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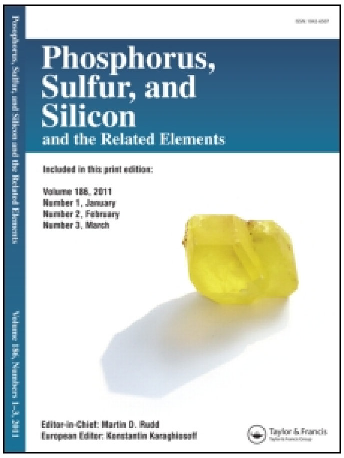

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Thermodynamic Properties and Molecular Dipole Moments of Antimony Compounds from Quantum Chemical Evaluations

Alexei N. Pankratov[a]; Inna M. Uchaeva[a]
[a] Department of Chemistry, N. G. Chernyshevskii Saratov State University, Saratov, Russia

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THERMODYNAMIC PROPERTIES AND MOLECULAR DIPOLE MOMENTS OF ANTIMONY COMPOUNDS FROM QUANTUM CHEMICAL EVALUATIONS

Alexei N. Pankratov and Inna M. Uchaeva
Department of Chemistry, N. G. Chernyshevskii Saratov State University, Saratov, Russia

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By the PM3 method, standard values of entropy, heats and Gibbs energies of formation and dipole moments of the molecules have been computed for a series of inorganic and organic antimony compounds. Linear dependences $P_{exper} = bP_{theor}$ (where P is any of the mentioned properties) have been stated, allowing a priori evaluation of thermodynamic characteristics and molecular dipole moments of Sb-containing substances. It has been concluded that triphenylstibinedichloride in benzene solution, as well as triphenylstibinehydroxychloride in dioxane medium, exist in the form of trigonal bipyramid with two axial chlorine and oxygen atoms.

Keywords: Antimony compounds; configuration; dipole moment; quantum chemical evaluation; theory—experiment correlation; thermodynamic properties

INTRODUCTION

Antimony serves as a component of alloys for battery plates, printing types, bearings, casting, and so on.[1] Inorganic compounds of antimony are used as mordant for dyeing, as pigments, catalysts in organic synthesis, selective cationites, ferroelectrics, optical glasses components, enamels, phosphors, semiconducting materials, match heads, pyrotechnic compositions.[1] Antimony halides are fluorinating and chlorinating

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Address correspondence to Alexei N. Pankratov, N. G. Chernyshevskii Saratov State University, 83 Astrakhanskaya Street, Saratov 410026, Russia. E-mail: PankratovAN@info.sgu.ru

agents, catalysts.[1] Potassium hexahydroxyantimonate is analytical reagent for detecting Na^+ ion.[1] Antimony organic substances are used as drugs, biocides, fungicides, components of polymerization catalysts, antioxidants, oil additives, and such.[1] The above list of antimony compounds applications is far from being comprehensive.

Trivalent antimony in the form of potassium antimony tartrate was found to be an inhibitor of glutathione-S-transferases from human erythrocytes with a 50% inhibition concentration of 0.05 mmol/l.[2]

Research into antimony compounds' stability, as well as into their reactivity, chemical reactions mechanisms and toxic effects, calls for information on relevant thermodynamic properties. For describing the substances reactivity in polar media, dipole moment is of importance. Dipole moment should be taken into consideration also in relation to the fact that molecular recognition, interaction of bioactive compounds with biosubstrates receptors are preceded by the chemical substances selection in accordance with electrostatic mechanism.[3–6]

Entropies, heats and free energies of formation and dipole moments are fundamental physicochemical characteristics of substances and molecules. Their measurements involve experimental difficulties and are not always feasible, and the corresponding methods have substantial restrictions.

It is of value to show a possibility of *a priori* estimation of the above characteristics, namely to establish quantitative interrelations possessing predictive power, between experimental and theoretical manifestations of the physicochemical properties under study.

For evaluating the energy characteristics, promising are methods of quantum chemistry. As for *ab initio* computations, in relation to compounds of antimony and other heavy elements only low level of sophistication is available in a number of cases. Therewith the results of such treatment depend significantly and not always monotonically on the selected basis and consideration of correlation effects.[7,8]

For rather simplified obtaining predictive quantitative relations, the semiempirical quantum chemical methods would be reasonable to use.

