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Stereoelectronic Structure of 1-Methyl-3-(trichlorogermyl)propionic Acid as Found by *Ab Initio* Calculations

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Abstract—Calculations of three structures of the 1-methyl-3-(trichlorogermyl)propionic acid molecule and its dimers were performed at the RHF/6-31G(d) level with the full geometry optimization. According to the calculations, in this molecule in a gaseous state the Ge atom is most likely pentacoordinated due to the Ge←O coordination interaction. The dimerization does not diminish, but slightly increases the strength of Ge←O coordination bond. At the formation of the Ge←O bond the electron density on the oxygen atom increases and on the Ge atom decreases. The comparison of the results of calculations with X-ray diffraction data and with the ^{35}Cl NQR spectrum shows that stereoelectronic structure of this compound in the crystalline and gaseous states are quite different.

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The XRD analysis of 1-methyl-3-(trichlorogermyl) propionic acid showed that Ge←:O interaction occurring in this molecule was much weaker than in the 3-(trichlorogermyl)propionamide, 2-methyl-3-(trichlorogermyl)propionic acid *N,N*-dimethylamide, and 1-(1-trichlorogermylethyl)pyrrolidone-2, but somewhat stronger than in the 3-(trichlorogermyl)propionic acid [1]. In the molecule of 1-methyl-3-(trichlorogermyl)propionic acid the coordination polyhedron of the Ge atom tends to transformation from the tetrahedral to a trigonal–bipyramidal structure, there is a noticeable trend to a differentiation of the bonds of Ge atom into axial and equatorial ones, namely, the Ge–Cl bond in *trans* position to oxygen atom is longer than the other two (Table 1). In the crystal, these molecules are bound into dimers by the O–H···O hydrogen bonds, which results in weakening of the coordination Ge←O bond in the dimer compared with the aforementioned molecule [1]. The nuclear quadrupole resonance (NQR) spectrum on the ^{35}Cl nuclei of this compound at 77 K (23.929, 22.870, and 22.078 MHz) indicates a substantial nonequivalence of all three Ge–Cl bonds. Such nonequivalence is not characteristic of the tetrahedral or trigonal–bipyramidal Ge atom. In this molecule the coordination polyhedron is of intermediate structure [2].

To examine further the stereoelectronic structure of 1-methyl-3-(trichlorogermyl)propionic acid, the nature of coordination Ge←O bond in it, and the effect on it of dimerization, we performed quantum-chemical calculations of three possible structures of this molecule and its dimers by RHF/6-31G(d) method with the full geometry optimization using the GAUSSIAN 03W software [3]. The XRD structural data and ^{35}Cl NQR spectra of the 1-methyl-3-(trichlorogermyl)propionic acid were obtained in the crystalline state, where the molecules not always are in the energetically most favorable form (e.g., see [4, 5]). Therefore, it seemed appropriate to explore stereoelectronic structure of this acid in the gaseous state and compare it with the existing XRD data and the ^{35}Cl NQR spectra. In the calculations, for the origin of the coordinate system the chlorine atom was chosen whose ^{35}Cl NQR parameters should be determined. The *Z*-axis of the system coincided with the direction of the corresponding Ge–Cl bond.

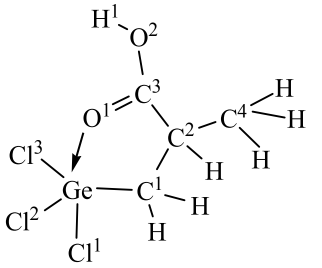
The ^{35}Cl NQR frequencies (ν) and asymmetry parameters (η) of the electric field gradient (EFG) at the ^{35}Cl nuclei were determined from the populations of less diffuse 3*p*-components of valence *p*-orbitals of the chlorine atom [6–8] using Eqs. (1) and (2), respectively [9].

