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Fourier transform Raman and infrared spectra and normal coordinate analysis of $(C_6H_5)_3Bi$ and $(C_6D_5)_3Bi$

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Abstract

The FT Raman and infrared spectra of triphenylbismuth $(C_6H_5)_3Bi$ and the perdeuterated molecule $(C_6D_5)_3Bi$ have been measured in the range $3600-100 \text{ cm}^{-1}$. A normal coordinate analysis has been performed for both substances using a modified valence force field. This leads to a complete assignment of all 96 vibrations of each of the two compounds. The complete molecule with 34 atoms and C_1 symmetry is calculated for the first time. Out-of-plane and in-plane vibrations are computed together in one step. For the perdeuterated isotopomer ²H NMR, ¹³C NMR and MS data are also given.

1. Introduction

Although Michaelis and Polis [1] prepared triphenylbismuth as early as 1887, the first IR data were not published until 1955 [2]. Today there are numerous IR data available [3–10]; however only one Raman spectrum of triphenylbismuth has been recorded in the range $530-100 \text{ cm}^{-1}$ by Shobatake et al. [7]. They performed a normal coordinate analysis for a simple BiX₃ model of triphenylbismuth, where each X group was given by the mass of a phenyl ring assuming C_{3v} symmetry. The Bi–C stretching-force constant was found to be $1.37 \times 10^2 \text{ N m}^{-1}$ and the C–Bi–C bending force constant to be $0.24 \times 10^{-18} \text{ N m}$.

Wetzel [11] determined the crystal structure of triphenylbismuth in 1942. Further investigations in the following years [12–14] showed that the BiC_3 skeleton is close to a pyramidal configuration with a C-Bi-C bond angle of 94°.

Perdeuterated triphenylbismuth $(C_6D_5)_3Bi$ has not yet been described. $(C_6T_5)_3Bi$ was prepared in 1989; however, no IR or Raman spectra were published for this substance [15].

With the complete structural data from X-ray structure analysis and both FT Raman and FT-infrared spectra, a normal coordinate analysis of the complete triphenylbismuth molecule and its deuterated species using a modified valence force field should establish the assignments of fundamental modes and supply a reasonable and transferable set of force constants.

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2. Experimental

The FT Raman and FT infrared spectra were recorded on a Perkin-Elmer 1760 × spectrometer. The 1.064 μ m line of a Nd:YAG (Spectron Laser Systems) was used as exciting radiation for Raman spectra registration. The laser power at the samples was 400 mW. A semiconductor InGaAs detector operating at room temperature and additionally, an FTIR spectrometer (Perkin-Elmer 1700) was used in the range 500–100 cm⁻¹ at a resolution of 2 cm⁻¹. Frequency accuracy was about ± 2 cm⁻¹.

Sample synthesis and spectroscopic preparation of $(C_6H_5)_3Bi$ and $(C_6D_5)_3Bi$ were carried out under an atmosphere of prepurified nitrogen.

 $(C_6H_5)_3$ Bi was prepared by the Grignard reaction of BiCl₃ with C_6H_5 MgBr in ether as reported previously [16,17]. Colourless crystals were recrystallized from dry ether; yield 75%, m.p. 71 °C. $(C_6D_5)_3$ Bi was prepared analogously to C_6D_5 MgBr. Colourless crystals were recrystallized from dry ether; yield 65%, m.p. 71–72 °C. Anal. found (calc. for $C_{18}D_{15}$ Bi): C, 46.9% (47.5%); D, 6.6% (6.6%).

²H NMR (400 MHz, CDCl₃): 7.35 (o^{-2} H, s); 7.41 (m^{-2} H, s); 7.77 (p^{-2} H, s). ¹³C NMR (400 MHz, CDCl₃): 154.9 (α -C, s); 137,35 (o-C.t); 127,47 (m-C, t); 130,18 (p-C,t). The NMR spectra were measured on a Bruker AM 400 NMR spectrometer using TMS as internal standard and were reported as δ .

