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Supplementary Material for "Reactivity of Permethylscandocene
Derivatives with Acetylene. Structure of *Bis* (permethylscandocene)

Acetylene-diyl, $(\eta^5\text{-C}_5\text{Me}_5)_2\text{Sc-C}\equiv\text{C-Sc}(\eta^5\text{-C}_5\text{Me}_5)_2$ "

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Abstract.

The structure of bis (bis (pentamethylcyclopentadienyl) scandium) acetylene, $(\text{C}_{10}\text{H}_{15})_2\text{Sc-C}\equiv\text{C-Sc}(\text{C}_{10}\text{H}_{15})_2 \cdot 1/2 \text{C}_7\text{H}_8$, has been determined. It crystallizes in the tetragonal system, in space group $P\bar{4}2_1c$ (#114), with $a=15.057(3)\text{\AA}$, $c=18.617(6)\text{\AA}$, volume = $4220.7(18)\text{\AA}^3$; $z=4$.

Experimental. A long prism was cleaved with a razor blade in an argon atmosphere and a fragment was placed with a little grease in a capillary. The crystal was centered on the diffractometer and preliminary cell dimensions plus an orientation matrix were calculated from the setting angles of 25 reflections. Two octants of data were collected and final cell dimensions were obtained from the setting angles of 24 reflections with $25^\circ < 2\theta < 38^\circ$. The data were corrected for a slight decay (2.2%) and Lorentz and polarization factors plus a Wilson scale factor were applied. The Laue group and the systematic absences in the diffractometer data were only consistent with the non-centrosymmetric space group $P\bar{4}2_1c$. The scandium atom was located from a Patterson map and the remaining atoms of the molecule found with

subsequent structure factor-Fourier cycles. Full matrix least squares converged with an R-index of 15%; the difference map had many peaks in it, but none greater than $|0.75| \text{ e}\text{\AA}^{-3}$. A region of positive density centered at $1/2, 1/2, 0$ (a $\bar{4}$ point) was interpreted as a disordered toluene molecule; because the atoms of the toluene all have z coordinates nearly equal to zero, the disorder is effectively four-fold. An idealized toluene was fitted to the map (C-C ring, 1.38\AA ; C-CH₃, 1.56\AA) with isotropic thermal parameters, B, of 10\AA^2 assigned; the toluene parameters were not refined, but were re-adjusted once toward the end of the refinement. Hydrogen atoms were introduced on the Cp* methyl groups at idealized positions based on difference maps calculated in the planes where they were expected; they were assigned isotropic thermal parameters 20% greater than the equivalent isotropic thermal parameter of their carbon atom. These hydrogen atoms were also adjusted once toward the end of the refinement. Refinement of the rest of the scandium dimer concluded smoothly, with the final R-index for reflections with $F_o^2 > 3\sigma(F_o^2)$ being 0.047. Crystal data are given in Table I, final parameters in Table II and selected distances and angles in Table III.

Calculations were done with programs of the CRYM Crystallographic Computing System and ORTEP. Scattering factors and corrections for anomalous scattering were taken from a standard reference (International Tables for X-ray Crystallography, Vol. IV, p. 71, p. 149; Birmingham, Kynoch Press, 1974). $R = \sum |F_o - |F_c|| / \sum F_o$, for only $F_o^2 > 0$, and goodness of fit = $[\sum w(F_o^2 - F_c^2)^2 / (n - p)]^{1/2}$ where n is the number of data and p the number of parameters refined. The function minimized in least squares was $\sum w(F_o^2 - F_c^2)^2$, where $w = 1/\sigma^2(F_o^2)$. Variances of the individual reflections were assigned based on counting statistics plus an additional term, $0.014I^2$. Variances of the merged reflections were determined by standard propagation of error plus another additional term, $0.014 \langle I \rangle^2$. The secondary extinction parameter (Larson, E. C. Acta Cryst. 1967, 23, 664, eqn. 3) refined to $0.08(6) \times 10^{-6}$.

