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Stereoelectronic Structure of Methoxyphenyltrichlorostannanes by the Results of *ab initio* Calculations

V. P. Feshin and E. V. Feshina

Institute of Technical Chemistry, Ural Branch, Russian Academy of Sciences,
ul. Akademika Koroleva 3, Perm', 614013 Russia
e-mail: itch-uro-ran@yandex.ru

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Abstract—The RHF/3-21G* and MP2/3-21G* levels were implemented for the study of the stereoelectronic structure of 2- and 4-methoxyphenyl- and 2,6-dimethoxyphenyltrichlorostannanes. In the 4-methoxyphenyltrichlorostannane the Sn atom is tetracoordinated, while in 2-methoxy- and 2,6-dimethoxyphenyltrichlorostannanes it is pentacoordinated due to the intramolecular interaction of the O atom with it. In this case a closure occurs of a 4-membered ring. In the last molecule, the Sn atom interacts almost exclusively with only one of the O atoms. The intramolecular interaction between the Sn and O atoms leads to the electron density transfer from C and H atoms of the methoxy groups as well as from the Sn atom to the atoms of its coordination polyhedron. As a result the electron density increases also on the O atom involved in this interaction.

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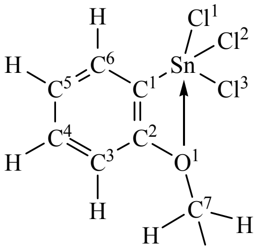
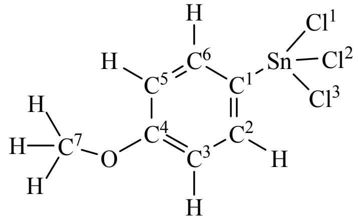
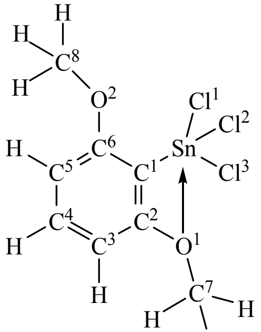
Investigation of 2-methoxyphenyltrichlorostannane by nuclear quadrupole resonance (NQR) on the ^{35}Cl nuclei has shown [1] that the Sn atom can be pentacoordinated through additional interaction with the oxygen atom of the methoxy group. For example, in the triplet ^{35}Cl NQR spectrum of 2-$CH_3OC_6H_4SnCl_3$ at 77 K the low-frequency line (20.070 MHz) is considerably removed from the high-frequency doublet (21.762 and 21.674 MHz). The expansion of the Sn atom coordination in such compounds may result in either intra- or intermolecular interaction of the Sn and O atoms. In the NQR spectrum of 4-$CH_3OC_6H_4SnCl_3$ which is incapable of such intramolecular interaction the splitting of the lines is relatively small (21.299, 21.204, 21.160, 21.008, 20.728 and 20.385 MHz). Apparently, the unit cell of this compound contains two crystallographically nonequivalent molecules. The relatively narrow range of frequencies of this spectrum and a small splitting of its lines indicate that the difference in the electron distribution of the chlorine atoms of this compound is insignificant. This allows us to conclude that the Sn atom is tetracoordinated and a significant intermolecular Sn←O interaction does not occur. Unfortunately, the asymmetry parameters of the electric field gradient (EFG) at the nuclei ^{35}Cl of these compounds were not measured.



I



II



III

Typically, in the case of significant intramolecular interaction of an atom of the element of Group IVA with the heteroatom of the carbofunctional substituent a 5- or 6-membered ring is closed [2–4]. In the 2-alkoxyphenyltrichlorostannane such interaction would lead to the closure of 4-membered ring.

To study the stereoelectronic structure of these compounds we performed quantum-chemical calculations by the RHF and MP2 methods with the 3-21G* basis set of the molecules of 2-$CH_3OC_6H_4SnCl_3$ (**I**), 4-$CH_3OC_6H_4SnCl_3$ (**II**) and 2,6-$(CH_3O)_2C_6H_3SnCl_3$ (**III**) with full geometry optimization using the Gaussian 03W software [5]. Unfortunately, it is impossible with this program to use a basic set of a higher level in the calculation of Sn compounds. However, the use of the 3-21G* basis set also leads to satisfactory agreement with experimental data [6]. We used the results of quantum-chemical calculations of electron distribution in the molecules to estimate the ^{35}Cl NQR parameters and to compare them with the available experimental data. Therefore, for the origin of coordinate system was chosen the chlorine atom whose NQR parameters should be determined. The system's *Z*-axis coincided with the corresponding Cl–Sn bond.

