Force constant calculations
for tricarbonyl(trichlorostibine)nickel(0), Ni(CO)$_3$SbCl$_3$

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Abstract

Force constant calculations have been carried out for the Ni(CO)$_3$SbCl$_3$ molecule by the FG-matrix method and a simplified valency force field (SVFF) with interaction constants. Some reassignments of the observed vibrational frequencies are proposed on the basis of these calculations. The ν(NiSb) stretching frequency at 232 cm^{-1} was confirmed and the force constant of 1.51 mdyne Å^{-1} evaluated. The k(NiSb) force constant is compared with k(NiP) in the related species Ni(PCl$_3$)$_4$. Bond stretching and bending force constants are compared for Ni(CO)$_3$SbCl$_3$ and the parent molecules SbCl$_3$ and Ni(CO)$_4$.

Introduction

The vibrational spectra of the tetrakis(trihalogenophosphine) compounds of nickel(0) have been well-characterised [1–4] and force constant calculations were recently undertaken for the Ni(PF$_3$)$_4$ and Ni(PCl$_3$)$_4$ species [5–7]. However, the reaction between tetracarbonyl nickel and arsenic(III) or antimony(III) chlorides proceeds to only the mono- or di-substitution stage, and the products are difficult to isolate. Compounds of the type Ni(CO)$_3$L, where L is SbEt$_3$ or SbPh$_3$, and Ni(CO)$_3$LL′, where L is SbEt$_3$ and L′ is SbEt$_2$Cl, have been reported [8,9], and partial assignments have been made of the vibrational spectra. Vibrational spectra of the monosubstituted phosphine nickel carbonyls of type Ni(CO)$_3$PX$_3$ where X is Cl, Me or Et, have been studied [8] in the ν(CO) stretching region only, and it has been concluded that the π-bonding in these compounds is very weak [10,11]. Recently, a full vibrational assignment of Ni(CO)$_3$SbCl$_3$ was made [12], and the Ni–Sb stretching vibration assigned to a band at 232 cm^{-1}.

In the present work, we report the results of the first force constant calculations on the Ni(CO)$_3$SbCl$_3$ species; these are used to check the vibrational assignment and to evaluate the force constant for Ni–Sb stretching. To assess the effect of the

substitution of $SbCl_3$ for a CO ligand in $Ni(CO)_4$, the force constants for $SbCl_3$ and $Ni(CO)_4$ were also evaluated.

Experimental: Force constant calculations

The structure of $Ni(CO)_3SbCl_3$ is shown in Fig. 1 and has been assigned to the molecular point group C_{3v}. The spectroscopic activity is as follows:

$$\Gamma_{vib} = 7A_1 + 2A_2 + 9E$$

for which $7A_1$ and $9E$ will be Raman and infra-red active and $2A_2$ will be inactive in both. The ligand $SbCl_3$ belongs to the point group C_{3v} and has the following activity, $2A_1 + 2E$, whereas $Ni(CO)_4$ has T_d symmetry with

$$\Gamma_{vib} = 2A_1 + 2E + F_1 + 4F_2$$

Of these, $2A_1 + 2E + 4F_2$ will be Raman active, $4F_2$ infra-red active and F_1 inactive in both the Raman and the infra-red.

The observed vibrational wavenumbers and assignments for the molecules $SbCl_3$ [13,14], $Ni(CO)_4$ [15,16] and $Ni(CO)_3SbCl_3$ [12] are given in Tables 1–3.

Force constant calculations were carried out with a modified form of the original programme of Snyder and Schachtschneider [17] with changes in formatting data input suggested by Fuhrer et al. [18] and further adapted for running on a Cyber 180-830 computer. The calculations used the Wilson FG-matrix method [19] and a simple valence force field with interaction constants. The input data consisted of molecular parameters, the number of symmetry elements, the number of atoms in the molecule, the molecular stereochemistry and the molecular vibrations. These were input in three stages, using the CART, GMAT and FPERT programmes. The vibrational wavenumbers were calculated and refined to give a best fit with the observed vibrational wavenumbers of the molecule. At each stage of the calculations various checks could be made to verify that the programme was reading the correct information and that the calculations had been performed correctly.

The molecular parameters used in the calculations were taken from the literature [20] and are given in Table 4. These parameters were transferred over to $Ni(CO)_3SbCl_3$ without change, in the absence of X-ray structural data for this molecule. The Ni–Sb bond length was estimated at 2.43 Å from calculations based on the sums of the covalent radii of Ni and Sb modified by comparison with the sums of the covalent radii of Ni and P atoms and the observed Ni–P bond length in
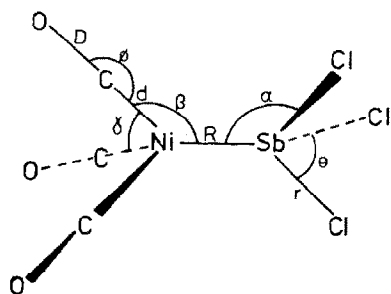

Fig. 1. Molecular structure and internal coordinates for $Ni(CO)_3SbCl_3$.