MS: 455, M⁺; 373, $(C_6D_5)_2Bi^+$; 291, $(C_6D_5)Bi^+$; 209, Bi^+ ; 164, $C_{12}D_{10}^+$; 160, $C_{12}D_8^+$; 82, $C_6D_5^+$; 54, $C_4D_3^+$.

3. Results and discussion

Most of the IR and Raman bands of $(C_6H_5)_3$ Bi (I) (Fig. 1) and $(C_6D_5)_3$ Bi (II) (Figs. 2 and 3) are caused by the phenyl substituents. They can be discussed as normal vibrations of monosubstituted benzene derivates, because the heavy bismuth central atom (208.98 g mol⁻¹) is an efficient coupling barrier of the phenyl rings. The nomenclature according to Whiffen [18] for such systems is used in this work.

Normal coordinate analysis is carried out by a computer program developed in our research group, based on the program by Shimanouchi [19]. The program PROMETHEUS[©] follows the GF matrix method according to Wilson et al. [20] and works on a normal PC under MS-WINDOWS[©]. It allows the calculation of molecules with more than 100 atoms



Fig. 1. FT Raman spectrum of (C₆H₅)₃Bi.



Fig. 2. FTIR spectrum of (C₆D₅)₃Bi (KBr disc).

even if the molecular structure is assumed as C_1 symmetry and has the possibility to calculate more isotopic molecules together. The vibrations (LX matrix) can be printed or animated on the screen. The experimental and calculated spectrum can be shown.

The vibrational problem was set up in internal coordinates; in-plane and out-of-plane vibrations were calculated together.

3.1. Normal coordinate analysis of $(C_6H_5)_3Bi$

In the first step a model calculation for the Bi-Ph one ring system was performed. The initial force constants were taken from normal coordinate analyses of other Ph-X systems [21-24]. After the refinement of the force constants a calculation for the complete molecules (I) and (II) with 34 atoms was carried out using the initial set of force



Fig. 3. FT Raman spectrum of $(C_6D_5)_3Bi$.

Parameter	Value	
d(Bi-C)	224.0	
d(C-C)	140.4	
d(C-H/D)	107.9	
$\angle (C-Bi-C)$	94.0	
\angle (Bi-C-C)	120.0	
$\angle (C - C - C)$	120.0	
∠(C-C-H/D)	120.0	

Table 1 Geometric parameters " for the normal coordinate analysis of $(C_6H_5)_3Bi$ and $(C_6D_5)_3Bi$

^a Distances in pm and angles in degrees.



Fig. 4. Calculated k-mode vibration at 1572 cm^{-1} (amplitude factor 40).



Fig. 5. Calculated g-mode vibration at 860 cm^{-1} (amplitude factor 40).

constants taken from the Bi-Ph calculation. The C-Bi-C in-plane bending force constant (f_4) was taken from a calculation with a CY₂ model [21]. The force constant were refined for (I) and (II) in one step.

The geometric parameters used were taken from the X-ray structure analysis of (I) [14] (see Table 1). For the complete molecules (I) and (II) C_1 symmetry was assumed because of the different torsion angles of the benzene rings (38°, 42° and 73°) [14].

In the calculation of the entire molecule all modes were found as triply degenerate vibrations according to expectation. The same characteristics of the modes appear in all three rings but with different amplitudes. The frequencies of these three modes are the same or nearly the same for the most vibrations and differ for f, u, t and y modes. The vibrations of the k and g modes are shown in Figs. 4 and 5.