For the series of organic and inorganic compounds belonging to different classes and possessing various functional groups, we have established a correctness of the most important thermodynamic and molecular characteristics reproduction by the MNDO, AM1 and PM3 methods,[9–15] as well as of electronegativity, inductive and mesomeric parameters of atomic groups.[16] Therewith the PM3 scheme[17,18] is the only among the mentioned ones which involves a set of parameters for antimony.[18] Stewart[18] pointing out that the average absolute error of Sb-containing substances' heats of formation consists 13.7 kcal/mol.

All the aforesaid has determined a choice of the PM3 method[17,18] for solving the problems of the present work, which is aimed at the evaluation of the standard gaseous-phase entropies (S), heats (ΔH_f) and Gibbs energies (ΔG_f) of formation, as well as first ionization potentials (I), dipole moments (μ) of the molecules of inorganic and organic antimony compounds in order to establish the correlations, having a predicting power, between the said values and experimental ones.

It is to be accentuated that in this paper not only $P = \Delta H_f$, I, μ (values usually treated), but also P=S, ΔG_f have been considered. For antimony-containing species, the heats of formation were only tested earlier.[18]

COMPUTATIONAL METHODS

The computations were performed using the software from the MOPAC package[19,20] with the complete geometry optimization (Broyden-Fletcher-Goldfarb-Shanno function minimizer[21] involving Thiel's fast minimization algorithm.[22] The preliminary optimization was realized by the molecular mechanics method (the MMX procedure)[23] with the software of the PCMODEL complex.[23] In quantum chemical computations, the condition of the gradient norm not exceeding 0.02 kcal/(molÅ) was preset. In some cases, the sufficient decrease in gradient norm was achieved by means of abandonment of the Thiel's fast minimization routine (the keyword NOTHIEL of the MOPAC package was applied), or under optimization with the Davidon-Fletcher-Powell method (keyword DFP),[21] or using combined approaches involving the keywords NOTHIEL and DFP.

For molecules with closed electronic shells, the restricted Hartree-Fock (RHF) formalism was used. Computations of the systems with open shells or the species, spin state of which was not so obvious, were conducted both in accordance with the RHF ideas and by the unrestricted Hartree-Fock (UHF) method.[7,20]

In calculating the rotational contributions to thermodynamic functions the symmetry number was taken as unity.

RESULTS AND DISCUSSION

The ΔG_f values were calculated from the relationship:

$$\Delta G_f = \Delta H_f - T\Delta S_f,$$

where the standard entropies of formation ΔS_f were calculated by the formula:

$$\Delta S_f = S - \sum_i S_i,$$

in which S_i are the entropies of the elements constituting molecule in their standard states[24–29] in view of hydrogen, oxygen, fluorine, chlorine, bromine, iodine being the two-atomic molecules; T = 298.15 K.

TABLE I Experimental and Computed Values of Standard Heats of Formation

Compound	$\Delta H_{f\,\mathrm{exper}}$, kcal/mol	Ref.	$\Delta H_{f\,\mathrm{theor}}$, kcal/mol RHF	 UHF
Sb	64.1	29	67.81	65.51
Sb^+	264.952	26	272.00	269.69
Sb^{2+}	646.0	18	616.85	616.85
Sb_2	57.1	26	70.45	70.45
$Sb_4{}^+$	245	29	270.85	270.01
$Sb_2H_4{}^+$	300	29	285.95	282.95
SbO	47.7	18	35.95	34.41
SbF	−11.3	18	−0.678	−2.83
SbCl	−2.549	26	13.32	11.33
$SbCl_2$	−18.5	18, 27, 29	−34.31	−34.54
InSb	82.3	18	80.08	80.08
$InSb_2$	75.0	18	58.58	72.49
Sb_2Te_2	51.1	29	27.21	—
$(CH_3)_2Sb$	31	30	19.31	19.19
			$\Delta H_{f\,\mathrm{theor}}$, kcal/mol (RHF)	
Sb_4	49.4	29	51.48	
SbH_3	34.681	27, 28	58.08	
Sb_2H_4	62	26, 29	80.57	
SbN	74.4	25	102.53	
Sb_2O_3	−109.9	29	−102.00	
$SbCl_3$	−75.0	18	−72.44	
SbOCl	−25.5	18, 27, 29	10.23	
$SbBr_3$	−43.18	26, 29	−36.49	
SbI_3	−1.9	26, 29	0.756	
Sb_3Bi	46.9	29	13.66	
$(CH_3)_3Sb$	7.75	26	−0.341	
$(C_2H_5)_3Sb$	10.4	18	−23.00	
$(C_6H_5)_3Sb$	104.1	18	98.67	