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

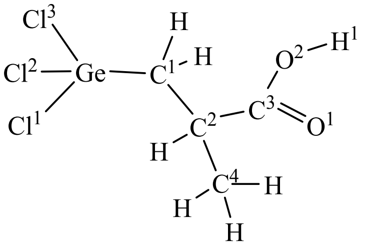
$$\eta = |3(N_x - N_y)/(2N_z - N_x - N_y)| \qquad (2)$$

Here e^2Qq_{at} is nuclear quadrupole coupling constant, h is the Planck constant; N_x, N_y and N_z are the populations of the 3p-components of valence p_x-, p_y-, and p_z-orbitals, respectively, of the indicator chlorine atom. The $e^2Qq_{\mathrm{at}}/2h$ value is found from the experimental NQR frequency of Cl_2 at 77 K, and the populations of 3p-components of valence p-orbitals of Cl atoms in this molecule are obtained by the calculation using an appropriate method [6–8].

To perform the calculations of the molecules we used the RHF/6-31G(d) method giving the results best consistent with the experimental ^{35}Cl NQR data. Quantum-chemical calculations of higher level do not improve the consistence [7, 8, 10].



I, II



III

The calculations showed at least three stable structures for the 1-methyl-3-(trichlorogermyl)propionic acid molecule close by the energy: **I**, **II** and **III**. For all the three structures no imaginary frequencies of stretching vibrations were detected. The total energy of the structure **I**, taking into account its zero point energy is by 0.55 and 1.42 kcal mol^{-1} lower than those of the structures **II** and **III,** respectively. In the gaseous state the 1-methyl-3-(trichlorogermyl)propionic acid molecule most likely corresponds to structure **I**.

In structure **I** the Ge···O distance is much shorter than the sum of the Ge and O van der Waals radii, which indicates that the Ge atom is pentacoordinated. The coordination polyhedron is a distorted trigonal bipyramid. One of the Ge–Cl bonds is much longer than the other two, which is typical for the compounds of the IVA group elements with trigonal–bipyramidal structure. The valence angles between the long Ge–Cl bond and two short ones, as well the Ge–C bond are substantially less than the tetrahedral angles. The valence angles of Ge atom with parti-cipation of its short Ge–Cl bonds differ appreciably: the Cl^{2}GeCl^3 angle is characteristic of a tetrahedron, while Cl^{2}GeCl^1 angle is typical of a trigonal bipyramid, and the Cl^{3}GeCl^1 angle has an intermediate value (Table 1).

The bond lengths and bond angles in structures **I** and **II** are similar, except for the Ge–Cl^1 bond and Ge···O distance, whereas the dihedral angles differ significantly (Table 1). Judging from the bond lengths values of the Ge atom and the value of its bond angles in the structure **II** we conclude that Ge atom retained the features of the trigonal–bipyramidal structure. However, they are considerably less pronounced than in structure **I**. The Ge···O distance in structure **II** is almost equal to the sum of the van der Waals radii of Ge and O (3.4 Å) [11, 12]. In structure **III** the zigzag fragment GeC^{1}C^{2}C^3 is almost flat, a possibility of the Ge←O interaction is excluded.

Thus, the coordination polyhedron of the Ge atom in structure **I** has the appearance of a distorted trigonal bipyramid, in **III** it is a tetrahedron, and in **II** it is of intermediate form between them. For structure **I** a coordination between Ge and O atoms can be assumed, whereas in structure **II** such bonding is practically absent. Nevertheless, the total energies of these structures are very close.

The bond lengths and the valence angles calculated for the structures **I–III** differ significantly from the XRD data (Table 1). Hence the 1-methyl-3-(trichlorogermyl)propionic acid structures are quite different in the crystalline and gaseous states.

