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Supplementary Material for "Reaction of Alkenylzirconocene with Dialkylzirconocene:
Unexpected Formation of Bimetallic (μ -Alkynyl)zirconocene Complexes."

Atomic Coordinates and Equivalent Isotropic Displacement Parameters (\AA^2)

| atom | <i>x</i> / <i>a</i> | <i>y</i> / <i>b</i> | <i>z</i> / <i>c</i> | U_{eq} |
|-------|---------------------|---------------------|---------------------|-----------------|
| Zr(1) | 0.30704(2) | 0.36835(3) | 0.29617(2) | 0.0323(1) |
| Zr(2) | 0.16826(2) | 0.65273(4) | 0.14760(2) | 0.0344(1) |
| Cl | 0.16959(6) | 0.3324(1) | 0.14443(6) | 0.0450(3) |
| C(1) | 0.2182(4) | 0.3875(6) | 0.3923(4) | 0.077(3) |
| C(2) | 0.1875(3) | 0.2408(6) | 0.3411(3) | 0.062(2) |
| C(3) | 0.2576(3) | 0.1281(5) | 0.3656(4) | 0.068(2) |
| C(4) | 0.3300(3) | 0.2000(7) | 0.4322(3) | 0.072(2) |
| C(5) | 0.3070(4) | 0.3597(7) | 0.4480(3) | 0.077(2) |
| C(6) | 0.4246(3) | 0.4016(6) | 0.2323(4) | 0.067(2) |
| C(7) | 0.4692(3) | 0.3679(7) | 0.3218(4) | 0.070(2) |
| C(8) | 0.4513(3) | 0.2076(7) | 0.3393(3) | 0.072(2) |
| C(9) | 0.3946(3) | 0.1370(5) | 0.2627(3) | 0.068(2) |
| C(10) | 0.3757(3) | 0.2500(6) | 0.1935(3) | 0.062(2) |
| C(11) | 0.0684(5) | 0.8674(6) | 0.1717(6) | 0.099(4) |
| C(12) | 0.0936(3) | 0.7675(7) | 0.2439(3) | 0.067(2) |
| C(13) | 0.0571(4) | 0.6128(7) | 0.2163(6) | 0.096(4) |
| C(14) | 0.0103(4) | 0.622(1) | 0.1269(7) | 0.140(5) |
| C(15) | 0.0158(5) | 0.771(2) | 0.1023(4) | 0.150(5) |
| C(16) | 0.2086(6) | 0.8807(6) | 0.0676(5) | 0.102(4) |
| C(17) | 0.1425(3) | 0.7746(9) | -0.0006(3) | 0.086(2) |
| C(18) | 0.1854(3) | 0.6245(7) | 0.0026(3) | 0.072(2) |
| C(19) | 0.2687(4) | 0.6284(6) | 0.0629(3) | 0.070(2) |
| C(20) | 0.2852(3) | 0.7804(6) | 0.1021(3) | 0.064(2) |
| C(21) | 0.2785(2) | 0.6620(4) | 0.2696(2) | 0.036(1) |
| C(22) | 0.3456(2) | 0.6348(4) | 0.3415(2) | 0.040(1) |
| C(23) | 0.4140(3) | 0.7257(5) | 0.4160(3) | 0.066(2) |

$$U_{\text{eq}} = 1/3 \{ \sum_i \sum_j U_{ij} a_i^* a_j^* a_i a_j \}$$

Atomic Coordinates and Equivalent Isotropic Displacement Parameters (\AA^2)

