ISSN 1070-3632, Russian Journal of General Chemistry, 2012, Vol. 82, No. 6, pp. 1073–1079. © Pleiades Publishing, Ltd., 2012.
Original Russian Text © V.P. Feshin, E.V. Feshina, 2012, published in Zhurnal Obshchei Khimii, 2012, Vol. 82, No. 6, pp. 914–920.

Steric and Electronic Structure of 2-Alkoxyphenyltrichlorostannanes according to 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

Received April 12, 2011

Abstract—Steric and electronic structure of 2-methoxy- and 2-ethoxyphenyltrichlorostannanes, as well as of 2-methoxyphenyltrichlorostannanes substituted in the ring, was studied using the RHF and B3LYP levels with the 3-21G* basis set. The results of calculations were compared with experimental ^{35}Cl NQR data. In all studied molecules the Sn atom is pentacoordinated. The structure of the coordination polyhedron is a highly distorted trigonal bipyramid. Replacing methyl group in the alkoxy substituent involved in the Sn←O coordinating interaction by a more electron-donor ethyl group increases the strength of the Sn←O coordination bond. The same occurs also at the introduction of an electron-releasing substituent in the aromatic ring.

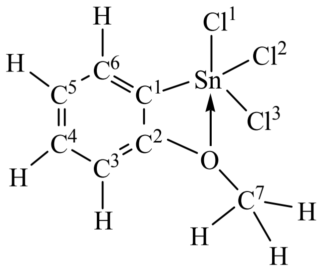
DOI: 10.1134/S1070363212060060

Earlier using the method of nuclear quadrupole resonance (NQR) on the ^{35}Cl nuclei it was found [1] that the tin atom in 2-alkoxyphenyltrichlorostannanes may be pentacoordinated through its interaction with the oxygen atom of the alkoxy group. For example, in the ^{35}Cl NQR spectrum of 2-$CH_3OC_6H_4SnCl_3$ **I** at 77 K the low-frequency line of the triplet (20.070 MHz) is considerably shifted from the high-frequency doublet (21.762 and 21.674 MHz). In the ^{35}Cl NQR spectrum of 2-$C_2H_5OC_6H_4SnCl_3$ **II** the low-frequency line (19.313 MHz) also is shifted significantly to lower frequencies as compared with the weakly split high-frequency doublet (21.880 and 21,475 MHz). In the doublet NQR spectrum of 2-methoxy-5-methylphenyltrichlorostannane **III** the low-frequency line (19.497 MHz) also is shifted considerably from the more intense high-frequency line (21.550 MHz). Such spectra are typical of the compounds of the IVA group elements with the trigonal–bipyramidal structure of the coordination polyhedron, in which one chlorine atom and the heteroatom of organic substituent occupy axial positions of the bipyramid, while the other two chlorine atoms are in the equatorial positions [1–3]. In the triplet NQR spectrum of 2-methoxy-3,5-dimethylphenyltrichlorostannane **IV** the low-frequency line (19.213 MHz) is in the same range as the low-frequency lines of the other alkoxyphenyltrichlorostannanes, the high-frequency line (22.119 MHz) is located at higher frequency by almost 3 MHz, and the third line (20.341 MHz) occupies an intermediate position [1].

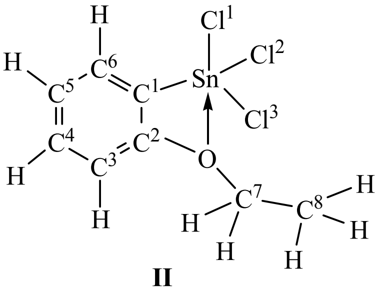
To study steric and electronic structure of these compounds and the influence of substituents on the strength of coordination Sn←O bond in them we calculated the corresponding molecules with full geometry optimization using the levels RHF and B3LYP with basis set 3-21G* by the Gaussian 03W software [4]. Unfortunately, this program does not allow calculation of Sn compounds using a basic set of a higher level. However, the calulation with 3-21G* set also leads to satisfactory agreement with the experimental data [5].