3.2. Phenyl ring in-plane vibrations

Most of the vibrations above 500 cm^{-1} were well known and assigned for monosubstituted benzene derivates. In the literature [7,21] the observed frequencies of 1327 and

1261 cm⁻¹ were assigned as in-plane C-C stretching (o-mode) and C-C-H bending (e-mode) vibrations respectively; however, a potential energy distribution has been calculated with δ (C-C-H/D) (88) and ν (C-C) (8) for the 1327 cm⁻¹ vibration, whereas the 1261 cm⁻¹ vibration shows a potential energy distribution with ν (C-C) (143) and δ (C-C-H/D) (35). This led us to conclude that the assignment of those two vibrations should be changed. In the deuterated species the 1263 cm⁻¹ vibration shows a potential energy distribution with δ (C-C-H/D) (94) and ν (C-C) (2) in contrast to the 1058 cm⁻¹ vibration with ν (C-C) (171) and δ (C-C-H/D) (12). On this basis the C-C-H/D bending (e-mode) has been assigned to the 1327 (I) and 1058 cm⁻¹ (II) vibrations and the C-C stretching (o-mode) to the 1261 (I) and 1263 cm⁻¹ (II) vibrations, which is the reverse of the earlier assignment [7,21]. This was in good agreement with the large shift of the C-C-H/D bending vibration due to deuteration, while the C-C stretching vibration shows almost no shift.

Table 2							
Assignment o	f observed	and calculated	IR a	nd Raman	frequencies of	(C ₆ H ₅) ₃ Bi and	$(C_6D_5)_3Bi$

Vibration ^a	(C ₆ H ₅) ₃	Bi/cm ⁻¹		$(C_6 D_5)_3 Bi/cm^{-1}$			
	Observed		Calculated	Observed		Calculated	
	IR	Raman		IR	Raman		
zl-mode	3057	3061	3060	2276	2275	2277	
z4-mode	3045		3046	2263	2262	2263	
z2-mode	3035	3039	3032	2263	2262	2257	
z3-mode	3018	3016	3017	2249	2248	2250	
z5-mode	3002		3008	2249	2248	2247	
k-mode	1567	1569	1572	1530	1531	1528	
1-mode	1567	1569	1570	1530	1531	1526	
m-mode	1474	1474	1476	1331	1331	1326	
n-mode	1431	1429	1444	1294	1296	1299	
e-mode	1327	1328	1337	1058		1043	
o-mode	1261	1263	1268	1263	1263	1254	
c-mode	1184	1189	1197	869	872	861	
a-mode	1158	1157	1177	869	872	854	
a-mode	1060		1064	1025		1021	
d-mode	1055	1055	1050	823	823	812	
b-mode	1014	1016	1009	803		794	
p-mode	998	999	996	954	956	954	
h-mode	984	985	1005	740	740	773	
i-mode	967		964	740	740	734	
i-mode	908	913	912	728	725	724	
g-mode	851	849	860	664	664	669	
f-mode	731	728	775, 741	545		530	
f-mode	723		736	537	539	529, 525	
v-mode	694		693	669		688	
r-mode	644	646	646	617	620	623	
s-mode	615	616	617	591	590	591	
x-mode	451	448	434	407		394	
w-mode	391	393	359	342	340	331	
u-mode	235	234	260, 247	225	223	246, 233	
			241			224	
t-mode	216	220	214	208	209	208	
t-mode	207	206	206	198	198	198	
t-mode	199	199	201	189	189	193	
v-mode	167	166	182, 177	155	158	171, 166	
,			175			163	
τ-Ring			74			67	
$\delta(C-Bi-C)$			35			34	

^a Assignment of the 30 phenyl vibrations according to Whiffen [18].

