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Structure and ^{35}Cl NQR parameters of 1,3-diphenyl-3-methyl-3-(trichlorogermyl)butanone-1 using *ab initio* calculations

Abstract: Quantum-chemical calculations at the RHF/6-31G(d) and MP2/6-31G(d) levels of two stable structures of 1,3-diphenyl-3-methyl-3-(trichlorogermyl)butanone-1 molecule were executed. According to calculations at the RHF/6-31G(d) level, the structure with pentacoordinated Ge atom is by 7.49 kJ/mol energetically more advantageous as compared with that with the tetracoordinated one. Using 3*p*-components of the Cl atom valence *p*-orbitals obtained from these calculations, the ^{35}Cl nuclear quadrupole resonance (NQR) parameters of this compound with the pentacoordinated Ge atom were assessed. Calculations performed at both the RHF/6-31G(d) and MP2/6-31G(d) levels do not differ principally and are close to experimental NQR data. Calculations at the RHF/6-31G(d) level performed at various Ge···O distances demonstrated that convergence of the Ge and O coordination centers leads to an increase in the positive charge at the Ge atom and in the negative charge at the O atom, and with that, electron density from the Ge atom shifts mainly to the axial Cl atom and from the C atom of carbonyl group to its O atom. On such convergence, the electron density of atoms directly bonded to those of the Ge coordination polyhedron decreases to some extent.

Keywords: structures of 1,3-diphenyl-3-methyl-3-(trichlorogermyl)butanone-1 molecule; quantum-chemical calculations; nuclear quadrupole resonance parameters; Ge←O coordination bond.

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Introduction

In organic compounds of elements of the IVA group, atoms of these elements can widen their coordination number as a result of intramolecular interaction with the heteroatom of an organic substituent. Some of the said compounds have been investigated by X-ray diffraction (Gar et al., 1982; Feshin et al., 1984, 1989; Gurkova et al., 1984a, b, 1985; Shipov et al., 2011), by nuclear quadrupole resonance (NQR) on the ^{35}Cl nuclei (Gar et al., 1982; Feshin et al., 1984, 1989, 1991), and by nonempirical methods of quantum chemistry (e.g., Feshin and Feshina, 2010, 2011).

In accordance with the X-ray diffraction data, the Ge atom in the 1,3-diphenyl-3-methyl-3-(trichlorogermyl) butanone-1 molecule is also pentacoordinated as a result of its interaction with the carbonyl O atom and of the locking of a five-nomial cycle (Feshin et al., 1984; Gurkova et al., 1984). The Ge···O distance in this compound (2.507 Å) is appreciably less than the sum of the van der Waals radii of the Ge and O atoms (3.6 Å) (Gurkova et al., 1984). In its ^{35}Cl NQR triplet spectrum (Feshin et al., 1984), one line is shifted to an appreciably lower frequency diapason (21.028 MHz) as compared with two others (23.139 and 24.040 MHz). As in other chlorine-containing molecules of trigonal-bipyramidal structure, the Ge-Cl axial bond in this molecule (2.181 Å) is appreciably longer than two equatorial bonds (2.138 and 2.144 Å) (Feshin et al., 1984; Gurkova et al., 1984), and the NQR frequency of its Cl atom is considerably lower than the NQR frequencies of equatorial Cl atoms (Feshin et al., 1984; Feshin and Polygalova, 1991).

On investigation in molecules of such a structure, e.g., 3-trichlorogermylpropionamide (Feshin and Feshina, 2010) and *N,N*-dimethylamide of 2-methyl-3-(trichlorogermyl) propionic acid (Feshin and Feshina, 2011), we have shown that, therein, oppositely charged Ge and O atoms initiate formation of the intramolecular Ge←O coordination bond and are the conductor of electron density from atoms nearest to the O atom to atoms belonging to the Ge coordination polyhedron. We suppose transfer of electron density from an electron-donor fragment of molecules to electron-acceptor one to be not a reason for the formation of such bond but a consequence. On its formation, the electron density of the O atom increases, whereas that of the Ge atom decreases. Similar results are to be expected for the 1,3-diphenyl-3-methyl-3-(trichlorogermyl)butanone-1 molecule. In addition, the study of the latter will enable

to ascertain whether the transfer of electron density takes place only from atoms nearest to the O atom to atoms belonging to the Ge coordination polyhedron or also from peripheral atoms of its electron-donor fragment.

