 175 (11), 174 (11), 173 (63), 152 (26), 151 (19), 146 (11), 145 (67), 133 (40), 131 (21) 126 (15), 125 (16), 121 (11), 119 (21), 103 (28), 102 (22), 101 (24), 95 (20), 89 (45), 88 (42), 87 (43), 77 (25), 75
(35) 73 (41), 72 (20), 69 (41), 59 (41), 58 (36), 57 (29); HRMS: m/z calcd [M+]: 352.1075, found 352.1076.

Crystallographic data for (Z)-3ae is as follows: C_{22}H_{15}F_{3}O, M_r = 352.36, colorless, block, 0.190 \times 0.180 \times 0.170 \text{ mm}, monoclinic, C-centered, a = 26.3108(9) Å, b = 8.0797(3) Å, c = 17.2065(5) Å, \beta = 110.2319(9) \degree, V = 3432.1(2) Å³, Z = 8, \rho_c = 1.364 g/cm³, \mu = 1.046 cm⁻¹, T = 123 K, \lambda = 0.71075 Å, 16564 reflections, 3934 unique [R(int) = 0.0230), Final GoF = 1.104, R₁ = 0.0610 ([I > 2.00σ(I)], wR₂ = 0.1563 (all data). CCDC No.: 982710.

Figure 7. ORTEP representation of (Z)-3ae (50% thermal ellipsoids)

\[(E)-2,3\text{-Diphenyl-1-(p-trifluorophenylphenyl)-2-propen-1-one (}(E)-3ae).\]

Colorless solid; mp 116.1-117.2 °C; R_f 0.17 (hexane/AcOEt = 30/1); $^1$H NMR (500 MHz, CDCl₃) δ: 7.09 (d, J = 8.0, 2H), 7.16–7.21 (m, 2H), 7.22–7.28 (m, 4H), 7.33–7.40 (m, 3H), 7.70 (d, J = 8.0, 2H), 7.91 (d, J = 8.0, 2H); $^{13}$C NMR (125 MHz, CDCl₃) δ: 123.7 (q, $^1$J_C-F = 273 Hz), 125.3 (q, $^2$J_C-F = 1.5 Hz), 128.2, 128.3, 128.8, 128.9, 129.4, 129.6, 129.8, 130.5, 133.3 (q, $^2$J_C-F = 32.6 Hz), 134.4, 135.9, 140.3, 141.5, 141.9, 196.4; IR (neat, cm⁻¹) 3052, 1650 (C=O), 1493, 1443, 1405, 1332, 1255, 1167, 1142, 1108,
1069, 1016; MS (EI): m/z (%) = 353 (11) [M+1⁺], 352 (36) [M⁺], 351 (11), 341 (11), 295 (12), 257 (13), 256 (16), 255 (12), 237 (15), 236 (32), 221 (26), 180 (19), 179 (71), 178 (86), 177 (22), 176 (21), 173 (45), 152 (38), 149 (31), 145 (51), 137 (71), 136 (49), 127 (53), 125 (50), 121 (52), 109 (53), 95 (100), 82 (85), 57 (80); HRMS: m/z calcd [M⁺]: 352.1075, found 352.1072.

Crystallographic data for (E)-3ae is as follows: C$_{22}$H$_{15}$F$_3$O, $M_r$ = 352.36, colorless, platelet, 0.140 × 0.050 × 0.010 mm, monoclinic, Primitive, $a = 5.7547(4)$ Å, $b = 8.6681(6)$ Å, $c = 34.026(3)$ Å, $\beta = 91.207(2)$ °, $V = 1696.9(2)$ Å$^3$, $Z = 4$, $\rho_c = 1.379$ g/cm$^3$, $\mu = 1.058$ cm$^{-1}$, $T = 123$ K, $\lambda = 0.71075$ Å, 23005 reflections, 3097 unique [$R$(int) = 0.1235), Final GoF = 1.064, $R_1 = 0.0752$ ([I > 2.00$\sigma$(I)], wR$_2 = 0.1983$ (all data). CCDC No.: 982712.

![Figure 8. ORTEP representation of (E)-3ae (50% thermal ellipsoids)](image)

(1-(4-(Trifluoromethyl)phenyl)ethene-1,2-diyl)dibenzene ((E)-4ae).

Colorless oil; $R_f$ 0.36 (Hexane); $^1$H NMR (500 MHz, CDCl$_3$) δ: 7.01-7.05 (m, 2H), 7.14-7.15 (m, 3H), 7.18-7.19 (m, 2H), 7.25-7.27 (m, 4H), 7.34-7.35 (m, 2H), 7.41-7.56 (m, 2H); $^{13}$C NMR (125 MHz, CDCl$_3$) δ: 124.2 (q, $^1$J$_{C-F}$ = 272 Hz), 125.1 (q, $^3$J$_{C-F}$ = 3.9
Hz), 125.5 (q, \(^{2}\text{J}_{\text{C-F}} = 3.9 \text{ Hz}\)) 127.3, 127.9, 127.8, 128.1, 128.9, 129.7, 130.0, 131.0, 136.8, 139.6, 141.3, 146.9; IR (neat, cm\(^{-1}\)) 3022, 2927, 1614, 1489, 1445, 1410, 1323, 1166, 1124, 1067, 1015, 845, 757, 721, 694; MS (EI): \(m/z\) (%) = 325 (21) [M+1\(^{+}\)], 324 (100) [M\(^{+}\)], 253 (26), 179 (26), 126 (11), 77 (3), 51 (3); HRMS: \(m/z\) calcd [M\(^{+}\)]: 324.1126, found 324.1129.

