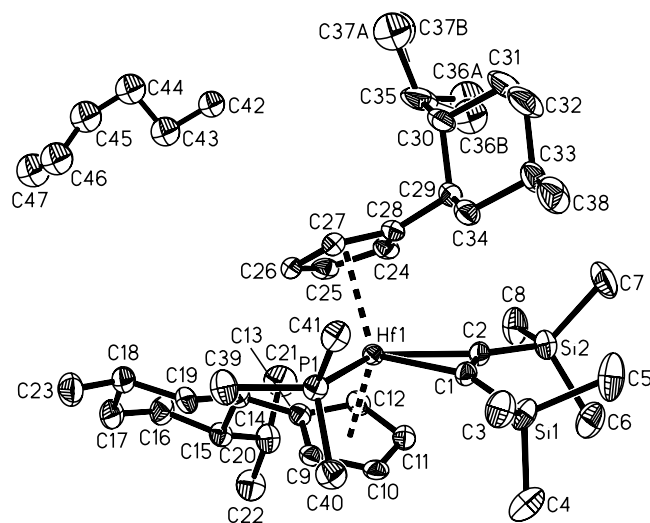


Crystal structure of 1-bis(((1*R*,2*S*,5*R*)-2-isopropyl-5-methylcyclohexyl)cyclopentadienyl)-1-trimethylphosphine-2,3-bis(trimethylsilyl)-1-hafnacycloprop-2-ene — hexane (1:0.5), (HfC₈H₁₈Si₂)(C₁₅H₂₂)₂(PC₃H₉) · 0.5C₆H₁₄

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Received January 11, 2010, accepted and available on-line January 30, 2010; CCDC no. 1267/2899



Abstract

C₄₄H₇₈HfPSi₂, tetragonal, *P*₄12₁2 (no. 92), *a* = 14.9634(2) Å, *c* = 44.9270(8) Å, *V* = 10059.3 Å³, *Z* = 8, *R*_g(*F*) = 0.026, *wR*_{ref}(*F*²) = 0.073, *T* = 200 K.

Source of material

(η^5 -menthyl-C₅H₄)₂HfCl₂ (0.650 g, 0.991 mmol) and magnesium turnings (0.025 g, 1.029 mmol) were dissolved in 15 ml of THF, followed by the addition of bis(trimethylsilyl)acetylene (0.23 ml, 1.015 mmol) and trimethylphosphine (1.0 ml, 1.0 mmol, *c* = 1 M in THF). The solution was stirred at 50 °C for 24 h, the color of the solution changed from colorless to brown. The solvent was removed under vacuum, and the obtained residue was extracted with 20 ml of *n*-hexane. Leaving the *n*-hexane solution at –78 °C gave fine, yellow crystals, which were dried under vacuum.

Discussion

For stoichiometric and catalytic reactions of organometallic compounds it is necessary to have suitable complex fragments that are coordinatively and electronically unsaturated. In group 4 chemistry such complex fragments are titanocene Cp*₂Ti, zirconocene Cp*₂Zr, and hafnocene Cp*₂Hf (Cp* = substituted or unsubstituted η^5 -cyclopentadienyl), which are considered as generally unstable 14-electron compounds having a *d*² configuration [1]. The aim is to find an adequate precursor that liberates the very re-

active core complex under mild conditions. Such suitable systems are metallocene alkyne complexes of the type Cp*₂M(η^2 -Me₃SiC₂SiMe₃) (Cp* = Cp or substituted cyclopentadienyl; M = Ti, Zr, Hf). Until recently, the hafnocene alkyne complexes have been unknown, as the first examples were reported by our group [2]. In a different paper, we showed the applicability of a chiral modification, namely, the menthyl substituted cyclopentadienyl ligand [3]. Throughout these investigations the new chiral-substituted hafnocene dichloride (η^5 -menthyl-C₅H₄)₂HfCl₂ was synthesized. The reaction of the titanium and zirconium analogues (η^5 -menthyl-C₅H₄)₂MCl₂ (M = Ti, Zr) with magnesium in THF in the presence of the bistrimethylsilylacetylene yielded the corresponding alkyne complexes (η^5 -menthyl-C₅H₄)₂M(η^2 -Me₃SiC₂SiMe₃) (M = Ti, Zr) [4]. Herein, we present the molecular structure of the first hafnocene alkyne complex with the menthyl substituted cyclopentadienyl ligand. Other than the titanium and zirconium analogues, an additional ligand is mandatory to form the title compound.