Table 1

Potential energy distributions (%) and wavenumbers for $SbCl_3$

ν	$\tilde{\nu}$ (cm^{-1})		Symm. class	Force constants			
	Obs	Calc		k_r	k_θ	k_{rr}	$k_{\theta\theta}$
ν_1	360	360	A_1	78.8	1.9	18.7	0.6
ν_2	165	165	A_1	2.0	74.0	0.5	23.5
ν_3	320	320	E	112.1	1.5	−13.3	−0.2
ν_4	134	134	E	1.4	117.4	−0.2	−18.6
Force constants ^{a}				1.79	0.27	0.21	0.04

^{a} Bond stretching and stretch–stretch interaction force constants have units of mdyne Å^{-1}; stretch–bend interaction force constants have units of mdyne Å^{-1} rad^{-1}; bending and bend–bend interaction force constants have units of mdyne Å^{-1} rad^{-2}.

$Ni(PF_3)_4$ [21].

For the $Ni(CO)_3SbCl_3$ species 40 internal coordinates were necessary for the generation of the full set of 18 normal vibrations. The internal coordinates used are shown in Fig. 1. In the SVFF force field ten primary force constants were used, namely:

k_r	SbCl stretching
k_R	SbNi stretching
k_d	NiC stretching
k_D	CO stretching
k_θ	ClSbCl deformation
k_α	NiSbCl deformation
k_β	CNiSb deformation
k_γ	CNiC deformation
$^\star k_\phi$	NiCO deformation
$^\star k_\tau$	CNiSbCl torsion

(*) kept fixed in final refinement

Since there were fourteen observed wavenumbers for $Ni(CO)_3SbCl_3$ [12], force field calculations would require normally the presence of a maximum of three or four interaction constants for effective refinement. However, the importance of the interaction constants and the use of all the available vibrational information for this type of molecule has already been demonstrated [5,7]. This situation arises because of the extensive mixing of the vibrational modes of the heavy ligands and the molecular skeleton. To achieve the necessary refinement with a realistic force field, therefore, several interaction and two primary (k_ϕ and k_τ) force constants were held constant at low values whilst other interaction constants were refined with the primary force constants. The effect of the presence of these fixed value interaction force constants on the refined force field could then be quantitatively assessed by allowing them to vary individually. It was found that some of the interaction constants, such as $k_{\theta\theta}$, were important for force-field stability even though their values were rather small.

Table 2

Potential energy distributions (%) and wavenumbers for Ni(CO)$_4$

ν	ν (cm^{-1})		Symm. class	Force constants								
	Obs	Calc		k_d	k_D	k_γ	k_ϕ	k_{dd}	$k_{d\gamma}$	k_{dD}	$k_{d\phi}$	$k_{\gamma\gamma}$
ν_1	2135	2136	A$_1$	4.1	95.1	0	0	0.7	0	−3.5	3.7	0
ν_2	381	381		81.2	4.9	0	0	14.0	0	3.6	−3.7	0
ν_3	459	458	E	0	0	11.0	87.0	0	0	0	0	2.0
ν_4	79	80		0	0	73.8	13.0	0	−0.1	0	0	13.3
ν_5	–	428	F$_1$	0	0	0	100.0	0	0	0	0	0
ν_6	2074	2073	F$_2$	4.1	101.0	0	0	−0.2	0	−3.7	−1.3	0
ν_7	461	462		3.2	0.1	10.0	91.2	−0.2	−6.0	−0.1	0	1.8
ν_8	422	422		111.8	0.5	0.5	0	−6.4	−8.3	1.3	0.4	0.1
ν_9	79	79		25.7	0.6	103.4	8.7	−1.5	−54.6	−0.7	−0.2	18.6
Force constants [a]				2.14	17.56	0.06	0.16	0.12	0.14	0.55	−0.10	−0.01

[a] Bond stretching and stretch–stretch interaction force constants have units of mdyne Å^{-1}; stretch–bend interaction force constants have units of mdyne Å^{-1} rad^{-1}; bend–bend interaction force constants have units of mdyne Å^{-1} rad^{-2}.