TABLE II Experimental and Computed Values of Standard Entropies

Compound	S_{exper}, cal/(mol·K)	Ref.	S_{theor}, cal/(mol K) RHF	UHF
Sb_2	61.38	26	62.64	62.64
SbO	56.94	26	55.49	55.51
SbF	56.1	26	56.26	56.26
SbS	58.431	28	57.36	58.68
SbSe	61.128	28	61.12	61.91
SbTe	62.71	28	61.46	63.84
			S_{theor}, cal/(mol·K) (RHF)	
Sb_4	84	27, 28	89.74	
SbH_3	55.68	26, 27	58.00	
SbN	55.2	27	55.11	
SbF_5	84.9	27	89.08	
$SbCl_3$	80.71	27, 28	84.76	
$SbBr_3$	89.09	27	93.25	
SbI_3	95.5	26	97.30	

The results obtained are presented in Tables I–IV.

For $P = \Delta H_f$, S, ΔG_f, μ we have established linear dependences of the type

$$P_{exper} = \mathbf{b}P_{theor}.$$

TABLE III Experimental and Computed Values of Standard Gibbs Energies of Formation

Compound	$\Delta G_{f\ exper}$, kcal/mol	Ref.	$\Delta G_{f\ theor}$, kcal/mol RHF	UHF
Sb_2	45.311	26	58.29	58.29
SbO	18.32	26	29.96	28.42
SbF	−6.0	27	−6.97	−9.12
SbCl	−8.939	26	6.95	4.96
			$\Delta G_{f\ theor}$, kcal/mol (RHF)	
Sb_4	37.08	27	37.75	
SbH_3	35.42	27	58.01	
$SbCl_3$	−71.59	26	−70.62	
$SbBr_3$	−50.19	26	−44.77	
SbI_3	−14.703	26	−12.58	

TABLE IV Experimental[31] and Computed Values of Dipole Moments (Gas and Liquid States, as well as Solvent, Specification is Attributed to Measurements by the Debye Methods)

Compound	μ_{exper}, D	Determination conditions	μ_{theor}, D
$SbCl_3$	4.11	Benzene, 289 K	4.28
$SbCl_5$	0	Liquid, 280–320 K	0.00171
$SbBr_3$	5.01	Dioxane, 298 K	4.84
SbI_3	1.58	Carbon disulphide, 298 K	3.50
$(C_6H_5)_3Sb$	0.57	Benzene, 287 K	0.416
$(4\text{-}CH_3C_6H_4)_3SbO$	2.0	Benzene, 298 K	4.81
$(C_6H_5)_3SbS$	5.66	Benzene, 298 K	6.10
$(C_6H_5)_3SbCl_2$	0	Benzene, 298 K	0.0124
$(C_6H_5)_3Sb(OH)Cl$	2.96	Dioxane, 313 K	2.99
$(C_2H_5O)_5Sb$	2.31	Benzene, 298 K	1.42
$(C_6H_5O)_5Sb$	2.31	Liquid	0.797

In Table V the values of **b**, correlation coefficients **r**, as well as the following conventional quantities: MS (mean signed)—average value for P_{theor}-P_{exper}, and MU (mean unsigned)—average value for $|P_{\mathrm{theor}}$-$P_{\mathrm{exper}}|$ are shown.