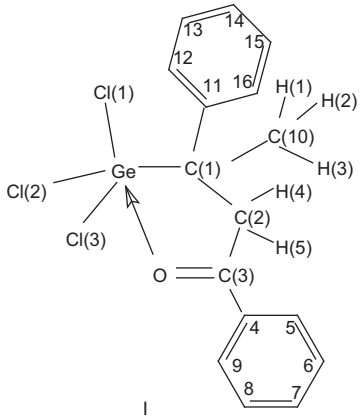
Results and discussion

In order to study the stereo-electronic structure of the 1,3-diphenyl-3-methyl-3-(trichlorogermyl)butanone-1 molecule and the mechanism and formation dynamic of the coordinated Ge←O bond therein, we performed quantum-chemical calculations at the RHF/6-31G(d) level with total optimization of its geometry, as well as at various Ge···O distances while using the Gaussian 03W program (Frisch et al., 2005). In accordance with these calculations and using equations (1) and (2) (Das et al., 1958), the ^{35}Cl NQR frequencies and asymmetry parameters of the electric field gradient (EFG) on the ^{35}Cl nuclei were assessed.

In the said calculations, not total populations of valence *p*-orbitals of Cl atoms but only their less diffusive 3*p*-components were used because the EFG quickly

Here, e^2Qq_{aT} is the atomic constant of the quadrupole interaction; h is the Planck constant; and N_x, N_y, and N_z are populations of 3*p*-components of valence p_x, p_y, and p_z, respectively, which are the orbitals of the indicative chlorine atom. The $e^2Qq_{aT}/2h$ value has been found using experimental NQR frequency of the Cl_2 compound at 77K and populations of 3*p*-components of the Cl atom valence *p*-orbitals in this molecule obtained from its calculation using the respective method (Feshin and Feshina, 2000; Shlyapnikov and Feshin, 2002; Feshin, 2009).

In order to calculate the 1,3-diphenyl-3-methyl-3-(trichlorogermyl)butanone-1 molecule, the RHF/6-31G(d) level giving the best correspondence with experimental NQR data was used. The use of quantum-chemical calculations of a higher level does not lead to any improvement of this correspondence (Shlyapnikov and Feshin, 2002; Feshin, 2009). Nonetheless, we have calculated this molecule at the MP2/6-31G(d) level. In these calculations, each Cl atom, the electron density of which was subsequently compared with experimental NQR data, was taken as a point of co-ordinates system origin. The Z axis of this system was directed along respective Cl-Ge bond.



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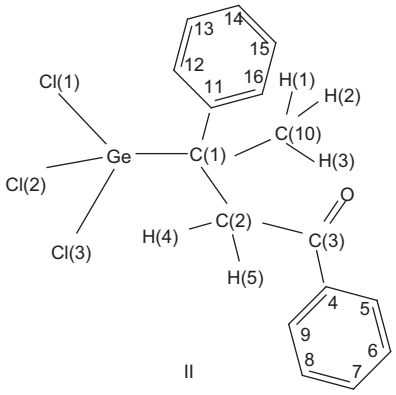

II

decreases with the increase in the distance to the charges that create it (Feshin and Feshina, 2000; Shlyapnikov and Feshin, 2002; Feshin, 2009). These characteristics had been compared with experimental NQR data (Feshin et al., 1984). Evaluation of the ^{35}Cl NQR data using total populations of the Cl atom valence *p*-orbitals does not lead to satisfactory accordance between calculated and experimental data (Feshin and Feshina, 2000; Shlyapnikov and Feshin, 2002; Feshin, 2009).

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

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

The calculation results of the 1,3-diphenyl-3-methyl-3-(trichlorogermyl)butanone-1 molecule have shown that it has two stable forms, I and II. Both structures I and II do not have imaginary frequencies of valence vibrations. Their calculation at the RHF/6-31G(d) level with total geometry optimization has demonstrated that structure I is somewhat more preferable. Its total energy (taking into account zero point energy) is 7.49 kJ/mol lower as compared with that of structure II. Therefore, structure I is typical also for the crystalline state of the substance. The calculation results of the said structures at the RHF and MP2 levels do not differ principally and are close to experimental data (Table 1). Quite naturally, calculation results