In structure **I** the electron distribution at the atom Cl^1 has axial symmetry: the full occupancies of its lone electron pair orbitals (p_x and p_y orbitals) as well as their 3p-components are nearly equal (Table 2). Almost identical population of the latter leads to nearly zero EFG asymmetry parameter at the nucleus of the Cl^1 atom. Total population of p_x and p_y orbitals of both Cl^2 and Cl^3 atoms differ somewhat more, but only slightly. The difference of the populations of 3p-

Table 1. Bond lengths (*d*, Å), bond angles (ω, deg), and torsion angles (τ, deg) in the molecule of 1-methyl-3-(trichlorogermyl)propionic acid (structures **I–VI**) calculated by the RHF/6-31G(d) method and determined by XRD analysis [1]

Parameter	**I**	**II**	**III**	**IV**[a]	**V**[a]	**VI**[a]	XRD
Bond							
Ge–Cl^1	2.171	2.159	2.144	2.168	2.156	2.143	2.140
Ge–Cl^2	2.145	2.141	2.142	2.147	2.142	2.143	2.127
Ge–Cl^3	2.140	2.139	2.139	2.145	2.140	2.138	2.122
Ge–C^1	1.942	1.937	1.930	1.941	1.937	1.93	1.926
C^1–C^2	1.531	1.532	1.543	1.531	1.531	1.543	1.528
C^2–C^3	1.510	1.516	1.518	1.510	1.516	1.518	1.501
C^2–C^4	1.538	1.536	1.528	1.539	1.536	1.528	1.521
O^1–C^3	1.192	1.189	1.186	1.207	1.203	1.200	1.218
O^2–C^3	1.320	1.325	1.331	1.297	1.302	1.308	1.304
O^2–H	0.953	0.953	0.953	0.965	0.966	0.966	1.040
Ge←O^1	2.777	3.376	5.165	2.720	3.349	–	3.075
Angle ω							
Cl^{1}GeCl^2	103.30	104.45	107.09	103.29	106.82	107.13	102.6
Cl^{1}GeCl^3	103.60	106.67	107.37	103.20	104.58	107.49	106.2
Cl^{1}GeC^1	104.68	108.51	112.42	104.82	108.74	112.39	108.0
Cl^{2}GeCl^3	109.22	107.36	106.63	108.83	107.17	106.68	106.2
Cl^{2}GeC^1	119.94	119.17	113.13	120.38	119.08	112.98	120.1
Cl^{3}GeC^1	114.04	109.93	109.86	114.16	109.76	109.87	112.5
GeC^{1}C^2	118.68	117.57	115.42	118.55	117.67	115.41	117.1
C^{1}C^{2}C^3	109.90	109.90	108.23	110.25	110.52	108.05	110.3
C^{2}C^{3}O^1	123.64	124.68	125.67	121.47	122.88	123.76	121.7
C^{2}C^{3}O^2	113.53	112.69	111.89	114.54	113.38	112.71	115.5
C^{3}O^{2}H	108.84	108.40	108.39	111.06	110.97	110.91	–
C^{1}C^{2}C^4	113.16	113.86	113.76	113.08	113.80	113.81	111.4
O^{1}C^{3}O^2	122.83	122.60	122.44	123.98	123.71	123.53	122.7
Angle τ							
Cl^{1}GeC^{1}C^2	142.34	95.57	–36.47	143.88	96.55	–36.44	–
Cl^{2}GeC^{1}C^2	27.16	–23.66	85.00	28.48	–22.97	84.94	–
Cl^{3}GeC^{1}C^2	–105.14	–148.12	–155.97	–103.83	–146.93	–156.07	–
GeC^{1}C^{2}C^3	47.06	71.51	173.95	46.05	70.96	173.55	–
C^{1}C^{2}C^{3}O^1	–15.86	4.08	113.84	–16.87	3.48	114.31	–
C^{1}C^{2}C^{3}O^2	164.70	–177.70	–65.75	163.97	–178.24	–65.25	–
GeC^{1}C^{2}C^4	–77.28	–56.37	–62.50	–77.86	–56.93	–62.35	–
O^{1}C^{3}O^{2}H	–1.15	–0.89	–0.22	–1.25	–0.85	–0.39	–
C^{2}C^{3}O^{2}H	178.28	–179.15	179.38	177.88	–179.11	179.18	–

[a] Geometric characteristics of both halves of the dimer are virtually identical.

