Electronic Supplementary Material (ESI) for Green Chemistry


# Supporting Information

# pH-Responsive Chelating Palladium(II) N-Heterocyclic Carbene Complexes：Recoverable Precatalysts for Suzuki-Miyaura Reaction in Pure Water

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**Table of Contents:**

**Characterization data for coupling products:**

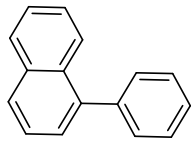
**4-Acetyldiphenyl**[1]

$^{1}$H NMR: δ 8.06 (d, *J* =8.4 Hz, 2H), 7.71 (d, *J* = 8.4Hz, 2H), 7.65 (d, *J* = 7.2 Hz, 2H), 7.50 (t, *J* = 7.2 Hz, 2H), 7.43 (t, *J* = 7.2 Hz, 1H), 2.67 (s, 3H); $^{13}$C NMR: δ 197.8, 145.8, 139.9, 135.9, 129.0, 128.9, 128.3, 127.3, 127.2, 26.7.

**Biphenyl-4-carbonitrile**[1]

$^{1}$H NMR: δ 7.80-7.70 (m, 4H), 7.68-7.60 (m, 2H), 7.55-7.40 (m, 3H); $^{13}$C NMR: δ 145.7, 139.2, 132.6, 129.2, 128.7, 127.7, 127.3, 119.0, 110.9.

**1-Phenylnaphthalene**[2]



$^{1}$H NMR: δ 8.10-7.99 (m, 3H), 7.70-7.50 (m, 2H); $^{13}$C NMR: δ 140.9, 140.4, 134.0, 131.8, 130.2, 128.4, 127.8, 127.4, 127.1, 126.2, 125.9, 125.6.

**2-Methylbiphenyl**[1]

$^{1}$H NMR: δ 7.59-7.51 (m, 2H), 7.50-7.49 (m, 3H), 7.44-7.40 (m, 4H), 2.45 (s, 3H); $^{13}$C NMR: δ 142.1, 142.1, 135.5, 130.5, 123.0, 129.4, 128.2, 127.4, 127.3, 126.9, 125.9, 20.6

**3-Methylbiphenyl** [1]

$^{1}$H NMR: δ 7.77-7.73 (m, 2H), 7.60-7.50 (m, 4H), 7.50-7.42 (m, 2H), 7.33-7.28 (m, 1H), 2.57 (d, *J* =3.6 Hz, 3H); $^{13}$C NMR: δ 141.5, 141.4, 138.5, 128.9, 128.8, 128.2, 128.1, 127.3, 124.4, 21.7.

**4-Methylbiphenyl** [1]

$^{1}$H NMR: δ 7.64 (d, *J* =8 Hz, 2H), 7.56 (d, *J* =8 Hz, 2H), 7.49 (t, *J* =7.2 Hz, 2H), 7.39 (t, *J* =7.6 Hz, 1H), 7.32(d, *J* =8 Hz, 2H), 2.26 (s, 3H); $^{13}$C NMR: δ 141.2, 138.4, 137.1, 129.5, 128.8, 127.1, 127.1, 21.2.

**1-(2'-Methylbiphenyl-4-yl)ethanone**[1]

$^{1}$H NMR: δ 8.05 (d, *J* =8.2 Hz, 2H), 7.57 (s, 1H), 7.45 (s, 1H), 7.35-7.25 (m, 4H), 2.68 (s, 3H), 2.31 (s, 3H); $^{13}$C NMR: δ 197.8, 147.0, 140. 8, 135.6, 135.2, 130.6, 129.5, 129.5, 128.3, 128.0, 126.0, 26.7, 20.4.

**4-Methoxybiphenyl** [1]

$^{1}$H NMR: δ 7.57 (t, *J* =8 Hz, 4H), 7.44 (t, *J* =7.4 Hz, 2H), 7.32 (t, *J* =7.4 Hz, 2H), 7.00 (d, *J* =8.8 Hz, 2H), 3.88 (s, 3H); $^{13}$C NMR: δ 159.2, 140.8, 133.8, 128.7, 128.2, 126.8, 126.7, 114.2, 55.4.

**4'-Methoxy-2-methylbiphenyl** [1]

$^{1}$H NMR: δ 7.40-7.30 (m, 6H), 7.07 (d, *J* =8.4 Hz, 2H), 3.94 (s, 3H), 2.40 (s, 3H); $^{13}$C NMR: δ 158.6, 141.7, 135.6, 134.5, 130.4, 130.4, 127.1, 125.9, 113.6, 55.3, 20.7.

**4-Nitrobiphenyl** [1]

$^{1}$H NMR: δ 8.32 (d, *J* =9.2 Hz, 2H), 7.76 (d, *J* =8.8 Hz, 2H), 7.65 (t, *J* =7.2 Hz, 2H), 7.55-7.42 (m, 3H); $^{13}$C NMR: δ 147.7, 147.1, 138.8, 129.2, 128.9, 127.8, 127.4, 124.1

**3-Phenylpyridine**[3]

$^{1}$H NMR: δ 8.87 (s, 1H), 8.62 (s, 1H), 7.90 (d, *J* =8 Hz, 1H), 7.65-7.58 (m, 2H), 7.51 (t, *J* =7.2 Hz, 2H), 7.46-7.43 (m, 1H), 7.42-7.37 (m, 1H); $^{13}$C NMR: δ 148.5, 148.4, 137.9, 136.7, 134.4, 129.1, 128.1, 127.2, 123.6.

**2-Phenylthiophene** [2]

$^{1}$H NMR: δ 7.68 (d, *J* =7.2 Hz, 2H), 7.44 (t, *J* =7.2 Hz, 2H), 7.38-7.31 (m, 3H), 7.14 (m, 1H); $^{13}$C NMR: δ 144.6, 134.5, 129.0, 128.1, 127.5, 126.0, 124.9, 123.2.

**1-(3'-Methylbiphenyl-4-yl)ethanone**[1]

$^{1}$H NMR: δ 8.05 (d, *J* =8.4 Hz, 2H), 7.70 (d, *J* =8.4 Hz, 2H), 7.50-7.42 (m, 2H), 7.39 (t, *J* =7.4 Hz, 1H), 7.27-7.23 (m, 1H), 2.66 (s, 3H),2.46 (s, 3H); $^{13}$C NMR: δ 197.8, 146.0, 139.9, 138.6, 135.8, 129.0, 128.9, 128.0, 127.2, 124.4, 26.7, 21.5.

**1-(4'-Methylbiphenyl-4-yl)ethanone** [1]

$^{1}$H NMR: δ 8.05 (d, *J* =8.4 Hz, 2H), 7.70 (d, *J* =8.4 Hz, 2H), 7.56 (d, *J* =8.4 Hz, 2H), 7.31 (d, *J* =8 Hz, 2H), 2.66 (s, 3H), 2.44 (s, 3H); $^{13}$C NMR: δ 197.8, 145.7, 138.3, 137.0, 135.6, 129.7 128.9, 127.1, 127.0, 26.7, 21.2.

**1-(4'-Methoxybiphenyl-4-yl)ethanone**[1]

$^{1}$H NMR: δ 8.03 (d, *J* =8.4 Hz, 2H), 7.67 (d, *J* =8.4 Hz, 2H), 7.60 (d, *J* =8.4 Hz, 2H), 7.03 (d, *J* =8.8 Hz, 2H), 3.89 (s, 3H), 2.65 (s, 3H); $^{13}$C NMR: δ 197.7, 159.9, 145.4, 135.3, 132.2, 129.0, 128.4, 126.6, 114.4, 55.4, 26.6.

**1-(4'-Fluorobiphenyl-4-yl)ethanone** [1]

$^{1}$H NMR: δ 8.04 (d, *J* = 8.6 Hz, 2H), 7.67-7.58 (m, 4H), 7.17 (t, J = 6.8 Hz, 2H), 2.65 (s, 3H); $^{13}$C NMR: δ 197.7, 164.2, 161.8, 144.7, 136.0, 135.8, 129.0, 128.9, 127.1, 116.0, 115.8, 26.7; $^{19}$F NMR: δ: -114.0.