The molecular structure shows a hafnacyclopropene unit with two bent cyclopentadienyl ligands and the attached phosphine. The alkyne is coordinated unsymmetrically to the hafnium shown by two different C—Hf distances (*d*(C1—Hf1) = 2.282(5) Å, *d*(C2—Hf1) = 2.211(5) Å). Also the C—C—Si angles ($\angle$ C2—C1—Si1 = 127.9(4)° and $\angle$ C1—C2—Si2 = 158.2(3)°) show a large deviation from each other. These differences are due to the steric influence of the additional ligand. The bond length C1—C2 with 1.312(8) Å is in the range of a double bond. These observations are in agreement with these found for Cp₂Hf(PMe₃)(η^2 -Me₃SiC₂SiMe₃) [2].

Table 1. Data collection and handling.

Crystal:	yellow prism, size 0.18 × 0.30 × 0.32 mm
Wavelength:	Mo <i>K</i> _α radiation (0.71073 Å)
μ :	2.178 cm ^{–1}
Diffractionmeter, scan mode:	STOE IPDS II, ω
2 θ _{max} :	50.04°
<i>N</i> (<i>hkl</i>) _{measured} , <i>N</i> (<i>hkl</i>) _{unique} :	52884, 8440
Criterion for <i>I</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} :	<i>I</i> _{obs} > 2 σ (<i>I</i> _{obs}), 7322
<i>N</i> (<i>param</i>) _{refined} :	441
Programs:	SHELXS-97 [5], SHELXL-97 [6], SHELXTL [7]