\((Z)-1-(m\text{-Methoxyphenyl})-2,3\text{-diphenyl-2-propen-1-one ((Z)-3af).}\)

![image](attachment:image.png)

Colorless solid; mp 71.2-72.8 °C; \(R_f\) 0.29; (hexane/AcOEt = 10/1); \(^{1}\text{H} NMR (500 MHz, CDCl\(_3\))\) \(\delta\): 3.80 (s, 3H), 7.01–7.05 (m, 1H), 7.14–7.25 (m, 5H), 7.27–7.37 (m, 5H), 7.46 (d, \(J = 7.5\), 2H), 7.53–7.57 (m, 2H); \(^{13}\text{C} NMR (125 MHz, CDCl\(_3\))\) \(\delta\): 55.3, 113.0, 120.4, 122.8, 126.3, 128.0, 128.1, 128.4, 128.8, 129.7, 130.0, 135.3, 137.6, 137.9, 140.8, 159.8, 199.1; IR (neat, cm\(^{-1}\)) 3056, 3024, 2938, 2835, 1666 (C=O), 1594, 1580, 1484, 1429, 1261, 1037; MS (EI): \(m/z\) (%) = 315 (40) [M+1\(^{+}\)], 314 (100) [M\(^{+}\)], 286 (18), 236 (14), 198 (15), 197 (95), 180 (13), 179 (94), 178 (96), 177 (40), 176 (47), 166 (10), 152 (47), 151 (25), 150 (10), 136 (37), 135 (98), 126 (14), 108 (25), 107 (95), 102 (20), 92 (94), 77 (95), 69 (73); HRMS: \(m/z\) calcd [M\(^{+}\)]: 314.1307, found 314.1310.

Crystallographic data for \((Z)-3af\) is as follows: \(\text{C}_{22}\text{H}_{18}\text{O}_{2}\), \(Mr = 314.38\), colorless, block, 0.180 × 0.170 × 0.170 mm\(^3\), monoclinic, C-centered, \(a = 27.3859(6)\) Å, \(b = 8.0159(2)\) Å, \(c = 17.9647(4)\) Å, \(\beta = 121.0707(7)^{\circ}\), \(V = 3377.8(2)\) Å\(^3\), \(Z = 8\), \(\rho_c = 1.236\) g cm\(^{-3}\), \(\mu = 0.779\) cm\(^{-1}\), \(T = 123(1)\) K, \(\lambda = 0.71075\) Å, 28309 reflections, 3877 unique \([R(int) = 0.0216]\), Final GoF = 1.083, \(R_1 = 0.0645 ([I > 2\sigma(I)])\), \(wR_2 = 0.1630\) (all data). CCDC No.: 982718.
Figure 9. ORTEP representation of (Z)-3af (50% thermal ellipsoids)

\[(E)-1-(m\text{-Methoxyphenyl})-2,3\text{-diphenyl-2-propen-1-one (}(E)-3af).\]

\[
\text{Ph} \quad \text{Ph} \\
\text{O} \\
\text{MeO} \quad (E)-3af
\]

Colorless solid; mp 88.4-89.5 °C; \(R_f\) 0.27; (hexane/AcOEt = 10/1); \(^1\)H NMR (500 MHz, CDCl\(_3\)) \(\delta\): 3.82 (s, 3H), 7.06–7.10 (m, 3H), 7.16-7.23 (m, 3H), 7.25-7.29 (m, 3H), 7.32-7.38 (m, 5H), 7.44 (d, \(J = 7.0\), 1H); \(^1\)C NMR (125 MHz, CDCl\(_3\)) \(\delta\): 55.4, 114.1, 118.6, 122.5, 126.3, 127.9, 128.2, 128.8, 128.9, 129.2, 129.6, 130.3, 134.7, 136.4, 139.4, 140.1, 140.7, 159.5, 197.3; IR (neat, cm\(^{-1}\)) 3057, 2923, 2852, 2362, 1653 (C=O), 1597, 1495, 1443, 1269; MS (El): \(m/z\) (%) = 315 (13) [M+1\(^+\)], 314 (59) [M\(^+\)], 197 (40), 179 (32), 178 (65), 177 (11), 176 (13), 152 (16), 136 (22), 135 (100), 108 (19), 107 (83), 92 (51), 86 (48), 84 (73), 77 (90), 69 (40); HRMS: \(m/z\) calcd [M\(^+\)]: 314.1307, found 314.1307.

Crystallographic data for (E)-3af is as follows: \(C_{22}H_{18}O_2\), \(Mr = 314.38\), colorless, block, 0.140 × 0.130 × 0.100 mm, triclinic, Primitive, \(a = 9.3539(3)\) Å, \(b = 9.8134(3)\) Å, \(c = 10.3948(4)\) Å, \(\alpha = 104.9234(8)\) \(^\circ\), \(\beta = 95.5597(8)\) \(^\circ\), \(\gamma = 111.7769(8)\) \(^\circ\), \(V = 836.28(5)\) Å\(^3\), \(Z = 2\), \(\rho_c = 1.248\) g/cm\(^3\), \(\mu = 0.786\) cm\(^{-1}\), \(T = 123\) K, \(\lambda = 0.71075\) Å, 8402 reflections, 3820 unique \([R(int) = 0.0146]\), Final GoF = 1.151, \(R_1 = 0.0492\) ([\(I >
2.00σ(I)), wR₂ = 0.1283 (all data). CCDC No.: 982714.