**4-Chlorobiphenyl** [1]

$^{1}$H NMR: δ7.64-7.54 (m, 4H), 7.52-7.37 (m, 5H); $^{13}$C NMR: δ140.0, 139.7, 133.4, 128.9, 128.9, 128.4, 127.6, 127.0

**Biphenyl-4-carbaldehyde** [3]

$^{1}$H NMR: δ 10.08 (s, 1H), 7.97 (d, *J* =8 Hz, 2H), 7.76 (d, *J* =8 Hz, 2H), 7.66 (d, *J* =6.8 Hz, 2H), 7.52-7.50 (m, 2H), 7.49-7.44 (m, 1H); $^{13}$C NMR: δ 191.9, 147.2, 139.7, 135.2, 130.3, 129.1, 128.5,

127.7, 127.4.

**4-Fluorobiphenyl** [2]

$^{1}$H NMR: δ 10.08 (s, 1H), 7.60-7.50 (m, 4H), 7.48 (t, *J* =7.2 Hz, 2H), 7.39 (t, *J* =7.2 Hz, 1H), 7.17 (t, *J* =8.8 Hz, 2H); $^{13}$C NMR: δ 161.3, 140.3, 137.4, 128.9, 128.8, 128.7, 127.3, 127.1, 115.6; $^{19}$F NMR: δ -115.8.

**1,4-Diphenylbenzene** [5]

$^{1}$H NMR: δ 7.71 (s, 4H), 7.68 (s, 2H), 7.67 (s, 2H), 7.49 (t, *J* =7.6 Hz, 4H), 7.39 (t, *J* =7.6 Hz, 2H); $^{13}$C NMR: δ 140.5, 140.1, 128.8, 127.5, 127.4, 127.1.

**4-(Trifluoromethyl)biphenyl** [1]

$^{1}$H NMR: δ 7.73 (s, 4H), 7.65-7.61 (m, 2H), 7.54-7.48 (t, *J* =7 Hz, 2H), 7.46-7.43 (m, 1H); $^{13}$C NMR: δ 144.8, 139.8, 129.0, 128.2, 127.4, 127.3, 125.7, 125.7,

**Diphenylmethane**[4]

$^{1}$H NMR: δ 7.45-7.40 (m, 4H), 7.35-7.20 (m, 6H), 4.09 (s, 2H); $^{13}$C NMR: δ 141.2, 129.0, 128.6, 126.2, 42.0.

**1-Benzyl-4-methoxybenzene**[4]

$^{1}$H NMR: δ 7.41 (t, *J* =7.2 Hz,2H), 7.34 (t, *J* =5.6 Hz, 3H), 7.26 (d, *J* =8.8 Hz, 2H), 6.98 (d, *J* =8.8 Hz, 2H), 4.08 (s, 2H), 3.90 (s, 3H); $^{13}$C NMR: δ 158.2, 141.8, 133.4, 130.1, 129.0, 128.6, 126.2, 114.1, 55.3, 41.2.

**References**:

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[3] J. V. Kingston and J. G. Verkade, *J. Org. Chem.*, 2007, **72**, 2816−2822

[4] G. A. Molander and M. D. Elia, *J. Org. Chem.*, 2006, **71**, 9198−9202

[5] J. F. Wei, J. Jiao, J. J. Feng, J. Lv, X. R. Zhang, X. Y. Shi and Z. G. Chen, *J. Org. Chem.*, 2009, **74**, 6283–6286

Geometry coordinates of **2**−**7** ：

**Compound 2**

| | | | |
|---|---|---|---|
| O | -8.85829800 | 0.87871400 | -0.29945000 |
| O | -7.54859800 | 2.66773200 | 0.17626400 |
| O | 6.63198300 | 3.42288100 | -0.69750800 |
| O | 8.20178000 | 1.95692000 | 0.03053900 |
| N | -3.05099500 | -1.85736300 | -0.20252900 |
| N | -1.17908100 | -2.81871100 | 0.37685800 |
| N | 1.25412800 | -2.93391100 | 0.62447900 |
| N | 3.08800200 | -1.87056600 | 0.10732700 |
| C | -0.04984200 | -3.24602800 | 1.20953100 |
| H | -0.13821900 | -2.75970400 | 2.18190800 |
| H | -0.10026700 | -4.32640200 | 1.35559600 |
| C | -2.12025200 | -1.92365400 | 0.75226400 |
| C | -1.54410700 | -3.34691200 | -0.85694300 |
| H | -0.95592200 | -4.09065400 | -1.37151300 |
| C | -2.70758000 | -2.73898000 | -1.21908000 |
| H | -3.31087200 | -2.84149100 | -2.10810100 |
| C | -4.23388100 | -1.01820800 | -0.17156300 |
| C | 1.91423700 | -1.75896600 | 0.73349800 |
| C | -5.47758200 | -1.60866500 | -0.40863300 |
| H | -5.56704500 | -2.67535000 | -0.58988500 |
| C | -6.61147400 | -0.80070800 | -0.37751200 |
| H | -7.59755400 | -1.21874800 | -0.55061700 |
| C | -6.49958700 | 0.57006500 | -0.10839300 |
| C | -5.24184700 | 1.14029600 | 0.12693600 |
| H | -5.16359700 | 2.20337900 | 0.32225600 |
| C | -4.09514100 | 0.34630700 | 0.09172400 |
| H | -3.11519100 | 0.79211900 | 0.23447900 |
| C | -7.77255900 | 1.37948400 | -0.09042200 |
| C | -8.72741700 | 3.54349900 | 0.21388400 |
| H | -9.22051800 | 3.47605300 | -0.75908700 |
| H | -9.40807700 | 3.14979600 | 0.97291000 |

| | | | |
|---|---|---|---|
| C | -8.24935600 | 4.94427400 | 0.52941100 |
| H | -7.75053600 | 4.98504800 | 1.50213200 |
| H | -9.11186400 | 5.61688900 | 0.56270800 |
| H | -7.56220500 | 5.31274100 | -0.23785400 |
| C | 2.05629200 | -3.82234300 | -0.08556400 |
| H | 1.75840500 | -4.84058900 | -0.28551900 |
| C | 3.19747800 | -3.15436000 | -0.41070100 |
| H | 4.06495000 | -3.46828400 | -0.97068600 |
| C | 4.08385200 | -0.82190300 | -0.00005100 |
| C | 3.69202100 | 0.43731100 | -0.46221400 |
| H | 2.67049300 | 0.62402200 | -0.77991200 |
| C | 4.65276300 | 1.44148800 | -0.55038000 |
| H | 4.39489100 | 2.43201000 | -0.91005100 |
| C | 5.98238200 | 1.18259100 | -0.19289100 |
| C | 6.35450800 | -0.09083700 | 0.25808700 |
| H | 7.38415700 | -0.28123100 | 0.53734100 |
| C | 5.40259500 | -1.10556700 | 0.36075000 |
| H | 5.68252100 | -2.08465000 | 0.73714200 |
| C | 6.96724900 | 2.31878400 | -0.31861600 |
| C | 9.24166600 | 2.99136600 | -0.05680800 |
| H | 9.27658000 | 3.33713200 | -1.09302500 |
| H | 8.93047600 | 3.82683300 | 0.57532600 |
| C | 10.54566800 | 2.37100300 | 0.39552600 |
| H | 10.48308100 | 2.02298300 | 1.43064100 |
| H | 11.33768100 | 3.12393000 | 0.33850500 |
| H | 10.83041300 | 1.53097800 | -0.24458500 |
| H | -2.14890600 | -1.38472000 | 1.68789200 |
| H | 1.57730000 | -0.88423800 | 1.26925900 |