Vibration	Calc./cn	n ⁻¹	PED % (I, II) ^a		
	(I)	(II)			
z1-mode (3) ^b	3060	2277	f ₃ (97, 94)		
z4-mode (3)	3046	2263	$f_3(98, 94)$		
z2-mode (3)	3032	2257	$f_3(99, 95)$		
z5-mode (3)	3017	2250	$f_3(100, 94)$		
z3-mode (3)	3008	2247	$f_3(100, 96)$		
k-mode (3)	1572	1528	$f_2(80, 91); f_5(10, 10); f_7(31, 16); f_{16}(-10, -12);$ $f_{-1}(-11, -11); f_{-1}(-14, -10); f_{-1}(6, 7)$		
I-mode (3)	1570	1526	$f_{18}(-10, -11), f_{22}(-10, -10), f_{24}(0, 7)$ $f_{2}(83, 90); f_{5}(10, 8); f_{7}(24, 10); f_{16}(-11, -12);$ $f_{18}(-10, -10); f_{22}(-8, -5); f_{24}(6, 7)$		
m-mode (3)	1476	1326	$f_2(32, 60); f_5(3, 5); f_7(72, 40); f_{16}(4, 8); f_{18}(-6, -11); f_{22}(-8, -7)$		
n-mode (3)	1444	1299	$f_2(32, 66); f_5(3, 3); f_7(72, 40); f_{16}(4, 6); f_{18}(-6, -11)$		
e-mode (3)	1337	1043	$f_2(7, 2); f_7(88, 95)$		
o-mode (3)	1268	1254	$f_2(143, 169); f_7(36, 13); f_{16}(-37, -42); f_{22}(-22, -14);$ $f_{22}(-11, -13); f_{22}(-10, -12)$		
c-mode (3)	1197	861	$f_{23}(-11, -15), f_{24}(-10, -12)$ $f_{2}(40, 4); f_{2}(58, 91); f_{2}(-10, -1); f_{22}(16, 6)$		
a-mode (3)	1177	854	$f_2(20, 9)$; $f_2(70, 81)$; $f_{22}(12, 8)$		
$a \operatorname{mode}(3)$	1064	1021	$f_1(8, 7)$; $f_2(70, 66)$; $f_2(4, 8)$; $f_{12}(18, 17)$; $f_{22}(-5, -5)$; $f_{24}(4, 5)$		
d-mode (3)	1050	812	$f_2(56, 25)$; $f_2(34, 66)$; $f_{12}(6, 2)$; $f_{12}(-10, -4)$; $f_{22}(10, 9)$		
b-mode (3)	1009	794	$f_2(40, 32); f_6(37, 4); f_6(5, 0); f_7(20, 59); f_{16}(6, 4);$		
0			$f_{10}(-6, -6); f_{20}(4.8)$		
p-mode (3)	996	954	$f_2(28, 8); f_2(2, 6); f_5(52, 75); f_6(2, 6); f_7(23, 14); f_{20}(-6, -9)$		
h-mode (3)	1005	773	$f_{0}(11, 9); f_{10}(38, 28); f_{11}(6, 4); f_{13}(53, 69); f_{27}(-6, -9)$		
j-mode (3)	964	734	$f_{9}(9, 5); f_{10}(45, 22); f_{12}(2, 14); f_{13}(57, 72); f_{27}(-7, -8)$		