Table 3

Potential energy distributions and wavenumbers for $Ni(CO)_3SbCl_3$

ν	$\tilde{\nu}$ (cm^{-1}) Obs	Calc	Symmetry class	k_r	k_R	k_d	k_D	k_θ	k_α	k_β	k_γ	k_ϕ
ν_1	2075	2075	A_1	0	0	4.0	95.1	0	0	0	0	0
ν_2	477	477		3.3	15.9	15.4	0.1	0.3	0.2	17.6	4.2	32.0
ν_3	424	424		0.5	0	52.9	1.8	0	0	2.8	0.7	12.9
ν_4	376	376		76.8	0.7	0.5	0	1.1	0.8	2.9	0.7	8.4
ν_5	232	232		4.3	42.8	2.9	0	5.5	3.9	0.9	0.2	60.5
ν_6	171	171		0.9	2.2	0	0	37.7	27.2	1.9	0.5	10.0
ν_7	(53)	48		0	164.9	17.8	0.2	0.5	0.4	181.7	43.6	7.8
ν_8	–	342	A_2	0	0	0	0	0	0	0	0	114.9
ν_9	–	83		0	0	0	0	0	0	0	0	16.9
ν_{10}	1992	1992	E	0	0	4.2	103.3	0	0	0	0	0
ν_{11}	376	376		4.8	0	0	0.2	0.1	0.6	1.8	11.7	89.2
ν_{12}	409	409		2.2	0	76.5	0.2	0	2.0	16.8	0	25.6
ν_{13}	351	351		38.1	0	20.2	0	0.2	1.1	6.7	1.1	54.8
ν_{14}	156	156		4.1	0	1.0	0.1	8.4	34.6	18.6	1.2	17.9
ν_{15}	74	85		0.2	0	6.5	0.1	0.1	33.2	14.4	17.8	17.7
ν_{16}	(119)	126		0.2	0	0	0	83.2	15.5	1.5	0.7	2.0
ν_{17}	(269)	358		59.4	0	32.4	0	0.5	0.1	3.1	3.3	24.5
ν_{18}	–	82		0	0	7.8	0.1	0.4	4.9	34.4	26.9	31.9
Force constants [a]				2.09	1.51	2.01	16.57	0.18	0.14	0.19	0.06	0.12

[a] Bond stretching and stretch–stretch interaction force constants have units of mdyne Å^{-1}; stretch–bend interaction force constants have units of mdyne Å^{-1} rad^{-1}, bend–bend interaction force constants have units of mdyne Å^{-1} rad^{-2}.

Force constants

k_r	k_{rr}	k_{dd}	k_{dD}	$k_{\theta\theta}$	$k_{\gamma\gamma}$	$k_{d\gamma}$	k_{DD}	$k_{R\beta}$	$k_{R\gamma}$	$k_{d\beta}$	$k_{\phi\phi}$
0	0	1.4	−4.3	0	0	0	3.8	0	0	0	0
0	0.6	5.6	0.3	0.2	−0.4	−16.2	0	−2.6	28.6	2.5	−7.7
0	0.1	19.4	2.2	0	−0.1	12.0	0.1	0	−0.3	−1.9	−3.1
0	12.6	0.2	0	0.5	−0.1	−1.2	0	0.2	−2.5	0.2	−2.0
0	0.7	1.1	0.1	2.7	0	−1.6	0	1.0	−10.6	0.2	−14.6
0	0.1	0	0	18.6	0	0.1	0	−0.3	3.5	0	−2.4
0	0	6.5	−0.4	0.3	−3.9	−56.1	0	26.6	−296.7	8.7	−1.9
12.8	0	0	0	0	0	0	0	0	0	0	−27.7
87.2	0	0	0	0	0	0	0	0	0	0	−4.1
0	0	−0.8	−4.6	0	0	0	−2.1	0	0	0	0
12.7	−0.4	0	0	0	0.5	0.2	0	0	0	0	−21.5
1.2	−0.2	−14.0	0.8	0	0	0.6	0	0	0	−5.5	−6.2
0.6	−3.1	−3.7	0.1	−0.1	0	−4.7	0	0	0	1.8	−13.2
19.0	−0.3	−0.2	0.1	−2.1	0.1	1.1	0	0	0	0.7	−4.3
27.2	0	−1.2	−0.2	0	0.8	−10.9	0	0	0	−1.5	−4.3
17.9	0	0	0	−20.5	0	0.1	0	0	0	0	−0.5
2.1	−4.9	−5.9	0.2	−0.1	0.1	−10.5	0	0	0	1.5	−5.9
13.9	0	−1.4	−0.2	−0.1	1.2	−14.6	0	0	0	2.5	−7.7
0.12	0.17	0.37	0.64	−0.03	−0.01	0.17	0.33	0.02	0.23	0.05	0.03

