

Vibrational and Quantum Chemical Study of Triphenylantimony (V) Benzilate $\text{SbPh}_3 [\text{O}_2\text{CC}(\text{OH})\text{Ph}_2]_2$

Tanveer Hasan^{1*}, P. K. Singh² and Shamoon Siddiqui³

ABSTRACT

A complete normal coordinate analysis was performed by two methods: a classical Wilson G-F matrix method and the Semi-empirical molecular orbital PM6 method, for a five coordinate Triphenylantimony (V) Benzilate $\text{SbPh}_3 [\text{O}_2\text{CC}(\text{OH})\text{Ph}_2]_2$, known to be an in vitro antitumour molecule

Keywords : FT-IR spectra, normal coordinate analysis, semi empirical, organometallic compounds.

I. INTRODUCTION

IN most of the organoantimony (V) compounds, the coordination number of antimony atom is five, whereas in some cases it may be six [1,2] or seven [3,4] also. The stretching vibrational frequencies of carbonyl groups in organoantimony carboxylates play vital role in the determination of their structures. If there are interactions between the antimony atom and the carbonyl oxygen atoms, the asymmetric absorption vibrational frequencies V_{sym} of carbonyl groups decrease, while the symmetric absorption vibrational frequencies V_{sym} increase, so the difference between these two frequencies Δ_V also decreases [5,6]. The title compound Triphenylantimony (V) Benzilate $\text{SbPh}_3 [\text{O}_2\text{CC}(\text{OH})\text{Ph}_2]_2$ shows a moderate value of Δ_V which indicates that there may be intermediate interaction between the antimony atom and the carbonyl oxygen atoms. In this study, experimental FT-IR is compared with theoretical frequencies obtained by normal coordinate analysis using two different methods: a classical mechanics Wilson G-F matrix method and the semi empirical quantum chemical molecular orbital PM3 method. Thus the advantages of the evaluation of both the methods are useful for obtaining a reliable assignment of the vibrational spec-

tra. To the best of our knowledge, the work on the normal coordinate analysis for the title compound is yet to be reported. The compound is reported to be antitumour active compound against MCF-7 cell line in vitro [7].

II. THEORY

The famous Wilson's G-F Matrix method [8] with Urey Bradley [9] force field has been used to evaluate the normal modes. These are given by the eigen values λ of the secular equation.

$$\text{GFL} = \lambda \text{L} \quad \text{where } \lambda = 4\pi^2 c^2 v^2$$

The potential energy distribution (PED) in the j^{th} internal coordinates for the i^{th} normal mode is given by

$$(\text{PED}) = \frac{L_{ji}^* L_{ij} F_{ji}}{\lambda_i}$$

III. EXPERIMENTAL DETAILS

A. Structure

The crystal structure of the title compound Triphenylantimony (V) Benzilate $\text{SbPh}_3 [\text{O}_2\text{CC}(\text{OH})\text{Ph}_2]_2$ is taken from the work of Barucki et al. [10]. The model molecular structure of the compound is given in Fig 1.

1* Tanveer Hasan, the corresponding author is Asst. Professor, Dept of Physics at Shia PG College Lucknow; (e-mail: tanveerhasan09@gmail.com).

2 P.K. Singh, is Reader, Dept of Applied sciences, SMS institute of Technology Lucknow.

3 Shamoon Siddiqui is PDF at Molecular Biophysics Unit, Indian Institute of Sciences, Bangalore.

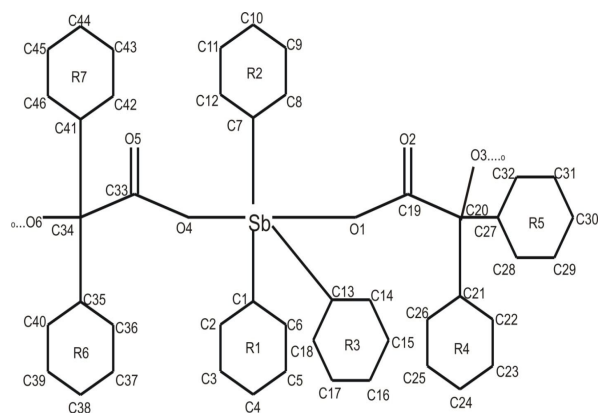


Fig. 1: Model Molecular Structure of Triarylorganantimony(V) $\text{SbPh}_3[\text{O}_2\text{CC}(\text{OH})\text{Ph}_2]_2$.

B. FTIR spectra

The FTIR spectra, given in Fig 2, have been recorded on a Perkin-Elmer Spectrum BX FTIR spectrophotometer in the frequency range 4000 to 400 cm^{-1} . X-ray data of the title compound has been taken from the CCDC [11].

