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Spatial and Electronic Structure and ^{35}Cl NQR Parameters of Ethyl(trichlorogermyl) Propionate According to Ab Initio Calculations

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Abstract—Two stable structures of ethyl(trichlorogermyl) propionate have been studied by RHF/6-31G(d) and MP2/6-31G(d) quantum-chemical caclulation with full geometry optimization. The structure with pentacoordinated Ge atom has been more stable than that with tetracoordinated Ge atom. Based on the computation results, the frequencies of ^{35}Cl nuclear quadrupole resonance of the studied compound with pentacoordinated Ge atom has been estimated, it has been in satisfactory agreement with the experimental data. Additionally, the calculations by means of the RHF/6-31G(d) method have been performed at various fixed Ge···O interatomic distances. When the Ge and O coordination centers get closer, both the positive charge on Ge and the negative charge on O increase. The electron density shifts from Ge atom to the axial Cl atom, and the electron density shifst from the carbonyl C atom to the carbonyl oxygen atom. The electron density charge trasfer from O to Ge does not occur.

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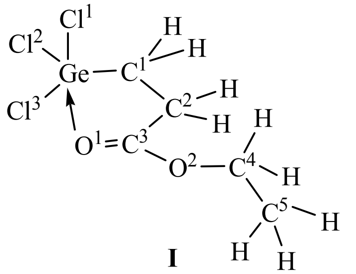
In organylgermanes containing the $Cl_3Ge–C–C–C=O$ fragment with Ge pentacoordination requirements fulfiled [1, 2], the intramolecular interaction of Ge with the organyl heteroatom is possible, and as a result their interatimic distance gets significantly smaller than the sum of their Van der Waals radii. In this case, the five-membered ring is formed, and Ge coordination polyhedron is transformed into a trigonal bipyramid. Some of such compounds have been studied by means of X-Ray diffraction analysis (XRD) [1–7] and ^{35}Cl nuclear quadrupole resonance (NQR) [1–3, 7, 8]. Their spacial and electronic structure has been studied by non-empirical quantum-chemical methods [9–11], the computation results have been compared with the experimental XRD and ^{35}Cl NQR data. To compare the theoretical results with the experimental NQR data we have developed [12–14] a procedure to estimate the ^{35}Cl NQR parameters according to the population density of less diffuse 3*p*-component of the valence p-orbitals of Cl atoms in chlorine-containing organic and organoelemental compounds, the orbital population being calculated by non-empirical quantum-chemical methods. According to Eqs. (1) and (2), from the populations determined by the RHF/6-31G(d) method the values of ^{35}Cl NQR frequency (ν) and the asymmerty parameter of electrical field gradient EFG (η), respectively, can be calculated in satisfactory agreement with the experimental data. Using quantum-chemical methods of higher level to estimate the Cl orbitals population does not lead to improvement of the result [15].

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

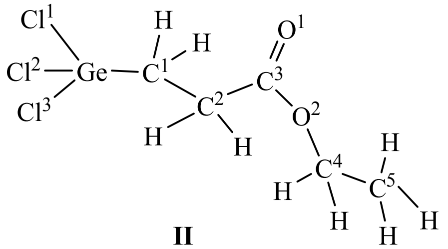
$$\eta = |3(N_x - N_y)/(2N_z - N_x - N_y)|. \quad (2)$$

In the equations, e^2Qq_{at} is the atomic constant of quadrupole interaction; h is the Planck constant; N_x, N_y, and N_z are polupations of $3p_x$-, $3p_y$-, and $3p_z$-orbitals, respectively, of the indicator Cl atom. The $e^2Qq_{\text{at}}/2h$ value was determined from the experimental NQR frequency of Cl_2 at 77 K and the populations of 3*p*-orbitals of the Cl atoms in Cl_2 were obtained from computations [12–15].

In this work, we extended the studies of spacial and electronic structure of organyltrichlorogermanes and the electron density rearrangement upon formation of the Ge←O coordination bond. Additionally, the parameters of ^{35}Cl NQR spectra of those compounds were computed by quantum-chemical calculations and compared with the respective experimental data. To do so, we performed quantum-chemical calculations of structures **I** and **II** of ethyl(trichlorogermyl) propionate using the RHF/6-31G(d) and MP2/6-31G(d) methods (utilizing GAUSSIAN 03W [16] software package) with full geometry optimization, and calculations of structure **I** by the RHF/6-31G(d) method at varied Ge···O distances. As the results of quantum-chemical calculations were then used to estimate the ^{35}Cl NQR parameters, the origin of coordinate system during the computation was set in succession on the chlorine atoms whose NQR characteristics should be estimated, and the *z* axis was directed along the Cl–Ge bond.