Reproducibility of the ΔH_f experimental value for elementary substance Sb on semiempirical computations is not surprising and originates from parameterization of the method. Nevertheless it should be noted the following: Tendencies in changing the experimental and

TABLE V Coefficients **b** in Equations $P_{\mathrm{exper}} = \mathbf{b}P_{\mathrm{theor}}$ and the **r**, MU, MS Values

P	Number of compounds	**b**	**r**	Error	
				MU	MS
ΔH_f^*	27	1.0129 ± 0.0462	0.9921	15.16	−0.04
ΔH_f^{**}	26	1.0137 ± 0.0449	0.9929	14.11	0.86
S^*	13	0.9732 ± 0.0175	0.9956	2.12	1.52
S^{**}	13	0.9695 ± 0.0145	0.9967	2.10	1.87
ΔG_f^*	9	0.8640 ± 0.1805	0.9868	8.13	7.91
ΔG_f^{**}	9	0.8684 ± 0.1736	0.9866	7.97	7.28
μ	11	0.8384 ± 0.2141	0.8410	0.74	0.24
μ^{***}	10	0.9333 ± 0.1907	0.9158	0.53	−0.02
μ^{+}	9	0.9984 ± 0.1568	0.9669	0.38	−0.23

[*] For molecular systems, the properties of which were computed in the RHF and UHF versions (Tables I–III), the RHF formalism is applied in the given case.

[**] For molecular systems, the properties of which were computed in the RHF and UHF versions (Tables I–III), the UHF formalism is applied in the given case.

[***] Data for $(4\text{-}CH_3C_6H_4)_3SbO$ are excluded.

[+] Data for $(4\text{-}CH_3C_6H_4)_3SbO$ and SbI_3 are excluded.

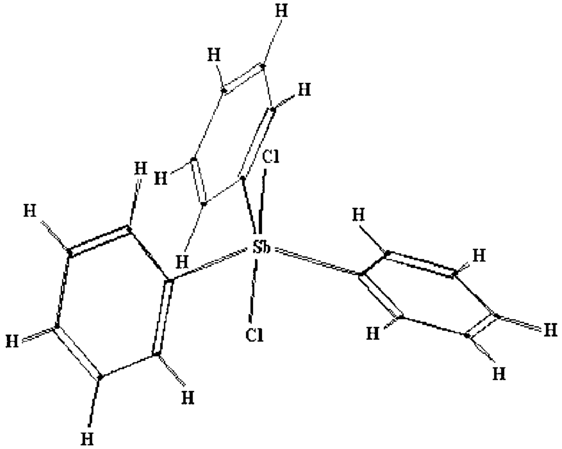
theoretical entropies, heats an free energies of formation of antimony compounds agree well with each other (**r** > 0.98) in spite of the fact that for a series of compounds (Sb^{2+}, SbN, SbOCl, Sb_3Bi, $(C_2H_5)_3Sb$) the difference $|\Delta H_{f\ \mathrm{theor}} - \Delta H_{f\ \mathrm{exper}}|$ is close to 30 kcal/mol or exceeds the aforesaid value to some extent.

Quantum chemical PM3 computations overestimate strongly the dipole moments of the $(4\text{-}CH_3C_6H_4)_3SbO$ and SbI_3 molecules.

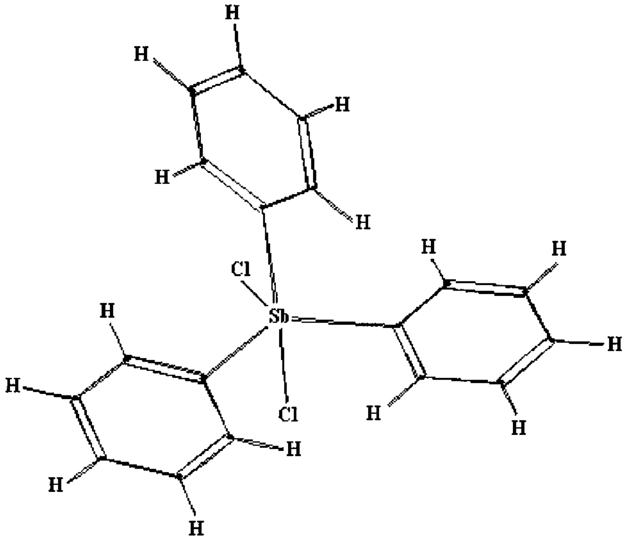
Consequtive exclusion from consideration of the results of quantum chemical computations and experiments on the above molecules' dipole moments leads to the considerable increase in correlation coefficient **r** and narrowed confidence limits about the slope. Therewith the **b** value in the equation $\mu_{\mathrm{exper}} = \mathbf{b}\mu_{\mathrm{theor}}$ becames progressively closer to unity. Thus agreement between experimental and computed dipole moments was used as criterion for whether the compounds are included in the correlation calculations.