**Complex 3**

| | | | |
|---|---|---|---|
| Pd | -0.27354900 | -1.57861700 | 0.66414500 |
| Br | -2.05041600 | -0.88277100 | 2.30514500 |
| Br | 1.64520400 | -1.08857900 | 2.21693000 |
| O | -6.23474400 | 3.72561800 | -0.28685600 |
| O | -4.11670900 | 4.51141600 | -0.38608500 |
| O | 4.52170400 | 3.91440500 | -0.93307000 |
| O | 6.31203100 | 2.71690600 | -0.24525500 |
| N | -2.87123900 | -1.71074100 | -1.12014300 |
| N | -1.63581800 | -3.47466000 | -1.10999000 |
| N | 0.74602900 | -3.65904500 | -1.13330900 |
| N | 2.23557400 | -2.10734700 | -1.17532800 |
| C | -0.50217700 | -4.33828200 | -0.80444000 |
| H | -0.51101300 | -4.58099800 | 0.26103300 |

| | | | |
|---|---|---|---|
| H | -0.57829200 | -5.25086600 | -1.39660800 |
| C | -1.72613700 | -2.21881900 | -0.58845400 |
| C | -2.71163700 | -3.76280100 | -1.94381600 |
| H | -2.82790100 | -4.70946900 | -2.44772100 |
| C | -3.49063500 | -2.65310200 | -1.94530000 |
| H | -4.40326400 | -2.43471000 | -2.47503000 |
| C | -3.38994500 | -0.38825200 | -0.91707200 |
| C | 1.03098400 | -2.42439400 | -0.63051400 |
| C | -4.76503300 | -0.21927500 | -0.73198000 |
| H | -5.42027600 | -1.08209700 | -0.67204700 |
| C | -5.28161700 | 1.06350500 | -0.57529600 |
| H | -6.34382900 | 1.21871100 | -0.42068600 |
| C | -4.42952900 | 2.17589500 | -0.58843400 |
| C | -3.05081800 | 1.99042700 | -0.76299400 |
| H | -2.38815200 | 2.84757100 | -0.75937300 |
| C | -2.53002900 | 0.71087900 | -0.93424900 |
| H | -1.46416200 | 0.56057300 | -1.05681400 |
| C | -5.03821300 | 3.52730200 | -0.40564700 |
| C | -4.61401600 | 5.85894100 | -0.18676900 |
| H | -5.31261000 | 6.09445400 | -0.99568300 |
| H | -5.16949600 | 5.88665600 | 0.75551900 |
| C | -3.41634900 | 6.79009700 | -0.17266800 |
| H | -2.72742200 | 6.53139400 | 0.63702100 |
| H | -3.75501400 | 7.82031600 | -0.01998400 |
| H | -2.87082300 | 6.74517600 | -1.12035800 |
| C | 1.76205900 | -4.12307900 | -1.96281800 |
| H | 1.72960000 | -5.08505800 | -2.44986600 |
| C | 2.70249600 | -3.14579200 | -1.98395800 |
| H | 3.63835100 | -3.07562600 | -2.51424900 |
| C | 2.93879200 | -0.86620400 | -1.01223100 |
| C | 2.28685500 | 0.33768200 | -1.28317400 |
| H | 1.24407800 | 0.33149400 | -1.57880600 |
| C | 2.98738200 | 1.53354100 | -1.16082800 |
| H | 2.50413500 | 2.48351800 | -1.36118200 |
| C | 4.33497200 | 1.52860000 | -0.77583700 |
| C | 4.97817600 | 0.31120600 | -0.51004400 |
| H | 6.01482300 | 0.30817100 | -0.19481900 |
| C | 4.28035300 | -0.88862800 | -0.62744500 |
| H | 4.75961800 | -1.83069400 | -0.38213300 |
| C | 5.03668100 | 2.84272800 | -0.66823200 |
| C | 7.06333000 | 3.94780000 | -0.09236500 |
| H | 7.09069200 | 4.46025500 | -1.05900200 |
| H | 6.53139300 | 4.59213300 | 0.61407800 |
| C | 8.44985000 | 3.57941400 | 0.40076300 |

| | | | |
|---|---|---|---|
| H | 8.40037500 | 3.06389900 | 1.36472600 |
| H | 9.04692700 | 4.48858700 | 0.52805700 |
| H | 8.96309500 | 2.92970500 | -0.31505300 |

**Complex 4**

| | | | |
|---|---|---|---|
| Pd | -0.01248400 | -1.04189600 | 0.66866300 |
| Br | -1.85810800 | -0.42375500 | 2.26267300 |
| Br | 1.83958600 | -0.38163100 | 2.23717400 |
| O | -6.34442400 | 3.77970600 | -0.36716400 |
| O | -4.31381500 | 4.72765700 | -0.59754000 |
| O | 4.48139100 | 4.72146400 | -0.85553500 |
| O | 6.34619300 | 3.63426600 | -0.21106800 |
| N | -2.57855900 | -1.40147800 | -1.12998200 |
| N | -1.21221800 | -3.06440300 | -1.08580100 |
| N | 1.17773100 | -3.07894300 | -1.07613800 |
| N | 2.56322500 | -1.43349700 | -1.11231800 |
| C | -0.02368500 | -3.84021100 | -0.75360100 |
| H | -0.02983500 | -4.06883500 | 0.31505300 |
| H | -0.02691700 | -4.76374100 | -1.33348700 |
| C | -1.39972400 | -1.81060500 | -0.58636100 |
| C | -2.26000300 | -3.44895800 | -1.91659900 |
| H | -2.30123000 | -4.41032200 | -2.40417200 |
| C | -3.12185100 | -2.40264900 | -1.93944900 |
| H | -4.04662200 | -2.26344900 | -2.47501600 |
| C | -3.19864000 | -0.12022900 | -0.95078300 |
| C | 1.36995900 | -1.82141000 | -0.58705600 |
| C | -4.57825200 | -0.05929700 | -0.73340300 |
| H | -5.15646800 | -0.97132600 | -0.62826800 |
| C | -5.19509600 | 1.18081000 | -0.60323800 |
| H | -6.26211300 | 1.25393400 | -0.42333100 |
| C | -4.43666500 | 2.35721200 | -0.67840100 |
| C | -3.05171700 | 2.28159700 | -0.88559800 |
| H | -2.46278700 | 3.19001700 | -0.93092800 |
| C | -2.43216900 | 1.04347300 | -1.02894700 |
| H | -1.36158800 | 0.97514300 | -1.17942800 |
| C | -5.14466200 | 3.65732600 | -0.52972800 |
| C | 2.23925700 | -3.48693700 | -1.87780000 |
| H | 2.27983300 | -4.45549800 | -2.35101300 |
| C | 3.11381000 | -2.45053200 | -1.89558300 |
| H | 4.05306900 | -2.32674700 | -2.40974900 |
| C | 3.18499800 | -0.15023900 | -0.94899500 |
| C | 2.45587100 | 1.01100100 | -1.21150900 |
| H | 1.41269900 | 0.93984300 | -1.49603600 |

| | | | |
|---|---|---|---|
| C | 3.07956800 | 2.24808800 | -1.09086600 |
| H | 2.53502900 | 3.16592100 | -1.28367500 |
| C | 4.42827400 | 2.32583000 | -0.71633600 |
| C | 5.15017200 | 1.15177500 | -0.45715900 |
| H | 6.18730900 | 1.21252700 | -0.14901900 |
| C | 4.52809700 | -0.08889000 | -0.57268500 |
| H | 5.06813500 | -0.99884100 | -0.33266500 |
| C | 5.04921600 | 3.67395100 | -0.61102300 |
| H | -4.86458900 | 5.51884600 | -0.47746700 |
| H | 6.65202700 | 4.55513800 | -0.16309100 |