Table SI. Crystal and Intensity Collection Data

Formula:	Formula Weight: 700.93
Crystal Color: pale yellow	Habit: prismatic
$a = 15.057(3) \text{ \AA}$	
$c = 18.617(6) \text{ \AA}$	
$v = 4220.7(18) \text{ \AA}^3$	$z = 4$
$\lambda = 0.71073 \text{ \AA}$	T: 22
Graphite monochromator	
Space group: $P\bar{4}2_1c$	Absences: $h00, h = 2n + 1; hhl, l = 2n + 1$
Crystal Size: .22 x .35 x .48mm	$\mu = 3.56 \text{ cm}^{-1} (\mu_{\text{max}} = 0.11)$
CAD-4 Diffractometer	ω scan
2θ range: $2^\circ - 40^\circ$	Octants collected: $h, k, \pm l$
Number reflections measured: 5284	
Number of independent reflections: 1460	
Number with $F_o^2 > 0$: 1327	
Number with $F_o^2 > 3\sigma(F_o^2)$: 894	
Goodness of fit for merging data: 0.967	
Final R-index: 0.0835	
Final goodness of fit: 1.71	

Table III. Final Parameters for $\text{Bis}[(\text{bis Cp}^*)\text{Sc}]$
Acetylene.

x, y, z and $U_{eq}^a \times 10^4$

Atom	x	y	z	U_{eq}
Sc	3220(.8)	537(.9)	1529(.8)	370(4)
C1	4616(4)	133(5)	1451(4)	439(21)
Cp1	1852(5)	275(5)	815(4)	409(24)
Cp2	2552(6)	346(6)	326(4)	444(24)
Cp3	3110(5)	-393(6)	427(4)	486(26)
Cp4	2767(5)	-887(5)	997(4)	436(25)
Cp5	1976(5)	-483(5)	1240(4)	437(24)
Me1	1018(5)	840(5)	785(4)	721(29)
Me2	2682(6)	1053(6)	-240(4)	837(32)
Me3	3899(5)	-667(6)	-31(4)	808(28)
Me4	3135(6)	-1757(5)	1285(5)	855(32)
Me5	1350(5)	-864(5)	1787(4)	714(27)
Cp6	3602(6)	2026(5)	1985(5)	502(29)
Cp7	3873(6)	1434(6)	2535(5)	490(26)
Cp8	3095(7)	1027(5)	2785(4)	484(24)
Cp9	2357(6)	1404(6)	2428(5)	500(26)
Cp10	2675(6)	2006(5)	1927(5)	521(29)
Me6	4237(5)	2603(5)	1563(6)	817(28)
Me7	4792(5)	1328(5)	2836(4)	679(27)
Me8	3049(6)	356(6)	3392(5)	889(29)
Me9	1391(5)	1264(6)	2637(4)	720(30)
Me10	2143(5)	2653(5)	1489(5)	794(28)

$$^a U_{eq} = \frac{1}{3} \sum_i \sum_j [U_{ij} (a_i^* a_j^*) (\vec{a}_i \cdot \vec{a}_j)]$$