Figure 10. ORTEP representation of (E)-3af (50% thermal ellipsoids)

(1-(3-Methoxyphenyl)ethene-1,2-diyl)dibenzene ((E)-4af).

Colorless oil; Rf 0.18 (Hexane/CH₂Cl₂ = 10/1); ¹H NMR (500 MHz, CDCl₃) δ: 3.78 (s, 3H), 6.84 (d, J = 8.0 Hz, 1H), 6.88 (s, 1H), 6.91 (d, J = 8.0 Hz, 1H), 6.97 (s, 1H), 7.02 (d, J = 7.0 Hz, 2H), 7.08-7.14 (m, 3H), 7.20-7.24 (m, 3H), 7.30-7.34 (m, 3H); ¹³C NMR (125 MHz, CDCl₃) δ: 55.2, 112.8, 113.4, 120.3, 126.8, 127.9, 128.3, 128.6, 129.5, 130.3, 137.3, 140.2, 142.4, 144.9, 159.5; IR (neat, cm⁻¹) 3024, 2927, 1614, 1489, 1445, 1323, 1166, 1124, 1067, 845, 757, 694; MS (EI): m/z (%) = 287 (22) [M⁺1⁺], 286 (80) [M⁺], 253 (15), 178 (13), 126 (5), 83 (13), 73 (6), 57 (4); HRMS: m/z calcd [M⁺]: 286.1358, found 286.1358.

(Z)-1-(o-Methoxyphenyl)-2,3-diphenyl-2-propen-1-one ((Z)-3ag).

(Z)-3ag
Colorless solid; mp 91.4-92.5 °C; $R_f$ 0.21; (hexane/AcOEt = 10/1); $^1$H NMR (500 MHz, CDCl$_3$) $\delta$: 3.75 (s, 3H), $\delta$: 6.82 (d, $J = 8.0$ Hz, 1H), $\delta$: 6.90 (t, $J = 7.0$ Hz, 1H), $\delta$: 7.00 (s, 1H), $\delta$: 6.82 (d, $J = 8.0$ Hz, 1H), $\delta$: 6.90 (t, $J = 7.0$ Hz, 2H), $\delta$: 7.14-7.33 (m, 5H), $\delta$: 7.39 (t, $J = 7.0$ Hz, 1H), $\delta$: 7.43-7.45 (m, 2H), $\delta$: 7.85 (d, $J = 9.0$ Hz, 1H); $^{13}$C NMR (125MHz, CDCl$_3$) $\delta$: 55.5, 111.9, 120.3, 126.8, 127.6, 127.8, 128.2, 128.5, 128.8, 132.0, 134.5, 136.0, 138.2, 144.3, 159.4, 197.6; IR (neat, cm$^{-1}$) 3021, 1650 (C=O), 1595, 1483, 1285, 1248, 1213, 1162, 1021, 757, 727, 694, 673, 566, 523, 514; MS (EI): $m/z$ (%) = 316 (3) [M+2$^+$], 315 (23) [M+1$^+$], 314 (94) [M$^+$], 178 (22), 135 (100), 92 (13), 77 (20), 51 (4); HRMS: $m/z$ calcd [M$^+$]: 314.1307, found 314.1305.

Crystallographic data for (Z)-3ag is as follows: C$_{22}$H$_{18}$O$_2$, $M_r = 314.38$, colorless, block, 0.120 $\times$ 0.100 $\times$ 0.090 mm, orthorhombic, Primitive, $a = 8.0194(2)$ Å, $b = 10.8524(3)$ Å, $c = 19.1356(4)$ Å, $V = 1665.37(7)$ Å$^3$, $Z = 4$, $\rho_c = 1.254$ g/cm$^3$, $\mu = 0.790$ cm$^{-1}$, $T = 123$ K, $\lambda = 0.71075$ Å, 16656 reflections, 3814 unique [$R$(int) = 0.0236], Final $GoF = 1.114$, $R_1 = 0.0376 ([I > 2.00\sigma(I)])$, $wR_2 = 0.0900$ (all data). CCDC No.: 982716.

Figure 11. ORTEP representation of (Z)-3ag (50% thermal ellipsoids)

1-($o$-Methoxyphenyl)-2,3-diphenyl-2-propen-1-one ((Z)- and (E)-3ag).

![Chemical structure of 1-($o$-Methoxyphenyl)-2,3-diphenyl-2-propen-1-one ((Z)- and (E)-3ag).]
Colorless oil; \( R_f \) 0.21; (hexane/AcOEt = 10/1); \(^1\)H NMR (500 MHz, CDCl\(_3\)) \( \delta \): 3.74 for \( E \) (s, 3H), 3.76 for \( Z \) (s, 3H); \(^{13}\)C NMR (125MHz, CDCl\(_3\)) \( \delta \): 55.5, 55.6, 111.2, 111.9, 120.3, 120.5, 127.7, 128.1, 128.4, 128.5, 128.9, 129.3, 130.0, 130.6, 131.5, 132.0, 134.6, 150.0, 136.0, 136.1, 138.2, 141.7, 142.2, 144.3, 157.0, 159.4, 197.6, 198.0.