I



II

The results of computation revealed that possessed two stable forms, **I** and **II**; none of them had imaginary frequencies of stretching vibrations. Structure **I** was somewhat more favorable, its total energy was by 0.870 kcal mol^{-1} (RHF) or 0.481 kcal mol^{-1} (MP2) lower than that of **II**. Thus, structure **I** should be found in the ethyl(trichlorogermyl) propionate crystals. The computation results did not significantly depend on the applied quantum-chemical method (Tables 1 and 2). The Ge···O distance in **I** as determined by means of MP2/6-31G(d) method was noticeably shorter than that from the RHF/6-31G(d) computations. This distance, as determined by both methods, was significantly less than the sum of Ge and O Van der Waals radii, indicating their interaction. Thus, Ge in this structure was pentacoordinated. One of the Ge–Cl^1 bonds in the structure was significantly longer than two others, the Cl^{2}GeC^1 and Cl^{3}GeC^1 bond angles were significantly larger than tetrahedral ones, and the Cl^{1}GeO^1 bond angle was close to 180°. These geometry parameters corresponded to trigonal bipyramid as a coordination polyhedron of pentacoordinated Ge. Other bond angles involving Ge atom (Table 1) revealed a pronounced distortion of the coordination polyhedron. according to the Cl^{1}GeC^1, Cl^{1}GeCl^2, and Cl^{1}GeCl^3 bond angles, all being more than 90°, Ge atom moved out of the equatorial plane of trigonal bipyramid towards the axial Cl^1; thus Ge atom was a vortex of the trigonal pyramid having C^1, Cl^2, and Cl^3 as a base.

Structure **II** differed from **I** in the Ge coordination number, in torsional and bond (to a some extent) angles, and in the Cl^1–Ge and Ge–C^1 bond lengths.

Table 1. Bond lengths (*d*), bond angles (α), and torsion angles (β) in **I**, as calculated by RHF/6-31G(d) and MP2/6-31G(d) methods

Bond	*d*, Å		Angle	α, deg		Angle	β, deg	
	RHF	MP2		RHF	MP2		RHF	MP2
Cl^1–Ge	2.169	2.181	Cl^{1}GeC^1	105.74	104.01	Cl^{1}GeC^{1}C^2	–137.46	–
Cl^2–Ge	2.131	2.139	Cl^{2}GeC^1	117.12	119.51	Cl^{2}GeC^{1}C^2	107.67	140.42
Cl^3–Ge	2.146	2.154	Cl^{3}GeC^1	114.32	114.13	Cl^{3}GeC^{1}C^2	–23.89	107.20
Ge–C^1	1.937	1.938	Cl^{1}GeCl^2	103.69	101.67	GeC^{1}C^{2}C^3	–55.57	–29.83
C^1–C^2	1.527	1.523	Cl^{1}GeCl^3	103.83	102.27	C^{1}C^{2}C^{3}O^1	13.57	–50.11
C^2–C^3	1.516	1.514	Cl^{2}GeCl^3	110.51	112.32	C^{1}C^{2}C^{3}O^2	–167.65	17.46
C^3–C^4	1.507	1.234	GeC^{1}C^2	115.06	112.39	C^{2}C^{3}O^{2}C^4	–0.37	–
C^3=O^1	1.190	1.227	C^{1}C^{2}C^3	110.73	109.23	C^{3}O^{2}C^{4}C^5	–173.13	163.93
C^3–O^2	1.318	1.342	C^{2}C^{3}O^1	120.33	120.30			–0.70
O^2–C^4	1.422	1.450	C^{2}C^{3}O^2	119.64	120.58			–
C^4–C^5	1.514	1.511	C^{3}O^{2}C^4	123.54	120.31			170.79
Ge···O^1	2.817	2.568	O^{2}C^{4}C^5	107.07	106.12			
			Cl^{1}GeO^1	171.94	–			
			GeO^{1}C^3	100.67	–			

Table 2. Bond lengths (*d*), bond angles (α), and torsion angles (β) in **II**, as calculated by RHF/6-31G(d) and MP2/6-31G(d) methods

