anti-Markovnikov addition of tellurium tetrachloride to trimethyl ethynyl silane

S.V. Amosova *, A.V. Martynov, V.A. Shagun, M.V. Musalov, L.I. Larina, L.B. Krivdin, L.V. Zhilitskaya, M.G. Voronkov

A.E. Favorsky Irkutsk Institute of Chemistry, Siberian Branch of the Russian Academy of Sciences, Irkutsk, 1, Favorsky Street 664033, Russia

ARTICLE INFO

ABSTRACT

An investigation of the $TeCl_4$ interaction with trimethyl ethynyl silane **1** in $CHCl_3$ has shown that anti-Markovnikov adduct [Z-1-(trimethylsilyl)-2-chlorovinyl]tellurium trichloride is formed as the only product. In time, it is hydrolyzed to give [Z-1-(trimethylsilyl)-2-chlorovinyl]tellurium (hydroxy) dichloride which, in turn, is dehydrated to afford bis[(2-chloro-1-trimethyl-silylvinyl)dichlorotellurium]oxide. These data revealed that the reaction studied was the first example of anti-Markovnikov syn-addition of $TeCl_4$ to terminal acetylenes. A computed simulation of the $TeCl_4$ interaction with ethynyl silane **1** in a gas state using PES method did not reveal dominating orientation of the addition but showed the conditions at which anti-Markovnikov addition can occur and which were probably met in carrying out the reaction in $CHCl_3$.

1. Introduction

It is known that interaction of tellurium tetrachloride or aryltellurium trichloride or tribromide with alkynes $RC≡CR^1$ (R = Ph, CH_2OH; R^1 = H, Alk, Ph) in apolar solvents (CCl_4, $CHCl_3$, C_6H_6) proceeds regio- and stereoselectively to furnish Z-$RCCl≡C(R^1)TeCl_3$ [1a,1b,1c,1d,1e,1f,1g,1h,1i,1j]. The interaction of $TeCl_4$ and $TeBr_4$ with twofold excess of terminal acetylenes $RC≡CH$ (R = Ph, C_5H_{11}) in benzene under reflux leads to formation of the 1:2 adducts – bis(α-organoyl-β-halogenovinyl)tellurium dichlorides $(RCX≡CH)_2TeX_2$ (X = Cl, Br) [1h,2a,2b]. When polar solvents (MeOH) are used, the reaction of aryl tellurium tribromides with terminal alkynes and phenylacetylene shows the same regioselectivity, but in this case E-isomers of monoadducts are formed due to anti-addition [1d]. In the reactions of $TeBr_4$ [2a,2b] and aryl tellurium tribromides [2b] with alkynes in benzene, anti-addition along with the syn-addition is realized, thus affording the mixtures of Z- and E-isomers of the corresponding adducts. It should be emphasized that these addition reactions obey the Markovnikov rule.

The reactions of tellurium tetrahalides with ethynyl silanes (silicon analogs of terminal alkynes) were unknown to date. Earlier, we have found a new cyclization reaction of $TeCl_4$ with diorganyl diethynyl silanes resulting in a new class of unsaturated silicon–tellurium containing heterocycles – 4,4-diorganyl-1,1,3,6-tetrachloro-1,4-tellurasilafulvenes [3]. To explain the formation of these heterocycles we have suggested that the anti-Markovnikov syn-

addition of $TeCl_4$ to ethynyl moiety of diethynyl silane occurs in the first stage of the reaction. Since the anti-Markovnikov orientation of the addition to acetylenic systems in a case of $TeCl_4$ is yet unknown, in this work we have computed probabilities of the Markovnikov and anti-Markovnikov modes of the $TeCl_4$ addition to trimethyl ethynyl silane, thus simulating a first stage of the aforementioned reaction, and then studied the interaction of $TeCl_4$ with $Me_3SiC≡CH$.

2. Results and discussion

2.1. Quantum-chemical simulation of the reaction

To elucidate the most possible direction of $TeCl_4$ addition to acetylenic moiety of trimethyl ethynyl silane **1** quantum chemical computations of the formation routes for the Markovnikov (α-) **2** and anti-Markovnikov (β-) **3** addition products were carried out (Scheme 1). For this purpose, within the framework of the molecular simulation methods we have investigated the potential energy surface (PES) of the mechanisms of interaction of **1** with $TeCl_4$ in order to choose the reaction channel that probably depends, first of all, on the topological and stereoelectronic characteristics of the pre-reaction bimolecular complex **1-TeCl_4**.