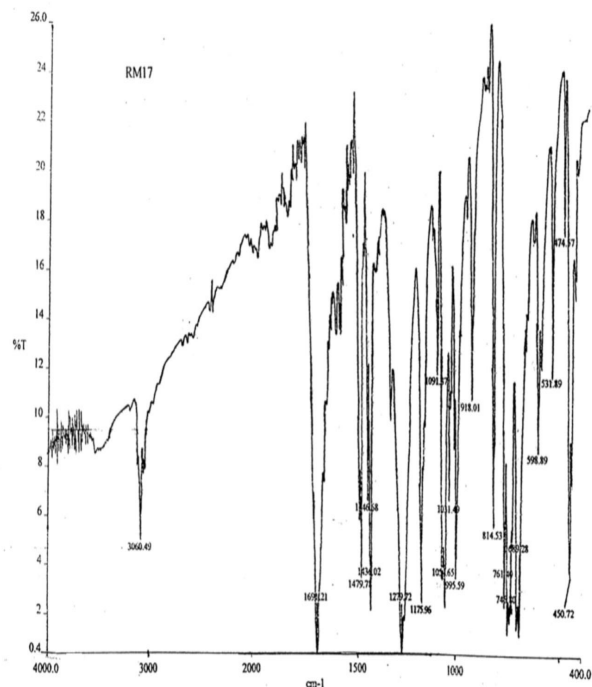


Fig 2 : FTIR spectra of Triphenyl antimony(v) benzilate $\text{SbPh}_3[\text{O}_2\text{CC}(\text{OH})\text{Ph}_2]_2$

C. Structure from Winmostar

The molecular structure as viewed from Winmostar of the title compound is given in Fig 3.

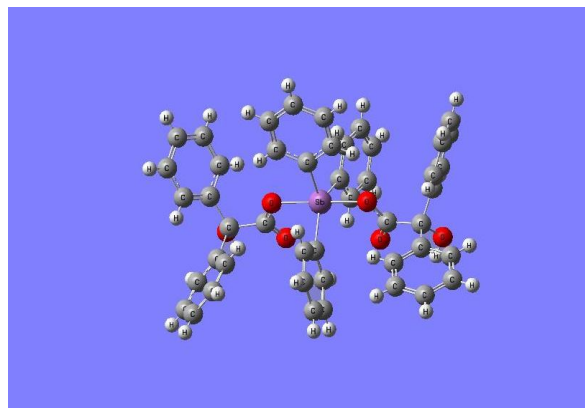


Fig. 3: Molecular Structure of Triphenylantimony (V) Benzilate $\text{SbPh}_3[\text{O}_2\text{CC}(\text{OH})\text{Ph}_2]_2$

IV. RESULTS AND DISCUSSION

Normal coordinate calculations were performed using the program developed by Shimanouchi [12] based on the Wilson's G-F matrix method [8]. We have used Urey Bradley force field [9] in our calculations, which takes into account both bonded, and non-bonded interactions and internal tensions. For the assignments, the force constants were initially transferred from our earlier work and literature [13-20] and were further refined by least square fit method to provide best match with the observed FT-IR spectra. In the assignment of the normal modes, as given in Table I, only the dominant potential energies distributions (PED's) are considered. All the force constants are presented in Table II. Identification with the experimental data has been made on the basis of potential energy distribution, line profile, line intensities and the presence/absence of a given mode in similar molecules [17-20]. Semi-empirical calculations are performed by Mopac 2007 software using PM6 method [21].

The observed frequencies agree with the calculated ones within 10 cm^{-1} . {Complete computational details can be obtained from corresponding author} Here we discuss only the conformationally important frequency modes they all are presented in the Table I.

A. C-H Stretching

The calculated frequencies from PM6 method of $\nu(\text{C-H})$ vibrations are found at 2768, 2764 and 2756 cm^{-1} and they can be assigned with the observed fre-

quencies at 3072, 3060 and 3048 cm^{-1} respectively. The $\nu(\text{C-H})$ vibration is reported in the range 3100-3000 cm^{-1} in the literature [22]. So these modes are found at lower values as reported earlier as shown in the Table I.

B. C=O Stretching

A highly intense peak is observed at 1692 cm^{-1} in the FTIR spectra, which is calculated by Wilson GF matrix method, at 1692 cm^{-1} attributed to the vibrational modes $\nu(\text{C=O})$ with [47%] PED mixed with $\nu(\text{C-C})_{\text{out-R}}$ [18%] and $\nu(\text{C-C})_{\text{adj-co}}$ [13%] PED, and it is calculated by PM6 method at 1744 cm^{-1} having vibrational mode as $\nu(\text{C=O})_{\text{adj-R6\&R7}}$ [71%]. The presence of $\nu(\text{C=O})$ double bond, makes the structure of the title compound fairly rigid and the formation of hydrogen bonds don't much disturb the charge distribution in the ring and side chains. The length of hydrogen bonds is also in support of this rigidity.