| atom | x/a | y/b | z/c | U_{eq} |
|--------|---------|--------|---------|-----------------|
| H(1) | 0.1803 | 0.5019 | 0.3899 | 0.077 |
| H(2) | 0.1204 | 0.2212 | 0.2905 | 0.062 |
| H(3) | 0.2564 | 0.0025 | 0.3371 | 0.069 |
| H(4) | 0.3945 | 0.1398 | 0.4655 | 0.070 |
| H(5) | 0.3509 | 0.4482 | 0.4952 | 0.076 |
| H(6) | 0.4267 | 0.5195 | 0.1992 | 0.066 |
| H(7) | 0.5120 | 0.4565 | 0.3697 | 0.071 |
| H(8) | 0.4768 | 0.1480 | 0.4039 | 0.073 |
| H(9) | 0.3684 | 0.0079 | 0.2572 | 0.068 |
| H(10) | 0.3326 | 0.2304 | 0.1238 | 0.061 |
| H(11) | 0.0854 | 0.9997 | 0.1681 | 0.105 |
| H(12) | 0.1362 | 0.8024 | 0.3118 | 0.068 |
| H(13) | 0.0636 | 0.5009 | 0.2565 | 0.099 |
| H(14) | -0.0260 | 0.5182 | 0.0838 | 0.135 |
| H(15) | -0.0166 | 0.8133 | 0.0333 | 0.149 |
| H(16) | 0.1982 | 1.0079 | 0.0849 | 0.101 |
| H(17) | 0.0741 | 0.8076 | -0.0436 | 0.085 |
| H(18) | 0.1550 | 0.5150 | -0.0389 | 0.071 |
| H(19) | 0.3162 | 0.5247 | 0.0779 | 0.071 |
| H(20) | 0.3488 | 0.8192 | 0.1539 | 0.065 |
| H(23A) | 0.3860 | 0.7902 | 0.4320 | 0.064 |
| H(23B) | 0.4551 | 0.8123 | 0.4100 | 0.064 |
| H(23C) | 0.4494 | 0.6405 | 0.4692 | 0.064 |

$$U_{\text{eq}} = 1/3 \{ \sum_i \sum_j U_{ij} a_i^* a_j^* a_i a_j \}$$

Atomic Anisotropic Displacement Parameters (\AA^2)

| atom | U_{11} | U_{22} | U_{33} | U_{12} | U_{13} | U_{23} |
|-------|----------|----------|----------|-----------|----------|-----------|
| Zr(1) | .0354(2) | .0279(1) | .0398(2) | -.0037(1) | .0214(1) | -.0055(1) |
| Zr(2) | .0351(2) | .0353(2) | .0321(2) | -.0066(1) | .0123(1) | -.0048(1) |
| Cl | .0477(4) | .0375(4) | .0495(5) | -.0128(3) | .0185(4) | -.0142(3) |
| C(1) | .117(4) | .065(3) | .097(4) | .014(3) | .092(4) | .017(3) |
| C(2) | .050(2) | .080(3) | .067(3) | -.009(2) | .037(2) | .015(2) |
| C(3) | .077(3) | .046(2) | .095(4) | -.005(2) | .048(3) | .018(2) |
| C(4) | .071(3) | .078(3) | .066(3) | -.004(3) | .027(2) | .030(3) |
| C(5) | .099(4) | .094(4) | .048(2) | -.033(3) | .041(3) | -.006(2) |
| C(6) | .055(2) | .073(3) | .100(4) | .014(2) | .059(3) | .018(3) |
| C(7) | .037(2) | .097(4) | .082(3) | .002(2) | .029(2) | -.020(3) |
| C(8) | .067(3) | .080(3) | .071(3) | .031(3) | .028(2) | -.004(3) |
| C(9) | .081(3) | .056(3) | .078(3) | .022(2) | .044(3) | -.009(2) |
| C(10) | .055(2) | .091(3) | .051(2) | .019(2) | .032(2) | -.009(2) |
| C(11) | .118(5) | .057(3) | .163(7) | .038(3) | .100(5) | .028(4) |
| C(12) | .053(2) | .100(4) | .055(2) | .010(2) | .027(2) | -.016(3) |
| C(13) | .084(4) | .066(3) | .185(7) | .015(3) | .105(5) | .026(4) |
| C(14) | .032(3) | .183(8) | .20(1) | -.021(4) | .035(4) | -.126(8) |
| C(15) | .096(5) | .29(1) | .059(3) | .123(7) | .019(3) | .016(6) |
| C(16) | .192(7) | .041(2) | .133(5) | .003(3) | .128(6) | .020(3) |
| C(17) | .070(3) | .126(5) | .063(3) | .016(3) | .027(2) | .048(3) |
| C(18) | .078(3) | .101(4) | .041(2) | -.024(3) | .028(2) | -.004(2) |
| C(19) | .087(3) | .078(3) | .062(3) | -.009(3) | .047(3) | .003(2) |
| C(20) | .073(3) | .071(3) | .060(2) | -.025(2) | .039(2) | -.002(2) |
| C(21) | .039(2) | .030(1) | .041(2) | -.004(1) | .018(1) | -.006(1) |
| C(22) | .046(2) | .031(1) | .043(2) | -.005(1) | .017(1) | -.007(1) |
| C(23) | .067(3) | .041(2) | .058(2) | -.007(2) | -.009(2) | -.009(2) |

