ORGANOMETALLICS
Organometallics, 1997, 16(10), 2216-2219, DOI:10.1021/om960414u

OM9604140

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

Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2)

atom	*x/a*	*y/b*	*z/c*	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)

$U_{eq}=1/3\{\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* a_i a_j\}$

Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^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

$U_{eq}=1/3\{\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* a_i a_j\}$

Atomic Anisotropic Displacement Parameters ($Å^2$)

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

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

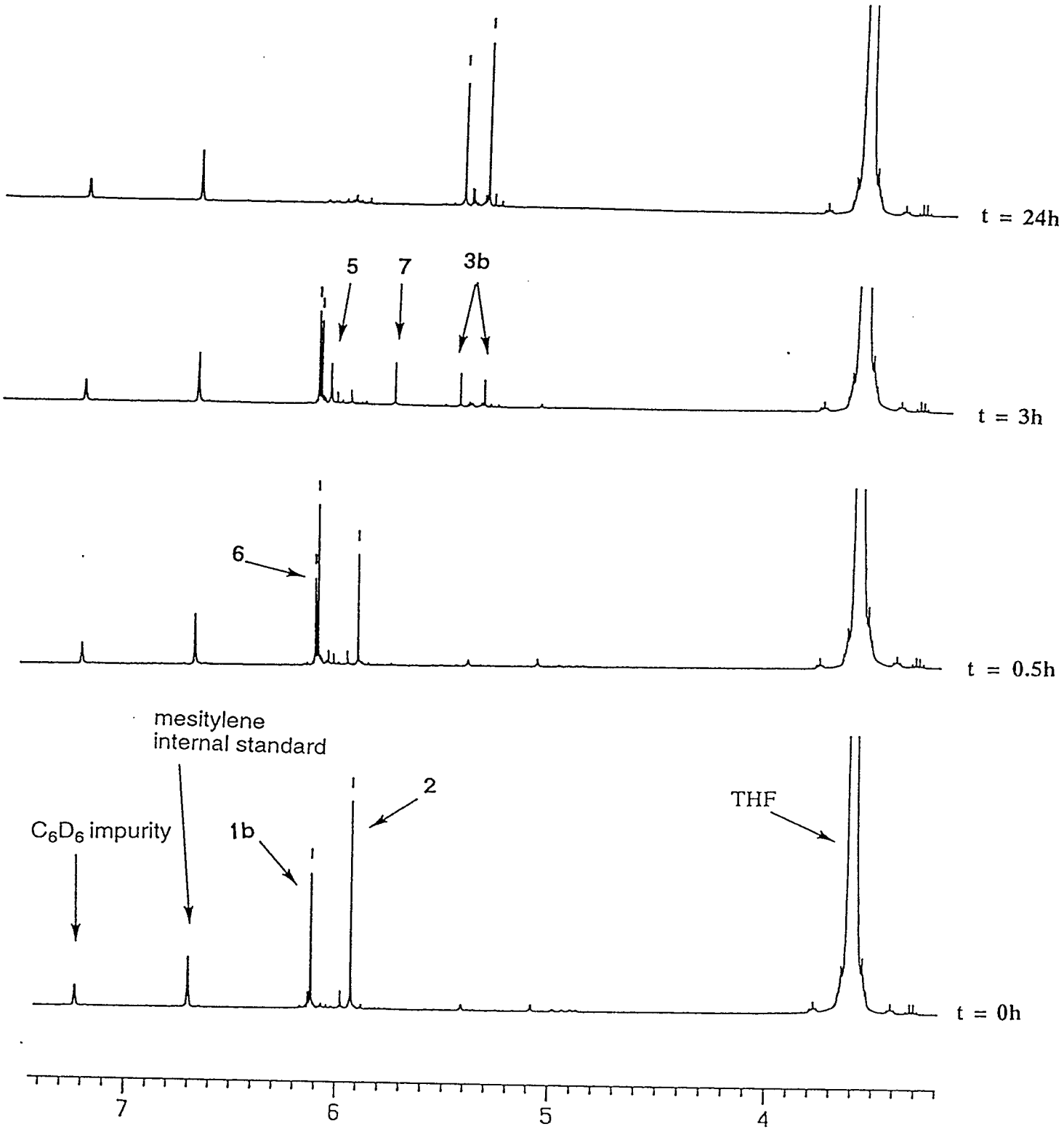

Fig. 1 ^{1}H-NMR spectra of the reaction mixture of **1b** and **2** (t = 0h, 0.5h, 3h and 24h).