Critical points and gradient channels connecting them were found using the density functional theory (DFT) with the three-parameter functional B3LYP [4a,4b,4c]. Taking into consideration the character of the electron shells of the atoms included into the systems under study, the basis set LANL2DZ was employed. Geometry full optimization of the molecular systems was carried

* Corresponding author.
E-mail address: amosova@irioch.irk.ru (S.V. Amosova).
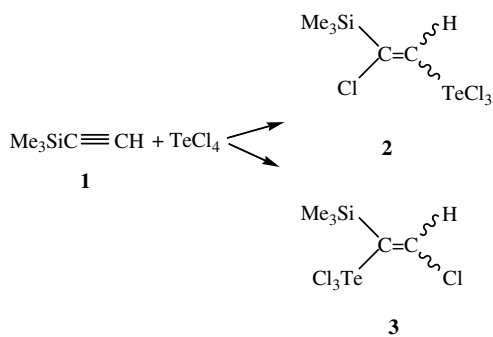
Scheme 1.

out till the value of 10^{-5} a.u./Bohr. On analyzing flat sites of the PES the gradient value has been installed at the level of 10^{-6} a.u./Bohr. Stationary points were identified by the analysis of the Gesse matrix. Search and localization of the transition states (TS) were carried out by method of linear and square-law synchronous transit QST2 and QST3 [5]. Analysis of the vibration frequencies in the Saddle point was performed, and conformity of the critical points with the gradient line connecting them was proved by the interior reaction coordinate method (IRC). All calculations were conducted using program complex GAUSSIAN-98 [6].

To examine the interaction of **1** with TeCl$_4$ as well as localize critical points corresponding to the most stable pre-reaction complexes, there have been computed the optimal structures of the isolated parent compounds used as starting materials for designing the bimolecular states. The basic geometrical and energy characteristics of the isolated ethynyl silane **1** and TeCl$_4$ are given in Fig. 1 and Table 1. Tellurium tetrachloride is represented according to the terminology of inorganic stereochemistry [7] as Te(monodental ligand)$_3$(LEP) and is capable of self-stabilizing in the configuration of both trigonal pyramid (T) with L$_a$TeL$_e$ equal to 91.2° (Fig. 1) which is close to the experimental values in RTeL$_3$ (for instance, R$_4$BTeMe$_3$ – 91.3° [8]), or square pyramid (S). The computations have shown insignificant (0.2 kcal/mol) predominance of the T-configuration (Table 1). Stabilization of TeCl$_4$ and formation of

the pre-reaction bimolecular complex on the interaction with silane **1** could occur with partial or complete reorganization of TeCl$_4$ configuration. Formally, configurational state of the complex – Te (monodentant ligand Cl)$_3$ (monodentant ligand silane **1**) (LEP) – can represent the spectrum of T–S configurations [7].

The topology of the complex could drastically influence the mechanism of the addition reaction. The calculations performed and the PES analysis of the TeCl$_4$ interaction with the acetylenic moiety of the ethynyl silane **1** allow us to localize four types of the complexes with different relative stabilities and probabilities of formation (Fig. 1, Table 2).

The structures **K$_1$** and **K$_4$** are related to the T configuration, while **K$_2$** and **K$_3$** are assigned to the S configuration. The values of thermodynamic stabilities of the complexes obtained (estimated as a difference between total energies of the optimal states of the parent compounds and the product) are 3.01, 9.08, 8.08 and 8.95 kcal/mol for **K$_1$**, **K$_2$**, **K$_3$** and **K$_4$** states, correspondingly. The structure **K$_3$** falls down from the total scheme of the complexes discussed. Despite the probability of the realization of the concerted reaction of the product **3** formation via the four-centered transition state (TS), the PES analysis has shown that the depth
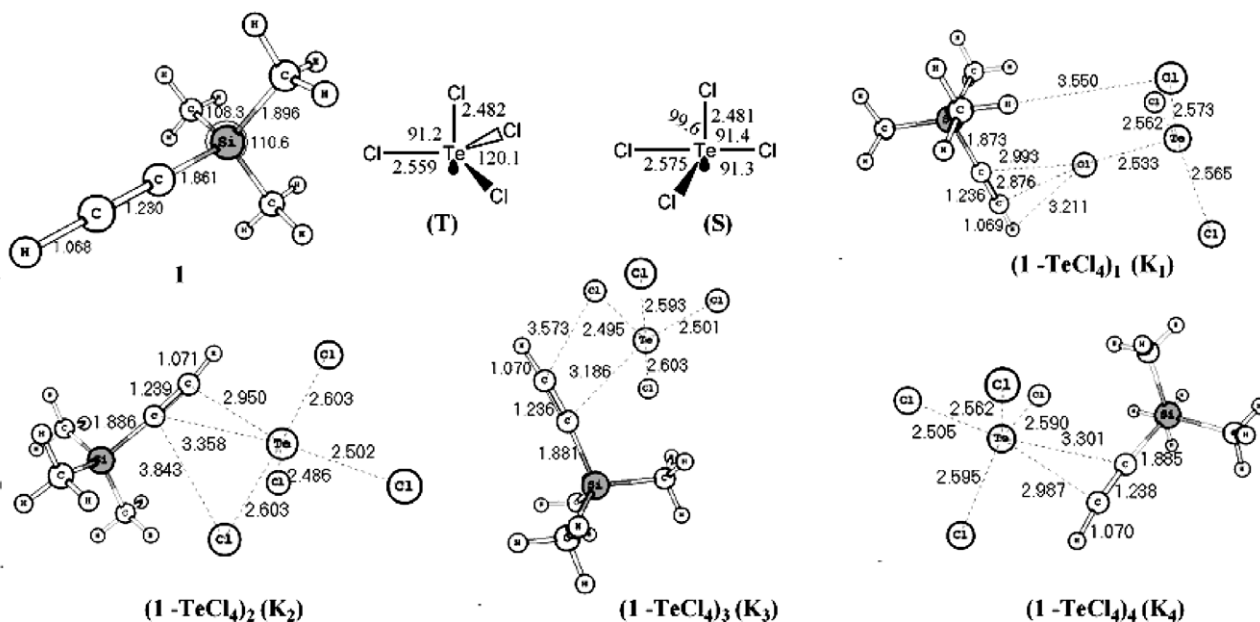