Expression for displacement parameters is

$$\exp[-2\pi^2(U_{11}h^2a^{*2}+U_{22}k^2b^{*2}+U_{33}l^2c^{*2}+2U_{12}hka^*b^*+2U_{13}hla^*c^*+2U_{23}klb^*c^*)]$$

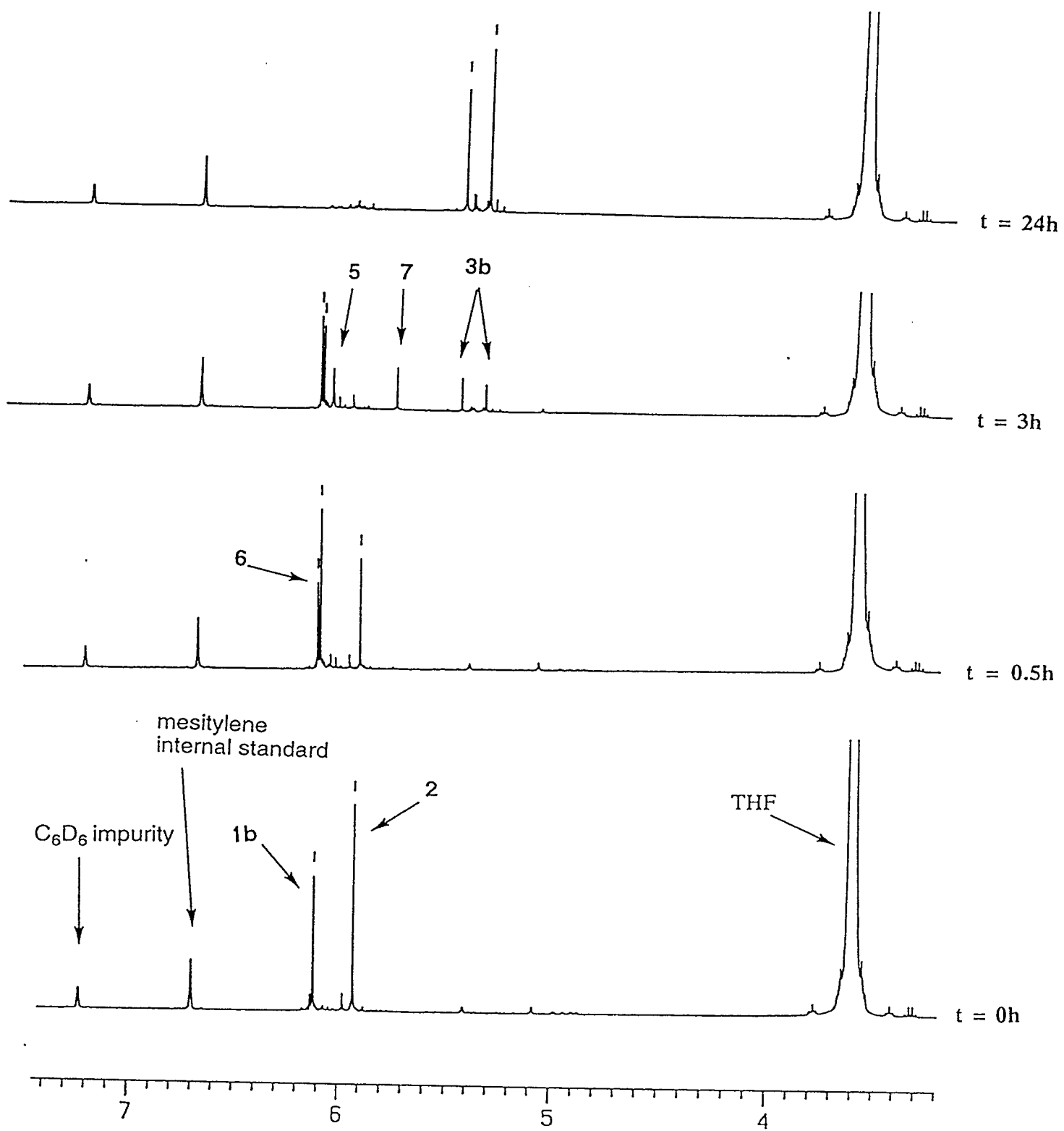


Fig. 1 $^1\text{H-NMR}$ spectra of the reaction mixture of 1b and 2 ($t = 0\text{h}$, 0.5h , 3h and 24h).