Table SIII. Assigned Parameters for $(Cp_2^*Sc)_2C_2$. x, y and $z \times 10^4$

Atom	x	y	z	B
C2	4608	4880	31	10.0
C3	5418	4475	95	10.0
C4	6170	5000	104	10.0
C5	6125	5920	48	10.0
C6	5290	6301	-17	10.0
C7	4530	5780	-25	10.0
C8	3741	4310	21	10.0
H 1A	645	717	1197	6.2
H 1B	689	699	360	6.2
H 1C	1171	1450	785	6.2
H 2A	2127	1166	-473	7.9
H 2B	3090	819	-600	7.9
H 2C	2916	1564	-35	7.9
H 3A	4394	-687	213	8.2
H 3B	3925	-221	-431	8.2
H 3C	3733	-1218	-267	8.2
H 4A	3748	-1640	1417	7.8
H 4B	3130	-2170	900	7.8
H 4C	2812	-1945	1675	7.8
H 5A	1679	-1274	2076	6.8
H 5B	898	-1185	1531	6.8
H 5C	1110	-409	2058	6.8
H6AA	4030	3209	1551	7.6
H6AB	4334	2395	1095	7.6
H6AC	4816	2619	1813	7.6
H6BA	4381	3136	1849	7.6
H6BB	4003	2787	1122	7.6
H6BC	4796	2299	1488	7.6
H 7A	4911	1799	3172	6.5
H 7B	5225	1344	2464	6.5
H 7C	4835	772	3087	6.5
H 8A	3638	189	3545	7.4
H 8B	2756	-184	3227	7.4
H 8C	2730	579	3793	7.4
H9AA	1348	693	2904	6.4
H9AB	1006	1253	2256	6.4
H9AC	1219	1716	2985	6.4
H9BA	1382	1136	3168	6.4
H9BB	1146	756	2413	6.4
H9BC	1046	1769	2564	6.4
H10A	1531	2502	1542	7.4
H10B	2330	2641	1021	7.4
H10C	2236	3233	1703	7.4
H10D	1830	3031	1834	7.4
H10E	1734	2344	1213	7.4
H10F	2533	3001	1219	7.4

Table SIV. Anisotropic Displacement Parameters for $(Cp_2Sc)_2C_2$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sc	284(9)	410(10)	415(8)	28(8)	-25(10)	-26(10)
Cl	395(53)	489(47)	434(49)	-26(47)	-97(43)	-28(48)
Cp1	222(46)	471(60)	534(56)	6(48)	-72(52)	-90(47)
Cp2	416(57)	519(67)	397(53)	-64(57)	-44(49)	-15(50)
Cp3	358(57)	686(71)	413(51)	-138(63)	3(51)	-192(54)
Cp4	388(58)	338(55)	581(59)	37(44)	-160(51)	-96(49)
Cp5	388(59)	377(54)	545(58)	-40(51)	-51(47)	32(50)
Me1	433(54)	711(70)	1018(72)	12(54)	-250(58)	-179(59)
Me2	927(81)	968(85)	615(63)	-14(62)	8(60)	355(65)
Me3	657(60)	1152(82)	616(58)	-14(70)	-60(54)	-414(63)
Me4	869(68)	510(57)	1187(97)	11(57)	-375(67)	-64(63)
Me5	673(60)	706(67)	763(68)	-201(53)	102(53)	-40(53)
Cp6	449(64)	361(63)	695(71)	10(51)	79(55)	-63(54)
Cp7	361(58)	512(61)	596(63)	-70(53)	22(56)	-234(53)
Cp8	581(65)	481(53)	391(55)	25(58)	98(60)	-174(46)
Cp9	377(61)	553(64)	570(62)	26(53)	47(56)	-180(53)
Cp10	478(68)	358(61)	727(68)	107(52)	-41(58)	-12(52)
Me6	711(64)	634(59)	1107(77)	-248(54)	98(72)	2(74)
Me7	590(67)	802(70)	645(57)	50(52)	-182(52)	-364(55)
Me8	1154(78)	913(73)	601(55)	-107(67)	149(76)	-189(67)
Me9	472(62)	740(71)	949(73)	-11(52)	165(57)	-164(63)
Me10	759(65)	545(57)	1078(74)	147(50)	-129(71)	-128(68)

The form of the displacement factor is:

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

Table SV. Complete Distances and Angles for $(\text{Cp}_2\text{Sc})_2\text{C}_2$.