The results of calculations of electronic distribution in molecules **I–IV** was used to estimate the parameters of the ^{35}Cl NQR and to compare them with experimental data. Therefore, we placed the coordinate system origin on the chlorine atom whose NQR parameters were determined. The *Z*-axis of the system coincided with the corresponding Cl–Sn bond.

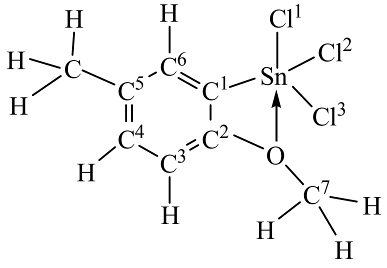
In the previous paper [6] we reported the results of the study of steric and electronic molecular structure of the compounds 2- and 4-$CH_3OC_6H_4SnCl_3$ and 2,6-$(CH_3O)_2C_6H_4SnCl_3$ by the RHF/3-21G* and MR2/3-



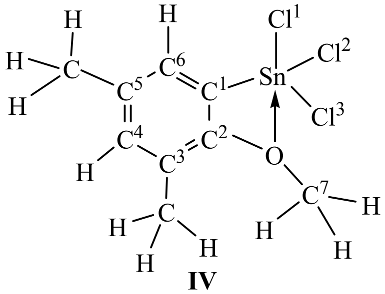
I



II



III



IV

21G* levels. The results obtained by these levels were fundamentally different. Moreover, the calcula-tion of the molecules by MR2/3-21G*, which is of higher level, but more expensive, has led to worse agreement of calculated and experimental ^{35}Cl NQR parameters than the calculation using RHF/3-21G* level. Therefore, in this paper in addition to the last level we used the level of density functional B3LYP/3-21G*.

The results of calculations of geometric characteristics of molecules **I–IV** by the RHF/3-21G* and B3LYP/3-21G* levels do not differ essentially (Table 1). In all studied molecules the Sn–C^1 bond in the *trans* position to the oxygen atom (C^{1}SnO angle is close to 180º) is longer than two others, which in the molecules **I** and **III** are identical. In molecule **IV** the lengths of all three bonds are quite different. Angles Cl^{1}SnC^1 and Cl^{3}SnC^1 in molecules **I** and **III** are identical, and in molecules **II** and **IV** they are some-what different. Their values are close to 120º. The ClSnC^1 angle is intermediate between the tetrahedral and right, but closer to tetrahedral. As in organyl-trichlorogermanes of the trigonal bipyramidal structure where the Ge atom becomes pentacoordinated at the closure of a five-membered ring as a result of its interaction with the heteroatom of the organic substituent [7, 8], the Sn atom in the studied molecules is shifted from the equatorial plane formed by the C^1, Cl^2, and Cl^{3}atoms to the axial Cl^1 atom: the angles C^{1}SnO, Cl^{2}SnO, and Cl^{3}SnO are less than 90º (Table 1). The sum of angles between the equatorial bonds of the Sn atom is less than 360º. This indicates a pyramidal structure of the equatorial fragment of the molecule with the Sn atom at the apex. In all the studied molecules the Sn···O distance is much less than the sum of Sn and O van der Waals radii (3.5 Å [9]). These geometric parameters of molecules **I–III** indicate a highly distorted trigonal–bipyramidal struc-ture of the coordination polyhedron of the tin atom. Judging from the dihedral angles ClSnC^{1}C^2, the Cl^2–Sn and Cl^3–Sn bonds are arranged symmetrically with respect to the plane of the aromatic ring in molecules **I** and **III** , and almost symmetrically in the molecules **II** and **IV** (especially in B3LYP/3-21G* calculations). The intramolecular Sn←O interaction in these molecules reduces substantially the angles SnC^{1}C^2 and C^{1}C^{2}O and increases the angles SnC^{1}C^6 and C^{3}C^{2}O (Table 1), compared to similar angles in aromatic molecules without a coordination interaction between the atoms in *ortho*-positions to each other. Therewith, the angles involving Sn–C^1 bond are changed much stronger than those involving the shorter C^2–O bond.