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Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	Occ.	x	y	z	<i>U</i> _{iso}
H(3A)	8 <i>b</i>		−0.0244	0.0060	0.5592	0.099
H(3B)	8 <i>b</i>		−0.0346	−0.0854	0.5411	0.099
H(3C)	8 <i>b</i>		0.0622	−0.0521	0.5514	0.099
H(4A)	8 <i>b</i>		0.0836	−0.2364	0.5805	0.119
H(4B)	8 <i>b</i>		−0.0163	−0.2612	0.5707	0.119
H(4C)	8 <i>b</i>		0.0131	−0.2694	0.6049	0.119
H(5A)	8 <i>b</i>		−0.1487	−0.1493	0.6193	0.136
H(5B)	8 <i>b</i>		−0.1703	−0.1368	0.5847	0.136
H(5C)	8 <i>b</i>		−0.1539	−0.0511	0.6053	0.136
H(6A)	8 <i>b</i>		−0.0991	−0.2562	0.6492	0.126
H(6B)	8 <i>b</i>		−0.1154	−0.2799	0.6835	0.126
H(6C)	8 <i>b</i>		−0.0180	−0.2912	0.6692	0.126
H(7A)	8 <i>b</i>		−0.1393	−0.0122	0.6893	0.132
H(7B)	8 <i>b</i>		−0.1934	−0.1025	0.6955	0.132
H(7C)	8 <i>b</i>		−0.1792	−0.0685	0.6621	0.132
H(8A)	8 <i>b</i>		0.0563	−0.1754	0.7183	0.111
H(8B)	8 <i>b</i>		−0.0436	−0.1744	0.7311	0.111
H(8C)	8 <i>b</i>		0.0086	−0.0824	0.7259	0.111
H(9)	8 <i>b</i>		0.3470	−0.1409	0.6270	0.048
H(10)	8 <i>b</i>		0.2017	−0.2239	0.6232	0.054
H(11)	8 <i>b</i>		0.1322	−0.2282	0.6741	0.054
H(12)	8 <i>b</i>		0.2299	−0.1402	0.7088	0.053
H(14)	8 <i>b</i>		0.3849	−0.0365	0.7000	0.054
H(15)	8 <i>b</i>		0.4856	−0.1958	0.6868	0.054
H(16A)	8 <i>b</i>		0.5228	−0.0595	0.7298	0.073
H(16B)	8 <i>b</i>		0.5816	−0.1482	0.7260	0.073
H(17A)	8 <i>b</i>		0.6234	−0.1059	0.6786	0.082
H(17B)	8 <i>b</i>		0.6480	−0.0280	0.7016	0.082
H(18)	8 <i>b</i>		0.5260	0.0586	0.6859	0.071
H(19A)	8 <i>b</i>		0.4219	0.0072	0.6511	0.058
H(19B)	8 <i>b</i>		0.4766	−0.0835	0.6463	0.058
H(20)	8 <i>b</i>		0.3600	−0.2367	0.7157	0.067
H(21A)	8 <i>b</i>		0.4318	−0.1376	0.7643	0.118
H(21B)	8 <i>b</i>		0.3425	−0.1965	0.7649	0.118
H(21C)	8 <i>b</i>		0.3460	−0.1061	0.7458	0.118
H(22A)	8 <i>b</i>		0.4891	−0.3249	0.7178	0.105
H(22B)	8 <i>b</i>		0.4408	−0.3263	0.7495	0.105
H(22C)	8 <i>b</i>		0.5278	−0.2659	0.7445	0.105
H(23A)	8 <i>b</i>		0.6512	0.0779	0.6547	0.120
H(23B)	8 <i>b</i>		0.5623	0.0860	0.6350	0.120
H(23C)	8 <i>b</i>		0.6201	−0.0039	0.6342	0.120
H(24)	8 <i>b</i>		0.0881	0.0327	0.7066	0.053
H(25)	8 <i>b</i>		0.2564	0.0313	0.7080	0.057
H(26)	8 <i>b</i>		0.3106	0.1066	0.6609	0.057
H(27)	8 <i>b</i>		0.1747	0.1610	0.6322	0.051
H(29)	8 <i>b</i>		−0.0381	0.0938	0.6711	0.055
H(30)	8 <i>b</i>		0.0206	0.2737	0.6621	0.079
H(31A)	8 <i>b</i>		−0.1523	0.2107	0.6801	0.114
H(31B)	8 <i>b</i>		−0.1266	0.3141	0.6771	0.114
H(32A)	8 <i>b</i>		−0.2040	0.2654	0.6344	0.102
H(32B)	8 <i>b</i>		−0.1055	0.2981	0.6257	0.102
H(33)	8 <i>b</i>		−0.1584	0.1169	0.6333	0.069

Table 2. Continued.