Distance(Å)		Distance(Å)	
Sc -C1	2.194(7)	Me6 -H6AA	0.964(9)
Sc -Cp1	2.483(8)	Me6 -H6AB	0.937(9)
Sc -Cp2	2.472(8)	Me6 -H6AC	0.989(9)
Sc -Cp3	2.490(8)	Me6 -H6BA	0.987(9)
Sc -Cp4	2.457(8)	Me6 -H6BB	0.936(9)
Sc -Cp5	2.480(8)	Me6 -H6BC	0.968(9)
Sc -Cp6	2.465(9)	Me7 -H 7A	0.963(8)
Sc -Cp7	2.510(9)	Me7 -H 7B	0.951(8)
Sc -Cp8	2.458(8)	Me7 -H 7C	0.961(8)
Sc -Cp9	2.488(9)	Me8 -H 8A	0.964(9)
Sc -Cp10	2.473(8)	Me8 -H 8B	0.975(9)
C1 -C1	1.224(9)	Me8 -H 8C	0.950(9)
Cp1 -Cp2	1.396(11)	Me9 -H9AA	0.995(8)
Cp1 -Cp5	1.401(11)	Me9 -H9AB	0.916(8)
Cp1 -Me1	1.518(11)	Me9 -H9AC	0.974(8)
Cp2 -Cp3	1.407(11)	Me9 -H9BA	1.007(8)
Cp2 -Me2	1.510(12)	Me9 -H9BB	0.946(8)
Cp3 -Cp4	1.396(11)	Me9 -H9BC	0.932(8)
Cp3 -Me3	1.520(12)	Me10-H10A	0.954(8)
Cp4 -Cp5	1.411(11)	Me10-H10B	0.916(8)
Cp4 -Me4	1.521(11)	Me10-H10C	0.970(8)
Cp5 -Me5	1.502(11)	Me10-H10D	0.979(8)
Me1 -H 1A	0.968(8)	Me10-H10E	0.928(8)
Me1 -H 1B	0.957(8)	Me10-H10F	0.933(8)
Me1 -H 1C	0.947(8)	C2 -C3	1.369(0)
Me2 -H 2A	0.956(9)	C2 -C7	1.364(0)
Me2 -H 2B	0.974(9)	C2 -C8	1.563(0)
Me2 -H 2C	0.928(9)	C3 -C4	1.381(0)
Me3 -H 3A	0.874(8)	C4 -C5	1.391(0)
Me3 -H 3B	1.004(8)	C5 -C6	1.387(0)
Me3 -H 3C	0.971(8)	C6 -C7	1.387(0)
Me4 -H 4A	0.971(8)		
Me4 -H 4B	0.949(8)		
Me4 -H 4C	0.919(8)		
Me5 -H 5A	0.957(8)		
Me5 -H 5B	0.961(8)		
Me5 -H 5C	0.925(8)		
Cp6 -Cp7	1.418(12)		
Cp6 -Cp10	1.401(12)		
Cp6 -Me6	1.512(12)		
Cp7 -Cp8	1.402(12)		
Cp7 -Me7	1.501(12)		
Cp8 -Cp9	1.415(12)		
Cp8 -Me8	1.517(12)		
Cp9 -Cp10	1.384(12)		
Cp9 -Me9	1.521(12)		
Cp10-Me10	1.503(12)		

Table SV. (Cont.)