The dihedral angles C^{1}C^{2}OC^7 in molecules **I** and **III** are 180º in the calculations by both methods. In molecule **II** the calculations using RHF/3-21G* gives this angle close to 180º, but the value significantly less than 180º was obtained in the calculations by B3LYP/3-21G* level. Calculation of molecule **IV** by both methods gave this angle significantly different from 180º. Apparently, a decrease in this angle allows the interaction of the groups Cl^{3}Sn and OCH$_3$ to occur directly through the field. The distance between the interacting Sn and O sites in this molecule is the

Table 1. Bond lengths (*d*), valence (ω), and torsion angles (β) in molecules **I–IV** calculated by the RHF/3-21G* and B3LYP/3-21G* levels

Bond	**I**		**II**		**III**		**IV**	
	RHF	B3LYP	RHF	B3LYP	RHF	B3LYP	RHF	B3LYP
	d, Å							
Cl^1–Sn	2.369	2.382	2.371	2.384	2.370	2.383	2.373	2.387
Cl^2–Sn	2.351	2.369	2.354	2.375	2.351	2.369	2.358	2.378
Cl^3–Sn	2.351	2.369	2.352	2.365	2.351	2.369	2.348	2.367
Sn–C^1	2.130	2.147	2.130	2.148	2.131	2.147	2.128	2.145
C^1–C^2	1.384	1.397	1.385	1.397	1.384	1.397	1.384	1.394
C^2–O	1.394	1.403	1.396	1.407	1.396	1.404	1.412	1.426
O–C^7	1.449	1.467	1.460	1.483	1.448	1.466	1.458	1.486
Sn←O	2.438	2.560	2.420	2.521	2.433	2.554	2.416	2.517
Angle	ω, deg							
Cl^{1}SnC^1	106.99	106.78	106.91	106.76	106.96	106.88	106.78	106.52
Cl^{2}SnC^1	117.71	117.13	117.72	116.47	117.82	117.24	116.81	116.63
Cl^{3}SnC^1	117.71	117.13	118.34	118.62	117.81	117.24	119.63	119.24
Cl^{1}SnCl^2	101.94	103.04	101.60	102.85	101.82	102.82	101.37	102.04
Cl^{1}SnCl^3	101.94	103.04	101.63	102.51	101.82	102.82	101.33	102.08
Cl^{2}SnCl^3	108.10	107.79	107.99	107.77	108.11	107.81	108.07	107.83
SnC^{1}C^2	102.70	105.09	102.32	104.13	102.53	104.89	102.58	103.78
SnC^{1}C^6	137.55	134.43	137.79	135.23	137.58	134.44	136.68	134.91
C^{1}C^{2}O	109.37	110.41	109.14	110.01	109.40	110.43	108.70	110.45
OC^{2}C^3	127.35	127.87	128.38	128.38	128.36	128.25	128.89	127.64
C^{2}OC^7	123.41	120.60	124.70	121.79	123.27	120.51	124.79	119.72
Cl^{1}SnO	166.09	164.47	166.21	165.04	166.14	164.71	166.38	165.45
Cl^{2}SnO	86.06	85.90	86.73	86.11	86.16	85.98	86.02	85.72
Cl^{3}SnO	86.06	86.03	85.94	86.03	86.16	85.98	86.98	86.92
C^{1}SnO	59.04	57.59	59.31	58.19	59.18	57.83	59.60	58.94
Angle	β, deg							
Cl^{1}SnC^{1}C^2	180.0	180.0	179.45	–179.18	180.0	180.0	179.85	179.13
Cl^{2}SnC^{1}C^2	–66.12	–65.21	–67.15	–65.45	–66.24	–65.35	67.32	66.04
Cl^{3}SnC^{1}C^2	66.12	65.21	65.67	65.87	66.24	65.35	–66.10	–66.28
SnC^{1}C^{2}O	0.0	0.0	–0.16	–1.92	0.0	0.0	–0.12	0.69
C^{1}C^{2}OC^7	180.0	180.0	178.84	167.98	180.0	180.0	–146.91	–133.69