i-mode (3)	912	724	$f_{11}(45, 26); f_{13}(67, 87); f_{27}(-8, -14); f_{29}(-9, -8)$		
g-mode (3)	860	669	$f_9(14, 15); f_{11}(17, 16); f_{13}(56, 56); f_{27}(7, 7)$		
f-mode	775	530	$f_9(2, 20); f_{12}(42, 1); f_{13}(43, 61); f_{25}(-8, 2); f_{27}(6, 13)$		
f-mode	743	529	$f_9(2, 20); f_{12}(40, 1); f_{13}(58, 60); f_{25}(-17, 2); f_{27}(8, 13)$		
f-mode	736	525	$f_9(4, 23); f_{12}(30, 3); f_{13}(65, 57); f_{25}(-16, 0); f_{27}(10, 12)$		
v-mode (3)	693	688	$f_9(18, 8); f_{10}(2, 38); f_{12}(39, 33); f_{13}(36, 16)$		
r-mode (3)	646	623	$f_1(14, 12); f_5(73, 72); f_6(9, 8); f_7(15, 20); f_{18}(7, 6); f_{19}(-11, -10); f_{19}(-6, -8)$		
s-mode (3)	617	591	$f_2(6, 5): f_2(78, 78): f_2(20, 22): f_{10}(8, 7): f_{20}(-5, -5): f_{20}(-7, -8)$		
x-mode (3)	434	394	$f_{10}(14, 19); f_{11}(56, 73); f_{12}(10, 8); f_{13}(42, 23); f_{27}(-9, -4);$ $f_{10}(14, 19); f_{12}(56, 73); f_{12}(10, 8); f_{13}(42, 23); f_{27}(-9, -4);$		
w-mode (3)	359	331	$f_{29}(-1, -26)$ $f_{9}(57, 42); f_{10}(8, 11); f_{11}(38, 49); f_{12}(8, 10); f_{26}(-7, -5);$ $f_{26}(-4, -5)$		
u-mode	260	246	$f_1(9, 13); f_2(10, 9); f_4(8, 8); f_6(69, 63)$		
u-mode	247	233	$f_1(11, 18); f_2(9, 8); f_4(1, 2); f_6(71, 62)$		
u-mode	241	224	$f_1(2,5); f_2(10,10); f_4(7,7); f_6(77,71)$		
t-mode	214	208	$f_1(68, 65); f_2(4, 5); f_6(4, 8); f_9(6, 4); f_{21}(8, 8)$		
t-mode	206	198	$f_1(61, 55); f_2(5, 6); f_6(15, 23); f_9(4, 2); f_{21}(8, 7)$		
t-mode	201	193	$f_1(68, 64); f_2(5, 5); f_6(11, 15); f_9(2, 0); f_{21}(8, 8)$		
y-mode	182	171	$f_1(7, 5); f_4(10, 11); f_9(52, 55); f_{11}(7, 10); f_{13}(20, 18)$		
y-mode	177	166	$f_1(9, 7); f_4(5, 5); f_9(53, 55); f_{11}(6, 9); f_{13}(20, 18)$		
y-mode	175	163	$f_1(2, 1); f_4(0, 0); f_9(60, 63); f_{11}(7, 10); f_{13}(22, 20)$		
τ -Ring (3)	74	67	$f_8(92, 92); f_{13}(5, 5)$		
$\delta(C-Bi-C)$ (3)	35	34	$f_4(86, 85); f_6(6, 7)$		