Bond	d (Å)			Angle	α (°)			Angle	β (°)	
	RHF	MP2	X-ray		RHF	MP2	X-ray		RHF	MP2
Cl(1)-Ge	2.178	2.190	2.181	Cl(1)GeCl(2)	103.02	101.93	101.73	Cl(1)GeC(1)C(2)	150.05	150.70
Cl(2)-Ge	2.160	2.169	2.144	Cl(1)GeCl(3)	99.71	98.55	97.64	Cl(1)GeC(1)C(10)	-91.11	-90.54
Cl(3)-Ge	2.152	2.162	2.138	Cl(1)GeC(1)	107.22	104.55	105.80	Cl(1)GeC(1)C(11)	30.37	31.35
Ge-C(1)	1.976	1.968	1.994	Cl(2)GeCl(3)	110.14	111.84	110.19	Cl(2)GeC(1)C(2)	36.13	39.28
C(1)-C(2)	1.543	1.532	1.534	Cl(2)GeC(1)	115.08	116.12	117.3	Cl(3)GeC(1)C(2)	-97.94	-100.23
C(2)-C(3)	1.514	1.512	1.496	Cl(3)GeC(1)	119.10	119.94	120.1	GeC(1)C(2)C(3)	45.92	43.15
C(3)=O	1.201	1.241	1.222	GeC(1)C(2)	112.02	110.48	109.6	C(1)C(2)C(3)C(4)	162.97	160.33
C(3)-C(4)	1.490	1.479	1.473	GeC(1)C(10)	104.97	104.45	104.3	C(1)C(2)C(3)O	-19.17	-22.01
C(1)-C(10)	1.540	1.534	1.532	GeC(1)C(11)	108.91	108.24	107.9	C(2)C(3)C(4)C(5)	2.42	2.05
C(1)-C(11)	1.534	1.516	1.514	C(1)C(2)C(3)	114.23	112.47	114.2	C(3)C(4)C(5)C(6)	179.43	179.27
Ge···O	2.645	2.452	2.507	C(2)C(3)O	118.47	117.99	117.9	GeC(1)C(11)C(12)	62.60	60.61
				C(2)C(3)C(4)	120.69	121.58	122.2	C(1)C(11)C(12)C(13)	178.24	178.25
				Cl(1)GeO	175.8	–	176.9	C(4)C(5)C(6)C(7)	0.27	0.65
								C(10)C(1)C(11)C(12)	178.94	176.38
								C(11)C(12)C(13)C(14)	-0.03	-0.67

Table 1 Bond lengths (d, Å), valence (α), and torsion (β) angles in structure I obtained from the RHF/6131G(d) and MP2/6-31G(d) calculations as well as from X-ray diffraction data (Feshin et al., 1984; Gurkova et al., 1984).

of the individual molecule's I geometry differ somewhat from X-ray diffraction data obtained for crystalline substance (Feshin et al., 1984; Gurkova et al., 1984).

The Ge···O distance as a result of calculations of structure I at the MP2/6-31G(d) level is appreciably less than that calculated at the RHF/6-31G(d) level. This distance determined at both levels is appreciably less than the sum of van der Waals radii of the Ge and O atoms and indicates an interaction between these atoms. Thus, the Ge atom in this structure is pentacoordinated. The Ce-Cl(1) bond in it is appreciably longer than two others, valence angles Cl(2)GeC(1) and Cl(3)GeC(1) considerably exceed tetrahedral angles, and the Cl(1)GeO angle is close to 180°. These geometrical parameters correspond to the trigonal-bipyramidal structure of the coordination polyhedron of the pentacoordinated Ge atom. Angles between the axial Cl-Ge bond and equatorial bonds of the Ge atom appreciably exceed 90° (Table 1); this indicates considerable distortion of its coordination polyhedron. Judging from the valence angles Cl(1)GeC(1), Cl(1)GeCl(2), and Cl(1)GeCl(3), the Ge atom oversteps the equatorial plane of the trigonal pyramid in the line of axial Cl(1) atom. It forms the vertex of the trigonal pyramid with C(1), Cl(2), and Cl(3) atoms forming the base of this pyramid.

The ^{35}Cl NQR frequencies of structure I calculated using equation (1) and populations of less diffusive 3*p*-components of valence *p*-orbitals of Cl atoms calculated at both levels are in accordance with the trigonal-bipyramidal structure of the coordination polyhedron of the Ge atom and with a ratio between experimental NQR frequencies of axial and equatorial Cl atoms in 1,3-diphenyl-3-methyl-3-(trichlorogermyl) butanone-1 (see above). These frequencies are close to experimental ^{35}Cl NQR data.