smallest compared to all the studied molecules. Perhaps this interaction is the main cause of the difference in all three Sn–Cl bond lengths and Cl^{2}Sn C^1 and Cl^{3}SnC^1 valence angles in molecule **IV** and, consequently, the electronic distribution on the chlorine atoms of these bonds and ^{35}Cl NQR frequencies of this compound. Significant deviation of the C^{1}C^{2}OC^7 angle from 180° in molecule **II** as calculated by the B3LYP/3-21G* level also leads to a noticeable difference in the Sn–Cl bond lengths and Cl^{2}SnC^1 and Cl^{3}SnC^1 bond angles (Table 1). The dihedral C^{2}OC^{7}C^8 angle in this molecule equals –80.11° (RHF) or –74.16° (B3LYP).

In molecule **II** the distance Sn···O is shorter than in **I**, that is, the replacement of the methyl group in the alkoxy substituent participating in the Sn←O coordination interaction by a more electron-donor ethyl group increases the strength of the Sn←O coordination bond. In molecules **III** and **IV** also the Sn···O distance is reduced compared with **I**, hence, the introduction of electron-donor substituent in the aromatic ring also increases the strength of the coordination Sn←O bond.

Earlier [10–12] we obtained satisfactory agreement between the experimental ^{35}Cl NQR frequencies (ν) and those calculated with Eq. (1) from the population of the less diffuse 3*p* components of valence *p* orbitals of chlorine atoms in organic and organometallic molecules calculated by the RHF/6-31G(d) level. A satisfactory agreement was obtained also between the experimental asymmetry parameters (η) of the electric field gradient (EFG) at the ^{35}Cl nuclei and those

Table 2. Populations of 3*p* components of valence *p* orbitals of Cl atoms in the molecules calculated by the RHF/3-21G* and B3LYP/3-21G* methods, the calculated ^{35}Cl NQR frequencies and experimental frequencies measured at 77 K [5, 16]

Run no.	Molecule	RHF				B3LYP				ν_{exp}, MHz
		$N3p_x$, *e*	$N3p_y$, *e*	$N3p_z$, *e*	ν_{calc}, MHz	$N3p_x$, *e*	$N3p_y$, *e*	$N3p_z$, *e*	ν_{calc}, MHz	
1	$(ClCH_2)_2SnCl_2$	1.102	1.110	0.785	35.961	1.121	1.133	0.804	36.151	36.708
2		1.059	1.059	0.894	18.480	1.081	1.081	0.907	19.409	18.030
3	$ClCH_3$	1.104	1.104	0.798	34.273	1.126	1.126	0.810	35.350	34.029
4	$ClC(O)CF_3$	1.131	1.091	0.812	33.713	1.143	1.086	0.845	30.649	33.432
5	$ClCH{=}CH_2$	1.113	1.096	0.813	32.690	1.134	1.109	0.836	32.029	33.411
6	$Cl(CH_2)_3SnCl_3$	1.089	1.108	0.816	31.696	1.105	1.131	0.833	31.981	31.750
7		1.063	1.067	0.889	20.389	1.084	1.089	0.894	21.540	20.352
8		1.061	1.066	0.886	19.888	1.081	1.088	0.899	20.762	20.160
9		1.059	1.056	0.897	17.980	1.081	1.077	0.910	19.298	19.668
10	$ClC(O)CH_3$	1.113	1.076	0.833	29.507	1.124	1.079	0.856	27.807	28.962[a]
11	$GeCl_4$	1.081	1.081	0.862	24.528	1.101	1.102	0.874	25.393	25.661[a]
12	$C_6H_5SnCl_3$	1.062	1.061	0.889	19.321	1.083	1.083	0.901	20.340	20.674[a]
13	CH_3SnCl_3	1.062	1.060	0.889	19.265	1.085	1.081	0.901	20.363	20.64[a]
14	$ClGe(CH_3)_3$	1.060	1.060	0.903	17.584	1.083	1.083	0.914	18.905	17.919
15	$SnCl_4$	1.068	1.068	0.873	21.840	1.091	1.091	0.883	23.268	24.095[a]
16	CH_3SiCl_3	1.074	1.070	0.918	17.253	1.093	1.088	0.933	17.625	19.043[a]
17	$ClSi(CH_3)_3$	1.062	1.062	0.933	14.375	1.083	1.083	0.945	15.437	16.506
18	$Cl_2Sn(CH_3)_2$	1.056	1.052	0.903	16.917	1.079	1.074	0.915	18.073	15.466
19	$ClSn(CH_3)_3$	1.049	1.049	0.913	15.232	1.073	1.073	0.921	17.004	11.73