**Complex 5**

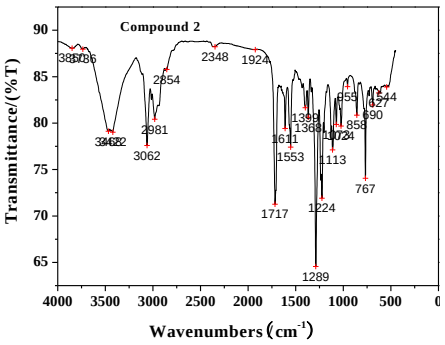
| | | | |
|---|---|---|---|
| Pd | -0.08277900 | -1.03277100 | 0.81413800 |
| Br | 1.80289300 | -0.33561700 | 2.32378700 |
| O | -6.52320400 | 3.66070000 | -0.03003500 |
| O | -4.54526000 | 4.62999100 | -0.50206600 |
| O | 4.31972600 | 4.71113900 | -0.93085000 |
| O | 6.21202700 | 3.64611000 | -0.33122000 |
| N | -2.72426800 | -1.48841100 | -0.84186300 |
| N | -1.32532400 | -3.12412500 | -0.83188900 |
| N | 1.06467000 | -3.11486900 | -0.90382100 |
| N | 2.43450900 | -1.45941700 | -1.01937200 |
| C | -0.11638600 | -3.88019100 | -0.52537700 |
| H | -0.08337500 | -4.08719700 | 0.54731300 |
| H | -0.12969500 | -4.81538000 | -1.08617200 |
| C | -1.50445200 | -1.85659300 | -0.36524400 |
| C | -2.41939700 | -3.55796800 | -1.57383300 |
| H | -2.47427100 | -4.53730500 | -2.02279400 |
| C | -3.30089300 | -2.52755800 | -1.57671600 |
| H | -4.26134000 | -2.42259000 | -2.05431800 |
| C | -3.35377800 | -0.20957300 | -0.67394200 |
| C | 1.26270100 | -1.84623300 | -0.44602200 |
| C | -4.70893000 | -0.16094200 | -0.33544000 |
| H | -5.25367900 | -1.07626100 | -0.12845400 |
| C | -5.33952000 | 1.07372800 | -0.21912900 |
| H | -6.38719700 | 1.13846400 | 0.05362600 |
| C | -4.61847000 | 2.25686400 | -0.43162800 |
| C | -3.25644700 | 2.19382200 | -0.75971900 |
| H | -2.69561500 | 3.10832500 | -0.91230300 |
| C | -2.62405300 | 0.96044300 | -0.88785800 |
| H | -1.57076100 | 0.90208500 | -1.13416600 |
| C | -5.34059100 | 3.55049700 | -0.29478200 |
| C | 2.10197700 | -3.53028300 | -1.73311400 |

| | | | |
|---|---|---|---|
| H | 2.13461400 | -4.50768200 | -2.18834300 |
| C | 2.96657800 | -2.48784400 | -1.80056000 |
| H | 3.88700200 | -2.36725400 | -2.34835900 |
| C | 3.05308300 | -0.16956800 | -0.90076200 |
| C | 2.30729500 | 0.98296200 | -1.15500900 |
| H | 1.25469100 | 0.90113000 | -1.39898300 |
| C | 2.92642300 | 2.22565200 | -1.07594600 |
| H | 2.36854600 | 3.13674800 | -1.26229600 |
| C | 4.28707200 | 2.31781300 | -0.75108300 |
| C | 5.02582200 | 1.15246700 | -0.50040900 |
| H | 6.07283000 | 1.22452400 | -0.23050900 |
| C | 4.40875500 | -0.09379600 | -0.57497000 |
| H | 4.96400600 | -0.99614900 | -0.34105700 |
| C | 4.90209200 | 3.67118400 | -0.68833200 |
| H | -5.10193100 | 5.41649700 | -0.37847700 |
| H | 6.51278100 | 4.56960600 | -0.30839400 |
| Cl | -1.78451500 | -0.32932800 | 2.32717700 |

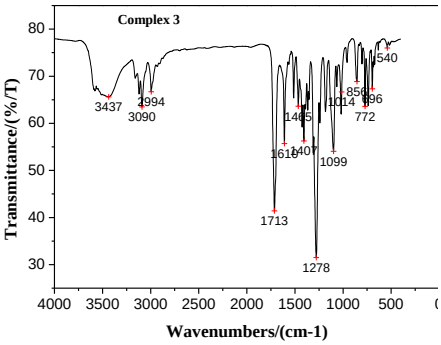
**Complex 7**

| | | | |
|---|---|---|---|
| Pd | -0.00932900 | -1.02696000 | 0.96831100 |
| O | -6.38621000 | 3.68102300 | -0.11965100 |
| O | -4.39550000 | 4.62928100 | -0.58047600 |
| O | 4.53922700 | 4.62639700 | -0.71396900 |
| O | 6.39357500 | 3.55093000 | -0.02165000 |
| N | -2.59985000 | -1.50401200 | -0.74008500 |
| N | -1.21246800 | -3.14819000 | -0.66573300 |
| N | 1.17930800 | -3.15635600 | -0.66634200 |
| N | 2.57676000 | -1.52150900 | -0.74181200 |
| C | -0.01931200 | -3.90793400 | -0.31415100 |
| H | -0.01978700 | -4.10187100 | 0.76159500 |
| H | -0.02266200 | -4.85005200 | -0.86343000 |
| C | -1.39703500 | -1.87290700 | -0.22182000 |
| C | -2.28719800 | -3.58571800 | -1.43348700 |
| H | -2.33523200 | -4.57108700 | -1.86979700 |
| C | -3.16127700 | -2.55006900 | -1.47674500 |
| H | -4.10693600 | -2.44587100 | -1.98315800 |
| C | -3.22553800 | -0.21830300 | -0.61248300 |
| C | 1.36948900 | -1.88011200 | -0.22753700 |
| C | -4.58650200 | -0.15545900 | -0.30082800 |
| H | -5.13956100 | -1.06321400 | -0.08280600 |
| C | -5.21261800 | 1.08462800 | -0.22524600 |
| H | -6.26477700 | 1.16089500 | 0.02646400 |
| C | -4.48168800 | 2.25895400 | -0.45251300 |

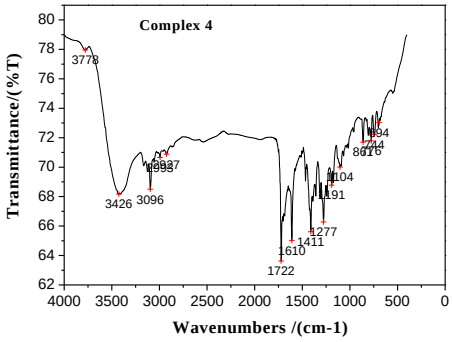
| | | | |
|---|---|---|---|
| C | -3.11434400 | 2.18181200 | -0.75439600 |
| H | -2.54613600 | 3.08967900 | -0.91883200 |
| C | -2.48613300 | 0.94269400 | -0.84157100 |
| H | -1.42891800 | 0.87358600 | -1.06778200 |
| C | -5.19966100 | 3.55883600 | -0.36047100 |
| C | 2.25572400 | -3.60467400 | -1.42544600 |
| H | 2.30005000 | -4.59270100 | -1.85612800 |
| C | 3.13656100 | -2.57450400 | -1.46934400 |
| H | 4.08619000 | -2.47789900 | -1.96999200 |
| C | 3.20487800 | -0.23601400 | -0.62219400 |
| C | 2.48428800 | 0.92026300 | -0.92697400 |
| H | 1.44002600 | 0.84742200 | -1.20671400 |
| C | 3.11704000 | 2.15616300 | -0.85166700 |
| H | 2.57845500 | 3.06978700 | -1.07810000 |
| C | 4.46627500 | 2.23863800 | -0.47964900 |
| C | 5.17842200 | 1.07005700 | -0.17385900 |
| H | 6.21551200 | 1.13454800 | 0.13370300 |
| C | 4.54757500 | -0.16972700 | -0.24476000 |
| H | 5.08156500 | -1.07353400 | 0.02977500 |
| C | 5.09756000 | 3.58479600 | -0.42612600 |
| H | -4.95045800 | 5.42106700 | -0.48646800 |
| H | 6.70628100 | 4.47065500 | -0.01017400 |
| Cl | -1.74351200 | -0.28859500 | 2.42456700 |
| Cl | 1.73771800 | -0.28142500 | 2.40666100 |