Table 2. The populations of valence *p*-orbitals of chlorine atoms (Σ*Np*) in structures **I–VI** calculated by the RHF/6-31G(d) method, of 3*p*-components of these orbitals (*N*3*p*), as well as calculated from the ^{35}Cl NQR frequencies (ν_{calc}) and asymmetry parameters (η_{calc}) of the electric field gradient at the ^{35}Cl nuclei

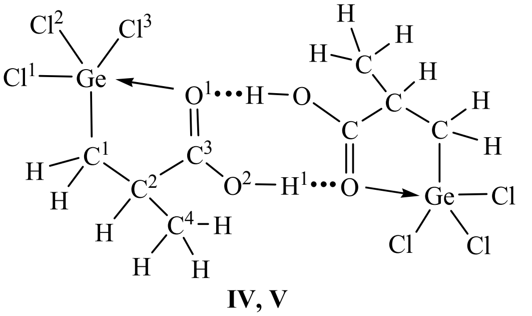
Structure	Atom	Orbital	N_x, e	N_y, e	N_z, e	ν_{calc}, MHz	η_{calc}, %
I	Cl^1	*N*3*p*	1.269	1.270	1.042	21.179	0.66
		Σ*Np*	1.928	1.929	1.447		
	Cl^2	*N*3*p*	1.273	1.284	1.024	23.709	6.48
		Σ*Np*	1.927	1.931	1.418		
	Cl^3	*N*3*p*	1.288	1.270	1.023	23.876	10.55
		Σ*Np*	1.929	1.924	1.412		
II	Cl^1	*N*3*p*	1.274	1.270	1.037	21.879	2.55
		Σ*Np*	1.930	1.923	1.435		
	Cl^2	*N*3*p*	1.276	1.274	1.030	22.808	1.22
		Σ*Np*	1.925	1.921	1.408		
	Cl^3	*N*3*p*	1.277	1.278	1.024	23.599	0.59
		Σ*Np*	1.928	1.926	1.408		
III	Cl^1	*N*3*p*	1.275	1.273	1.032	22.529	1.24
		Σ*Np*	1.925	1.921	1.423		
	Cl^3	*N*3*p*	1.276	1.273	1.031	22.669	1.85
		Σ*Np*	1.924	1.921	1.408		
IV	Cl^1	*N*3*p*	1.272	1.268	1.041	21.321	2.62
		Σ*Np*	1.930	1.925	1.442		
	Cl^3	*N*3*p*	1.275	1.281	1.025	23.557	3.56
		Σ*Np*	1.928	1.929	1.418		
V	Cl^1	*N*3*p*	1.274	1.270	1.036	21.972	2.54
		Σ*Np*	1.929	1.922	1.431		
	Cl^3	*N*3*p*	1.276	1.273	1.031	22.669	1.85
		Σ*Np*	1.925	1.921	1.409		
VI	Cl^1	*N*3*p*	1.276	1.274	1.031	22.715	1.23
		Σ*Np*	1.924	1.921	1.406		

components of p_x and p_y orbitals of these atoms is much larger compared with Cl^1, which leads to much larger values of the calculated parameters of EFG asymmetry at their nuclei. The p_σ-electron density on the atom Cl^2 (the population of p_z orbitals) is reduced significantly compared with Cl^1, whereas in going from Cl^2 to Cl^3 it varies only slightly. The half-sums of the populations of 3*p*-components of p_x and p_y orbitals of atoms Cl^2 and Cl^3 are practically identical. The populations of 3*p*-components of p_z orbitals differ slightly. This leads to a small difference in their calculated ^{35}Cl NQR frequencies [see Eq. (1)]. Slight increase in the half-sums of the populations of p_x and p_y orbitals, as well as a significant decrease in the population of p_z orbitals of the chlorine atom in going from the axial Cl^1 atom to the equatorial atoms Cl^2 and Cl^3 leads to a significant increase in the ^{35}Cl NQR frequencies of the two latter. The ratio of the populations of 3*p*-components of valence *p*-orbitals of atoms Cl^1, Cl^2 and Cl^3 and calculated ^{35}Cl NQR parameters of these nuclei corresponds to the trigonal–bipyramidal structure of the Ge coordination polyhedron in structure **I**.