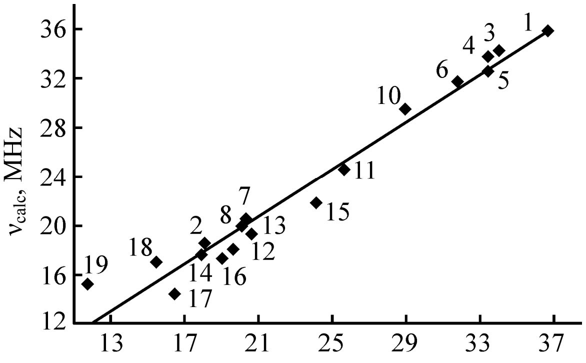
[a] Mean value of the NQR frequency.

calculated from the 3*p* components with Eq. (2) for a number of organic molecules.

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

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

Here e^2Qq_{at} is atomic nuclear quadrupole coupling constant, *h* is the 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 indicatory chlorine atom. The value of $e^2Qq_{at}/2h$ is found from the experimental NQR frequency of Cl_2 at 77K and the population of the 3*p* components of valence *p* orbitals of Cl atoms of the molecule are derived from a calculation by an appropriate method [10–12].



Correlation between the experimental ^{35}Cl NQR frequencies (ν_{exp}) and the frequencies (ν_{calc}) derived from the populations of 3*p* components of valence *p* orbitals of chlorine atoms in these molecules calculated by the RHF/3-21G* method. The numbering of points corresponds to the numbers in Table 2.

As we have to use the 3-21G* basis set to study the steric and electronic structure of the Sn compounds by the methods of quantum chemistry and to estimate the results of these calculations comparing them with experimental data on the ^{35}Cl NQR it was interesting to consider the experimental ^{35}Cl NQR frequencies of a series of chlorine-containing organic and organometallic compounds comparing them with the data derived from the populations of 3*p* components of valence *p* orbitals of chlorine atoms in these molecules calculated by the RHF/3-21G* and B3LYP/3-21G* levels (Table 2). For most molecules, including those containing the Sn–Cl bonds, the agreement between the experimental and calculated NQR frequencies is quite satisfactory. Linear correlation between the experimental (ν_{exp}) and calculated (ν_{calc}) ^{35}Cl NQR frequencies is satisfactory:

$$\nu_{calc} = (1.015\pm0.063)\nu_{exp} - (0.736\pm1.712), \quad (3)$$

$$r\ 0.996,\ n\ 1\text{–}14\ (\text{RHF}),$$

$$\nu_{calc} = (0.916\pm0.093)\nu_{exp} + (2.059\pm2.481), \quad (4)$$

$$r\ 0.987,\ n\ 1\text{–}14\ (\text{B3LYP}).$$

Table 3. Populations of valence *p* orbitals of Cl (ΣNp) and their 3*p* components ($N3p$) in the molecules **I–IV** calculated by the RHF/3-21G* and B3LYP/3-21G* methods, and ^{35}Cl NQR frequencies (ν_{calc}) and asymmetry parameters (η_{calc}) of electric field gradient on the ^{35}Cl nuclei calculated from the populations of 3*p* components