Angle(°)			Angle(°)		
C1 -C1 -Sc	175.1(6)		Me6 -Cp6 -Cp7	123.7(8)	
Cp5 -Cp1 -Cp2	109.3(7)		Me6 -Cp6 -Cp10	127.1(8)	
Me1 -Cp1 -Cp2	123.9(7)		Cp8 -Cp7 -Cp6	105.9(7)	
Me1 -Cp1 -Cp5	125.9(7)		Me7 -Cp7 -Cp6	127.0(8)	
Cp3 -Cp2 -Cp1	107.6(7)		Me7 -Cp7 -Cp8	126.9(8)	
Me2 -Cp2 -Cp1	127.4(7)		Cp9 -Cp8 -Cp7	108.9(7)	
Me2 -Cp2 -Cp3	124.9(7)		Me8 -Cp8 -Cp7	125.2(8)	
Cp4 -Cp3 -Cp2	107.6(7)		Me8 -Cp8 -Cp9	125.6(8)	
Me3 -Cp3 -Cp2	127.4(7)		Cp10 -Cp9 -Cp8	107.9(8)	
Me3 -Cp3 -Cp4	124.8(7)		Me9 -Cp9 -Cp8	125.1(8)	
Cp5 -Cp4 -Cp3	109.1(7)		Me9 -Cp9 -Cp10	126.4(8)	
Me4 -Cp4 -Cp3	126.3(7)		Cp9 -Cp10-Cp6	107.9(7)	
Me4 -Cp4 -Cp5	124.5(7)		Me10 -Cp10-Cp6	123.9(7)	
Cp4 -Cp5 -Cp1	106.4(7)		Me10 -Cp10-Cp9	127.3(8)	
Me5 -Cp5 -Cp1	127.7(7)		H6AA-Me6 -Cp6	110.6(8)	
Me5 -Cp5 -Cp4	125.6(7)		H6AB-Me6 -Cp6	112.9(8)	
H 1A-Me1 -Cp1	110.2(7)		H6AC-Me6 -Cp6	109.1(8)	
H 1B-Me1 -Cp1	109.6(7)		H6BA-Me6 -Cp6	109.0(8)	
H 1C-Me1 -Cp1	110.0(7)		H6BB-Me6 -Cp6	112.9(8)	
H 1B-Me1 -H 1A	108.2(8)		H6BC-Me6 -Cp6	110.7(8)	
H 1C-Me1 -H 1A	109.0(8)		H6AB-Me6 -H6AA	110.1(9)	
H 1C-Me1 -H 1B	109.9(8)		H6AC-Me6 -H6AA	105.8(8)	
H 2A-Me2 -Cp2	109.2(8)		H6AC-Me6 -H6AB	108.0(8)	
H 2B-Me2 -Cp2	107.9(8)		H6BB-Me6 -H6BA	108.3(8)	
H 2C-Me2 -Cp2	110.3(8)		H6BC-Me6 -H6BA	105.7(8)	
H 2B-Me2 -H 2A	107.7(9)		H6BC-Me6 -H6BB	109.9(9)	
H 2C-Me2 -H 2A	111.7(9)		H 7A -Me7 -Cp7	109.6(7)	
H 2C-Me2 -H 2B	110.1(9)		H 7B -Me7 -Cp7	111.0(7)	
H 3A-Me3 -Cp3	112.6(8)		H 7C -Me7 -Cp7	109.7(7)	
H 3B-Me3 -Cp3	105.3(7)		H 7B -Me7 -H 7A	109.1(8)	
H 3C-Me3 -Cp3	106.4(7)		H 7C -Me7 -H 7A	108.2(7)	
H 3B-Me3 -H 3A	112.1(8)		H 7C -Me7 -H 7B	109.3(8)	
H 3C-Me3 -H 3A	115.3(9)		H 8A -Me8 -Cp8	110.6(8)	
H 3C-Me3 -H 3B	104.3(8)		H 8B -Me8 -Cp8	110.0(8)	
H 4A-Me4 -Cp4	106.2(7)		H 8C -Me8 -Cp8	111.9(8)	
H 4B-Me4 -Cp4	107.1(7)		H 8B -Me8 -H 8A	107.0(8)	
H 4C-Me4 -Cp4	110.5(8)		H 8C -Me8 -H 8A	109.0(8)	
H 4B-Me4 -H 4A	108.5(8)		H 8C -Me8 -H 8B	108.3(8)	
H 4C-Me4 -H 4A	111.2(8)		H9AA-Me9 -Cp9	108.1(7)	
H 4C-Me4 -H 4B	113.1(8)		H9AB-Me9 -Cp9	114.1(8)	
H 5A-Me5 -Cp5	107.6(7)		H9AC-Me9 -Cp9	109.1(7)	
H 5B-Me5 -Cp5	107.5(7)		H9BA-Me9 -Cp9	106.9(7)	
H 5C-Me5 -Cp5	109.3(7)		H9BB-Me9 -Cp9	111.9(8)	
H 5B-Me5 -H 5A	108.8(8)		H9BC-Me9 -Cp9	112.5(8)	
H 5C-Me5 -H 5A	111.8(8)		H9AB-Me9 -H9AA	109.3(8)	
H 5C-Me5 -H 5B	111.6(8)		H9AC-Me9 -H9AA	104.7(8)	
Cp10-Cp8 -Cp7	109.2(8)		H9AC-Me9 -H9AB	111.1(8)	