Atom	Site	Occ.	x	y	z	<i>U</i> _{iso}
H(34A)	8 <i>b</i>		−0.0092	0.0795	0.6190	0.058
H(34B)	8 <i>b</i>		0.0164	0.1833	0.6176	0.058
H(35A)	8 <i>b</i>		0.0768	0.2179	0.7085	0.114
H(35B)	8 <i>b</i>		0.0779	0.2204	0.7075	0.114
H(38A)	8 <i>b</i>		−0.2086	0.1776	0.5885	0.113
H(38B)	8 <i>b</i>		−0.1325	0.1050	0.5819	0.113
H(38C)	8 <i>b</i>		−0.1093	0.2093	0.5804	0.113
H(39A)	8 <i>b</i>		0.3602	0.0571	0.5717	0.092
H(39B)	8 <i>b</i>		0.3939	−0.0024	0.5991	0.092
H(39C)	8 <i>b</i>		0.3574	0.0966	0.6048	0.092
H(40A)	8 <i>b</i>		0.1846	−0.1203	0.5690	0.087
H(40B)	8 <i>b</i>		0.2840	−0.1407	0.5802	0.087
H(40C)	8 <i>b</i>		0.2680	−0.0743	0.5528	0.087
H(41A)	8 <i>b</i>		0.1858	0.0754	0.5556	0.078
H(41B)	8 <i>b</i>		0.1952	0.1425	0.5832	0.078
H(41C)	8 <i>b</i>		0.1113	0.0765	0.5812	0.078
C(42)	8 <i>b</i>	0.50	0.7503(9)	0.256(1)	1.0024(4)	0.085(4)
H(42A)	8 <i>b</i>	0.50	0.7181	0.1996	1.0045	0.128
H(42B)	8 <i>b</i>	0.50	0.7289	0.2877	0.9846	0.128
H(42C)	8 <i>b</i>	0.50	0.7400	0.2933	1.0200	0.128
C(43)	8 <i>b</i>	0.50	0.8483(9)	0.238(1)	0.9993(5)	0.106(3)
H(43A)	8 <i>b</i>	0.50	0.8728	0.2048	1.0165	0.128
H(43B)	8 <i>b</i>	0.50	0.8629	0.2062	0.9806	0.128
C(44)	8 <i>b</i>	0.50	0.8779(9)	0.334(1)	0.9988(5)	0.114(3)
H(44A)	8 <i>b</i>	0.50	0.8604	0.3666	1.0170	0.137
H(44B)	8 <i>b</i>	0.50	0.8572	0.3659	0.9809	0.137
C(45)	8 <i>b</i>	0.50	0.9758(9)	0.313(2)	0.9979(5)	0.124(3)
H(45A)	8 <i>b</i>	0.50	0.9856	0.2756	1.0158	0.148
H(45B)	8 <i>b</i>	0.50	1.0047	0.3708	1.0023	0.148
C(46)	8 <i>b</i>	0.50	1.036(1)	0.272(2)	0.9750(3)	0.130(4)
H(46A)	8 <i>b</i>	0.50	1.0544	0.3143	0.9594	0.156
H(46B)	8 <i>b</i>	0.50	1.0098	0.2172	0.9658	0.156
C(47)	8 <i>b</i>	0.50	1.109(1)	0.251(2)	0.9967(5)	0.144(5)
H(47A)	8 <i>b</i>	0.50	1.1536	0.2124	0.9872	0.215
H(47B)	8 <i>b</i>	0.50	1.0839	0.2202	1.0141	0.215
H(47C)	8 <i>b</i>	0.50	1.1376	0.3067	1.0031	0.215
C(36A)	8 <i>b</i>	0.50	−0.042(2)	0.198(1)	0.7315(4)	0.098(4)
H(36A)	8 <i>b</i>	0.50	−0.0438	0.1336	0.7284	0.147
H(36B)	8 <i>b</i>	0.50	−0.1023	0.2228	0.7310	0.147
H(36C)	8 <i>b</i>	0.50	−0.0144	0.2110	0.7509	0.147
C(37A)	8 <i>b</i>	0.50	0.020(2)	0.3442(5)	0.7104(5)	0.105(5)
H(37A)	8 <i>b</i>	0.50	0.0560	0.3695	0.6943	0.158
H(37B)	8 <i>b</i>	0.50	0.0474	0.3586	0.7296	0.158
H(37C)	8 <i>b</i>	0.50	−0.0405	0.3695	0.7096	0.158
C(36B)	8 <i>b</i>	0.50	−0.038(2)	0.177(1)	0.7267(4)	0.096(4)
H(36D)	8 <i>b</i>	0.50	−0.0407	0.1179	0.7171	0.144
H(36E)	8 <i>b</i>	0.50	−0.0991	0.1994	0.7295	0.144
H(36F)	8 <i>b</i>	0.50	−0.0086	0.1713	0.7460	0.144
C(37B)	8 <i>b</i>	0.50	0.017(2)	0.3367(6)	0.7201(5)	0.107(5)
H(37D)	8 <i>b</i>	0.50	0.0506	0.3764	0.7069	0.160
H(37E)	8 <i>b</i>	0.50	0.0453	0.3350	0.7397	0.160
H(37F)	8 <i>b</i>	0.50	−0.0445	0.3592	0.7222	0.160

Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
C(1)	8 <i>b</i>	0.0528(4)	−0.0781(4)	0.6248(1)	0.034(3)	0.039(3)	0.043(3)	−0.002(2)	−0.006(3)	−0.001(2)
C(2)	8 <i>b</i>	0.0371(4)	−0.0900(3)	0.6532(1)	0.032(3)	0.039(3)	0.051(3)	−0.003(2)	−0.003(3)	0.001(3)
C(3)	8 <i>b</i>	−0.0012(5)	−0.0548(5)	0.5569(2)	0.062(4)	0.081(5)	0.055(4)	−0.009(4)	−0.021(3)	0.002(4)
C(4)	8 <i>b</i>	0.0207(6)	−0.2350(5)	0.5865(2)	0.105(7)	0.061(5)	0.072(5)	−0.025(4)	−0.017(4)	−0.006(4)
C(5)	8 <i>b</i>	−0.1363(5)	−0.1132(6)	0.6016(2)	0.062(5)	0.130(7)	0.081(6)	−0.033(5)	−0.026(5)	0.030(6)
C(6)	8 <i>b</i>	−0.0727(6)	−0.2552(5)	0.6691(2)	0.084(6)	0.073(5)	0.094(6)	−0.033(5)	0.008(5)	0.012(4)
C(7)	8 <i>b</i>	−0.1520(4)	−0.0725(6)	0.6819(2)	0.040(4)	0.114(7)	0.111(7)	0.007(4)	0.023(4)	0.006(6)
C(8)	8 <i>b</i>	−0.0007(5)	−0.1432(6)	0.7183(1)	0.060(4)	0.111(7)	0.050(4)	−0.022(4)	0.010(3)	0.015(4)
C(9)	8 <i>b</i>	0.3069(4)	−0.1518(3)	0.6430(1)	0.037(3)	0.037(3)	0.044(3)	0.007(2)	0.000(2)	−0.002(2)
C(10)	8 <i>b</i>	0.2258(4)	−0.1981(4)	0.6408(1)	0.044(3)	0.032(3)	0.058(4)	0.013(3)	−0.008(3)	−0.006(3)
C(11)	8 <i>b</i>	0.1868(4)	−0.1997(3)	0.6690(1)	0.038(3)	0.033(3)	0.064(4)	0.004(3)	−0.005(3)	0.013(3)
C(12)	8 <i>b</i>	0.2420(4)	−0.1519(4)	0.6884(1)	0.041(3)	0.049(4)	0.043(3)	0.007(3)	−0.004(3)	0.006(3)
C(13)	8 <i>b</i>	0.3193(4)	−0.1238(3)	0.6726(1)	0.034(3)	0.039(3)	0.041(3)	0.005(3)	−0.006(3)	0.003(2)

Table 3. Continued.