A strong band with two peaks in the range 1446-1436 cm^{-1} is observed in FTIR spectra and it is calculated.

C. C-C Stretching

From classical method at 1437 cm^{-1} and 1446 cm^{-1} with modes of vibrations as $\nu(\text{C-C})_{\text{R-adj-Sb}}$ [98%] and $\nu(\text{C-C})_{\text{R-adj-C=O}}$ [95%] PED's respectively, these peaks are calculated by PM6 method at 1481 and 1456 cm^{-1} with vibrational modes as $\nu(\text{C-C})_{\text{R7}}$ [39%] and $\nu(\text{C-C})_{\text{R2}}$ [42%]. The $\nu(\text{C-C})$ mode is reported in the range of 1488- 1632 cm^{-1} in the literature [22, 23].

D. C-O Stretching

A very intense absorption band is obtained in the FTIR spectra, containing two peaks at frequencies 1279 cm^{-1} and 1267 cm^{-1} , this band is calculated at 1272 and 1266 cm^{-1} frequencies from Wilson GF method, having $\nu(\text{C-O})_{\text{adj-R}}$ [30%] and $\nu(\text{C-O})_{\text{adj-R}}$ [22%] as vibrational modes. This band is calculated at frequencies 1267 and 1260 cm^{-1} from PM6 method with vibrational modes as $\phi(\text{C-C-H})_{\text{R4}}$ [51%] and $\phi(\text{O-H-C})_{\text{R4\&R5}}$ [48%]. The value of frequency difference for asymmetric and symmetric stretching $\Delta\nu$ for $\nu(\text{CO}_2)_{\text{asym}}$ and $\nu(\text{CO}_2)_{\text{sym}}$ is calculated as 1629-1279=350 cm^{-1} as shown in Table I.

E. Sb-O Stretching

An absorption band is observed in the spectra with three peaks obtained at 1100, 996 and 918 cm^{-1} ,

these are calculated at 1090, 1005 and 918 cm^{-1} from Wilson GF matrix method and at 1113, 996 and 930 cm^{-1} with PM6 method respectively. The concerned Vibrational modes from GF matrix method are $\nu(\text{Sb-O})$ [22%], $\nu(\text{Sb-O})$ [41%] and $\nu(\text{Sb-O})$ [31%] mixed with PM6 modes also as shown in Table I. The stretching vibration, $\nu(\text{Sb-O})$ is reported in the range 561-585 cm^{-1} by Khosa et al. [24] and at 755 cm^{-1} by Shanker et al.[25], indicating that this mode is obtained at considerable higher frequencies. This increase in wave number may be attributed to the replacement of antimony of organic group R by more electrons withdrawing oxygen atom [26].

F. In-plane and out of plane bending and torsional modes

A very sharp band with three peaks are observed in FTIR spectra at 761, 746 and 689 cm^{-1} which are calculated at 761, 743 and 688 cm^{-1} by Wilson GF matrix method and it is attributed to the mode $\phi(\text{C-C-C})_{\text{R-adj-C=O}}$ [30%], $\phi(\text{C-C-C})_{\text{R-adj-C=O}}$ [30%] and $\phi(\text{C-C-C})_{\text{R-adj-Sb}}$ [60%] respectively. This intense band is calculated at 772, 698 and 689 cm^{-1} by PM6 method having modes of vibration as $\phi(\text{O=C-C})_{\text{adj-R5}}$ [51%], $\phi(\text{C-C-O})$ [73%] and $\nu(\text{CC})$ [56%] respectively. The in-plane bending mode $\phi(\text{C-C-C})_{\text{R}}$ is reported in literature[27] at 522 cm^{-1} and 495 cm^{-1} . A sharp band is obtained in the FTIR spectra with two peaks observed at 599 cm^{-1} and 451 cm^{-1} and these are calculated at 591 and 458 cm^{-1} by GF matrix method, having modes of vibrations as $\omega(\text{O=C})$ [37%] and $\nu(\text{C-C-C})_{\text{R-adj-C=O}}$ [80%], and by PM6 method these are calculated at 599 and 452 cm^{-1} having vibrational modes as $\phi(\text{C-C-C})_{\text{R-6}}$ [106%] and $\phi(\text{C-C-C})_{\text{R4}}$ [61%] respectively. A medium shoulder peak is observed at 438 cm^{-1} in FTIR spectra and it is calculated at 435, 489 cm^{-1} with classical and PM6 method respectively having vibrational motions from first method as $\tau(\text{Sb-C})$ [10%] mixed with $\tau(\text{C-C})_{\text{r-adj-co}}$ [12%], $\tau(\text{C-C})_{\text{r-adj-Sb}}$ [42%] and in-plane bending $\phi(\text{C-Sb-O})$ [21%] and $\nu(\text{Sb-O})_{\text{adj-R}}$ [52%] from PM6 method. Here PM6 method gives better assignment of the mode $\nu(\text{Sb-O})$, as it is much closer to the reported [24,25,28] $\nu(\text{Sb-O})$ mode. This mode seems to be the characteristic mode of the present compound. A weak shoulder peak is observed in far infra red region of the spectra at 426 cm^{-1} which is calcu-

lated at 422 cm⁻¹ by classical method with Vibrational modes $\varphi(\text{C-Sb-O})$ [60%] PED, and it is calculated at 426 cm⁻¹, having modes of vibration as $\varphi(\text{C-C-C})\text{R3}$ [71%]. This mode suggests the participation of oxygen atom in (C-Sb-O) bonding [29,30]. This mode also seems to be one of the characteristic modes of the title compound.