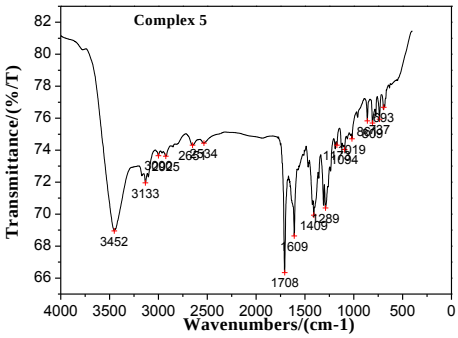

Compound **2**



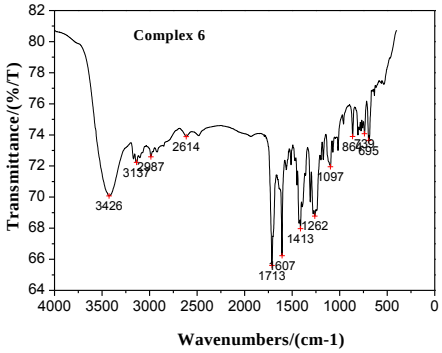

Complex **3**



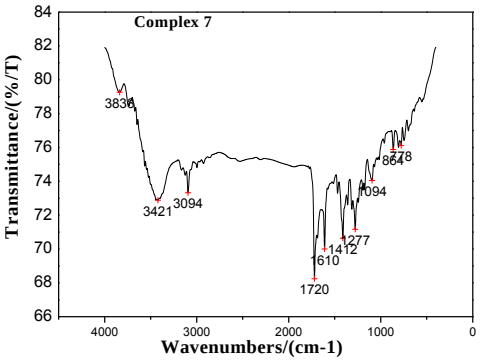

Complex **4**




Complex **5**




Complex **6**




Complex **7**

**Figure S1** the measured IR spectra of **2**–**7**

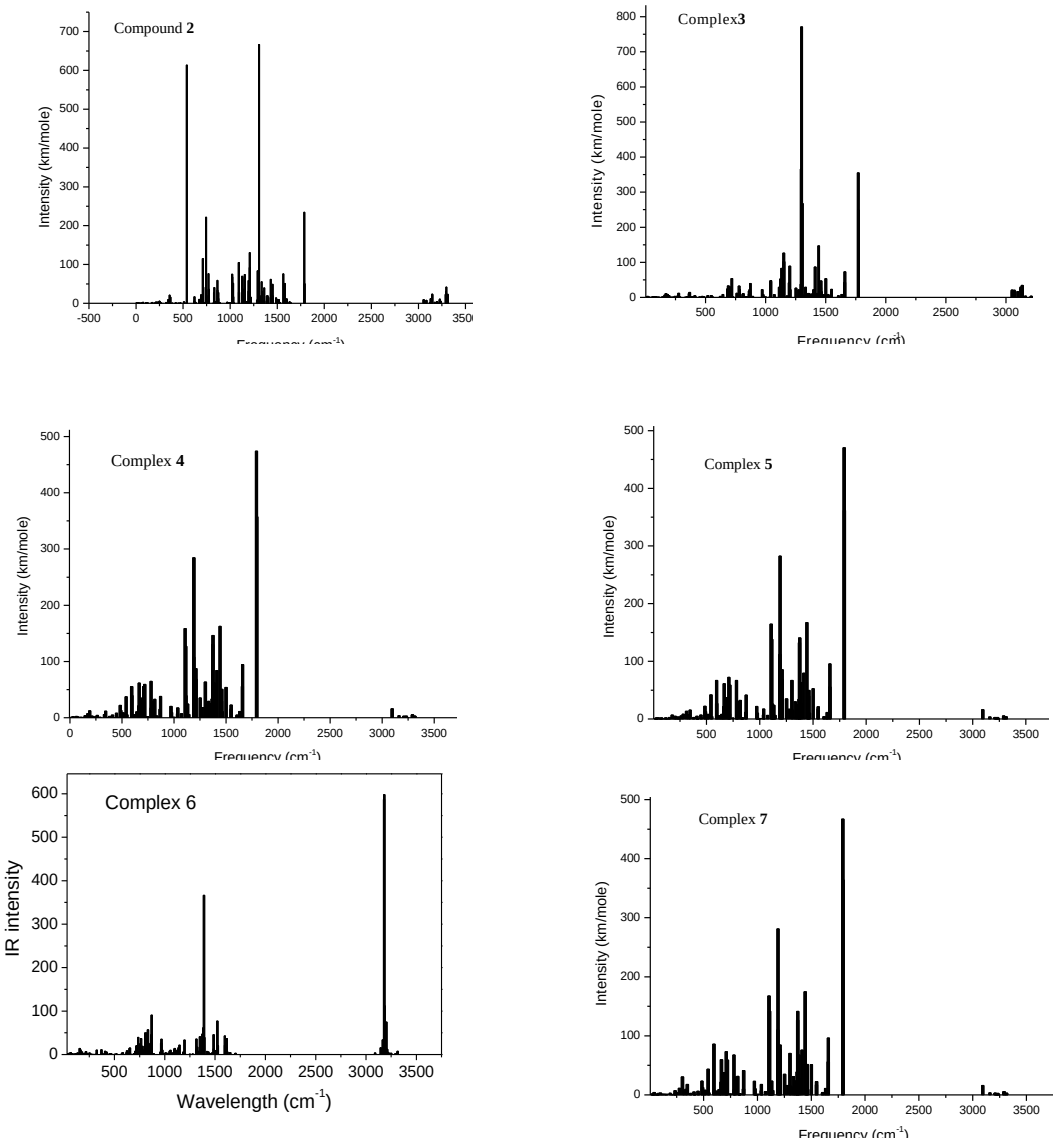
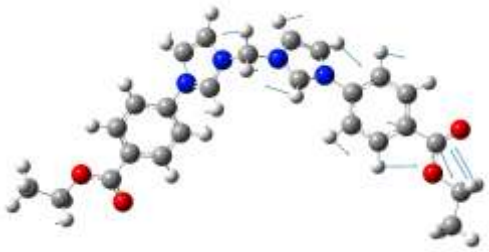


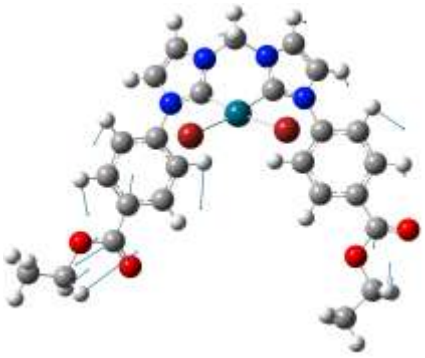

**Figure S2.** The calculated IR spectra of **2**–**7**.

Table S1. Calculated (unscaled) vibration wavenumbers ($cm^{-1}$) and intensities of the strongest vibrations for **2**–**7**.

| Compound | Wavenumber ($cm^{-1}$) | IR intensity |
|---|---|---|
| **2** | 1306.6695 | 666.8305 |
| **3** | 1298.9788 | 771.2047 |
| **4** | 1792.9253 | 474.1367 |
| **5** | 1792.7335 | 470.3788 |
| **6** | 1703.4328 | 598.1502 |
| **7** | 1792.7088 | 467.114 |