(1-(2-Methoxyphenyl)ethene-1,2-diyl)dibenzene ((\(E\))-4ag).

\[
\begin{array}{c}
\text{Ph} \\
\text{OMe} \\
\text{Ph} \\
\end{array}
\]

\((E\)-4ag\)

Colorless oil; \( R_f \) 0.18 (hexane/\(CH_2Cl_2\) = 10/1); \(^1\)H NMR (500 MHz, CDCl\(_3\)) \( \delta \): 3.53 (s, 3H), 6.72 (s, 1H), 6.81 (d, \( J = 8.0 \text{ Hz} \), 1H), 6.88 (t, \( J = 7.0 \text{ Hz} \), 1H), 7.00-7.01 (m, 2H), 7.05-7.07 (m, 3H), 7.12-7.21 (m, 7H); \(^{13}\)C NMR (125 MHz, CDCl\(_3\)) \( \delta \): 55.6, 111.8, 120.5, 126.6, 126.7, 127.8, 128.0, 128.7, 129.4, 129.6, 130.2, 131.0, 133.7, 137.5, 140.3, 141.1, 157.3; IR (neat, cm\(^{-1}\)) 3053, 3020, 2957, 1595, 1487, 1456, 1433, 1253, 1110, 1026, 776, 753, 719, 696; MS (EI): \( m/z \) (\%) = 287 (20) [M+1\(^+\)], 286 (99) [M\(^+\)], 165 (45), 126 (12), 83 (15), 77 (6), 51 (4); HRMS: \( m/z \) calcd [M\(^+\)]: 286.1358, found 286.1355.

\((Z\)-1,2,3-Tris(4-methoxyphenyl)prop-2-en-1-one ((\(Z\))-3bb).

\[
\begin{array}{c}
\text{OMe} \\
\text{MeO} \\
\text{OMe} \\
\end{array}
\]

\((Z\)-3bb\)

Yellow oil; \( R_f \) 0.20; (hexane/AcOEt = 10/1); \(^1\)H NMR (500 MHz, CDCl\(_3\)) \( \delta \): 3.73 (s,
3H), 3.79 (s, 3H), 3.81 (s, 3H), 6.85 (t, \( J = 8.5 \) Hz, 3H), 7.009 (s, 1H), 7.08 (d, \( J = 8.5 \) Hz, 2H); \(^{13}\)C NMR (125 MHz, CDCl\(_3\)) \( \delta \): 55.0, 55.1, 55.3, 113.9, 114.1, 127.2, 128.3, 129.5, 130.0, 130.1, 132.0, 138.3, 158.9, 159.2, 163.8, 198.5; FTIR (neat, cm\(^{-1}\)) 3024, 2958, 2928, 2836, 1656 (C=O), 1597, 1572, 1511, 1461, 1421, 1302, 1029, 904, 831; MS (EI): \( m/z \) (%): 374 (88) \([M^+]\), 355 (35), 295 (15), 281 (25), 266 (32), 239 (30), 227 (48), 221 (30), 169 (45), 149 (99), 135 (84), 113 (28), 83 (11), 71 (33), 57 (45); HRMS: \( m/z \) calcd \([M^+]\): 374.1518; found 374.1517.

\((E)-1,2,3\)-Tris(4-methoxyphenyl)prop-2-en-1-one (((E)-3bb)).

![Chemical structure of (E)-3bb](image)

Yellow oil; \( R_f \) 0.20; (hexane/AcOEt = 10/1); \(^1\)H NMR (500 MHz, CDCl\(_3\)) \( \delta \): 3.77 (s, 3H), 3.82 (s, 3H), 3.86 (s, 3H), 6.70-6.73 (m, 7H), 6.90 (t, \( J = 8.5 \) Hz, 3H), 7.11 (s, 1H), 7.85 (d, \( J = 9.0 \) Hz, 2H); \(^{13}\)C NMR (125 MHz, CDCl\(_3\)) \( \delta \): 55.06, 55.09, 55.3, 113.3, 113.6, 114.2, 127.2, 127.6, 129.3, 130.1, 132.0, 138.2, 159.0, 159.8, 162.7, 196.6; IR (neat, cm\(^{-1}\)) 3024, 2958, 2928, 2836, 1656 (C=O), 1597, 1572, 1511, 1461, 1421, 1302, 1029, 904, 831; MS (EI): \( m/z \) (%): 374 (88) \([M^+]\), 355 (35), 295 (15), 281 (25), 266 (32), 239 (30), 227 (48), 221 (30), 169 (45), 149 (99), 135 (84), 113 (28), 83 (11), 71 (33), 57 (45); HRMS: \( m/z \) calcd \([M^+]\): 374.1518; found 374.1517.

\((Z)-1-(4\text{-Methoxyphenyl})\text{-2,3-bis(4-(trifluoromethyl)phenyl)prop-2-en-1-one} (((Z)-3cb)).