The results of calculations of geometric characteristics of the studied molecules by the RHF and MP2 methods are close enough to each other (Table 1). The calculation of molecule **I** indicates that the Sn atom is pentacoordinated in agreement with the experimental ^{35}Cl NQR spectrum of this compound at 77 K. The Sn ← O^1 distance in the molecule is much shorter than the sum of the Sn and O van der Waals radii (3.5 Å [7]) The Cl^1–Sn bond is longer than the bonds Cl^2–Sn and Cl^3–Sn. The angle Cl^{1}SnO^1 is close to 180º, which is characteristic of the angle between the axial bonds of the central Sn atom in a trigonal–bipyramidal coordination polyhedron. The angles Cl^{2}SnC^1 and Cl^{3}SnC^1 are close to 120º, that is characteristic of the angles between the equatorial bonds in such structure, whereas the angle Cl^{1}SnC^1 is more closer to tetrahedral than to a right angle. The values of the angles Cl^{1}SnCl^2 and Cl^{1}SnCl^3 are intermediate between the right and the tetrahedral, and the angle Cl^{2}SnCl^3 is close to the tetrahedral. The equatorial Cl^1–Sn, Cl^2–Sn and Cl^3–Sn bonds of this molecule do not lie in one plane: the sum of the angles between these bonds is less than 360º (343.52º by RHF and 344.05º by MP2). The Cl^1–Sn bond lies in the plane of the aromatic ring, the Cl^2–Sn and Cl^3–Sn bonds are arranged symmetrically with respect to the plane.

In molecule **II**, the Sn–Cl bond lengths are identical, and the angles ClSnC^1 are close to the tetrahedral. This corresponds to ^{35}Cl NQR data indicating the tetrahedral coordination of the tin atom in this compound and the lack of intermolecular interactions between the Sn and the O atoms.

The calculated geometric characteristics of the molecule **III**, the Sn–Cl bond lengths in particular, differ somewhat from the experimental ones [7]. According to the calculations by both methods the lengths of the three Sn–Cl bonds are virtually identical, as well as the bond angles Cl^{1}SnC^1, Cl^{2}SnC^1, and Cl^{3}SnC^1. The dihedral angles Cl^{2}SnC^{1}C^2 and Cl^{3}SnC^{1}C^2 are also equal. Consequently, the electron distribution on the Cl^2 and Cl^3 atoms in this molecule is the same. Therefore, Table 2 shows the population of the valence *p*-orbitals and their 3*p*-components and the ^{35}Cl NQR parameters calculated from them only for one of these atoms. At the same time, the experimental ^{35}Cl NQR data indicate the inequivalence of electron distribution of all three chlorine atoms in this compound [1, 7]. This discrepancy between the calculated and experimental data may indicate a different structure and, consequently, electron distribution in the molecule **III** in the gaseous and crystalline states of matter. However, the difference between the calculated and experimental geometric characteristics of the molecule is relatively small and is not of fundamental nature. Somewhat different are the calculated and experimental distances Sn···O^1 and Sn···O^2. The former, both calculated and experimental, is much less than the sum of the van der Waals radii of these atoms, while the last calculated is almost equal to the sum while the experimental distance is somewhat shorter (Table 1). These data indicate that in molecule **III** there is a coordination interaction of Sn with the O^1 atom while interaction with the O^2 atom is practically absent. As a result, the Sn atom is pentacoordinated, but the structure of its coordination polyhedron differs from the trigonal–bipyramidal, which is characteristic of the other tin compounds with intra- and intermolecular coordination.

The rapprochement of Sn and O^1 atoms resulting from the intramolecular Sn ← O interactions in molecules **I** and **III** leads to a decrease in the SnC^{1}C^2 and C^{1}C^{2}O^1 bond angles and an increase in the angles SnC^{1}C^6 and O^{1}C^{2}C^3 compared to the corresponding angles in molecule **II**. The change in the SnC^{1}C^2 and SnC^{1}C^6 angles is much larger than in the corresponding angles involving the C^2–O^1 bond. In molecule

Table 1. Bond lengths (*d*), bond angles (ω), and torsion angles (β) in molecules **I–III**[a] calculated by the RHF/3-21G* and MP2/3-21G* levels, and X-ray diffraction data [7] for molecule **III**