V. CONCLUSIONS

Normal coordinate analysis data performed for the title compound from both Wilson G F matrix method and Semi-empirical PM6 method shows close resemblance of the calculated & observed vibrational bands. The value of frequency difference for asymmetric and symmetric stretching $\Delta\nu$ for $\nu(\text{CO}_2)_{\text{asym}}$ and $\nu(\text{CO}_2)_{\text{sym}}$ is calculated as $1629-1279 = 350 \text{ cm}^{-1}$ (from Table I), which is greater than 300 cm^{-1} , this suggests that the coordination number of antimony is five confirming the trigonal bipyramidal (TBPY) structure of the title compound. This also indicates that there will be at least moderate if not strong secondary bonding interactions between carbonyl oxygen atoms of carboxylate group and the central antimony atom.

APPENDIX

Tables - I

1. Back Bone & Mixed Mode

Calculated Freq (cm-1)	Observed Freq (cm-1)	Assignment (% Potential energy distribution)
1514	1512	$\nu(\text{C-C})_{\text{out-r}}[95]$
1272	1279	$\nu(\text{C-O})_{\text{adj-r}}[30] + \nu(\text{C-C})_{\text{r-ad-co}}[34] + \nu(\text{C-C})[15]$
1266	1267	$\nu(\text{C-O})_{\text{adj-r}}[22] + \nu(\text{C-C})_{\text{adj-r}}[12] + \nu(\text{C-O})_{\text{ad-sb}}[10]$
1090	1100	$\nu(\text{O-Sb})[22] + \nu(\text{C-C})_{\text{r-ad-co}}[18]$
1005	996	$\nu(\text{O-Sb})[41] + \nu(\text{C-C})_{\text{r-ad-co}}[17]$
980	983	$\nu(\text{O-Sb})[31] + \nu(\text{C-C})_{\text{r-ad-co}}[21]$
435	438	$\tau(\text{C-C})_{\text{adj-sb}}[42] + \phi(\text{C-Sb-O})[21] + \tau(\text{C-C})_{\text{r-ad-o}}[12] + \tau(\text{Sb-C})[10]$

2. Side Chain Modes

Calculated Freq (cm-1)	Observed Freq (cm-1)	Assignment(% Potential energy distribution)
1692	1692	$\nu(\text{O=C})[47] + \nu(\text{C-C})_{\text{adj-r}}[18] + \nu(\text{C-C})_{\text{adj-o}}[13]$
1667	1666	$\nu(\text{O=C})[54] + \nu(\text{C-C})_{\text{adj-r}}[15] + \nu(\text{C-C})_{\text{adj-o}}[17]$
1642	1652	$\nu(\text{C-C})[67]$
1602	1604	$\nu(\text{C-C})_{\text{adj-r}}[24] + \nu(\text{C=O})[22] + \nu(\text{C-O})_{\text{adj-r}}[17]$
761	761	$\phi(\text{C-C-C})_{\text{r-adj-c}}[30] + \nu(\text{C-O})_{\text{ad-sb}}[19] + \phi(\text{O-C=O})_{\text{ad-Sb}}[16] + \phi(\text{O=C-C})_{\text{ad-c}}[10]$
591	599	$\omega(\text{O=C})[37] + \phi(\text{C-C-C})_{\text{r-adj-c}}[24] + \phi(\text{C-C-C})_{\text{ad-o-r}}[9]$
583	586	$\phi(\text{C-C-C})_{\text{r-adj-c}}[35] + \omega(\text{O=C})[15] + \nu(\text{C-C})_{\text{ad-r}}[8] + \nu(\text{C-C})_{\text{adj-r}}[6]$
422	426	$\phi(\text{C-Sb-O})[60]$