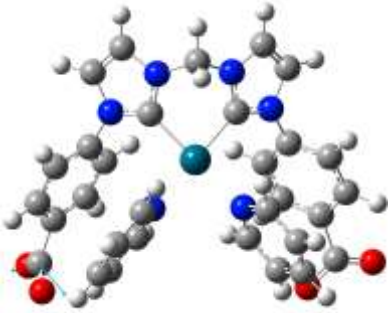
**Compound 2**



**Complex 3**

**Complex 4**

**Complex 5**

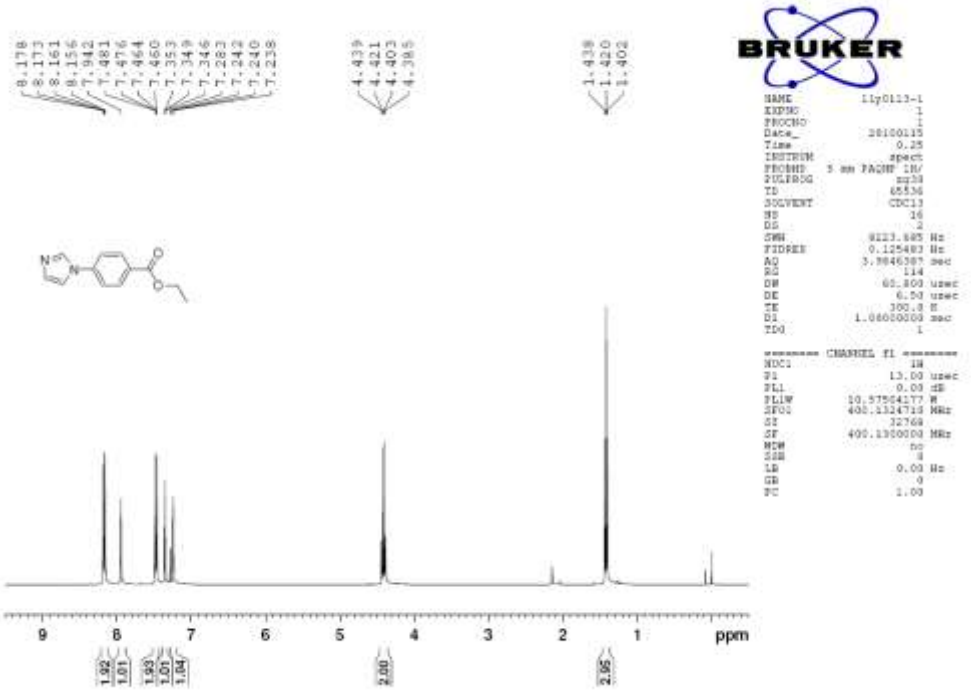


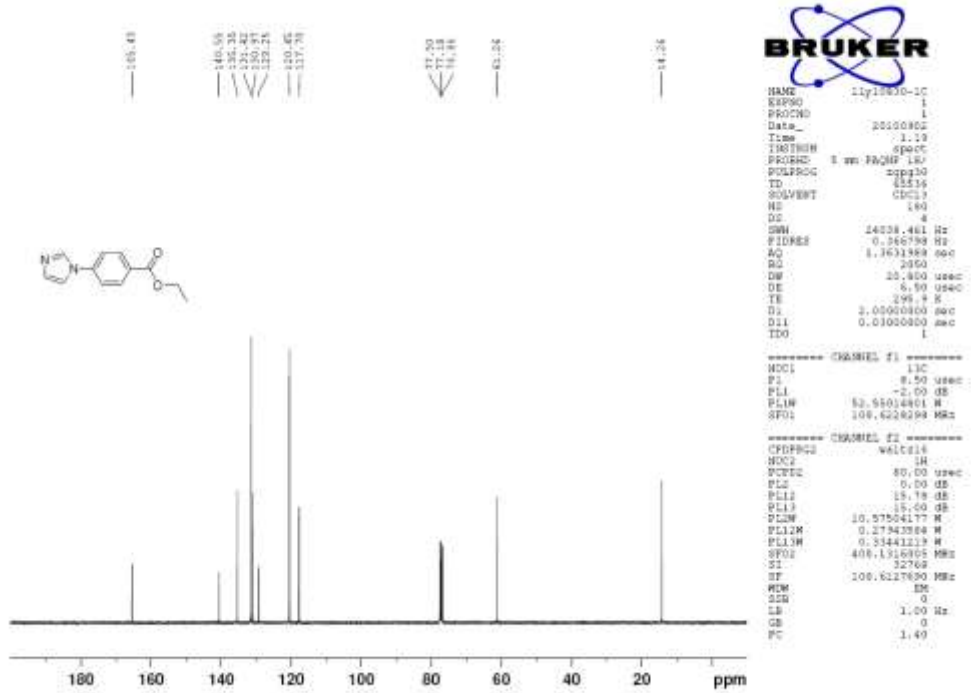
**Complex 6**

**Complex 7**

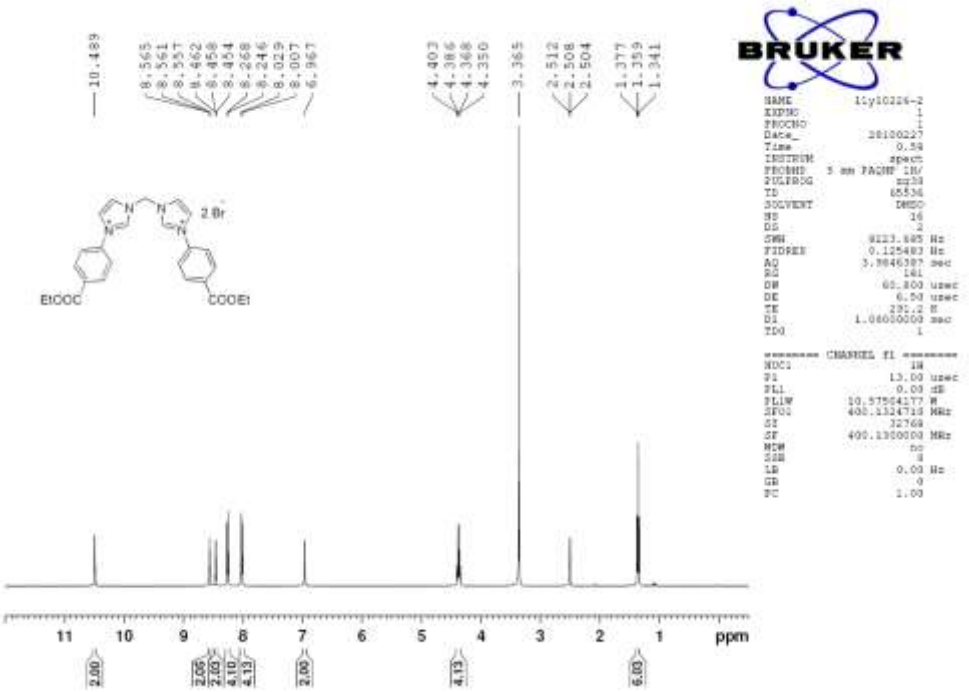
**Figure S3**. The investigated vibration modes of **2**−**7**.

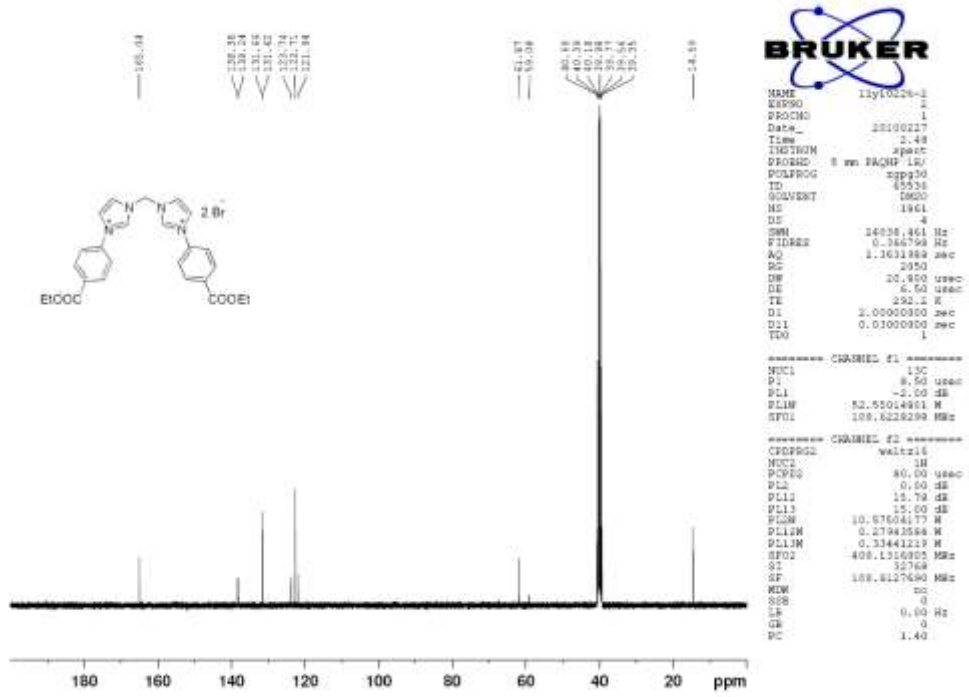
**Ethyl 4-(1H-imidazol-1-yl)benzoate (1)**