Molecule	Atom	Orbital	Np_x, *e*	Np_y, *e*	Np_z, *e*	ν_{calc}, MHz	η_{calc}, %
				RHF			
I	Cl^1	$N3p$	1.057	1.055	0.900	17.473	1.92
		ΣNp	1.967	1.964	1.592	–	–
	Cl^2	$N3p$	1.061	1.064	0.889	19.435	2.59
		ΣNp	1.966	1.970	1.571	–	–
II	Cl^1	$N3p$	1.057	1.055	0.901	17.371	1.94
		ΣNp	1.968	1.964	1.593	–	–
	Cl^2	$N3p$	1.061	1.064	0.889	19.433	1.73
		ΣNp	1.966	1.970	1.572	–	–
III	Cl^1	$N3p$	1.056	1.055	0.901	17.304	0.97
		ΣNp	1.968	1.965	1.593	–	–
	Cl^2	$N3p$	1.061	1.064	0.889	19.433	2.59
		ΣNp	1.966	1.970	1.572	–	–
IV	Cl^1	$N3p$	1.056	1.055	0.901	17.305	0.97
		ΣNp	1.968	1.965	1.596	–	–
	Cl^2	$N3p$	1.060	1.062	0.893	18.817	1.79
		ΣNp	1.967	1.971	1.583	–	–
	Cl^3	$N3p$	1.062	1.065	0.887	19.770	2.55
		ΣNp	1.965	1.968	1.567	–	–
				B3LYP			
I	Cl^1	$N3p$	1.080	1.078	0.910	18.906	1.75
		ΣNp	1.953	1.947	1.545	–	–
	Cl^2	$N3p$	1.085	1.086	0.898	19.284	3.34
		ΣNp	1.951	1.954	1.522	–	–
II	Cl^1	$N3p$	1.080	1.078	0.911	18.793	1.79
		ΣNp	1.953	1.947	1.546	–	–
	Cl^2	$N3p$	1.084	1.086	0.900	20.696	1.62
		ΣNp	1.952	1.956	1.530	–	–
	Cl^3	$N3p$	1.085	1.086	0.897	21.087	0.80
		ΣNp	1.951	1.953	1.521	–	–
III	Cl^1	$N3p$	1.079	1.078	0.910	18.849	0.89
		ΣNp	1.953	1.948	1.546	–	–
	Cl^2	$N3p$	1.085	1.086	0.898	20.975	0.80
		ΣNp	1.952	1.954	1.523	–	–
IV	Cl^1	$N3p$	1.079	1.077	0.911	18.683	1.80
		ΣNp	1.954	1.948	1.550	–	–
	Cl^2	$N3p$	1.082	1.084	0.903	20.136	0.94
		ΣNp	1.954	1.956	1.538	–	–
	Cl^3	$N3p$	1.085	1.088	0.897	21.201	2.37
		ΣNp	1.950	1.952	1.519	–	–

The correspondence between these NQR frequencies is better when the calculation is based on the results of RHF/3-21G* calculations. The NQR frequencies only of a few (15–19) molecules deviate from the correlation line corresponding to Eq. (3). In Eq. (3) the coefficient at ν_{exp} is close to unity and the absolute term differs from zero. Consequently, the ^{35}Cl NQR frequencies derived from the results of calculations of the molecules by RHF/3-21G* level usually are lower than the experimental values by the value of the absolute term in Eq. (3). Apparently, the steric and electronic structures of molecules in the gaseous and crystalline states are quite different. The obtained correlation indicates that the comparison of the ^{35}Cl NQR frequencies derived from the results of calculations of the molecules by RHF/3-21G* level with experimental data is quite acceptable.