3. Ring Modes

Calculated Freq (cm-1)	Observed Freq (cm-1)	Assignment(% Potential energy distribution)
1639	1629	$\nu(\text{C-C})_{\text{adj-r}}[63] + \nu(\text{C-C})_{\text{r-adj-co}}[22]$
1576	1566	$\nu(\text{C-C})_{\text{r-adj-Sb}}[83]$
1557	1560	$\nu(\text{C-C})_{\text{r-adj-co}}[51] + \nu(\text{C-C})_{\text{adj-o}}[16] + \nu(\text{C-O})_{\text{adj-sb}}[11]$
1446	1446	$\nu(\text{C-C})_{\text{r-adj-sb}}[98]$
1437	1436	$\nu(\text{C-C})_{\text{r-adj-co}}[95]$
1314	1305	$\nu(\text{C-C})_{\text{r-adj-sb}}[74]$
1292	1294	$\nu(\text{C-C})_{\text{r-adj-sb}}[37]$
1176	1176	$\nu(\text{C-C})_{\text{r-adj-sb}}[88]$
1165	1162	$\nu(\text{C-C})_{\text{r-adj-co}}[88]$
1084	1091	$\nu(\text{C-C})_{\text{r-ad-co}}[36]$
1053	1054	$\nu(\text{C-C})_{\text{r-adj-sb}}[71] + \nu(\text{C-C-C})_{\text{r-ad-sb}}[18]$
1033	1032	$\nu(\text{C-C})_{\text{r-adj-sb}}[72] + \nu(\text{C-C-C})_{\text{r-ad-sb}}[10]$
918	918	$\nu(\text{C-C})_{\text{r-adj-sb}}[47] + \nu(\text{C-C-C})_{\text{r-adj-sb}}[43]$
897	893	$\nu(\text{C-C})_{\text{r-ad-co}}[68]$
821	815	$\nu(\text{C-C-C})_{\text{r-adj-c}}[33] + \nu(\text{C-O})_{\text{ad-sb}}[18] + \nu(\text{C-C})_{\text{r-ad-co}}[14]$
743	746	$\nu(\text{C-C-C})_{\text{r-adj-c}}[30] + \nu(\text{C-C-C})_{\text{ad-r}}[9] + \nu(\text{C-C-C})_{\text{ad-o-r}}[6]$
688	689	$\nu(\text{C-C-C})_{\text{r-adj-sb}}[60] + \nu(\text{C-Sb})[21] + \nu(\text{C-C})_{\text{r-ad-sb}}[17]$
531	531	$\nu(\text{C-C-C})_{\text{r-adj-sb}}[85] + \nu(\text{C-C})_{\text{r-ad-sb}}[7]$
474	475	$\nu(\text{C-C-C})_{\text{r-adj-c}}[46] + \nu(\text{C-C-C})_{\text{adj-r}}[16] + \nu(\text{O=C})[37]$
458	451	$\nu(\text{C-C-C})_{\text{r-adj-c}}[88]$

Notes:

1. Here the abbreviation ad means adjacent outside.
2. r-stands for the ring one ,two etc.

Only the dominant modes are taken in most of the cases

Tables - II

Internal Co-ordinates and Urey Bradley Force Constants (md/A⁰)