Bond	*d*, Å		Angle	α, deg		Angle	β, deg	
	RHF	MP2		RHF	MP2		RHF	MP2
$\mathrm{Cl^1{-}Ge}$	2.146	2.150	$\mathrm{Cl^1GeC^1}$	111.37	110.47	$\mathrm{Cl^1GeC^1C^2}$	–59.44	–58.80
$\mathrm{Cl^2{-}Ge}$	2.134	2.136	$\mathrm{Cl^2GeC^1}$	111.97	113.53	$\mathrm{Cl^2GeC^1C^2}$	180.0	–
$\mathrm{Cl^3{-}Ge}$	2.146	2.150	$\mathrm{Cl^3GeC^1}$	111.38	110.48	$\mathrm{Cl^3GeC^1C^2}$	59.44	179.99
$\mathrm{Ge{-}C^1}$	1.922	1.918	$\mathrm{Cl^1GeCl^2}$	107.67	107.77	$\mathrm{GeC^1C^2C^3}$	180.0	58.81
$\mathrm{C^1{-}C^2}$	1.527	1.525	$\mathrm{Cl^1GeCl^3}$	106.61	106.52	$\mathrm{C^1C^2C^3O^1}$	–0.01	180.0
$\mathrm{C^2{-}C^3}$	1.520	1.520	$\mathrm{Cl^2GeCl^3}$	107.62	107.77	$\mathrm{C^1C^2C^3O^2}$	179.98	–0.03
$\mathrm{C^3{=}O^1}$	1.184	1.217	$\mathrm{GeC^1C^2}$	112.28	109.98	$\mathrm{C^2C^3O^2C^4}$	0.07	179.99
$\mathrm{C^3{=}O^2}$	1.328	1.359	$\mathrm{C^1C^2C^3}$	111.22	110.57	$\mathrm{C^3O^2C^4C^5}$	179.97	–0.10
$\mathrm{O^2{-}C^4}$	1.419	1.445	$\mathrm{C^2C^3O^4}$	116.28	116.47			179.98
$\mathrm{C^4{-}C^5}$	1.514	1.512	$\mathrm{C^2C^3O^1}$	122.35	122.78			
$\mathrm{Ge\cdots O^1}$	4.651	4.648	$\mathrm{C^2C^3O^2}$	117.87	117.91			
			$\mathrm{C^3O^2C^4}$	124.04	120.96			
			$\mathrm{O^2C^4C^5}$	107.07	106.18			

Other bond lengths in **I** and **II** were respectively similar (Tables 1 and 2). Computations of **II** by both methods revealed that its $\mathrm{Cl^2}$, Ge, $\mathrm{C^1}$–$\mathrm{C^5}$, $\mathrm{O^1}$, $\mathrm{O^2}$, and one of the methyl group hydrogens were located almost in the same plane, thus forming a zigzag of $\mathrm{Cl^2}$, Ge, $\mathrm{C^1}$–$\mathrm{C^3}$, and $\mathrm{O^2}$. Other Cl and H atoms were located almost symmetrically with respect to that plane; the coordination polyhedron of Ge was a tetrahedron.

In order to study the character of electron density rearrangement upon formation of the $\mathrm{Ge{\leftarrow}O^1}$ coordination bond in **I**, its structure was computed by the RHF/6-31G(d) method at several fixed $\mathrm{Ge\cdots O}$ distances, other geometry parameters being optimized. The varied distance was chosen between 3.5 Å, a sum of Ge and O Van der Waals radii, and 2.5 Å, below the result of full optimization (Table 1).