Table SV. (Cont.)

Angle(°)

H9BB-Me9 -H9BA	105.9(8)
H9BC-Me9 -H9BA	107.0(8)
H9BC-Me9 -H9BB	112.2(8)
H10A -Me10-Cp10	107.6(7)
H10B -Me10-Cp10	109.8(8)
H10C -Me10-Cp10	106.5(7)
H10D -Me10-Cp10	106.1(7)
H10E -Me10-Cp10	109.2(8)
H10F -Me10-Cp10	108.7(7)
H10B -Me10-H10A	113.0(8)
H10C -Me10-H10A	108.2(8)
H10C -Me10-H10B	111.4(8)
H10E -Me10-H10D	109.6(8)
H10F -Me10-H10D	109.3(8)
H10F -Me10-H10E	113.7(9)
C7 -C2 -C3	121.7(0)
C8 -C2 -C3	120.1(0)
C8 -C2 -C7	118.2(0)
C4 -C3 -C2	118.4(0)
C5 -C4 -C3	121.9(0)
C6 -C5 -C4	117.6(0)
C7 -C6 -C5	121.0(0)
C6 -C7 -C2	119.3(0)

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Bis ((bis Cp*)Sc} Acetylene										Page	2				
4	665	671	-9	16	213	198	10	17	-96	60	-8				
5	306	284	35	17	-97	4	-6					1	339	323	25
6	514	540	-44					6	3	1		2	476	469	12
7	402	413	-18		5	5	1					3	463	450	21
8	430	429	1					0	278	278	0	4	261	247	18
9	365	366	-1	0	308	300	9	1	461	453	15	5	126	121	3
10	382	393	-15	2	326	296	33	2	288	315	-43	6	92	82	4
11	201	200	0	4	355	316	42	3	299	279	30	7	-80	1	-16
12	237	255	-16	6	625	627	-2	4	145	190	-43	8	114	108	2
13	304	309	-5	8	182	181	0	5	291	283	12	9	-29	56	-8
14	235	237	-1	10	257	243	9	6	235	232	3	10	192	187	4
15	247	236	8	12	309	305	3	7	235	227	8	11	38	71	-7
16	261	267	-5	14	236	249	-7	8	290	275	18	12	62	43	3
17	330	349	-6	16	239	150	14	9	140	123	9	13	157	166	-4
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				14	0	1		6	160	129	5	2	158	170	-2
								7				3	199	198	0
				0	402	396	6					4	160	144	3
				1	229	223	4	14	5	1		5	-79	35	-4
				2	107	130	-10								
				3	74	17	9	0	91	106	-1	15	4	1	
				4	212	180	21	1	203	99	21				
				5	27	54	-1	2	116	39	9	0	-155	30	-15
				6	196	171	5	3	92	82	1	1	328	299	10
				7	67	6	3	4	94	45	4	2	61	65	0
				8	-64	33	-3	5	270	212	17	3	134	150	-3
				9	191	167	5	6	147	72	10	4	-30	32	-1
				14	1	1		14	6	1		15	5	1	
								0	118	74	5				
				0	265	247	14	1	100	102	0	0	-115	29	-8
				1	322	326	-3	2	-175	73	-23	1	155	124	5
								3	116	44	7				