INTERNAL COORDINATE	FORCE CONSTANT	INTERNAL COORDINATE	FORCE CONSTANT
1. $\nu(\text{Sb-C1})$	5.510	41. $\nu(\text{C31-C32})$	5.690
2. $\nu(\text{Sb-O4})$	6.785	42. $\nu(\text{O4-C33})$	4.565
3. $\nu(\text{Sb-C7})$	5.510	43. $\nu(\text{C33=O5})$	8.740
4. $\nu(\text{Sb-O1})$	6.785	44. $\nu(\text{C33-C34})$	4.552
5. $\nu(\text{Sb-C13})$	5.510	45. $\nu(\text{C34-C41})$	6.212
6. $\nu(\text{C1-C2})$	5.659	46. $\nu(\text{C34-O6})$	6.950
7. $\nu(\text{C1-C6})$	5.659	47. $\nu(\text{C34-C35})$	6.212
8. $\nu(\text{C2-C3})$	5.659	48. $\nu(\text{C35-C36})$	5.690
9. $\nu(\text{C3-C4})$	5.659	49. $\nu(\text{C35-C40})$	5.690
10. $\nu(\text{C4-C5})$	5.659	50. $\nu(\text{C36-C37})$	5.690
11. $\nu(\text{C5-C6})$	5.659	51. $\nu(\text{C37-C38})$	5.690
12. $\nu(\text{C7-C8})$	5.659	52. $\nu(\text{C38-C39})$	5.690
13. $\nu(\text{C7-C12})$	5.659	53. $\nu(\text{C39-C40})$	5.690
14. $\nu(\text{C8-C9})$	5.659	54. $\nu(\text{C41-C42})$	5.690
15. $\nu(\text{C9-C10})$	5.659	55. $\nu(\text{C41-C46})$	5.690
16. $\nu(\text{C10-C11})$	5.659	56. $\nu(\text{C42-C43})$	5.690
17. $\nu(\text{C11-C12})$	5.659	57. $\nu(\text{C43-C44})$	5.690
18. $\nu(\text{C13-C14})$	5.659	58. $\nu(\text{C44-C45})$	5.690
19. $\nu(\text{C13-C18})$	5.659	59. $\nu(\text{C45-C46})$	5.690
20. $\nu(\text{C14-C15})$	5.659	60. $\phi(\text{C7-Sb-O4})$	0.665 (0.420)
21. $\nu(\text{C15-C16})$	5.659	61. $\phi(\text{C7-Sb-C1})$	0.500 (0.300)
22. $\nu(\text{C16-C17})$	5.659	62. $\phi(\text{C7-Sb-C13})$	0.500 (0.300)
23. $\nu(\text{C17-C18})$	5.659	63. $\phi(\text{C7-Sb-O1})$	0.665 (0.420)
24. $\nu(\text{O1-C19})$	4.565	64. $\phi(\text{O4-Sb-C1})$	0.665 (0.420)
25. $\nu(\text{C19-O2})$	8.740	65. $\phi(\text{O4-Sb-C13})$	0.665 (0.420)
26. $\nu(\text{C19-C20})$	4.552	66. $\phi(\text{O4-Sb-O1})$	0.427 (0.250)
27. $\nu(\text{C20-O3})$	6.950	67. $\phi(\text{C1-Sb-C13})$	0.500 (0.300)
28. $\nu(\text{C20-C27})$	6.212	68. $\phi(\text{C1-Sb-O1})$	0.665 (0.420)
29. $\nu(\text{C20-C21})$	6.212	69. $\phi(\text{C13-Sb-O1})$	0.665 (0.420)
30. $\nu(\text{C21-C22})$	5.690	70. $\phi(\text{Sb-C1-C2})$	0.885 (0.500)
31. $\nu(\text{C21-C26})$	5.690	71. $\phi(\text{Sb-C1-C6})$	0.885 (0.500)
32. $\nu(\text{C22-C23})$	5.690	72. $\phi(\text{C2-C1-C6})$	0.695 (0.350)
33. $\nu(\text{C23-C24})$	5.690	73. $\phi(\text{C1-C2-C3})$	0.695 (0.350)
34. $\nu(\text{C24-C25})$	5.690	74. $\phi(\text{C2-C3-C4})$	0.695 (0.350)
35. $\nu(\text{C25-C26})$	5.690	75. $\phi(\text{C3-C4-C5})$	0.695 (0.350)
36. $\nu(\text{C27-C28})$	5.690	76. $\phi(\text{C4-C5-C6})$	0.695 (0.350)
37. $\nu(\text{C27-C32})$	5.690	77. $\phi(\text{C5-C6-C1})$	0.695 (0.350)
38. $\nu(\text{C28-C29})$	5.690	78. $\phi(\text{Sb-C7-C8})$	0.885 (0.500)
39. $\nu(\text{C29-C30})$	5.690	79. $\phi(\text{Sb-C7-C12})$	0.885 (0.500)
40. $\nu(\text{C30-C31})$	5.690	80. $\phi(\text{C8-C7-C12})$	0.695 (0.350)