Fig. 1. Molecular structures and salient geometrical parameters of the compound **1** and TeCl$_4$ and their bimolecular complexes (**1-TeCl$_4$**)$_n$. Bond lengths are in Å, bond angles – in grad.

Table 2
Spin–spin coupling constants $^1J_{CH}$ of the four possible isomers of 1-silyl-2-chlorovinyl tellurium trichloride calculated at the DFT-B3LYP/aug-cc-pVTZ-J/6-311G** level[a]

Compound	J_{DSO}	J_{PSO}	J_{SD}	J_{FC}	J	Experiment
Z-$H_3SiC(TeCl_3)$=CHCl	1.27	−0.36	0.44	197.88	199.2	201.6[b]
E-$H_3SiC(TeCl_3)$=CHCl	1.50	−0.45	0.61	194.10	195.8	
E-H_3SiCCl=CHTeCl_3	1.72	−0.35	0.33	180.88	182.6	
Z-H_3SiCCl=CHTeCl_3	1.67	−0.45	0.31	185.85	187.35	

[a] All couplings and their contributions are in Hz; Equilibrium HF/6-31G** geometries were used throughout.
[b] Measured in compound **3**.

of the potential well, where complex K_3 is situated from the side of its possible transition to the more stable state K_2, does not exceed 1.7 kcal/mol. The interconversion activation parameters of other computed complexes exceed 17 kcal/mol, which as will be shown below, surpass the activation barriers for the product **2** and **3** formation. The most stable is the square pyramid complex K_2, where the interaction of $TeCl_4$ with the π-system of the acetylenic moiety delivers the appreciable deformation of the valence angle CCH to 170.6°. Complex K_2 through TS1 (Fig. 2) with the activation barrier 12.48 kcal/mol affords product **2**. In the stationary state K_4 that is slightly weaker in relative stability than complex K_2 (0.57 kcal/mol) transition to the product **2** occurs via the same transition state (TS1) with the activation barrier of 11.91 kcal/mol.

All attempts to localize in the state K_2 and K_4 gradient channels leading to the *anti*-Markovnikov adduct **3** failed. The PSE analysis shows that in the less stable complex K_1 realization of two independent gradient channels leading to the products **2** and **3** turns to be possible. Firstly, as a main component of the reaction coordinate in both channels, an interatomic distance between C_β atom and axial chlorine atom acts. In the next stage, the reaction channel is capable of shifting both to concerted or ionic addition. The former through TS2 results in the product **2**, the latter through TS3 gives the product **3**. Thus, formation of the *anti*-Markovnikov adduct **3** in the reaction directly relates to accumulation in the reaction mixture of sterically favorable bimolecular complexes from those considered above. Increase in the thermolysis rate probably shifts reaction channel towards ionic component, which results in a positive effect for the product **3** formation. It is necessary to note also, that formation of the compound **3** will take place on transition to a polar phase state, which is capable of increasing the stability of the complex K_3 since a degree of its charge separation, judging by the values of dipole moments, is higher than in the complex K_2 (Table 1). Based on slight distinction in relative stabilities of the complexes K_2 and K_3, complex K_3 could become dominating, which also rises the probability of the adduct **3** formation.