![Chemical structure of (Z)-3cb](image)
Colorless solid; 103.9-105.2 °C; \( R_f \) 0.25; (hexane/AcOEt = 10/1); \(^1\)H NMR (500 MHz, CDCl\(_3\)) \( \delta \): 3.83 (s, 3H), 6.87 (d, \( J = 8.5 \) Hz, 2H), 7.22 (s, 1H), 7.42-7.48 (m, 4H), 7.59-7.63 (m, 4H), 7.93 (d, \( J = 8.5 \) Hz, 2H); \(^13\)C NMR (125 MHz, CDCl\(_3\)) \( \delta \): 55.3, 114.3, 123.8 (q, \( J_{C,F} = 270.6 \) Hz), 123.9 (q, \( J_{C,F} = 269.5 \) Hz), 125.4 (q, \( J_{C,F} = 3.6 \) Hz), 125.8 (q, \( J_{C,F} = 3.6 \) Hz) 126.6, 129.7, 129.9 (q, \( J_{C,F} = 53.6 \) Hz), 130.2 (q, \( J_{C,F} = 53.6 \) Hz), 132.0, 138.4, 140.9, 141.9, 164.5, 196.4; IR (neat, cm\(^{-1}\)) 2934, 2843, 1655 (C=O), 1614, 1596, 1573, 1462, 1322, 1237, 1164, 1015, 907, 781; MS (EI): \( m/z \) (%): 450 (80) [M\(^+\)], 431 (20), 422 (9), 315 (8), 295 (20), 265 (23), 246 (22), 225 (11), 196 (8), 176 (9), 135 (99), 107 (38), 84 (72), 77 (69), 57 (18); HRMS: \( m/z \) calcd [M\(^+\)]: 450.1054, found 450.1055.

Crystallographic data for (Z)-3cb is as follows: C\(_{24}\)H\(_{16}\)F\(_6\)O\(_2\), \( M_r = 450.38 \), colorless, platelet, 0.100 \( \times \) 0.060 \( \times \) 0.010 mm, monoclinic, Primitive, \( a = 13.789(1) \) Å, \( b = 8.2551(6) \) Å, \( c = 17.588(2) \) Å, \( \beta = 96.860(2) ^\circ \), \( V = 1987.6(3) \) Å\(^3\), \( Z = 4 \), \( \rho_c = 1.505 \) g/cm\(^3\), \( \mu = 1.326 \) cm\(^{-1}\), \( T = 123 \) K, \( \lambda = 0.71075 \) Å, 23005 reflections, 3630 unique \( [R(int) = 0.0586] \), Final \( GoF \) = 1.070, \( R_1 = 0.0592 \) ([\( I > 2.00\sigma(I) \)]), \( wR_2 = 0.1702 \) (all data). CCDC No.: 982720.
(E)-1-(4-Methoxyphenyl)-2,3-bis(4-(trifluoromethyl)phenyl)prop-2-en-1-one ((E)-3cb).

Colorless solid; 98.3-100.2 °C; Rf 0.16; (hexane/AcOEt = 10/1); $^1$H NMR (500 MHz, CDCl$_3$) δ: 3.89 (s, 3H), 6.96 (d, $J = 8.0$ Hz, 2H), 7.18-7.20 (m, 3H), 7.41 (d, $J = 8.0$ Hz, 2H), 7.48 (d, $J = 8.0$ Hz, 2H), 7.61 (d, $J = 8.0$ Hz, 2H), 7.91 (d, $J = 8.5$ Hz, 2H); $^{13}$C NMR (125 MHz, CDCl$_3$) δ: 55.5, 113.8, 123.9 (q, $^1J_{C,F} = 270.6$ Hz), 125.4 (q, $^3J_{C,F} = 3.5$ Hz), 125.8 (q, $^3J_{C,F} = 3.6$ Hz) 129.5, 129.9, 130.1, 130.5 (q, $^2J_{C,F} = 26.3$ Hz), 132.4, 136.5, 138.0, 139.8, 141.6, 163.6, 195.0; IR (neat, cm$^{-1}$) 2926, 1653 (C=O), 1597, 1573, 1419, 1322, 1256, 1164, 1016, 907, 839; MS (EI): m/z (%) = 450 (25) [M$^+$], 431 (5), 422 (4), 315 (10), 295 (30), 265 (12), 246 (26), 225 (11), 196 (8), 176 (6), 135 (99), 107 (28), 92 (42), 77 (48), 57 (14); HRMS: m/z calcd [M$^+$]: 450.1054, found 450.1060.

Crystallographic data for (E)-3cb is as follows: C$_{24}$H$_{16}$F$_6$O$_2$, Mr = 450.38, colorless, block, 0.130 × 0.040 × 0.020 mm, monoclinic, Primitive, $a = 9.234(1)$ Å, $b$
= 5.6213(7) Å, \( c = 20.157(3) \) Å, \( \beta = 98.054(3) \) °, \( V = 1036.0(2) \) Å³, \( Z = 2 \), \( \rho_c = 1.444 \) g/cm³, \( \mu = 1.272 \) cm⁻¹, \( T = 123 \) K, \( \lambda = 0.71075 \) Å, 14482 reflections, 3739 unique \([R(int) = 0.0534]\), Final GoF = 1.023, \( R_1 = 0.0689 \) ([\( I > 2.00\sigma(I) \)], \( wR_2 = 0.1750 \) (all data). CCDC No.: 982717.

Figure 13. ORTEP representation of \((E)-3cb\) (50% thermal ellipsoids)

\((Z)-1-(4-Methoxyphenyl)-2-propylhex-2-en-1-one (\(Z\)-3db).