For comparison with experimental NQR data, we estimated ^{35}Cl NQR frequencies and asymmetry parameters of the electric field gradient on the ^{35}Cl nuclei from the results of quantum chemical calculations of the studied molecules **I–IV** by the RHF/3-21G* and B3LYP/3-21G* levels (Table 3). Given the similarity of Sn–Cl^2 and Sn–Cl^3 bond lengths in molecules **I** and **III**, as well as valence and dihedral angles involving them, we can assume that the electronic distribution on their chlorine atoms is also the same. This is valid also for the molecule **II** calculated by RHF/3-21G* level. Therefore, Table 3 includes the populations of valence *p* orbitals and the 3*p* components of these orbitals, as well as calculated from them ^{35}Cl NQR parameters for only one of these chlorine atoms. For the molecule **II** calculated by the B3LYP/3-21G* level these data are shown for the three chlorine atoms. Unfortunately, the NQR frequencies of all studied molecules derived from the results of RHF/3-21G* calculations were significantly lower than the experimental data obtained at 77 K. At the same time, the ratio of the calculated NQR frequencies for axial and equatorial chlorine atoms in these molecules corresponds to the experimental one. The ^{35}Cl NQR frequencies derived from the populations of 3*p* components of valence *p* orbitals of chlorine atoms in molecules **I–IV** calculated by B3LYP/3-21G* are slightly lower than experimental ones, but close to them (the difference is within 1.0 MHz), with the exception of the axial Cl^1 atom in molecule **I**. Apparently, the steric and electronic structure of the studied molecules in the crystalline state, characteristic of the sample during measuring the NQR spectra, differs markedly from that of individual molecules, for which the quantum-chemical calculations were performed. Therewith, the steric and electronic structure of the studied molecules in the crystalline state is better described by B3LYP/3-21G* level.

Lower NQR frequencies of the axial chlorine atoms Cl^1 compared with the equatorial Cl^2 and Cl^3 in the studied molecules are due both to a higher half-sum of the populations of 3*p* components of valence p_x and p_y orbitals of the equatorial chlorine atoms and lower occupancy of the 3*p* components of their valence p_z orbitals (Table 3).

Usually, when the structure of coordination polyhedron of an atom of IVA group element is a trigonal bipyramid, the parameter of asymmetry of electric field gradient on the ^{35}Cl nucleus of equatorial chlorine atoms is rather large, while on the axial it is close to zero [13–15]. In the studied molecules **I–IV** the parameters of the electric field gradient asymmetry on ^{35}Cl nuclei of both axial and equatorial chlorine atoms are close to zero (Table 3). This is due to the close value of the populations of p_x and p_y orbitals and their 3*p* components for all three chlorine atoms in each studied molecule. In turn, this is due to the pyramidal structure of the equatorial fragment of trigonal-bipyramidal coordination polyhedron of Sn atom and indicates a significant distortion of the structure of this polyhedron. Unfortunately, the experimental asymmetry parameters of the electric field gradient on the ^{35}Cl nuclei of the studied compounds have not been measured. Therefore, no data exist for comparison with the calculated asymmetry parameters.

ACKNOWLEDGMENTS

This work was supported by the Russian Foundation for Basic Research (project no. 10-03-00131a), as well as by the basic research program carried out jointly with the organizations of Siberian and Far East branches of Russian Academy of Sciences “Study of steric and electronic structures of compounds of the Mendeleev’s Table IVA and VA groups elements in different states of aggregation.”