Thus, calculations made have not reveal dominating orientation of the addition in the reaction of $TeCl_4$ with ethynyl silane **1**, while in a gas phase a certain preference of the Markovnikov addition is observed.
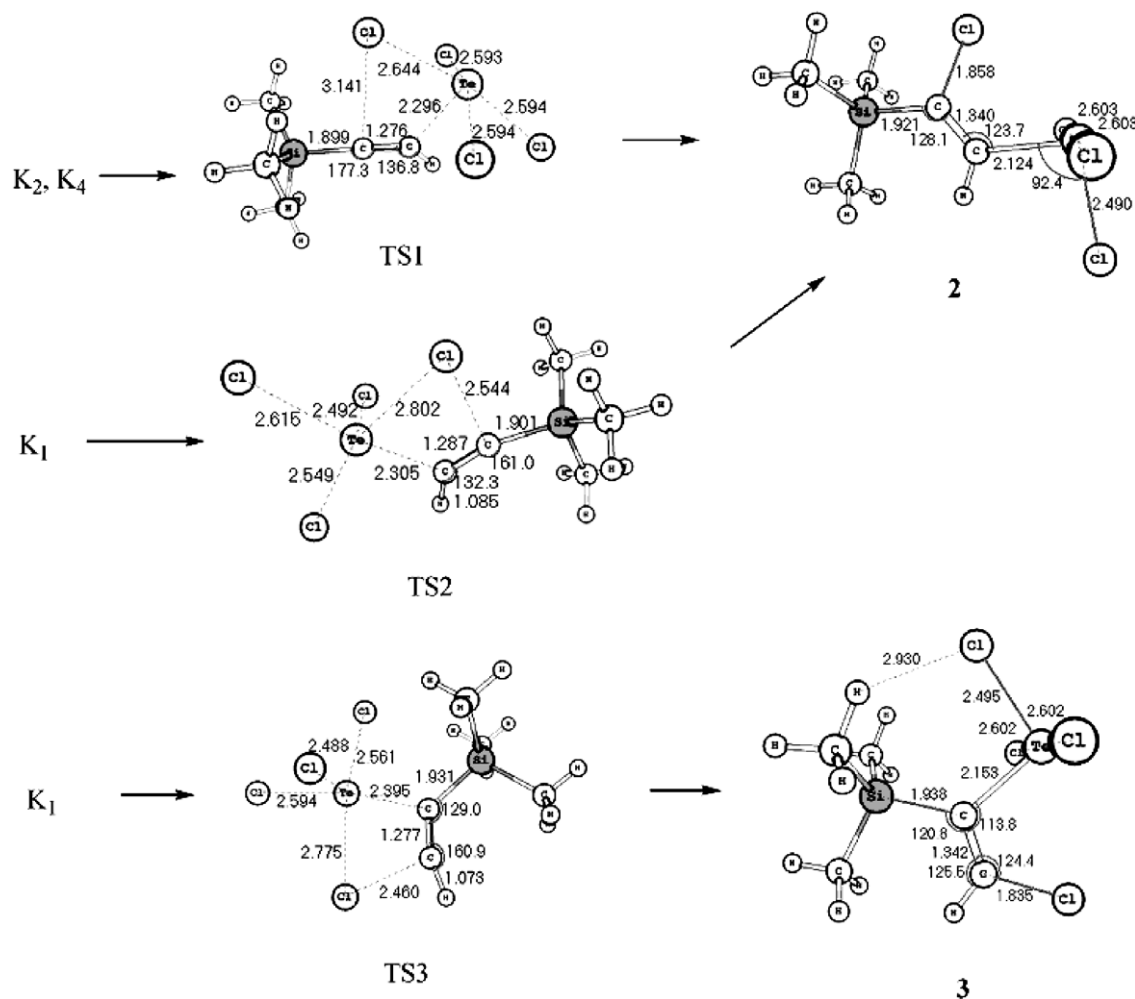

Fig. 2. Molecular structures and salient geometry parameters of the addition reaction products (**2** and **3**) and transition states (TS1–3) connecting them with the parent complexes K_n. Bond lengths are in Å, bond angles – in grad.

2.2. Experimental investigation of the reaction

We have established that the interaction of tellurium tetrachloride with trimethyl ethynyl silane **1** in chloroform at room temperature is a first example of *anti*-Markovnikov *syn*-addition of TeCl$_4$ to terminal acetylenes. As a result of this reaction, both in equimolar ratio of TeCl$_4$ and Me$_3$SiC≡CH and in 1:2 ratio, a monoadduct – [Z-1-(thimethylsilyl)-2-chlorovinyl]tellurium trichloride **3** – is formed (Scheme 2).

In the ^{1}H NMR spectra, vinyltellurium trichloride **3** manifests itself as a low-field singlet signal of olefinic proton (=CH) at δ 8.00 ppm (in CDCl$_3$) ($^3J_{\text{Te–H}}$ 28.2 Hz) and a singlet signal of trimethyl silyl group at δ 0.54 ppm (CDCl$_3$). The ^{13}C NMR spectra are characterized by a doublet signal of sp^2-hybridized carbon atom =CH at δ 144.31 ppm ($^1J_{\text{C–H}}$ 201.6 Hz), a singlet signal of =C(Si)Te at δ 148.62 ppm and a quartet signal of Me$_3$Si group at δ −0.76 ppm ($^1J_{\text{C–H}}$ 121.14 Hz), the ^{125}Te NMR spectra show a signal at δ 1407 ppm. In the ^{29}Si NMR spectra the Me$_3$Si group appears as a signal at δ 7.3 ppm. The presence in 2D NOESY NMR spectra of the cross peaks, induced by the dipole–dipole interaction between =CH and methyl protons of Me$_3$Si group, points to *cis*-arrangement of an olefinic proton and Me$_3$Si group. Formation of the 1:1 adduct is supported by the elemental analysis data.