Colorless oil; \( R_f 0.33; \) (hexane/AcOEt = 15/1); \( ^1\)H NMR (500 MHz, CDCl₃) \( \delta \): 0.81 (t, \( J = 7.5 \) Hz, 3H), 0.91 (t, \( J = 7.5 \) Hz, 3H), 1.29–1.38 (m, 2H), 1.39–1.47 (m, 2H), 1.83 (q, \( J = 7.5 \) Hz, 2H), 2.27 (t, \( J = 7.5 \) Hz, 2H), 3.88 (s, 3H), 5.61 (t, \( J = 8.0 \) Hz, 1H), 6.94 (d, \( J = 9.5 \) Hz, 2H), 7.91 (d, \( J = 8.5 \) Hz, 2H); \(^{13}\)C NMR (125 MHz, CDCl₃) \( \delta \): 13.7, 13.8, 21.5, 22.7, 31.7, 37.6, 55.5, 113.8, 130.1, 130.3, 131.7, 140.4, 163.7, 199.5; IR (neat, cm⁻¹) 3024, 2959, 2928, 2872, 1660 (C=O), 1600, 1574, 1508, 1463, 1258, 1160, 1030; MS (EI): \( m/z (%) = 246 (M^+, 22), 245 (13), 217 (34), 215 (54), 203 (70), 190 (15), 189 (20), 176 (15), 175 (23), 141 (25), 136 (10), 135 (100), 92 (18), 85 (31), 83 (50), 77 (18); HRMS: \( m/z \) calcd [M⁺]: 246.1620, found 246.1622.

\((E)-1-(4-Methoxyphenyl)-2-propylhex-2-en-1-one ((E)-3db).\)
Colorless oil; \( R_f \) 0.30; (hexane/AcOEt = 15/1); \(^1\)H NMR (500 MHz, CDCl\(_3\)) \( \delta \): 0.95 (q, \( J = 7.0 \) Hz, 6H), 1.42–1.51 (m, 4H), 2.26 (q, \( J = 8.0 \) Hz, 2H), 2.46 (t, \( J = 8.0 \) Hz, 2H), 3.86 (s, 3H), 6.11 (t, \( J = 7.5 \) Hz, 1H), 6.92 (d, \( J = 8.5 \) Hz, 2H), 7.72 (d, \( J = 8.5 \) Hz, 2H); \(^{13}\)C NMR (125 MHz, CDCl\(_3\)) \( \delta \): 14.0, 14.1, 22.1, 22.3, 29.1, 30.6, 55.4, 113.2, 131.3, 131.8, 141.0, 143.2, 162.5, 196.0; IR (neat, cm\(^{-1}\)) 3024, 2959, 2932, 2871, 1644 (C=O), 1601, 1575, 1508, 1463, 1255, 1162, 1031; MS (EI): \( m/z \) (%) = 246 (12) [M\(^+\)], 217 (16), 203 (11), 175 (10), 135 (100), 121 (11), 108 (15), 92 (67), 79 (15), 78 (12), 77 (67), 55 (33); HRMS: \( m/z \) calcd [M\(^+\)]: 246.1620, found 246.1618.

\((Z)\)-1-(4-Methoxyphenyl)-2-methyl-3-phenylprop-2-en-1-one ((\(Z\))-3eb).

Colorless oil; \( R_f \) 0.24 (hexane/AcOEt = 10/1); \(^1\)H NMR (500 MHz, CDCl\(_3\)) \( \delta \): 2.16 (d, \( J = 1.5 \) Hz, 3H), 3.81 (s, 3H), 6.67 (d, \( J = 1.0 \) Hz, 1H), 6.82 (d, \( J = 9.5 \) Hz 2H), 7.05–7.35 (m, 5H), 7.88 (d, \( J = 8.5 \) Hz, 2H). \(^{13}\)C NMR (125 MHz, CDCl\(_3\)) \( \delta \): 197.5, 163.8, 137.4, 135.8, 131.8, 129.2, 128.2, 128.0, 127.2, 126.1, 113.8, 55.4, 29.7; IR (neat, cm\(^{-1}\)) 3024, 2921, 1652 (C=O), 1558, 1507, 1465, 1396, 1260, 1027, 801; MS (EI): \( m/z \) (%) = 253 (7) [M+1\(^+\)], 252 (33) [M\(^+\)], 251 (16), 237 (14), 221 (16), 136 (7), 135 (80), 115 (28), 92 (26), 83 (100), 57 (55); HRMS: \( m/z \) calcd [M\(^+\)]: 252.1150, found 252.1151.

\((E)\)-1-(4-Methoxyphenyl)-2-methyl-3-phenylprop-2-en-1-one ((\(E\))-3eb).
Colorless oil; \( R_f \) 0.21 (hexane/AcOEt = 10/1); \(^1\)H NMR (500 MHz, CDCl\(_3\)) \( \delta \): 2.26 (d, \( J = 1.5 \) Hz, 3H), 3.88 (s, 3H), 6.96 (d, \( J = 9.0 \) Hz, 2H), 7.11 (d, \( J = 1.0 \) Hz 1H), 7.31–7.37 (m, 1H), 7.38–7.44 (m, 4H), 7.81 (d, \( J = 8.5 \) Hz, 2H); \(^{13}\)C NMR (125 MHz, CDCl\(_3\)) \( \delta \): 14.9, 55.4, 113.5, 128.3, 128.4, 129.6, 130.6, 132.0, 135.9, 136.9, 140.0, 162.8, 198.3; IR (neat, cm\(^{-1}\)) 3022, 2958, 1641 (C=O), 1599, 1508, 1444, 1306, 1254, 1172, 1145, 1031, 1018; MS (EI): \( m/z \) (%) = 253 (28) [M+1\(^+\)], 252 (97) [M\(^+\)], 251 (52), 237 (34), 221 (36), 136 (12), 135 (100), 114 (30), 92 (32), 77 (57), 64 (18); HRMS: \( m/z \) calcd [M\(^+\)]: 252.1150, found 252.1147.