Upon transition from structure **II** (with no $\mathrm{Ge{\leftarrow}O^1}$ coordination interaction) to structure **I** with $\mathrm{Ge{\leftarrow}O^1}$ of 3.5 Å (similarly, the coordination interaction was almost absent), the total charge at the Cl atoms was somewhat decreased (Table 3). However, with decreasing the varied interatomic distance to 2.5 Å, the partial charges of all Cl atoms increased, especially that of $\mathrm{Cl^1}$, located at the axial position of the trigonal bipyramid. The negative charges of the equatorial Cl atoms were only slightly increased. Upon transition from structure **II** to structure **I** with $\mathrm{Ge\cdots O^1}$ of 3.5 Å, the partial positive charge of Ge practically did not change. However, with decreasing varied interatomic distance to 2.5 Å, the Ge partial charge increased by 0.091 *e*, a value very close to the total increase in the charge of three Cl atoms (0.097 *e*). The same transition from **II** to **I** with decreasing $\mathrm{Ge\cdots O^1}$ distance led to an increase in the partial negative charge on $\mathrm{O^1}$ by 0.032 *e*, a value close to the increase in the positive charge at $\mathrm{C^3}$ (0.029 *e*). Upon transition from structure **II** to structure **I** with $\mathrm{Ge\cdots O^1}$ of 3.5 Å, the partial negative charge at $\mathrm{C^1}$ increased and did not change much with shortening of $\mathrm{Ge\cdots O^1}$. In cotrast to that, the partial negative charge at $\mathrm{C^2}$ first increased and then was practically constant. Simultaneously, the charge at $\mathrm{O^2}$ was only slightly decreased, whereas those of $\mathrm{C^4}$ and $\mathrm{C^5}$ changed even less.

Table 3. Mulliken charges (*q*, e) at atoms in **I** as calculated by RHF/6-31G(d) method at varied $\mathrm{Ge\cdots O}$ [*r*($\mathrm{Ge\cdots O}$), Å] distances and in **II** as calculated by the same method with full geometry optimization [*r*($\mathrm{Ge\cdots O}$) 4.651 Å]

Atom	*r*($\mathrm{Ge\cdots O}$), Å				
	2.5	2.817	3.0	3.5	4.651
$\mathrm{Cl^1}$	–0.282	–0.253	–0.238	–0.218	–0.227
$\mathrm{Cl^2}$	–0.205	–0.198	–0.194	–0.189	–0.196
$\mathrm{Cl^3}$	–0.242	–0.237	–0.235	–0.225	–0.227
Ge	0.759	0.729	0.707	0.668	0.666
$\mathrm{C^1}$	–0.546	–0.539	–0.537	–0.541	–0.505
$\mathrm{C^2}$	–0.471	–0.471	–0.470	–0.468	–0.497
$\mathrm{C^3}$	0.849	0.835	0.828	0.820	0.823
$\mathrm{O^1}$	–0.568	–0.551	–0.543	–0.536	–0.534
$\mathrm{O^2}$	–0.598	–0.605	–0.607	–0.609	–0.613
$\mathrm{C^4}$	–0.026	–0.021	–0.018	–0.018	–0.016
$\mathrm{C^5}$	–0.494	–0.493	–0.492	–0.491	–0.491

Table 4. Selected bond lengths (d, Å) and bond angles (α, deg) in **I** as calculated by RHF/6-31G(d) method at varied Ge···O [r(Ge···O), Å] distances

Parameters	r(Ge···O), Å			
	2.5	2.817	3.0	3.5
d(Ge–Cl^1)	2.191	2.169	2.161	2.150
d(Ge–Cl^2)	2.136	2.131	2.130	2.131
d(Ge–Cl^3)	2.149	2.146	2.147	2.147
d(Ge–C^1)	1.939	1.937	1.937	1.940
d(O^1=C^3)	1.195	1.190	1.188	1.186
d(O^2–C^3)	1.310	1.318	1.321	1.325
d(O^2–C^4)	1.425	1.422	1.421	1.419
α(Cl^{1}GeO^1)	174.84	171.94	169.78	161.60
α(Cl^{1}GeC^1)	102.40	105.74	107.19	109.51
α(Cl^{2}GeC^1)	119.60	117.13	115.91	113.42
α(Cl^{3}GeC^1)	115.74	114.31	113.63	113.00
α(O^{1}GeC^1)	72.66	66.30	62.67	52.52
α(O^{1}GeCl^2)	80.67	79.79	79.90	86.51
α(O^{1}GeCl^3)	82.24	81.37	81.62	81.29
α(GeO^{1}C^3)	107.97	100.67	95.78	81.58

Thus, upon the described transition mainly changed the polarity of Ge–Cl, especially that of the axial Ge–Cl^1, and of the O^1=C^3 bonds. The partial positive charge at Ge increased, and so did the negative charges at Cl^1 and O^1. The electron density transfer from O^1 to Ge was not observed. As the Cl^{1}GeO^1 and GeO^{1}C^3 bond angles were obtuse (Table 1), the increase of electron density at the axial Cl accompanied by shortening of the Ge···O^1 distance occurred probably due to the direct through-field geminal interaction [13, 14] of partially negative O^1 with the axial Cl^1–Ge bond and of partially positive Ge with the O^1=C^3 bond (Table 3). Another reason of the electron density increase at the axial Cl could be due to the polarization of the Cl^1–Ge bond by partially negative C^1, Cl^2, and Cl^3, their bonds angles with Ge–Cl^1 being obtuse as well.