The computations of dipole moments have allowed us to conclude on geometry of triphenylstibinedichloride $(C_6H_5)_3SbCl_2$ and triphenylstibinehydroxychloride $(C_6H_5)_3$ Sb(OH)Cl molecules as solutes.

In the case of $(C_6H_5)_3SbCl_2$, two trigonal-bipyramidal configurations were investigated. Configuration (**I**) with two axial chlorine atoms corresponds to a dipole moment of 0.0124 D. For the structure (**II**), in which one chlorine atom occupies equatorial, and another axial position, dipole moment consisits 6.60 D. The hypothetical structure (**III**) with two equatorial chlorine atoms unlikely exists. Being simulated by means of the PCMODEL package, it rearranges into the system **I** on optimization by the molecular mechanics (MMX) or quantum chemistry (PM3) method.



I



II

Experiment[31] gives for the molecule $(C_6H_5)_3SbCl_2$ in benzene a zero dipole moment.

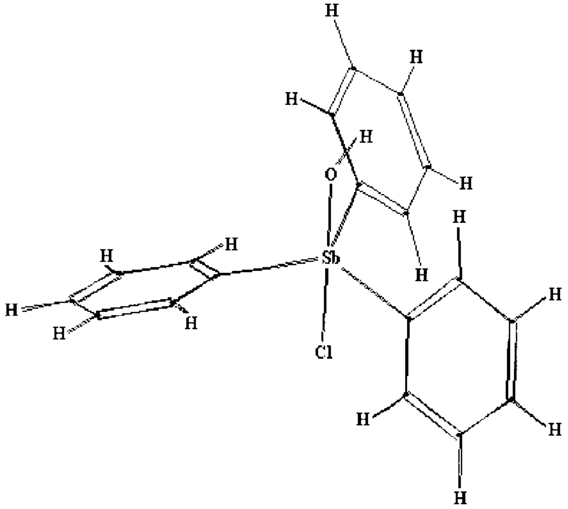
Consequently, it is configuration **I** that is realized in benzene solution. Two factors that favour this are:

1. The form **I** is more stable thermodynamically as compared to **II** and, likely, to **III**:

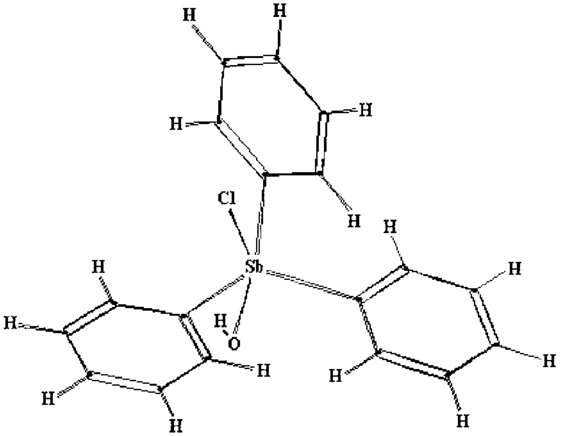
Configuration	ΔH_f, kcal/mol	S, cal/(mol. K)	ΔG_f, kcal/mol
I	95.29	148.75	147.18
II	107.34	151.75	158.34

2. Solvent is non-polar.

For triphenylstibinehydroxychloride, three possible trigonal bipyramidal configurations have been considered: 1) structure **IV** with axial hydroxy and chloro ligands; 2) configuration **V**, in which hydroxy group is axial, and chlorine atom occupies equatorial position; 3) form **VI**, for which equatorial position of OH group is characteristic, and chlorine occupies axial position. Structure **VII**, in which both inorganic ligands OH and Cl are equatorial, can be simulated within the PCMODEL software package. However, it transforms into the form **VI** in the course of molecular-mechanical or quantum chemical optimization.