In time, tellurium trichloride **3** is hydrolyzed on air to give [Z-1-(trimethylsilyl)-2-chlorovinyl]tellurium(hydroxy) dichloride (**4**), which is registered in the ^{1}H NMR spectra by a singlet signal of an olefinic proton at δ 7.23 ppm (in CDCl$_3$) and a singlet signal of Me$_3$Si group at δ 0.42 ppm. In the IR spectra of the product an intensive band of the OH group appears at v 3352 cm^{-1}.

In turn, due to intermolecular dehydration in chloroform the compound **4** turns into bis[(2-chloro-1-trimethylsilylvinyl)dichlorotellurium]oxide **5** within several hours (Scheme 3).

Formation of the compound **5** is well explained by the common trend of diaryltellurium dichlorides and dibromides Ar^{1}Ar^{2}TeX$_2$ to yield bis(diaryldihalogenotellurium)oxides (Ar^{1}Ar^{2}TeX)$_2$O (X = Cl, Br) as a result of hydrolysis [9].

Bis(dichlorotellurium)oxide **5** manifests itself in the ^{1}H NMR spectra by a high-field singlet signal of an olefinic proton at δ 7.22 ppm (in CDCl$_3$) ($^3J_{\text{Te–H}}$ 24.7 Hz) and a singlet signal of the Me$_3$Si group at δ 0.49 ppm (CDCl$_3$). In the ^{13}C NMR spectra there are a doublet signal of =CH at δ 133.13 ppm ($^1J_{\text{C–H}}$ 206.8 Hz), a doublet signal of =C(Si)Te at δ 157.21 ppm ($^2J_{\text{C–H}}$ 15.1 Hz) and a quartet of the Me$_3$Si group at δ 0.23 ppm ($^1J_{\text{C–H}}$ 121.3 Hz), in the
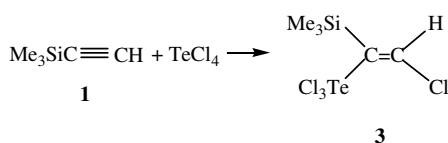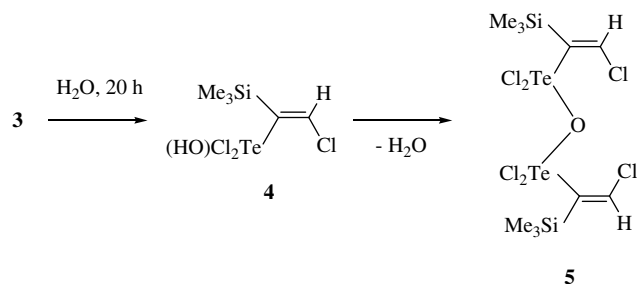
^{29}Si NMR spectra – a signal at 6.44 ppm, in the ^{125}Te NMR spectra – a doublet signal at δ 1371.6 ppm ($^3J_{\text{Te–H}}$ 21.8 Hz). In the IR spectra no absorption of the OH group is observed. As distinct from the IR spectra of the compounds **3** and **4**, which are characterized by two strong absorption bands at v 1542–1547 and 1248–1255 cm^{-1}, the compound **5** in the same region shows four strong absorption bands: 1540, 1464, 1378 and 1254 cm^{-1}. Elemental analysis of the compound **5** corresponds to the structure of bis-Z,Z-[(2-chloro-1-trimethylsilylvinyl)dichlorotellurium]oxide.

2.3. Structure assignment of the reaction products by the fine structure of the ^{13}C NMR spectra

Comparison of the coupling constants of an olefinic proton and tellurium atom in the compounds **3** and **5** with the data for divinyl telluride [10a,10b] as well as the experimental value of $^2J_{\text{Te–H}}$ for Z-2-chlorostyryl-1-tellurium trichloride obtained from the ^{1}H NMR spectra of this compound, synthesized by us using the known reaction of TeCl$_4$ with phenylacetylene [1a,1b,1c,1d,1e,1f,1g], does not allow to unambiguously judge about regio- and stereoisomerism of these compounds only on the basis of these spectral data. In particular, large difference in the values of the $^2J_{\text{Te–H}}$ constant for Z-2-chlorostyryl-1-tellurium trichloride (5.6 Hz) and the $^2J_{\text{Te–H}}$ constant for divinyl telluride (48.8 Hz) almost coinciding with the *trans*-vicinal constant $^3J_{\text{Te–H}}$ (41.8 Hz) for the same compound, testifies to ambiguity of these values application to determine the isomerism of the unsaturated tellurium trichloride and dichloride **3** and **5** on the basis of fine structure of the ^{125}Te or ^{1}H spectra. In contrast, for similar selenium analogs the regularities associating the $J_{\text{Se–H}}$ constants with relative arrangements of the hydrogen and selenium atoms at a double bond have been found [11a,11b,11c,11d].