Unfortunately, the asymmetry parameters of the EFG on the ^{35}Cl nuclei of 1,3-diphenyl-3-methyl-3-(trichlorogermyl) butanone-1 have not been measured. These parameters evaluated using equation (2) and populations of 3*p*-components of the Cl atom valence *p*-orbitals obtained from the structure I calculation at the MP2/6-31G(d) level (Table 2) are in accordance with experimental data obtained for other Cl-containing compounds of trigonal-bipyramidal structure (e.g., Feshin et al., 1981, 1985, 1988; Feshin and Voronkov, 1990); they are close to zero for axial Cl atoms, whereas for equatorial atoms, the electron distribution of which considerably differs from axially symmetrical, these parameters are markedly larger than zero. The asymmetry parameters and ^{35}Cl NQR frequencies evaluated using the results of the structure I calculations at the RHF/6-31G(d) level correspond to a more distorted trigonal-bipyramidal structure of the Ge atom coordination polyhedron.

According to calculations of molecule I at the MP2/6-31G(d) level with total optimization of its geometry, the Mulliken's charge of the axial Cl(1) atom (-0.263 e) is close to the charge of the equatorial Cl(2) atom, whereas when calculated at the RHF/6-31G(d) level, these charges are equal (-0.250 e). At the same time, according to calculations at both levels, the spatial distribution of electron density of these atoms (populations of their p_x, p_y, and p_z orbitals) differs appreciably. The population of the p_z orbital of the axial chlorine atom is markedly larger, whereas that of the p_y orbital is less as compared with

Structure	Level	Atom	Orbital	N_x (e)	N_y (e)	N_z (e)	ν_c (MHz)	η_c (%)
I	RHF	Cl(1)	N3p	1.270	1.274	1.036	21.972	5.25
			∑Np	1.925	1.929	1.443	–	–
		Cl(2)	N3p	1.269	1.283	1.029	23.022	8.50
			∑Np	1.927	1.933	1.435	–	–
		Cl(3)	N3p	1.272	1.288	1.018	24.424	9.16
			∑Np	1.928	1.934	1.406	–	–
	MP2	Cl(1)	N3p	1.268	1.273	1.039	21.215	3.24
			∑Np	1.926	1.931	1.452	–	–
		Cl(2)	N3p	1.266	1.286	1.027	22.870	12.05
			∑Np	1.926	1.936	1.438	–	–
		Cl(3)	N3p	1.269	1.290	1.017	24.109	12.00
			∑Np	1.928	1.939	1.411	–	–
II	RHF	Cl(1)	N3p	1.272	1.272	1.035	22.063	0.0
			∑Np	1.926	1.922	1.437	–	–
		Cl(2)	N3p	1.273	1.275	1.031	22.622	1.23
			∑Np	1.925	1.923	1.425	–	–
		Cl(3)	N3p	1.276	1.276	1.027	23.180	0.0
			∑Np	1.923	1.920	1.411	–	–

Table 2 Populations of the Cl atom valence *p*-orbitals (∑Np) and their 3*p*-components (N3p) in structures I and II obtained from the RHF/6-31G(d) and MP2/6-31G(d) calculations, as well as the ^{35}Cl NQR frequencies (ν_c) and asymmetry parameters (η_c) of the EFG at the ^{35}Cl nuclei obtained using the populations of 3*p*-components.

equatorial atoms (Table 2). Therefore, the axial Ge-Cl bond is considerably longer than two equatorial bonds (Table 1), and the NQR frequency of the axial Cl atom and the asymmetry parameter of the EFG on its nucleus resulted from these calculations are considerably less than respective values for equatorial Cl atoms (Table 2).

The ^{35}Cl NQR frequencies and asymmetry parameters of the EFG on the ^{35}Cl nuclei of structure II calculated at the RHF/6-31G(d) level (Table 2) are in accordance with these characteristics for the compounds in which the Cl atom is bonded to the tetracoordinated atom (e.g., Feshin et al., 1981; Feshin and Voronkov, 1990): the NQR frequencies of all the three Cl atoms are close to one another, with their asymmetry parameters being close or equal to zero.

To study the redistribution of electron density in the 1,3-diphenyl-3-methyl-3-(trichlorogermyl)butanone-1 molecule on formation of the Ge←O coordination bond, structure I was calculated at the RHF/6-31G(d) level at various fixed Ge···O distances and optimization of its remaining geometrical parameters. These distances were varied from 3.6 Å (the sum of van der Waals radii of the Ge and O atoms) to 2.2 Å. The latter distance is less than that obtained on the total optimization of this molecule geometry (Table 1).