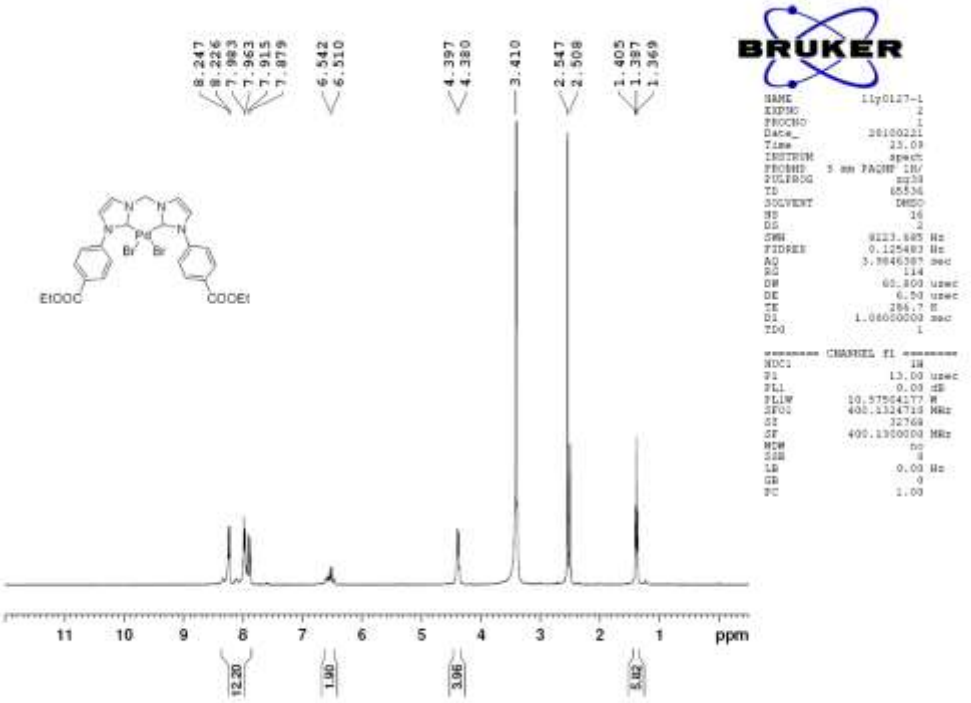



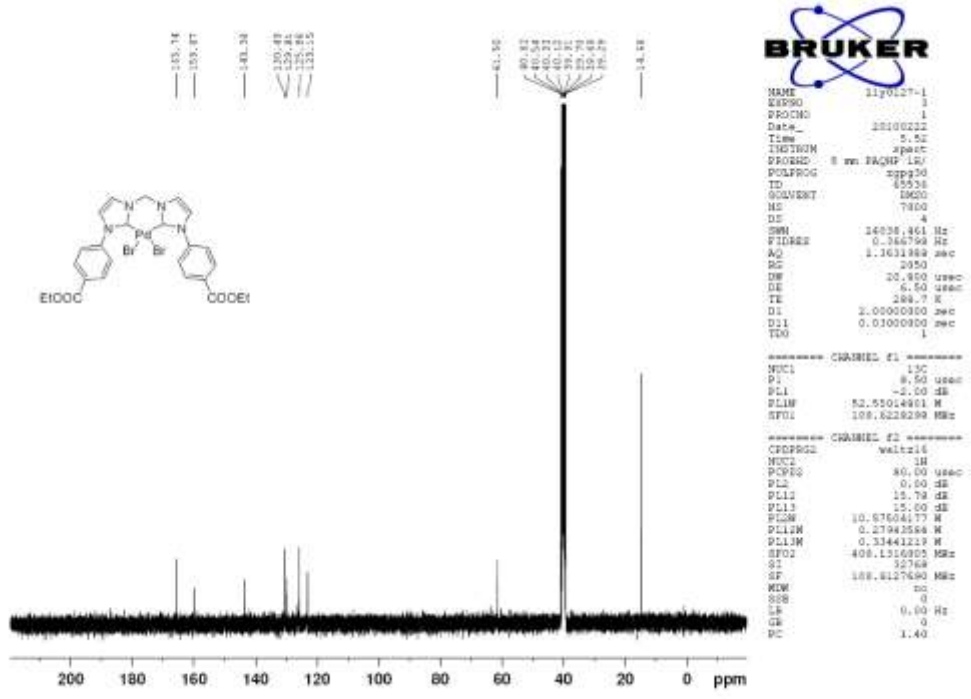
**1,1-Bis[1-(4-ethylcarboxyphenyl)]-3,3'-methylenimidazolium dibromide (2)**