Bond	**I**		**II**		**III**		
	RHF	MP2	RHF	MP2	RHF	MP2	X-ray diffraction data
	d, Å						
Cl^1–Sn	2.369	2.365	2.346	2.345	2.358	2.357	2.311
Cl^2–Sn	2.351	2.350	2.345	2.345	2.356	2.354	2.293
Cl^3–Sn	2.351	2.350	2.346	2.346	2.356	2.354	2.303
Sn–C^1	2.130	2.152	2.121	2.132	2.118	2.140	2.082
C^1–C^2	1.384	1.405	1.400	1.420	1.380	1.399	1.401
C^2–O^1	1.394	1.428	1.360	1.392	1.383	1.423	1.346
O^1–C^7	1.449	1.482	1.440	1.478	1.447	1.480	1.449
Sn←O^1	2.438	2.427	–	–	2.529	2.470	2.85
Angle	ω, deg						
Cl^1SnC^1	106.99	106.55	114.03	113.63	114.12	112.69	113.2
Cl^2SnC^1	117.71	117.89	112.91	113.63	115.36	115.95	118.4
Cl^3SnC^1	117.71	117.89	110.63	109.77	115.36	115.95	115.1
Cl^1SnCl^2	101.94	101.82	104.71	104.82	101.04	100.74	102.8
Cl^1SnCl^3	101.94	101.82	106.35	107.29	101.04	100.74	104.2
Cl^2SnCl^3	108.10	108.27	107.73	107.29	108.09	108.71	101.3
SnC^1C^2	102.70	101.96	120.79	120.89	105.42	103.60	113.0
SnC^1C^6	137.55	138.15	120.62	119.84	134.42	136.01	125.3
Cl^1SnO^1	166.05	166.55	–	–	171.63	171.86	–
$C^1C^2O^1$	109.37	108.63	–	–	109.93	108.72	114.2
$O^1C^2C^3$	127.95	128.42	–	–	127.52	128.37	124.4
$C^2O^1C^7$	123.41	120.36	–	–	123.32	120.10	120.7
Angle	β, deg						
$Cl^1SnC^1C^2$	180.0	180.0	–69.74	–59.88	180.0	180.0	–
$Cl^2SnC^1C^2$	–66.12	–66.48	49.62	59.86	–63.62	–64.65	–
$Cl^3SnC^1C^2$	66.12	66.48	170.44	179.99	63.62	64.65	128.5
$SnC^1C^2O^1$	0.0	0.0	–	–	0.0	0.0	–
$C^1C^2O^1C^7$	180.0	180.0	–	–	180.0	180.0	–

[a] In molecule **II** by the RHF and MP2 calculations the angles are, respectively: $O^1C^4C^3$ 115,94° and 115.17°; $C^7O^1C^4$ 121.40° and 117.19°; $SnC^1C^2C^3$ 179.75° and 180.0°; $O^1C^4C^3C^2$ 180.0° and 180.0°; $C^7O^1C^4C^3$ –179.94° and 180.0°. In molecule **III** the bond lengths are: C^6–O^2 1.355Å and 1.389Å; O^2–C^8 1.442 Å and 1.479 Å; distance Sn ← O^2 3.485 Å and 3.559 Å; angles $O^2C^6C^1$ 116.75° and 116.10°; $C^8O^2C^6$ 122.11° and 117.60°.

III the Sn···O distance increases, the strength of the Sn ← O coordination bond decreases, and respective changes occur in the values of these angles, as compared with **I** (Table 1). In addition, the axial Sn–Cl^1 bond length is reduced.

Earlier [8–10] we have obtained satisfactory agreement between both the experimental and calculated with Eq. (1) ^{35}Cl NQR frequencies ν and the calculated by the RHF/6–31G(d) method populations of less diffuse 3*p* components of valence *p* orbitals of chlorine atoms in organic and organometallic molecules containing Cl–M bond (M = C, Si, P, As). Also, a satisfactory agreement has been obtained between the experimental asymmetry parameters η of the electric field gradient (EFG) at the ^{35}Cl nuclei calculated from these 3*p*-components with Eq. (2) for a number of organic molecules with C–Cl bond.

$$\nu = (e^2Qq_{\mathrm{at}}/2h[-N_z + (N_x + N_y)/2](1 + \eta^2/3)^{1/2}, \qquad (1)$$

$$\eta = |\,3(N_x - N_y)/(2N_z - N_x - N_y)\,|. \qquad (2)$$

Here e^2Qq_{at} is nuclear quadrupole coupling constant, *h* is Planck's constant, N_x, N_y, and N_z are the populations of 3*p*-components of valence p_x, p_y, and p_z orbitals respectively of the indicator chlorine atom. The value of e^2Qq_{at} / 2*h* is found from the experimental NQR frequency of Cl_2 at 77 K, and the population of 3*p* components of valence *p* orbitals of Cl atoms of the molecule is derived from a calculation with the corresponding method [8–10].