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
C(14)	8b	0.4031(4)	−0.0833(4)	0.6854(1)	0.043(3)	0.047(3)	0.045(3)	0.001(3)	0.001(3)	−0.001(3)
C(15)	8b	0.4622(4)	−0.1536(4)	0.7022(1)	0.039(3)	0.051(4)	0.045(3)	0.006(3)	−0.010(3)	0.003(3)
C(16)	8b	0.5436(5)	−0.1047(5)	0.7153(2)	0.049(4)	0.067(4)	0.066(4)	−0.006(4)	−0.018(4)	0.000(3)
C(17)	8b	0.5977(4)	−0.0598(5)	0.6919(2)	0.037(4)	0.073(5)	0.095(6)	0.001(3)	−0.021(4)	−0.007(4)
C(18)	8b	0.5443(4)	0.0076(4)	0.6729(2)	0.043(3)	0.053(4)	0.082(5)	−0.001(3)	0.000(4)	−0.001(3)
C(19)	8b	0.4593(4)	−0.0381(4)	0.6613(1)	0.033(3)	0.056(4)	0.055(3)	0.005(3)	0.000(3)	0.004(3)
C(20)	8b	0.4138(4)	−0.2105(5)	0.7256(1)	0.050(4)	0.070(5)	0.049(4)	−0.001(3)	−0.011(3)	0.010(3)
C(21)	8b	0.3806(6)	−0.1579(6)	0.7526(2)	0.095(6)	0.095(7)	0.046(4)	0.006(5)	−0.005(4)	0.003(4)
C(22)	8b	0.4733(5)	−0.2890(5)	0.7352(2)	0.070(5)	0.074(5)	0.067(4)	0.010(4)	−0.020(4)	0.023(4)
C(23)	8b	0.5995(5)	0.0453(5)	0.6468(2)	0.054(4)	0.067(4)	0.118(7)	−0.004(4)	0.013(4)	0.021(5)
C(24)	8b	0.1262(4)	0.0591(4)	0.6921(1)	0.050(4)	0.048(4)	0.036(3)	0.006(3)	0.006(3)	−0.011(3)
C(25)	8b	0.2201(4)	0.0568(4)	0.6928(1)	0.055(4)	0.049(4)	0.040(3)	0.009(3)	−0.012(3)	−0.018(3)
C(26)	8b	0.2501(4)	0.0994(4)	0.6668(2)	0.034(3)	0.040(3)	0.069(4)	−0.004(3)	0.000(3)	−0.018(3)
C(27)	8b	0.1737(4)	0.1301(3)	0.6506(1)	0.041(3)	0.037(3)	0.050(3)	−0.003(3)	0.003(3)	−0.004(3)
C(28)	8b	0.0970(4)	0.1067(4)	0.6668(1)	0.038(3)	0.039(3)	0.043(3)	0.005(3)	0.004(3)	−0.008(3)
C(29)	8b	0.0030(4)	0.1369(4)	0.6610(1)	0.037(3)	0.050(4)	0.051(3)	0.005(2)	0.001(3)	−0.007(3)
C(30)	8b	−0.0151(4)	0.2304(5)	0.6741(2)	0.043(4)	0.064(5)	0.091(5)	0.019(3)	−0.004(4)	−0.031(4)
C(31)	8b	−0.1145(5)	0.2538(7)	0.6691(2)	0.062(5)	0.113(7)	0.108(7)	0.044(5)	−0.007(5)	−0.048(6)
C(32)	8b	−0.1396(5)	0.2516(6)	0.6365(2)	0.058(5)	0.099(7)	0.099(6)	0.043(5)	−0.018(4)	−0.022(5)
C(33)	8b	−0.1207(4)	0.1627(5)	0.6231(2)	0.036(3)	0.070(5)	0.067(4)	0.010(3)	−0.008(3)	0.001(4)
C(34)	8b	−0.0215(4)	0.1388(4)	0.6279(1)	0.039(3)	0.050(3)	0.055(3)	0.010(3)	−0.003(3)	−0.003(3)
C(35)	8b	0.0147(5)	0.2419(4)	0.7068(2)	0.080(6)	0.092(6)	0.114(7)	0.039(5)	−0.027(5)	−0.067(6)
C(38)	8b	−0.1449(5)	0.1637(6)	0.5907(2)	0.054(4)	0.094(6)	0.078(5)	0.016(4)	−0.019(4)	0.000(5)
C(39)	8b	0.3503(4)	0.0426(5)	0.5927(1)	0.055(4)	0.079(5)	0.049(4)	−0.005(4)	0.005(3)	0.016(4)
C(40)	8b	0.2443(5)	−0.0949(5)	0.5719(1)	0.065(4)	0.066(4)	0.044(3)	0.001(3)	0.003(3)	−0.003(3)
C(41)	8b	0.1753(4)	0.0829(4)	0.5770(1)	0.058(4)	0.055(3)	0.042(3)	−0.006(3)	−0.005(3)	0.004(3)
Hf(1)	8b	0.17726(2)	−0.04329(1)	0.651719(5)	0.0319(1)	0.0341(1)	0.03199(9)	0.0012(1)	−0.0007(1)	−0.0015(1)
P(1)	8b	0.2374(1)	−0.0015(1)	0.59749(3)	0.0453(8)	0.0458(8)	0.0359(7)	−0.0034(7)	0.0004(7)	−0.0007(7)
Si(1)	8b	−0.0142(1)	−0.1178(1)	0.59292(4)	0.055(1)	0.056(1)	0.051(1)	−0.0146(8)	−0.0168(8)	0.0000(8)
Si(2)	8b	−0.0455(1)	−0.1378(1)	0.67954(4)	0.0399(9)	0.063(1)	0.057(1)	−0.0056(9)	0.0048(9)	0.0059(8)

Acknowledgments. This work was supported by the Deutsche Forschungsgemeinschaft (grant no. GRK 1213). Funding and facilities provided by the Leibniz-Institut für Katalyse e.V. an der Universität Rostock are gratefully acknowledged.

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