With the decreasing distance between the coordination centers in **I** from 3.5 to 2.5 Å, the Ge–Cl^1 and O^1=C^3 were elongated, the length of the O^2–C^4 was slightly increased as well; the O^2–C^3 bond was shortened. Simultaneously, the Cl^{1}GeC^1, O^{1}GeC^1, Cl^{2}GeC^1, Cl^{3}GeC^1, and Cl^{1}GeO^1 bond angles approached 90°, 90°, 120°, 120°, and 180°, respectively (Table 4). These limiting values of the bond angles were characteristic of the ideal trigonal bipyramid as Ge coordination polyhedron. The other bond lengths and bond angles in **I** changed only slightly and irregularly.

Table 5. Population density of 3p components of the valence p-orbitals of chlorine (N) in **I** as calculated by RHF/6-31G(d) and MP2/6-31G(d) methods; ^{35}Cl NQR frequencies (ν_c) and EFG at ^{35}Cl asymmetry parameters (η_c) as calculated from the population density

Method	Atom	N_x, e	N_y, e	N_z, e	ν_c, MHz	η_c, %
RHF	Cl^1	1.271	1.268	1.042	21.180	1.98
	Cl^2	1.276	1.285	1.019	24.355	5.16
	Cl^3	1.270	1.282	1.029	23.014	7.29
MP2	Cl^1	1.268	1.266	1.046	20.250	1.36
	Cl^2	1.273	1.290	1.016	24.364	9.60
	Cl^3	1.267	1.286	1.028	22.819	11.47

Previously, we reported on the ^{35}Cl NQR spectrum of ethyl(trichlorogermyl) propionate registered at 77 K [1]. The features of the spectrum confirmed the pentacoordination of Ge due to its interaction with O and the formation of the 5-membered cycle; the non-equivalence of the three Ge–Cl was also revealed. The coordination polyhedron of Ge was a highly distorted trigonal bipyramid. The low-frequency spectral line (21.754 MHz) corresponded to the axial Cl, whereas a pair of high-frequency lines (22.611 and 23.454 MHz) was assigned to the equatorial atoms. The above-discussed quantum-chemical calculations were in line with the experimental spectral data for the crystalline state. From the populations of the less diffuse 3p-orbitals, we estimated the values of ^{35}Cl NQR frequency and the asymmerty parameter of EFG (Table 5).

The ^{35}Cl NQR frequencies as calculated according to the RHF/6-31G(d) results were close to the experimental values (deviations were less than 1 MHz), whereas the results of MP2/6-31G(d) computation only led to satisfactory prediction for the equatorial Cl atoms. The NQR frequency for the axial Cl thus calculated was significantly underestimated. That was due to lower half-sum of 3p_x- and 3p_y-orbitals population of the axial Cl in the case of MP2/6-31G(d) model than that of RHF/6-31G(d) model, as well as to higher 3p_z-orbital population (Table 5).

The populations of the 3p_x-orbitals of the axial and equatorial Cl atoms were virtually the same as obtained with the RHF/6-31G(d) method, whereas the population of 3p_y-orbital was significantly lower in the case of the axial Cl (Table 5). That was one of the reasons for the lower NQR frequency in the case of the axial Cl. However, the main reason was much higher population of the 3p_z(p_σ)-orbital of the axial Cl [see Eq. (1)]. That was in line with the higher electron density on the axial Cl atom mainly due to the axial Ge–Cl^1 bond polarization under the action of partially negative O^1, C^1, Cl^2, and Cl^3 [13, 14].

The EFG asymmetry parameters at ^{35}Cl of ethyl(trichlorogermyl) propionate were not unfortunately measured. The values calculated according to the populations of 3*p*-orbitals derived from both computational methods (Table 5) were in line with experimental data for other chlorine-containing compounds of trigonal bipyramid coordination [17–20]. In particular, the asymmetry parameters were close to zero in the case of axial Cl atom and positive in the cases of equatorial Cl atoms.

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