For comparison with experimental NQR data and the results of quantum chemical calculations of the

Table 2. Populations of valence *p* orbitals of chlorine atoms (Σ*Np*) and 3*p*-components (N_{3p}) in molecules **I–III**, calculated by the RHF/3-21G* and MP2/3-21G* levels, and calculated from these populations the ^{35}Cl NQR frequencies (ν_{calc}) and asymmetry parameters (η_{calc}) of electric field gradient on the nuclei ^{35}Cl of these molecules

Molecule	Atom	Orbital	Np_x, *e*	Np_y, *e*	Np_z, *e*	ν_{calc}, MHz	η_{calc}, %
				RHF			
I	Cl^1	N3*p*	1.057	1.055	0.900	17.473	1.92
		ΣN*p*	1.967	1.964	1.952	–	–
	Cl^2	N3*p*	1.061	1.064	0.889	19.435	2.59
		ΣN*p*	1.966	1.970	1.571	–	–
II	Cl^1	N3*p*	1.063	1.060	0.888	19.435	2.59
		ΣN*p*	1.963	1.957	1.558	–	–
III	Cl^1	N3*p*	1.057	1.057	0.892	18.885	6.23
		ΣN*p*	1.969	1.964	1.574	–	–
	Cl^2	N3*p*	1.062	1.062	0.890	19.264	0.0
		ΣN*p*	1.968	1.970	1.579	–	–
				MP2			
I	Cl^1	N3*p*	1.057	1.055	0.901	17.078	1.94
		ΣN*p*	1.968	1.964	1.591	–	–
	Cl^2	N3*p*	1.061	1.065	0.888	19.284	3.34
		ΣN*p*	1.966	1.970	1.570	–	–
II	Cl^1	N3*p*	1.064	1.060	0.888	19.174	3.45
		ΣN*p*	1.963	1.958	1.557	–	–
III	Cl^1	N3*p*	1.064	1.057	0.893	18.466	6.27
		ΣN*p*	1.969	1.964	1.575	–	–
	Cl^2	N3*p*	1.061	1.063	0.890	18.950	0.87
		ΣN*p*	1.968	1.971	1.578	–	–

studied molecules, we implemented the levels RHF/3-21G* and MP2/3-21G* to evaluate the ^{35}Cl NQR frequencies and asymmetry parameters of the examined molecules (Table 2). Unfortunately, the calculated NQR frequencies were significantly lower than the experimental ones obtained at 77 K. At the same time, the ratio of the calculated NQR frequencies for different Cl atoms in these molecules corresponds to the experimental ratio. It can be assumed that the low values of the calculated NQR frequencies are due to inaccuracy of the estimated populations of the valence *p* orbitals 3*p*-components of Cl atoms with the 3-21G* basis set. However, using this basis set to calculate the γ-chloropropyltrichlorstannane we obtained a satisfactory agreement between the experimental and calculated by similar way ^{35}Cl NQR frequencies of this molecule (the C–Cl and Sn–Cl bonds), with the exception of the NQR frequency of the axial chlorine atom [6]. Apparently, the discrepancy between the calculated and experimental NQR frequencies of the compounds studied is due mainly to the distinctions in the stereoelectronic structure of their molecules in either gaseous, or crystalline states.

The higher values of the NQR frequencies of equatorial than axial chlorine atoms in the molecules **I** and **III** is due to a larger half-sum of the populations of 3*p*-components of valence p_x and p_y orbitals of the equatorial chlorine atoms and a smaller population of the 3*p*-components of their p_z orbitals [Eq. (1), Table 2]. The same ratio is observed for the total populations of the relevant orbitals.

The EFG asymmetry parameters η at the ^{35}Cl nuclei of the axial and equatorial Cl atoms in the molecule **I** differ only slightly, while the η value of equatorial Cl atom is too small, which is not characteristic of such atoms in the molecules of trigonal-bipyramidal structure [11–13]. According to the ^{35}Cl NQR spectrum registered at 77 K, the electron distribution of the equatorial chlorine atoms in this molecule differs only slightly.