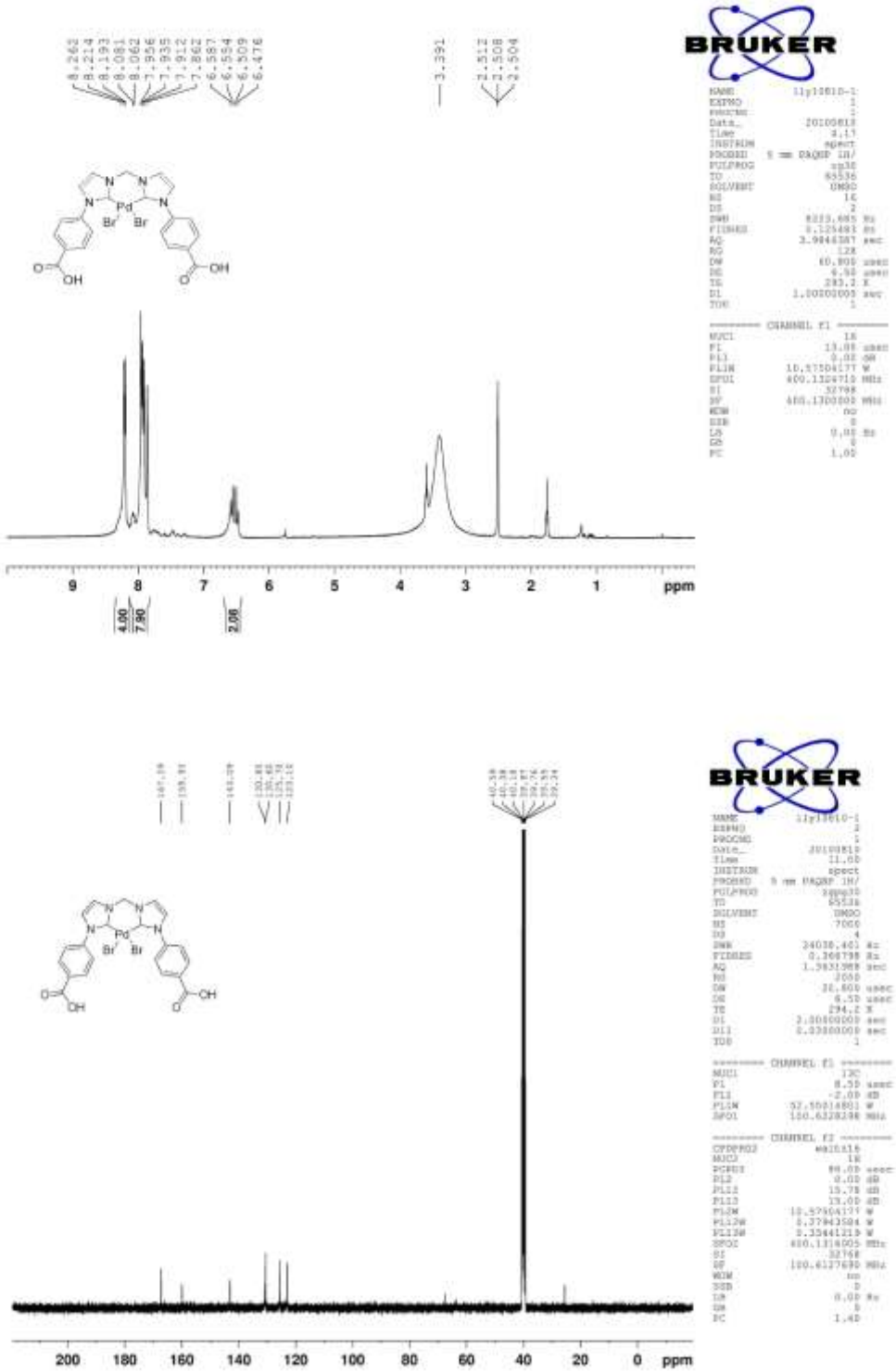



**Palladium(II) Complex (3)**

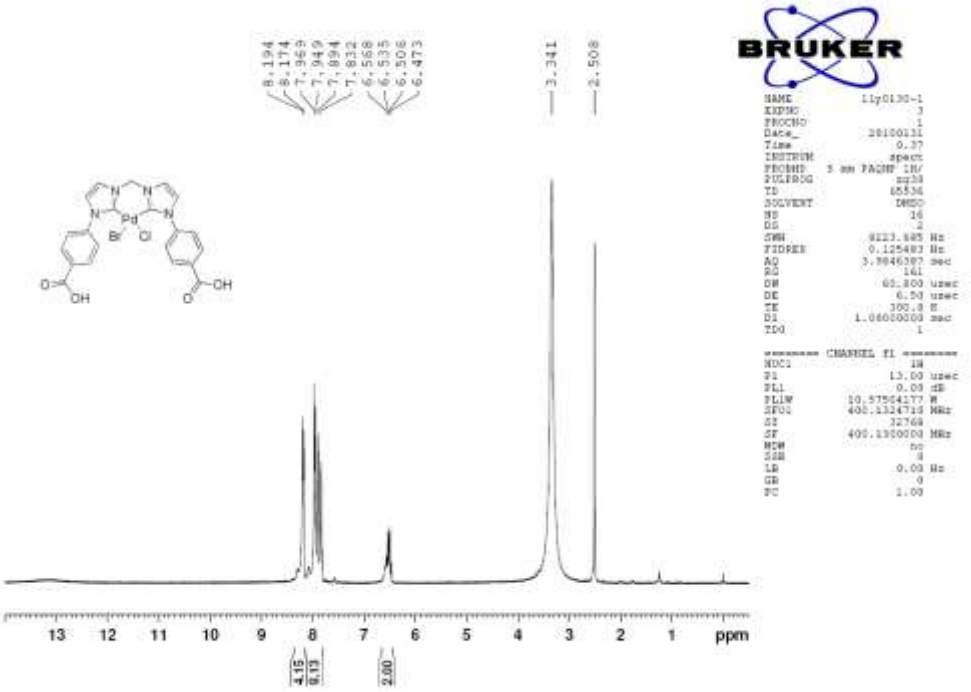


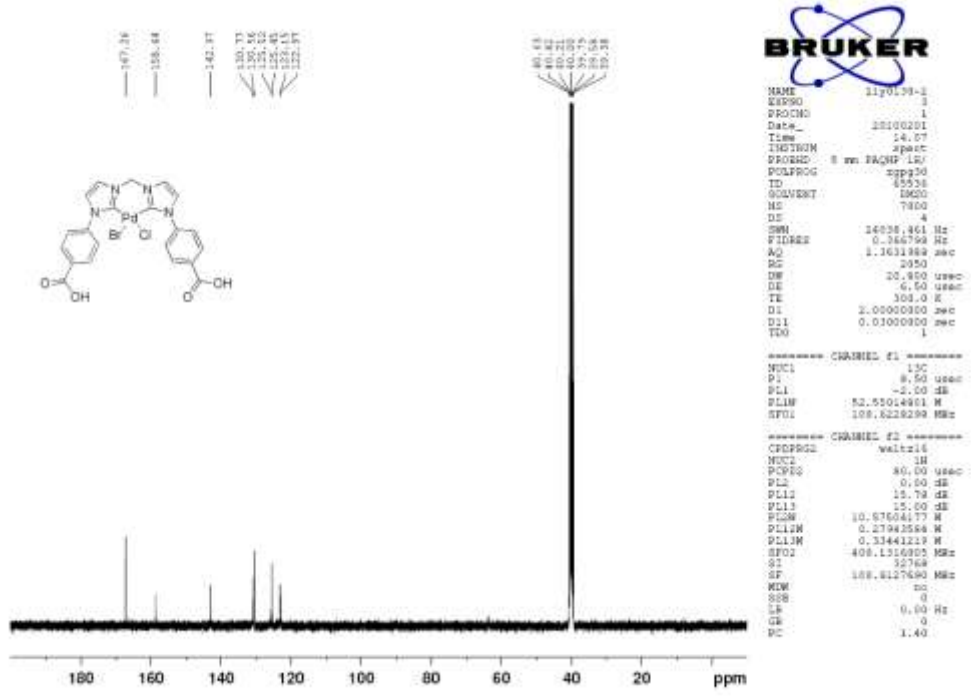



**Palladium(II) Complex (4)**

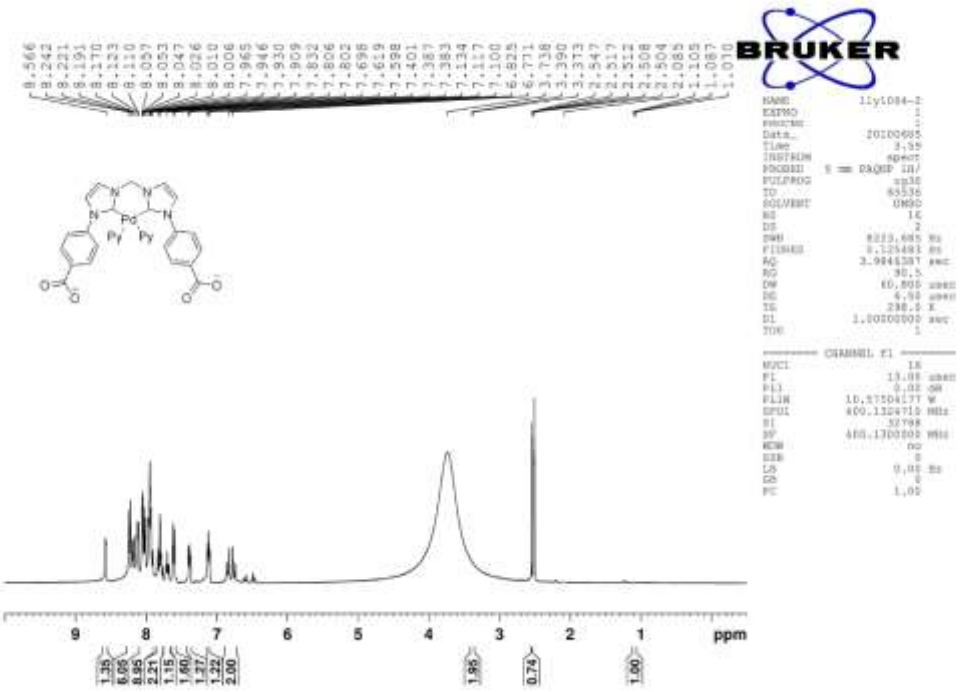


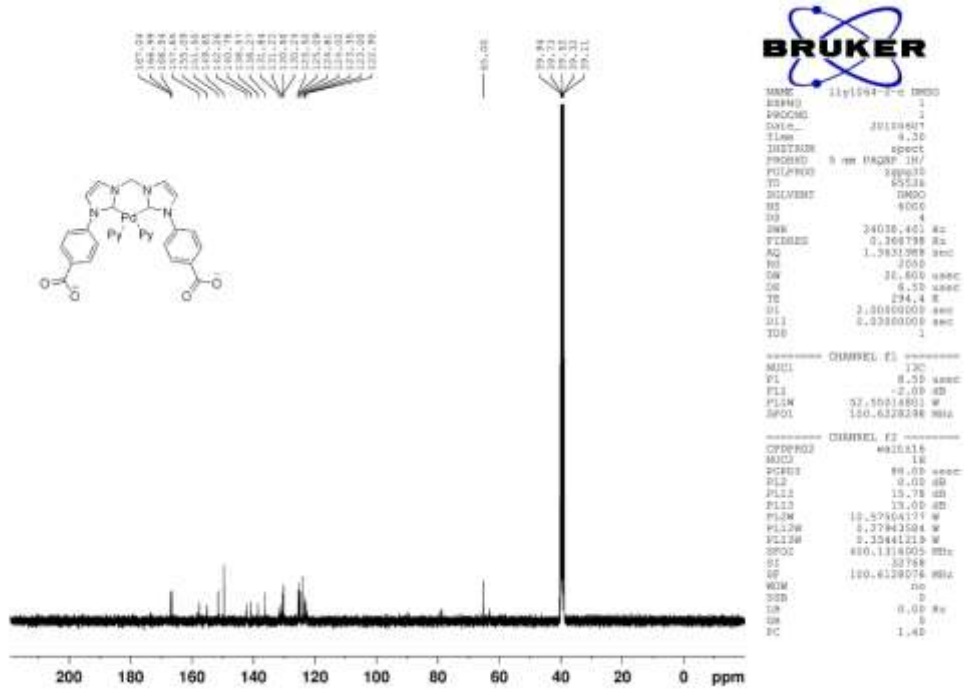
**Palladium(II) Complex (5)**



**Palladium(II) Complex (6)**



**Palladium(II) Complex (7)**