REFERENCES

1. Feshin, V.P., Dolgushin, G.V., Lazarev, I.M., and Voronkov, M.G., *Zh. Strukt. Khim.*, 1989, vol. 30, no. 1, p. 169.
2. Feshin, V.P., Nikitin, P.A., Voronkov, M.G., Gar, T.K., Viktorov, N.A., Gurkova, S.N., Gusev, A.I., and Shiryaev, V.I., *Zh. Obshch. Khim.*, 1984, vol. 54, no. 3, p. 646.
3. Feshin, V.P. and Polygalova, G.A., *J. Organometal. Chem.*, 1991, vol. 409, no. 1, p. 1.
4. Frisch, M.J., Trucks, G.W., Schlegel, H.B., Scuseria, G.E., Robb, M.A., Cheeseman, J.R., Montgomery, J.A., Jr., Vreven, T., Kudin, K.N., Burant, J.C., Millam, J.M., Iyengar, S.S., Tomasi, J., Barone, V., Mennucci, B., Cossi, M., Scalmani, G., Rega, N., Petersson, G.A., Nakatsuji, H., Hada, M., Ehara, M., Toyota, K., Fukuda, R., Hasegawa, J., Ishida, M., Nakajima, T., Honda, Y., Kitao, O., Nakai, H., Klene, M., Li, X., Knox, J.E., Hratchian, H.P., Cross, J.B., Bakken, V., Adamo, C., Jaramillo, J., Gomperts, R., Stratmann, R.E., Yazyev, O., Austin, A.J., Cammi, R., Pomelli, C., Ochterski, J.W., Ayala, P.Y., Morokuma, K., Voth, G.A., Salvador, P., Dannenberg, J.J., Zakrzewski, V.G., Dapprich, S., Daniels, A.D., Strain, M.C., Farkas, O., Malick, D.K., Rabuck, A.D., Raghavachari, K., Foresman, J.B., Ortiz, J.V., Cui, Q., Baboul, A.G., Clifford, S., Cioslowski, J., Stefanov, B.B., Liu, G., Liashenko, A., Piskorz, P., Komaromi, I., Martin, R.L., Fox, D.J., Keith, T., Al-Laham, M.A., Peng, C.Y., Nanayakkara, A., Challacombe, M., Gill, P.M.W., Johnson, B., Chen, W., Wong, M.W., Gonzalez, C., and Pople, J.A., *Gaussian 03*, Revision, D.1. Gaussian, Inc., 2003.

5. Feshin, V.P. and Feshina, E.V., *Zh. Obshch. Khim.*, 2010, vol. 80, no. 8, p. 1298.
6. Feshin, V.P. and Feshina, E.V., *Zh. Obshch. Khim.*, 2012, vol. 82, no. 5, p. 747.
7. Gurkova, S.N., Gusev, A.I., Alekseev, N.V., Gar, T.K., and Viktorov, N.A., *Zh. Strukt. Khim.*, 1985, vol. 26, no. 5, p. 183.
8. Tandura, S.N., Gurkova, S.N., Gusev, A.I., and Alekseev, N.V., *Zh. Strukt. Khim.*, 1985, vol. 26, no. 6, p. 136.
9. Gurkova, S.N., Gusev, A.I., Alekseev, N.V., Feshin, V.P., Lazarev, I.M., Dolgushin, G.V., and Voronkov, M.G., *Zh. Strukt. Khim.*, 1987, vol. 28, no. 4, p. 180.
10. Feshin, V.P. and Feshina, E.V., *Z. Naturforsch., A*, 2000, vol. 55, no. 2, p. 555.
11. Feshin, V.P., *Elektronnye effekty v organicheskikh i elementoorganicheskikh molekulakh* (Electronic Effects in Organic and Organoelement Molecules), Yekaterinburg: Izd. Ural. Otd. Ross. Akad. Nauk, 1997.
12. Feshin, V.P., *Geminal'noe vzaimodeistvie v organicheskoi i elementoorganicheskoi khimii* (Geminal Interaction in Organic and Organoelement Chemistry), Yekaterinburg: Izd. Ural. Otd. Ross. Akad. Nauk, 2009.
13. Feshin, V.P., Dolgushin, G.V., Lazarev, I.M., Sapozhnikov, Yu.E., Yasman Ya.B., Voronkov, M.G., Dokl. Akad. Nauk SSSR, 1988, vol. 300, no. 5, p. 1181.
14. Buslaev, Yu.A., Kravchenko, E.A., Morgunov, V.G., Burtsev, M.Yu., Feshin, V.P., Dolgushin, G.V., Lazarev, I.M., and Voronkov, M.G., *Dokl. Akad. Nauk SSSR*, 1988, vol. 300, no. 6, p. 1408.
15. Feshin, V.P. and Voronkov, M.G., *Z. Naturforsch., A,* 1990, vol. 45, no. 1, p. 213.