\((Z)-1-(4-Methoxyphenyl)-2-phenylbut-2-en-1-one ((Z)-3eb').\)

Colorless oil; \( R_f \) 0.24 (hexane/AcOEt = 10/1); \(^1\)H NMR (500 MHz, CDCl\(_3\)) \( \delta \): 1.76 (d, \( J = 7.5 \) Hz, 3H), 3.85 (s, 3H), 6.31 (q, \( J = 7.5 \) Hz, 1H), 6.90 (d, \( J = 8.5 \) Hz 2H), 7.05–7.35 (m, 5H), 7.95 (d, \( J = 8.5 \) Hz, 2H). \(^{13}\)C NMR (125 MHz, CDCl\(_3\)) \( \delta \): 199.7, 163.9, 141.9, 137.5, 132.1, 129.8, 128.7, 128.2, 127.5, 125.8, 113.9, 55.5, 23.0; IR (neat, cm\(^{-1}\)) 3024, 2921, 1653 (C=O), 1597, 1507, 1165, 1029, 800, 582, 520; MS (EI): \( m/z \) (%) = 253 (7) [M+1\(^+\)], 252 (33) [M\(^+\)], 251 (16), 237 (14), 221 (16), 136 (7), 135 (80), 115 (28), 92 (26), 83 (100), 57 (55); HRMS: \( m/z \) calcd [M\(^+\)]: 252.1150, found 252.1151.

\((E)-1-(4-Methoxyphenyl)-2-phenylbut-2-en-1-one ((E)-3eb).\)
Colorless oil; \( R_f \) 0.18 (hexane/AcOEt = 10/1); \(^1\)H NMR (500 MHz, CDCl\(_3\)) \( \delta \): 1.89 (d, \( J = 7.0 \) Hz, 3H), 3.85 (s, 3H), 6.48 (q, \( J = 7.0 \) Hz, 1H), 6.88 (d, \( J = 9.0 \) Hz 2H), 7.25–7.40 (m, 5H), 7.80 (d, \( J = 8.5 \) Hz, 2H); \(^1^3\)C NMR (125 MHz, CDCl\(_3\)) \( \delta \): 15.3, 55.4, 113.4, 127.4, 128.2, 129.4, 130.7, 132.1, 136.1, 136.7, 142.7, 162.9, 196.0; IR (neat, cm\(^{-1}\)) 3023, 2931, 1650 (C=O), 1599, 1509, 1441, 1311, 1256, 1169, 1028; MS (EI): \( m/z \) (%): 253 (21) [M+1\(^+\)], 252 (100) [M\(^+\)], 251 (13), 237 (11), 235 (14), 221 (32), 178 (11), 165 (17), 136 (12), 135 (88), 115 (26), 92 (43), 91 (31), 77 (83), 64 (20); HRMS: \( m/z \) caled [M\(^+\)]: 252.1150, found 252.1146.

\((Z)-2\)-Benzyldiene-1-(4-methoxyphenyl)hexan-1-one ((\(Z\))-3fb).

Pale yellow oil; \( R_f \) 0.24 (hexane/AcOEt = 20/1); \(^1\)H NMR (500 MHz, CDCl\(_3\)) \( \delta \): 0.90 (t, \( J = 7.0 \) Hz, 3H), 1.35-1.44 (m, 2H), 1.46-1.54 (m, 2H), 2.47 (td, \( J = 7.5, 1.5 \) Hz, 2H), 3.80 (s, 3H), 6.65 (s, 1H), 6.80 (d, \( J = 8.5 \) Hz, 2H), 7.03–7.35 (m, 5H), 7.87 (d, \( J = 9.0 \) Hz, 2H). \(^1^3\)C NMR (125 MHz, CDCl\(_3\)) \( \delta \): 13.8, 22.4, 29.6, 31.5, 55.3, 113.7, 125.8, 127.1, 128.0, 128.3, 128.6, 129.9, 131.7, 132.0, 137.4, 141.9, 163.6, 199.6. IR (neat) 2956, 2929, 2857, 1654 (C=O), 1597, 1507, 1258, 1165, 1028, 842, 696; MS (EI): \( m/z \) (%): 295 (M+1\(^+\), 8), 294 (M\(^+\), 30), 263 (7), 251 (11), 237 (3), 203 (3), 135 (100), 115 (50), 92 (32), 77 (35), 64 (10); Exact mass EI caled for C\(_{20}\)H\(_{22}\)O\(_2\) 294.1620, found 294.1613.