Choice in favor of the *anti*-Markovnikov structure of the compounds prepared was made on the basis of $^1J_{\text{CH}}$ experimental coupling constant of the compound **3** in comparison with the calculated values in the four possible isomers of the model compound – 1-silyl-2-chlorovinyl tellurium trichloride (Table 2). Calculations of the $^1J_{\text{CH}}$ were performed at the DFT-B3LYP level with the basis set aug-cc-pVTZ-J [13] including four tight *s*-functions for both hydrogen and carbon. All four non-relativistic coupling contributions were taken into account, namely, Fermi contact, J_{FC}, spin–dipolar, J_{SD}, diamagnetic spin–orbital, J_{DSO}, and paramagnetic spin–orbital, J_{PSO}. Calculations of spin–spin coupling constants have been carried out using the DALTON package [14] while geometrical optimizations were performed with the GAMESS code [15]. The calculations of $^1J_{\text{CH}}$ point to the large differences in the values of these coupling constants in relation to the electronegativity of the element (Cl 2.83, Te 2.01) attached to the coupled carbon atom as well as to the spatial arrangement of the adjacent substituents at the C=C bond giving rise to the unambiguous assignment of the *anti*-Markovnikov structure.

Thus, the reaction of tellurium tetrachloride with trimethyl ethynyl silane represents the first example of unusual *anti*-Markovnikov addition of tellurium tetrahalide to terminal acetylenes.

3. Experimental

3.1. General

The ^{1}H (400 MHz), ^{13}C (100.6 MHz), ^{29}Si (79.5 MHz) and ^{125}Te (126.4 MHz) NMR spectra were taken in the CDCl$_3$ solutions on a Bruker DPX-400 spectrometer. HMDS was used as an inner standard for the ^{1}H NMR spectra; the ^{125}Te NMR spectra were recorded relative to Me$_4$Te. The IR spectra were recorded on a Bruker IPS 25 spectrometer. Trimethyl ethynyl silane **1** was prepared according to the procedure [12]. TeCl$_4$ was obtained from Aldrich.

Scheme 2.

Scheme 3.

3.2. Interaction of trimethyl ethynyl silane 1 with TeCl₄ at ratio 1:1 and 2:1

To $TeCl_4$ (2.72 g, 10.1 mmol) in 10 ml $CHCl_3$ was added in argon atmosphere ethynyl silane **1** (1.00 g, 10.1 mmol) in 10 ml $CHCl_3$, the resulting mixture was stirred at 20 °C for 6 h in daylight. A dark gray inorganic deposit (Te, unreacted $TeCl_4$) blurring on air was filtered off. After evacuation of the solvent from the filtrate was obtained 1.45 g (39%) of the product **3** as a white crystalloid matter, m.p. 80.5–81 °C. ^1H NMR ($CDCl_3$, 25 °C, δ, ppm): 8.00 (s, =CH, 1H, $^2J_{Si-H}$ 7.7 Hz, $^3J_{Te-H}$ 28.4 Hz), 0.54 (s, 9H, Me_3Si, $^4J_{TeH}$ 10.6 Hz, $^2J_{Si-H}$ 6.9 Hz); ^{13}C NMR ($CDCl_3$, 25°C, δ, ppm): 144.3 (d, =CH, $^1J_{CH}$ 201.6 Hz), 148.6 (s, =C), −0.76 (q, CH_3, $^1J_{CH}$ 121.1 Hz); ^{29}Si NMR ($CDCl_3$, 25 °C, δ, ppm): 7.33s; ^{125}Te NMR ($CDCl_3$, 25 °C, δ, ppm): 1317. IR (KBr) 3049 (=CH), 2940, 2902, 1547s, 1520w, 1413, 1283w, 1284s, 869s, 845s, 822, 764, 709, 630, 506, 415s cm^{-1}. Anal. Calc. for $C_5H_{10}SiTeCl_4$: C, 16.35; H, 2.74; Cl, 38.57; Si, 7.64; Te, 34.71. Found: C, 16.11; H, 2.52; Cl, 38.29; Si, 7.42; Te, 33.56%.

Similarly, the product **3** in 35% yield was prepared by the reaction of equimolar mixture of $TeCl_4$ and trimethyl ethynyl silane **1** in chloroform in argon atmosphere at darkness.