In an individual molecule **I** the calculated length of the two equatorial bonds Cl–Sn, bond angles Cl^2SnC^1 and Cl^3SnC^1, as well as dihedral angles $Cl^2SnC^1C^2$ and $Cl^3SnC^1C^2$ are identical (Table 1). Therefore, we should assume that the electron density distribution over these bonds, as well as the calculated NQR parameters of the chlorine atoms also is identical. Therefore, in Table 2 the populations of 3*p*-components of valence *p* orbitals of chlorine atoms in this molecule, the calculated from them NQR frequencies and the EFG asymmetry parameters on the ^{35}Cl nuclei are listed for only one of them.

Table 3. Charges (q) of atoms in molecules **I–III** calculated by the RHF/3-21G* and MP2/3-21G* method[a]

Atom	**I**		**II**		**III**	
	RHF	MP2	RHF	MP2	RHF	MP2
Cl^1	–0.423	–0.421	–0.375	–0.375	–0.405	–0.404
Cl^2	–0.406	–0.405	–0.379	–0.375	–0.417	–0.416
Cl^3	–0.406	–0.405	–0.386	–0.386	–0.417	–0.416
Sn	1.481	1.476	1.370	1.364	1.484	1.486
C^1	–0.443	–0.430	–0.365	–0.362	–0.488	–0.471
C^2	0.442	0.403	0.440	0.409	0.481	0.434
O^1	–0.767	–0.730	–0.735	–0.692	–0.764	–0.727
C^7	–0.269	–0.280	–0.278	–0.298	–0.269	–0.280
H	0.261	0.261	0.243	0.243	0.261	0.262
H	0.224	0.226	0.206	0.208	0.221	0.223
H	0.224	0.226	0.206	0.208	0.221	0.223

[a] In molecule **III** the charges (q, e) calculated by the RHF/3-21G* and MP2/3-21G* levels are, respectively: O^2 –0.730 and –0.682; C^6 –0.280 and –0.299, H 0.254, and H 0.252, H 0.207 and 0.208, H 0.207 and 0.208.

The asymmetry parameters calculated for the chlorine atoms of the molecule **II** are typical for the M–Cl bonds of tetracoordinated M atom [8–10].

Judging from the dihedral angles $Cl^1SnC^1C^2$ and $SnC^1C^2O^1$, the atoms Cl, Sn, and O in the molecule **III** lie in one plane. The Cl^1 atom is in the *trans* position to the O^1 atom as indicates the value of $Cl^1SnO^{1,}$ close to 180º (Table 1). Nevertheless, the ratio of asymmetry parameters of EFG on the nuclei of atoms Cl^1 and Cl^2 (Cl^3) is opposite to those of axial and equatorial Cl atoms in the molecules of trigonal–bipyramidal structure [11–13]. This may be due to the influence of the O^2 atom in molecule **III** affecting the populations of 3p-components of valence p_x and p_y orbitals which in the Cl^1 atom become substantially different, while in Cl^2 and Cl^3 atoms are identical (Table 2). This effect leads also to the practical equality of the lengths of three Sn–Cl bonds and similarity of the Sn bond angles in molecule **III**, in contrast to **I**.

In molecules **I** and **III** the partial positive charge of the Sn atom and the negative charge of O atom involved in the coordination interaction with Sn atom increase compared to the molecule **II** (Table 3). This does not correspond to the electron density transfer from the O atom to Sn at the formation of coordination Sn ← O bond. In the molecules **I** and **III** the electron density of all atoms of the Sn coordination polyhedron increases while that of the atoms C and H of methoxy group decreases compared to **II**. Hence, the intramolecular interaction between the Sn and O atoms results in the transfer of the electron density from C and H atoms of methoxy group, as well as from the Sn atom, to the atoms of its coordination polyhedron. This leads also to increase in the electron density of O atom involved in the interaction. Electron distribution of the atoms of methoxy group in molecule **III**, where the oxygen is not involved in the interaction with the Sn atom, practically corresponds to the electron distribution of this group in molecule **II**.

Thus, in the studied molecules **I** and **III** the tin atom is pentacoordinated. However, stereoelectronic structure of its coordination polyhedron differs significantly from the trigonal–bipyramidal structure of the coordination polyhedron of other pentacoordinated atoms of the group IVA elements, formed by the intermolecular interaction of the atom with the heteroatom of the organic ligand or as a result of intramolecular closure of a 5- or 6-membered ring. In molecule **III** only one oxygen atom is involved in the interaction with the Sn atom. The intramolecular interaction between Sn and O atoms in molecules **I** and **III** results in the transfer of the electron density from the C and H atoms of the methoxy group in 2 position of aromatic rings and from the Sn atom to the atoms of its coordination polyhedron. This increases also the electron density of the O atom involved in this interaction.

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