While decreasing the Ge···O distances, the partial positive charge of the Ge atom and the partial negative charges of its coordination polyhedron's atoms—of Cl atoms, especially the Cl(1) atom, which in trigonal-bipyramidal structure I becomes axial, as well as of O and C(1) atoms—increase (Table 3). At this point, the electron density of the C(2), C(3), and C(5) atoms directly bonded to atoms of the Ge coordination polyhedron decreases somewhat. The charge of the C(4) atom, also directly bonded to this coordination polyhedron atom, does not change. On the decrease of the Ge···O distance, redistribution of electron density also in the methyl and methylene groups, in the aromatic ring bonded to the carbonyl group, takes place. At this point, the electron density of this ring decreases. In another aromatic ring, changes are practically absent (Table 3).

Thus, on convergence of the Ge and O coordination centers, the partial negative charge of the oxygen atom and the partial positive charge of the Ge atom increase; this phenomenon contradicts ideas on the transfer of electron density from the oxygen atom to the vacant d-orbitals of the Ge atom on the formation of coordination bond between these. Apparently, electrostatic interaction exists between them. Under the action of the partial negative charge of the oxygen atom, as well as of equatorial Cl and C(1) atoms, the Ge-Cl(1) axial bond becomes polarized and leads to the increase of electron density on its Cl atom. The partial negative charge of the latter polarizes equatorial bonds O=C(3), C(1)-C(2), and C(1)-C(5) and leads to the increase in electron density of oxygen and C(1) atoms.

Conclusions

In accordance with performed calculations, 1,3-diphenyl-3-methyl-3-(trichlorogermyl)butanone-1 has two stable

Atom	2.2	2.5	2.644	2.8	3	3.2	3.4	3.6
Ge	0.783	0.755	0.740	0.721	0.694	0.671	0.656	0.649
Cl(1)	-0.296	-0.264	-0.250	-0.236	-0.220	-0.208	-0.204	-0.204
Cl(2)	-0.255	-0.250	-0.250	-0.250	-0.248	-0.245	-0.241	-0.238
Cl(3)	-0.243	-0.224	-0.217	-0.211	-0.203	-0.197	-0.193	-0.192
O	-0.604	-0.585	-0.576	-0.567	-0.558	-0.552	-0.548	-0.546
C(1)	-0.265	-0.258	-0.254	-0.249	-0.243	-0.238	-0.233	-0.229
C(2)	-0.413	-0.414	-0.416	-0.417	-0.419	-0.420	-0.420	-0.422
C(3)	0.593	0.582	0.577	0.574	0.570	0.568	0.567	0.566
C(4)	-0.125	-0.117	-0.115	-0.113	-0.112	-0.112	-0.112	-0.114
C(5)	-0.191	-0.199	-0.201	-0.204	-0.206	-0.208	-0.208	-0.208
C(6)	-0.215	-0.213	-0.212	-0.211	-0.211	-0.210	-0.210	-0.210
C(7)	-0.170	-0.175	-0.177	-0.178	-0.180	-0.181	-0.181	-0.181
C(8)	-0.215	-0.212	-0.212	-0.211	-0.210	-0.210	-0.209	-0.209
C(9)	-0.156	-0.164	-0.166	-0.168	-0.170	-0.171	-0.172	-0.172
C(10)	-0.526	-0.526	-0.526	-0.526	-0.525	-0.525	-0.526	-0.527
C(11)	0.083	0.074	0.071	0.067	0.063	0.059	0.055	0.049
H(1)	0.196	0.209	0.216	0.223	0.232	0.240	0.248	0.256
H(2)	0.216	0.206	0.202	0.198	0.194	0.191	0.188	0.186
H(3)	0.183	0.183	0.183	0.182	0.181	0.180	0.180	0.180
H(4)	0.215	0.211	0.211	0.211	0.213	0.215	0.217	0.220
H(5)	0.239	0.232	0.230	0.227	0.225	0.222	0.219	0.216

Table 3 The Mulliken's charges (q, e) at the atoms in structure I obtained from the RHF/6-31G(d) calculations at different Ge···O distances [r(Ge···O), Å].

forms: the one with the pentacoordinated Ge atom and the other one with the tetracoordinated Ge atom. The first structure is more preferable. Assessment results of its geometrical characteristics and of ^{35}Cl NQR parameters judging from calculations performed at the RHF/6-31G(d) and MP2/6-31G(d) levels do not differ principally and are close to experimental data. On convergence of the Ge and O coordination centers in this molecule, the partial negative charge of the oxygen atom and the partial positive charge of the Ge atom increase; this phenomenon contradicts ideas on the transfer of electron density from the oxygen atom to the Ge atom on the formation of coordination bond between these. On such convergence, the electron density of all atoms of the Ge coordination polyhedron increases as a result of its shift from neighboring C atoms and from the Ge atom.

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