Similarly, the product **3** in 50% yield was prepared in the reaction of $TeCl_4$ and silane **1** in darkness at the reagent ratio 1:2, correspondingly.

Similarly, from $TeCl_4$ (0.94 g, 3.5 mmol) and silane **1** (0.34 g, 3.5 mmol) in 20 ml of $CHCl_3$ after stirring for 2.5 h at 20 °C in argon atmosphere on daylight and keeping the solution overnight was obtained 0.31 g of the mixture of the compounds **3**, **4** and **5** in ratio 1:10:10 (according to the ^1H NMR data).

*Compound **4**:* ^1H NMR ($CDCl_3$, 25 °C, δ, ppm): 7.24s (=CH), 0.42s(CH_3). IR (Vasiline oil) 3352 (OH), 3011, 2959, 2930, 2902, 2855, 1541s, 1444, 1411, 1385, 1255s, 1216, 1050, 849s, 760s, 692s, 510, 446 cm^{-1}.

*Compound **5**:* ^1H NMR ($CDCl_3$, 25 °C, δ, ppm): 7.22s (=CH, $^3J_{TeH}$ 25.7 Hz, $^1J_{CH}$ 206.6 Hz), 0.49s (CH_3, $^2J_{SiH}$ 6.9 Hz), $^4J_{TeH}$ 10.6 Hz); ^{13}C NMR ($CDCl_3$, 25°C, δ, ppm): 133.1d (=CH, $^1J_{CH}$206.8 Hz), 157.2d (=C, $^2J_{CH}$ 15.1 Hz), 0.23q (CH_3, $^1J_{CH}$ 121.3 Hz); ^{29}Si NMR ($CDCl_3$, 25 °C, δ, ppm): 6.44; ^{125}Te NMR ($CDCl_3$, 25 °C, δ, ppm): 1371.8d ($^3J_{Te-H}$ 25.2 Hz).

Similarly, from $TeCl_4$ (1.69 g, 6.25 mmol) and silane **1** (1.23 g, 12.5 mmol) in 40 ml of $CHCl_3$ in argon atmosphere at 20 °C after stirring in darkness for 11 h was obtained 1.39 g of the 1:3 mixture of the compounds **3** and **5** (according to the ^1H NMR data). Recrystallization from chloroform/hexane (1:4) afforded compound **5** as white fine crystals, m.p. 154.5 °C. The ^1H, ^{13}C, ^{29}Si, ^{125}Te NMR see above. IR (vaseline oil) 3010, 2964, 2924, 2853, 1649, 1572, 1540, 1465, 1377, 1254, 887, 849, 827, 764, 738, 700, 626, 447 cm^{-1}. Anal. Calc. for $C_{10}H_{20}Cl_6Te_2Si_2O$: C, 17.65; H, 2.96; Cl, 31.27; Si, 8.26; Te 37.51. Found: C, 17.85; H, 3.26; Cl, 31.71; Si, 7.89; Te 37.67%.