Table 3 Vibrational frequencies and potential energy distribution (PED) of $(C_6H_5)_3Bi$ (I) and $(C_6D_5)_3Bi$ (II)

^a Only PED values greater than $\pm 5\%$ in (I) or (II) are given in the table. ^b These vibrations appear three times at equal frequencies.

3.3. Phenyl ring out-of-plane vibrations and skeletal vibrations

The nine out-of-plane vibrations according to Whiffen [18] are also well known, although it is more difficult to find a good force field for these vibrations.

The assignment of the vibration below 500 cm^{-1} has already been discussed controversially in the literature [7,9,10,21]; only the vibration at 359 cm^{-1} was assigned as w-mode

Force constant ^a		Value	Forc	Value	
f_1	ν(B i-C)	1.620	f_{16}	$v(C-C)/v(C-C)_0$	0.848
f	v(C-C)	6.551	f_{17}	v(C-H)/v(C-C)	0.037
fa	$v(C-H)^{b}$	4.979	f_{18}	$v(C-C)/\delta(C-C-C)$	0.505
f_	$\delta (C-Bi-C)^{c}$	0.420	f19	$v(C-H)/\delta(C-C-H)$	-0.099
fs	$\delta(C-C-C)$	1.119	f_{20}	$\delta(C-C-C)/\delta(C-C-C)_0$	0.065
Ĵ6	$\delta(C-C-Bi)$	0.985	f_{21}	$v(Bi-C)/\delta(C-C-Bi)$	0.446
f_7	$\delta(C-C-H)$	0.512	f_{22}	$v(C-C)/\delta(C-C-H)$	0.231
$f_{\rm R}$	$\tau (C_2 - Bi - C - C_2)^{\circ}$	0.300	f23	$v(C-C/v(C-C)_m)$	-0.258
f9	$\tau(C/Bi-C-C-C/H)$	0.420	f_{24}	$v(C-C)/v(C-C)_p$	0.478
f_{10}	$\tau (C/H-C-C-C/H)_{\alpha(Bi)}$	0.461	f25	$\gamma(C_3 - Bi) / \gamma(C_3 - H)_0$	0.086
f_{11}	$\tau(C/H-C-C-C/H)_{\omega(Bi)}$	0.346	f_{26}	$\delta(C-C-C)/\delta(C-C-H)$	0.064
f12	$\gamma(C_3 - Bi)$ out-of-plane wag	0.955	f27	$\gamma(C_3 - H(/\gamma(C_3 - H)_0))$	0.037
f13	$\gamma(C_3 - H)$ out-of-plane wag	0.296	f_{28}	$C/Bi-C-C-C/H)/\tau(C/H-C-C-C/H)_0$	0.030
f_{14} f_{15}	$\gamma(C_2H-C)$ out-of-plane wag $\nu(C-H)/\nu(C-H)_0$	0.060 0.063	f ₂₉	$\tau(C/H-C-C-C/H)/\tau(C/H-C-C-C/H)_0$	0.065

Table 4 Force constants of $(C_6H_5)_3Bi$ and $(C_6D_5)_3Bi$

^a Force constant dimension: valence 10^2 N m⁻¹; deformation 10^{-18} N m; valence/valence 10^2 N m⁻¹; valence/deformation 10^{-8} N; deformation/deformation 10^{-18} N m. ^b All force constants containing hydrogen (H) are also used for deuterium (D). ^c Not refined, see text.

by all authors. We assigned these vibrations on the basis of their potential energy distributions and LX matrices as shown in Tables 2 and 3. In particular the assignments for the x- and y-mode vibrations at 451 cm^{-1} and 167 cm^{-1} differ from the literature for Ph₃Bi [7,9,10,21].

There are six calculated vibrations below 100 cm^{-1} but we are not able to measure vibrations in that region. Because it is difficult to find force constants for the torsion of the rings around the bismuth central atom we gave the force constant f_8 a value of 0.300 (Table 4). For the out-of-plane bismuth vibration a force constant f_4 was given [21]. Neither force constant f_4 nor f_8 were refined in our calculation. Hence the calculated wavenumber for the ring torsion is questionable and in further research spectra in the region below 100 cm^{-1} must be included.

3.4. Vibrational spectra and normal coordinate analysis of $(D_6D_5)_3Bi$

The assignment of the vibrations of the deuterated molecule is shown in Table 2 and is in good agreement with the assignment for other deuterated benzene derivates [23,25].

The C-H/D stretching vibrations show an isotopic shift quotient of 1.34-1.35, the C-C-H/D bending vibrations a shift of 1.25-1.33 and the C-H/D out-of-plane wagging vibrations one of 1.23-1.35. The C-C stretching vibrations show almost no shift in the deuterated molecule.

With the deuteration of the molecule the l-, k-, m- and n-mode vibrations change their potential energy distribution characteristics from $\delta(C-C-H/D)$ in-plane bending (f_7) to $\nu(C-C)$ stretching (f_2) , whereas the a-, c-, d- and b-mode vibrations change from $\nu(C-C)$ stretching to $\delta(C-C-H/D)$ in-plane bending. This means, that the C-C-H/D in-plane bending vibrations and the C-C stretching vibrations become stronger in their characteristics, respectively, due to the isotopic substitution. The interaction force constant f_{22} has a positive value in the potential energy distribution of the l-, k-, m- and n-mode vibrations and a negative value for the a-, c-, d- and b-mode vibrations.

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