81. ϕ (C7-C8-C9)	0.695 (0.350)	126. ϕ (C41-C34-C35)	0.795 (0.250)
82. ϕ (C8-C9-C10)	0.695 (0.350)	127. ϕ (O6-C34-C35)	0.250 (0.250)
83. ϕ (C9-C10-C11)	0.695 (0.350)	128. ϕ (C34-C35-C36)	0.680 (0.025)
84. ϕ (C10-C11-C12)	0.695 (0.350)	129. ϕ (C34-C35-C40)	0.680 (0.025)
85. ϕ (C11-C12-C7)	0.695 (0.350)	130. ϕ (C36-C35-C40)	0.499 (0.250)
86. ϕ (Sb-C13-C14)	0.885 (0.500)	131. ϕ (C35-C36-C37)	0.499 (0.250)
87. ϕ (Sb-C13-C18)	0.885 (0.500)	132. ϕ (C36-C37-C38)	0.499 (0.250)
88. ϕ (C14-C13-C18)	0.695 (0.350)	133. ϕ (C37-C38-C39)	0.499 (0.250)
89. ϕ (C13-C14-C15)	0.695 (0.350)	134. ϕ (C38-C39-C40)	0.499 (0.250)
90. ϕ (C14-C15-C16)	0.695 (0.350)	135. ϕ (C39-C40-C45)	0.499 (0.250)
91. ϕ (C15-C16-C17)	0.695 (0.350)	136. ϕ (C34-C41-C42)	0.680 (0.025)
92. ϕ (C16-C17-C18)	0.695 (0.350)	137. ϕ (C34-C41-C46)	0.680 (0.025)
93. ϕ (C17-C18-C13)	0.695 (0.350)	138. ϕ (C42-C41-C46)	0.680 (0.250)
94. ϕ (O1-C19=O2)	1.525 (0.350)	139. ϕ (C41-C42-C43)	0.680 (0.250)
95. ϕ (O1-C19-C20)	0.450 (0.450)	140. ϕ (C42-C43-C44)	0.680 (0.250)
96. ϕ (O2=C19-C20)	1.755 (0.020)	141. ϕ (C43-C44-C45)	0.680 (0.250)
97. ϕ (C19-C20-O3)	0.410 (0.525)	142. ϕ (C44-C45-C46)	0.680 (0.250)
98. ϕ (C19-C20-O3)	0.660 (0.525)	143. ϕ (C45-C46-C41)	0.680 (0.250)
99. ϕ (C19-C20-C21)	0.660 (0.025)	144. ϕ (Sb-O1-C19)	0.435 (0.525)
100. ϕ (O3-C20-C27)	0.250 (0.025)	145. ϕ (Sb-O4-C33)	0.435 (0.525)
101. ϕ (O3-C20-C21)	0.250 (0.025)	146. ω (O2-C19)	0.318
102. ϕ (C27-C20-C21)	0.795 (0.255)	147. ω (O3-C20)	0.200
103. ϕ (C20-C21-C22)	0.680 (0.255)	148. ω (O5-C33)	0.318
104. ϕ (C20-C21-C26)	0.680 (0.255)	149. ω (O6-C34)	0.200
105. ϕ (C22-C21-C26)	0.499 (0.250)	150. τ (Sb-C1)	0.045
106. ϕ (C21-C22-C23)	0.499 (0.250)	151. τ (C1-C2)	0.020
107. ϕ (C22-C23-C24)	0.499 (0.250)	152. τ (C2-C3)	0.020
108. ϕ (C23-C24-C25)	0.499 (0.250)	153. τ (C3-C4)	0.020
109. ϕ (C24-C25-C26)	0.499 (0.250)	154. τ (C4-C5)	0.020
110. ϕ (C25-C26-C21)	0.499 (0.250)	155. τ (C5-C6)	0.020
111. ϕ (C20-C27-C28)	0.680 (0.255)	156. τ (C6-C1)	0.020
112. ϕ (C20-C27-C32)	0.680 (0.255)	157. τ (Sb-C7)	0.045
113. ϕ (C28-C27-C32)	0.499 (0.250)	158. τ (C7-C8)	0.020
114. ϕ (C27-C28-C29)	0.499 (0.250)	159. τ (C8-C9)	0.020
115. ϕ (C28-C29-C30)	0.499 (0.250)	160. τ (C9-C10)	0.020
116. ϕ (C29-C30-C31)	0.499 (0.250)	161. τ (C10-C11)	0.020
117. ϕ (C30-C31-C32)	0.499 (0.250)	162. τ (C11-C12)	0.020
118. ϕ (C31-C32-C27)	0.499 (0.250)	163. τ (C12-C7)	0.020
119. ϕ (O4-C33=O5)	1.525 (0.350)	164. τ (Sb-C13)	0.045
120. ϕ (O4-C33-C34)	0.450 (0.250)	165. τ (C13-C14)	0.020
121. ϕ (O5=C33-C34)	1.755 (0.350)	166. τ (C14-C15)	0.020
122. ϕ (C33-C34-C41)	0.660 (0.025)	167. τ (C15-C16)	0.020
123. ϕ (C33-C34-O6)	0.250 (0.250)	168. τ (C16-C17)	0.020
124. ϕ (C33-C34-C35)	0.660 (0.255)	169. τ (C17-C18)	0.020
125. ϕ (C41-C34-O6)	0.250 (0.250)	170. τ (C18-C13)	0.020

171. τ (Sb-O1)	0.041
172. τ (O1-C19)	0.030
173. τ (C19-C20)	0.040
174. τ (C20-C21)	0.020
175. τ (C21-C22)	0.022
176. τ (C22-C23)	0.022
177. τ (C23-C24)	0.022
178. τ (C24-C25)	0.022
179. τ (C25-C26)	0.022
180. τ (C26-C21)	0.022
181. τ (C20-C27)	0.020
182. τ (C27-C28)	0.022
183. τ (C28-C29)	0.022
184. τ (C29-C30)	0.022
185. τ (C30-C31)	0.022
186. τ (C31-C32)	0.022
187. τ (C32-C27)	0.022
188. τ (Sb-O4)	0.041
189. τ (O4-C33)	0.030
190. τ (C33-C34)	0.040
191. τ (C34-C35)	0.020
192. τ (C35-C36)	0.022
193. τ (C36-C37)	0.022
194. τ (C37-C38)	0.022
195. τ (C38-C39)	0.022
196. τ (C39-C40)	0.022
197. τ (C40-C35)	0.022
198. τ (C34-C41)	0.020
199. τ (C41-C42)	0.022
200. τ (C42-C43)	0.022
201. τ (C43-C44)	0.022
202. τ (C44-C45)	0.022
203. τ (C45-C46)	0.022
204. τ (C46-C41)	0.022

Note:

- ν (X-Y) represents the stretching between the atoms X and Y etc.
- ϕ (X-Y-Z) represents the in plane bending be-

tween the atoms X, Y and Z.