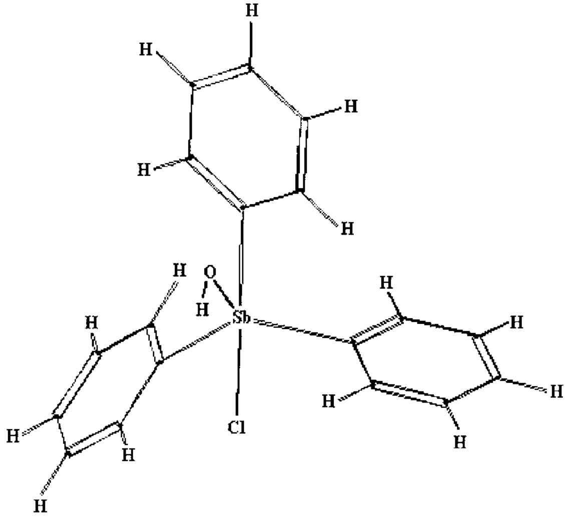
IV



V

Given below are thermodynamic characteristics and dipole moments of the molecules **IV–VI** computed by the PM3 method.

Configuration	ΔH_f, kcal/mol	S, cal/(mol. K)	ΔG_f, kcal/mol	μ,D
IV	85.74	147.65	141.98	2.99
V	91.64	147.82	147.83	5.22
VI	88.12	149.23	143.88	5.51



VI

The experimental value of the dipole moment of the $(C_6H_5)_3Sb(OH)Cl$ molecule in dioxane is equal to 2.96 D,[31] that is in well agreement with axial disposition of hydroxy and chloro groups.

The dipole moment of dioxane molecule in benzene at 298 K consists 0.34 to 0.45 D,[31] that is, the solvent is low-polar. Therefore, for triphenylstibinehydroxychloride, as in the case of triphenylstibinedichloride, the preferable configuration of the molecule with axial inorganic ligands is determined by both thermodynamic considerations and the relationship among the polarities of solvent and solute molecules.

Configuration preference of trigonal-bipyramidal molecules $(C_6H_5)_3SbCl_2$ and $(C_6H_5)_3Sb(OH)Cl$ could be explained by the sterically hindered axial positions pointed out in monograph.[32] In this connection the bulky phenyl groups tend to occupy equatorial positions. The analogous spatial structure with axial inorganic and OCH_3 ligands is peculiar for the $(CH_3)_3SbF_2$, $(CH_3)_3SbCl_2$, $(C_6H_5)_3Sb(NCO)_2$, $(C_6H_5)_3Sb(OH)_2$, $(C_6H_5)_3Sb(OCH_3)_2$, $(C_6H_5)_4SbOH$, $(C_6H_5)_4SbOCH_3$ molecules[32–37] in crystal state.

CONCLUSION

The existence of quantitative relations P_{exper} *vs* P_{theor} as such (different from previous[17,18,38–46] analysis of PM3, SAM1 absolute errors by the data of the MNDO, AM1, SAM1, PM3 methods) shows that the semiempirical quantum chemical PM3 method does reproduce correctly alteration trends of thermodynamic and molecular properties of antimony compounds.

Using the correlations found one could predict the properties not always available to the experimental measurement. In doing so, the computed values have to be corrected by the multiplier **b**. For $P = \Delta H_f$, μ (linear dependence with excluding the data for $(4\text{-}CH_3C_6H_4)_3SbO$ and SbI_3), the **b** values are close to unity, that allows one to calculate the corresponding characteristics directly, without any correlation equations.

A priori evaluation of the said parameters by quantum chemical methods is important for molecular design of compounds with given properties, may serve as a base for expert decision on reasonability of synthesis that is sometimes labor- and time-consuming, requiring complicated device, rigid conditions, expensive and toxic chemicals.

The trigonal bipyramidal configuration of the triphenylstibinedichloride and triphenylstibinehydroxychloride molecules in solutions has been revealed.

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