\((E)-2\)-Benzyldiene-1-(4-methoxyphenyl)hexan-1-one ((\(E\))-3fb).
Pale yellow oil; \( R_f 0.22 \) (hexane/AcOEt = 20/1). \(^1\)H NMR (500 MHz, CDCl\(_3\)) \( \delta \): 0.90 (t, \( J = 7.0 \) Hz, 3H), 1.35-1.44 (m, 2H), 1.48-1.55 (m, 2H), 2.73 (t, \( J = 8.0 \) Hz, 2H), 3.88 (s, 3H), 6.95 (d, \( J = 9.0 \) Hz, 2H), 6.97 (s, 1H), 7.30-7.42 (m, 5H), 7.85 (d, \( J = 8.5 \) Hz, 2H); \(^{13}\)C NMR (125 MHz, CDCl\(_3\)) \( \delta \): 13.8, 22.9, 27.9, 30.8, 55.4, 113.4, 128.1, 128.4, 128.5, 129.0, 130.9, 132.0, 135.8, 138.3, 142.4, 162.9, 198.2; IR (neat) 2958, 2918, 2858, 1645 (C=O), 1600, 1507, 1457, 1170, 1028, 767, 700; MS (EI): \( m/z \) (%) = 295 (M+1\(^+\), 13), 294 (M\(^+\), 50), 263 (13), 251 (11), 237 (8), 203 (6), 135 (100), 115 (57), 92 (28), 77 (33), 64 (10); Exact mass EI calcd for C\(_{20}\)H\(_{22}\)O\(_2\) 294.1620, found 294.1615.

\((Z)-1-(4-Methoxyphenyl)-2-phenylhept-2-en-1-one ((Z)-3\textsuperscript{fb}).\)

Pale yellow oil; \( R_f 0.24 \) (hexane/AcOEt = 20/1); \(^1\)H NMR (500 MHz, CDCl\(_3\)) \( \delta \): 0.83 (t, \( J = 7.5 \) Hz, 3H), 1.24-1.32 (m, 2H), 1.35-1.44 (m, 2H), 2.09 (q, \( J = 7.0 \) Hz, 2H), 3.85 (s, 3H), 6.23 (t, \( J = 8.0 \) Hz, 1H), 6.90 (d, \( J = 9.5 \) Hz, 2H), 7.03-7.35 (m, 5H), 7.95 (d, \( J = 9.0 \) Hz, 2H). \(^{13}\)C NMR (125 MHz, CDCl\(_3\)) \( \delta \): 13.8, 22.2, 30.2, 36.7, 55.4, 113.8, 127.4, 128.1, 128.5, 128.8, 129.3, 131.7, 135.9, 140.7, 163.6, 197.3. IR (neat) 2956, 2929, 2857, 1654 (C=O), 1597, 1507, 1258, 1165, 1028, 842, 696; MS (EI): \( m/z \) (%) = 295 (M+1\(^+\), 8), 294 (M\(^+\), 30), 263 (7), 251 (11), 237 (3), 203 (3), 135 (100), 115 (50), 92 (32), 77 (35), 64 (10); Exact mass EI calcd for C\(_{20}\)H\(_{22}\)O\(_2\) 294.1620, found 294.1613.
(E)-1-(4-Methoxyphenyl)-2-phenylhept-2-en-1-one ((E)-3′fb).

Pale yellow oil; \( R_f = 0.16 \) (hexane/AcOEt = 20/1); \(^1\)H NMR (500 MHz, CDCl\(_3\)) \( \delta \): 0.86 (t, \( J = 7.0 \) Hz, 3H), 1.28-1.37 (m, 2H), 1.41-1.48 (m, 2H), 2.26 (q, \( J = 7.5 \) Hz, 2H), 3.85 (s, 3H), 6.36 (t, \( J = 7.5 \) Hz, 1H), 6.90 (d, \( J = 8.5 \) Hz, 2H), 7.26-7.31 (m, 5H), 7.81 (d, \( J = 9.0 \) Hz, 2H); \(^1^3\)C NMR (125 MHz, CDCl\(_3\)) \( \delta \): 13.8, 22.4, 29.1, 31.4, 55.4, 113.4, 113.9, 127.3, 128.2, 128.6, 129.4, 130.8, 132.1, 136.5, 141.4, 142.5, 162.8, 196.1; IR (neat) 2957, 2918, 2849, 1652 (C=O), 1699, 1541, 1507, 1310, 1257, 1167, 1026, 702; MS (EI): \( m/z \) (%) = 295 (M\(^+\), 6), 294 (M\(^+\), 30), 251 (10), 237 (2), 157 (2), 135 (100), 115 (15), 92 (15), 77 (18), 64 (5); Exact mass EI calcd for C\(_{20}\)H\(_{22}\)O\(_2\) 294.1620, found 294.1617.

References:

Supporting Information 2

Rh(I)-Catalyzed Carbonylative Arylation of Alkynes with Arylboronic Acids using Formaldehyde as a Carbonyl Source

Chuang Wang,\(^a\) Tsumoru Morimoto,*\(^a\) Hiroyuki Kanashiro,\(^a\) Hiroki Tanimoto,\(^a\) Yasuhiro Nishiyama,\(^a\) Kiyomi Kakiuchi,\(^a\) and Levent Artok\(^b\)
a Graduate School of Materials Science, Nara Institute of Science and Technology (NAIST)
Ikoma, Nara 630-0101, Japan

b Department of Chemistry, Faculty of Science, Izmir Institute of Technology,
Urla 35430, Izmir, Turkey

E-mail: morimoto@ms.naist.jp
MeO

1b
3aa
E: 76% of D
PhO
BuMeO\((E)\)-3'fb