- ω (X-Y) represents the out of plane bending (wagging) between the atoms X and Y.
- τ (X-Y) represents the torsion of the atoms X and Y.
- The number in parenthesis represents the non-bonded value of the atoms X, Y and Z

REFERENCES

- K. Hartke and H. Wolff, M. Chem. Ber., 113, 1394 (1980).
- P. L. Millington and D. B. Sowerby, J. Chem. Soc. Dalton Trans., 1199 (1992).
- M. Dogamala, F. Huber and H. Preut, Z. Anorg. Allg. Chem., 571, 130 (1989).
- Y. Q. Ma, J. S. Li, Z. N. Xuan and R. C. Liu, J. Organomet. Chem., 620, 235 (2001).
- K. Singhal, R. Rastogi and P. Raj, Indian J. Chem., 26A, 146 (1987).
- A. Glowacki, F. Huber and H. Preut, Recl. Trav. Chim. Pays-Bas., 107, 278 (1988).
- K. Chandarshekhkar, H.M. Behl, K. Vishal, O.P. Sidhu, P. Pushpangadan, C.V. Rao, S.K. Shukla, A. Ranjan, R. Kant, K. Singhal and P. Raj, Triorganoantimony compounds for pesticidal use, PCT/IN2004/000407;WO/2006/067800.
- E.B. Wilson Jr., J.C. Decius and P.C. Cross, Molecular Vibrations, (Dover Publications), pp.11-31 (1980).
- H.C. Urey and C.A. Bradley, Phys. Rev., 38, 1969-1975 (1931).
- H. Barucki, S.J. Coles, J.F. Costello, T. Gelbrich and M.B. Hursthouse, J. Chem Soc. Dalton Trans., 2319-2325 (2000).
- The Royal society of chemistry, CCDC no. (2000) 186/1998.
- T. Shimanouchi, in Computer program for normal coordinate treatment of Polyatomic molecules, (University of Tokyo, 1968).
- N. Misra, O. Prasad and L. Sinha, Indian Journal of Biochemistry & Biophysics., 43, 173-181 (2006).
- T. Hasan, P.K. Singh, K. Singhal, P. Raj and N. Misra, Pramana J. of Physics, 69 No.4, 675-680 (2007).
- T. Hasan, P.K. Singh, K. Singhal, P. Raj and N. Misra, E journal of Chem., vol. 5 No5, 723-735 (2008).
- P.K. Singh, T. Hasan, O. Prasad, L. Sinha, K. Raj and N. Misra, Spectroscopy., 20(5-6), 275-283 (2006).
- J. H.J. Gotze, P. Lemannzich and B. Schaaf, Spectrochim. Acta Part A 50, 1871 (1994).
- J.R. Scherer, Spectrochim. Acta, 20, 345 (1964).
- M. Tasumi, T. Urano and M. Nakata, J. Mol. Structure, 146, 383 (1986).
- C.L. Lau and R.G. Snyder, Spectrochim. Acta Part A 27, 2073 (1971).
- J.J.P. Stewart, MOPAC 2007, Stewart Computational Chemistry, version 7.075W.

- [22] N.B. Colthup, L.H. Daly and S.E. Wiberley, Introduction to Infrared and Raman Spectroscopy, Academic Press, New York, 1964, p. 74; N.B. Colthup, L.H. Daly and S.E. Wiberley, Introduction to Infrared and Raman Spectroscopy, Academic Press, New York, p.199,212,225,249 (1964).
- [23] K. Shobatake, C. Postmus, J.R. Ferraro and K. Nakamoto, Appl. Spectrosc., 23(1), 12 (1969).
- [24] M.K. Khosa, M. Mazhar, S. Ali, K. Shahid and F. Malik, Turk. J. Chem., 30, 345- 354 (2006).
- [25] D. Shankar, A.K. Rai., Y.P. Singh, H. Rehwani, V. Khushalani and R.S. Gupta, Bioorgan.Chem. and Appl., 2006, 1-7 (2006).
- [26] H.A. Meinema, A. Mackor and J.G. Noltes, J. Organometal. Chem., 37, 285, (1972).
- [27] C. Ludwig, M. Dolny and H.J. Gotze, Spectrochim. Acta Part A 53, 2363- 2372 (1997).
- [28] P. Raj, S. Agnihotri and K. Singhal, Syn. & Reactivity in Inorg, Metal-Org, Nanometal Chemistry.,32, 569-581 (2002).
- [29] N.S.Biradar and V.K. Kulkarni, J. Inorgnucl. Chem., 33, 3781 (1971).
- [30] J.N.R. Ruddick and J.R. Sames, J. Organometal. Chem., 60, 233 (1973).