Acknowledgement

References

[1] (a) M. Moura Campos, N.P. Petragnani, Tetrahedron 18 (1962) 527;
(b) S. Uemura, H. Miyoshi, M. Okano, Chem. Lett. (1979) 1357;
(c) A. Chieffi, P.H. Menezes, J.V. Comasseto, Organometallics 16 (1997) 809;
(d) X. Huang, Y.P. Wang, Tetrahedron Lett. 37 (1996) 7417;
(e) R.A. Zingaro, N. Petragnani, J.V. Comasseto, Organomet. Synth. 3 (1986) 649;
(f) J.V. Comasseto, H.A. Stefani, A. Chieffi, J. Zukerman-Schpector, Organometallics 10 (1991) 845;
(g) J. Zukerman-Schpector, E.E. Castellano, G. Oliva, J.V. Comasseto, H.A. Stefani, Acta Cryst. C47 (1991) 960;
(h) J. Zukerman-Schpector, I. Haiduc, M.J. Dabdoub, J.C. Biazzotto, A.L. Braga, L. Dornelles, I. Caracelli, Z. Kristallogr. 217 (2002) 1;
(i) J. Zukerman-Schpector, R.L. Camillo, J.V. Comasseto, R.A. Santos, I. Caracelli, Acta Cryst. C55 (1999) 1577;
(j) B.I. Pak, I.M. Balog, V.G. Lendel, Yu.V. Migalina, Abstracts of the 16 Ukrainian Conference on Organic Chemistry, Ternopol, 1992, p. 278.
[2] (a) H.A. Stefani, I.P. Campos de Arruda, L.C. Roque, M.A. Montoro, A.L. Braga, J. Chem. Res. (S) (1996) 54;
(b) H.A. Stefani, N. Petragnani, J. Zukerman-Schpector, L. Dornelles, D.O. Silva, A.L. Braga, J. Organomet. Chem. 562 (1998) 127.
[3] S.V. Amosova, N.A. Makhaeva, A.V. Martynov, A.I. Albanov, O.G. Yarosh, M.G. Voronkov, Abstracts of International Symposium on Advanced Science in Organic Chemistry, Sudak, Crimea, 2006, P. C-009.
[4] (a) A.D. Becke, J. Chem. Phys. 98 (1993) 5648;
(b) C. Lee, W. Yang, R.G. Parr, Phys. Rev. (B) 37 (1988) 785;
(c) B. Miehlich, A. Savin, H. Stoll, H. Preuss, Chem. Phys. Lett. 157 (1989) 200.
[5] A.P. Scott, L. Radom, J. Phys. Chem. 100 (1996) 16502.
[6] M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, V.G. Zakrzewski, J.A. Montgomery, R.E. Stratmann, J.C. Burant, S. Dapprich, J.M. Millam, A.D. Daniels, K.N. Kudin, M.C. Strain, O. Farkas, J. Tomasi, V. Barone, M. Cossi Mennucci, B. Mennucci, C. Pomelli, C. Adamo, S. Cliord, J. Ochterski, G.A. Petersson, P.Y. Ayala, Q. Cui, K. Morokuma, D.K. Malick, A.D. Rabuck, K. Raghavachari, J.B. Foresman, J. Cioslowski, J.V. Ortiz, B.B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. Comperts, R.L. Martin, D.J. Fox, T. Keith, M.A. Al-Laham, C.Y. Peng, A. Nanayakkara, C. Gonzalez, M. Challacombe, P.M.W. Gill, B. Johnson, W. Chen, M.W. Wong, J.L. Andres, C. Gonzalez, M. Head-Gordon, E.S. Replogle, J.A. Pople, GAUSSIAN 98, Revision A. u6, Gaussian, Ltd., Pittsburgh, PA, 1998.
[7] D. Kipert, Inorganic Stereochemistry, Mir, Moscow, 1985, p. 276.
[8] R.F. Ziolo, J.M. Troup, Inorg. Chem. 18 (1979) 2271.
[9] I.D. Sadekov, A.V. Zakharov, A.A. Maksimenko, Sulfur Reports 23 (2002) 125.
[10] (a) V.M. Bzhezovskii, D.F. Kushnarev, B.A. Trofimov, G.A. Kalabin, N.K. Gusarova, G.G. Efremova, Izv. AN SSSR. Ser. Khim. (1981) 2507;
(b) B.A. Trofimov, S.V. Amosova, Divinyl Sulfide and Its Derivatives, Nauka, Novosibirsk, 1983, 264p.
[11] (a) I. Johannsen, H. Eggert, J. Am. Chem. Soc. 106 (1984) 1240;
(b) I. Johannsen, L. Henriksen, H. Eggert, J. Org. Chem. 51 (1986) 1657;
(c) W. McFarlane, D.S. Rycroft, J. Chem. Soc., Chem. Commun. (1973) 10;
(d) N.P. Luthra, J.D. Odom, in: S. Patai, Z. Rappoport (Eds.), The Chemistry of Organic Selenium and Tellurium Compounds, vol. 1, Wiley, 1986, p. 190.
[12] N.V. Komarov, O.G. Yarosh, Zh. Obshch. Khim. 37 (1967) 264.
[13] P.F. Provasi, G.A. Aucar, S.P.A. Sauer, J. Chem. Phys. 115 (2001) 1324.
[14] C. Angeli, K.L. Bak, V. Bakken, O. Christiansen, R. Cimiraglia, S. Coriani, P. Dahle, E.K. Dalskov, T. Enevoldsen, B. Fernandez, C. Haettig, K. Hald, A. Halkier, H. Heiberg, T. Helgaker, H. Hettema, H.J.A. Jensen, D. Jonsson, P. Joergensen, S. Kirpekar, W. Klopper, R. Kobayashi, H. Koch, A. Ligabue, O.B. Lutnaes, K.V. Mikkelsen, P. Norman, J. Olsen, M.J. Packer, T.B. Pedersen, Z. Rinkevicius, E. Rudberg, T.A. Ruden, K. Ruud, P. Salek, A. Sanchez de Meras, T. Saue, S.P.A. Sauer, B. Schimmelpfennig, K.O. Sylvester-Hvid, P.R. Taylor, O. Vahtras, D.J. Wilson, H. Ågren, Dalton, A Molecular Electronic Structure Program, Release 2.0, 2005. <http://www.kjemi.uio.no/software/dalton/dalton.html>.
[15] M.W. Schmidt, K.K. Baldridge, J.A. Boatz, S.T. Elbert, M.S. Gordon, J.H. Jensen, S. Koseki, N. Matsunaga, K.A. Nguyen, S.J. Su, T.L. Windus, M. Dupuis, J.A. Montgomery, J. Comp. Chem. 14 (1993) 1347.