The calculated ^{35}Cl NQR frequencies of structure **I** differ considerably from the experimental ones. Close to the latter are the calculated ^{35}Cl NQR frequencies of structure **II** (Table 2). Consequently, the electron distribution on the chlorine atoms in this structure virtually corresponds to the experimental ^{35}Cl NQR data. The populations of 3*p*-components of valence p_x and p_y orbitals of each of its chlorine atoms differ slightly. Therefore, the calculated asymmetry parameters are close to zero. The half-sums of these populations increase slightly in going from the Cl^1 atom to the atoms Cl^2 and then to Cl^3. This change contributes little to the ^{35}Cl NQR frequency in this series. The main contribution to this increase occurs from a larger decrease in the populations of 3*p*-components of p_z orbitals [Eq. (1)]. Full populations of the valence p_σ (p_z) orbitals of Cl^2 and Cl^3 atoms in structure **II** are identical, whereas the populations of 3*p*-components differ significantly (Table 2). This indicates a difference in the polarization of these orbitals.

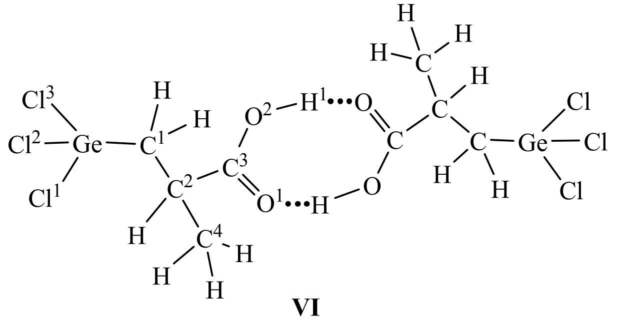
The Ge–Cl bond lengths in structure **III** differ slightly. Given the existence of a correlation between the length and ^{35}Cl NQR frequency for these bonds in organyltrichlorogermanes [2, 13], we can assume that the ^{35}Cl NQR frequency of the structure **III** will also vary slightly. Therefore, we calculated the ^{35}Cl NQR parameters only for the two chlorine atoms forming the bonds of different length with the Ge atom (Table 2). The total populations of p_x and p_y orbitals are almost identical, as well as the populations of 3*p*-components of these orbitals. The populations of 3*p*-components of the valence p_z orbitals of these atoms are also nearly identical. Therefore, their ^{35}Cl NQR frequencies and asymmetry parameters of EFG on the ^{35}Cl nuclei also differ very slightly. The values of the latter are close to zero. Such ^{35}Cl NQR parameters are characteristic of the Cl atoms associated with the tetrahedral atoms of the group IVA elements. The calculated ^{35}Cl NQR frequencies of structure **III** differ significantly from the experimental ones.

As noted above, in a crystal the molecules of 1-methyl-3-(trichlorogermyl)propionic acid are joined by the O–H···O hydrogen bonds to form dimers, and this reduces the strength of the coordination Ge←O bond [1]. To elucidate the nature of the influence of dimerization on the Ge←O bond strength we calculated the dimer **IV** and **V** with the full geometry optimization setting the initial geometric characteristics of the structures **I** and **II**, respectively, as the input parameters.



IV, V

According to the calculations, the total energy of the dimer **IV** with accounting its in the zero point is lower by 2 kcal mol^{-1} than that of the dimer **V**. For both these dimers the imaginary frequencies of stretching vibrations are absent. The total energies of the dimers **IV** and **V** are by 15.3 and 14.13 kcal mol^{-1} lower than the doubled energies of the structures **I** and **II**, respectively. This is consistent with the existence of 1-methyl-3-(trichlorogermyl)propionic acid in the gaseous state also as a dimer. In both dimers the geometric characteristics are slightly different from the characteristics of the monomer molecules (Table 1). Quite naturally, the largest differences are observed in the COOH group directly involved in the formation of the hydrogen bonds. The length of the O–H···O hydrogen bond in the dimer **IV** is 1.838 Å, while in the dimer **V,** 1.831 Å. The Ge···O distance in both dimers is not larger, but by contrast is less than in the respective monomeric molecules (Table 1). Consequently, dimerization does not diminish, but slightly increases the strength of the Ge←O coordination bond in 1-methyl-3-(trichlorogermyl)propionic acid, like in the case of unsubstituted 3-(trichlorogermyl)propionic acid [14].



VI

Dimer **VI** formed through the O–H···O hydrogen bonding of two molecules of **III** also has minimum on potencial energy surface. The imaginary frequencies of stretching vibrations for it were not revealed. Its total energy at the accounting for the zero point energy is by 4.0 kcal mol^{-1} higher than that of the dimer **IV** and by 13.89 kcal mol^{-1} less than the doubled energy of structure **III**.

The ^{35}Cl NQR frequencies of the dimers calculated from populations of 3*p*-components of valence *p*-orbitals of chlorine atoms are slightly different from the ^{35}Cl NQR frequencies of the monomeric molecules. The lengths two Ge–Cl bonds in the dimers **IV** and **V** are almost identical and of three Ge–Cl bonds in the dimer **VI** are also practically equal. Therefore,

Table 3. Atomic charges (q, e) in structures **I–VI** calculated by the RHF/6-31G(d) method

Atom	**I**	**II**	**III**	**IV**[a]	**V**[a]	**VI**[a]
Ge	0.724	0.662	0.666	0.724	0.659	0.665
Cl^1	–0.253	–0.238	–0.219	–0.246	–0.232	–0.217
Cl^2	–0.215	–0.198	–0.198	–0.226	–0.200	–0.212
Cl^3	–0.227	–0.208	–0.212	–0.229	–0.209	–0.195
C^1	–0.546	–0.532	–0.557	–0.546	–0.531	–0.559
C^2	–0.266	–0.276	–0.268	–0.268	–0.279	–0.268
C^3	0.797	0.793	0.771	0.829	0.824	0.800
O^1	–0.565	–0.558	–0.545	–0.656	–0.640	–0.625
O^2	–0.694	–0.699	–0.704	–0.720	–0.723	–0.730
H^1	0.477	0.474	0.471	0.551	0.543	0.541

[a] The charge on the atoms of the two halves of the dimers **IV–VI** are identical.

the parameters of the ^{35}Cl NQR for these dimers were calculated only for one of them (Table 2). The ^{35}Cl NQR parameters of the dimer **IV** are characteristic of the chlorine-containing compounds of the IVA group elements with trigonal–bipyramidal structure (e.g., see [15, 16]). The parameters calculated for the dimers **V** and **VI** are typical of the chlorine atoms bonded with tetracoordinated atoms of these elements.

In going from structure **III**, where the coordination interaction of Ge←O is impossible, to structure **I,** where such interaction is quite probable, the partial positive charge on the Ge atom and the negative charge on the O^1 atom increase. The same occurs in going from dimer **VI** to dimer **IV** (Table 3). This is not consistent with the transfer of electron density from the oxygen atom on the Ge atom and with the formation of the Ge←:O coordination bond through the transfer of the oxygen lone pair to the Ge vacant *d*-orbitals. The increase in the partial negative charge on the atom O^1 in structures **I** and **IV** is due to a shift in them of the electron density from the C^3 atom and, to some extent, from the atoms O^2 and H^1 under the influence of the partial positive charge on the Ge atom. Since the negative charge of the atom O^1 increases considerably less than it decreases summarily on the atoms C^3, O^2, and N^1, probably it is distributed partially over the chlorine atoms to which a charge is passed also from the Ge atom as a result of polarization of the Ge–Cl bond under the influence of the negative charge of the O^1 atom.

In going from structure **III** to **II,** the partial negative charge on the atom O^1 increases slightly as a result of polarization of the O^1–C^3 bond, while the positive charge on the Ge atom remains virtually unchanged. Also, the negative charge on the atom Cl^1 slightly increases and the negative charge on the C^1 decreases. No regularity is observed therewith in the change of atomic charges. Similar changes in the charges are observed in going from dimer **VI** to dimer **V**.

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