Table 4

Molecular parameters [20] for $Ni(CO)_4$ and $SbCl_3$

Atomic masses	
Sb = 121.750; Cl = 35.453; Ni = 58.710;	
C = 12.011; O = 15.990.	
Bond lengths and angles	
$r(Sb-Cl)$	2.35 Å
$r(Ni-C)$	1.84 Å
$r(C-O)$	1.15 Å
$\angle ClSbCl$ 99.5, $\angle NiCO$ 180, $\angle CNiC$ 109.5°	

For $Ni(CO)_3SbCl_3$ the following interaction constants were used in several combinations; the final force-field pattern was selected with those interaction constants marked (*) held fixed:

$^*k_{rr}$ SbCl–SbCl stretch–stretch interaction

k_{dd} NiC–NiC stretch–stretch interaction

k_{dD} NiC–CO stretch–stretch interaction

$^*k_{\alpha\alpha}$ $SbCl_2$–$SbCl_2$ angle–angle interaction

$^*k_{\gamma\gamma}$ NiC_2–NiC_2 angle–angle interaction

$k_{d\gamma}$ NiC–NiC_2 stretch–angle interaction

$^*k_{DD}$ CO–CO stretch–stretch interaction

$^*k_{R\beta}$ NiSb–SbNiC stretch–angle interaction

$^*k_{R\gamma}$ SbNi–NiC_2 stretch–angle interaction

$^*k_{d\beta}$ NiC–SbNiC stretch–angle interaction

$^*k_{\phi\phi}$ NiCO–NiCO angle–angle interaction

For the $SbCl_3$ species the k_r (SbCl stretching), k_θ ($SbCl_2$ deformation), k_{rr} (SbCl–SbCl stretch–stretch interaction) and $k_{\theta\theta}$ ($SbCl_2$–$SbCl_2$ angle–angle deformation interaction) force constants were used to fit the four observed vibrational fundamentals. For the $Ni(CO)_4$ species, the four primary force constants k_d (NiC stretching), k_D (CO stretching), k_ϕ (NiCO deformation) and k_γ (NiC_2 deformation) were used with the interaction constants k_{dd} (NiC–NiC stretch–stretch interaction), k_{dD} (NiC–CO stretch–stretch interaction), $k_{\gamma\gamma}$ (NiC_2–NiC_2 angle–angle deformation interaction), $k_{d\gamma}$ (NiC–NiC_2 stretch–angle deformation interaction) and $k_{\gamma\phi}$ (NiC_2–NiCO angle–angle deformation interaction). These force constants were used to fit eight observed vibrational fundamentals for $Ni(CO)_4$, keeping $k_{\gamma\phi}$ fixed at a selected low value. Reasons for this have been described earlier; the inclusion of $k_{\gamma\phi}$ resulted in a more realistic and acceptable force field.

The rms errors in the final best-fit force constant calculations between observed and calculated frequencies were 0.0, 0.2 and 0.1%, for $SbCl_3$, $Ni(CO)_4$ and $Ni(CO)_3SbCl_3$, respectively.

The potential energy distributions for the best-fit situations in $SbCl_3$, $Ni(CO)_4$ and $Ni(CO)_3SbCl_3$ are given in Tables 1–3, respectively. The observed and calcu-

Table 5

Observed [12] and calculated wavenumbers and proposed new vibrational assignments for $Ni(CO)_3SbCl_3$

ν	Symmetry class	Approximate description of mode	Calculated $\tilde{\nu}$ (cm^{-1})
ν_1	A_1	CO symmetric stretch	2075
ν_2		NiCO symmetric deformation	477
ν_3		NiC symmetric stretch	424
ν_4		SbCl symmetric stretch	376
ν_5		NiSb stretch	232
ν_6		$SbCl_3$ symmetric deformation	171
ν_7		NiC_3 symmetric deformation	48
ν_8	A_2	NiCO rock	342
ν_9		NiCO torsion	83
ν_{10}	E	CO asymmetric stretch	1992
ν_{11}		NiCO asymmetric deformation	376
ν_{12}		NiC asymmetric stretch	409
ν_{13}		SbCl asymmetric stretch	351
ν_{14}		$SbCl_3$ asymmetric deformation	156
ν_{15}		NiC_3 asymmetric deformation	85
ν_{16}		$SbCl_3$ asymmetric deformation	126
ν_{17}		NiCO rock	358
ν_{18}		NiC_3 rock	82

lated wavenumbers are shown in these Tables, and the proposed re-assignment of $Ni(CO)_3SbCl_3$ is given in Table 5.

Discussion of results

The refined calculations fitted the observed vibrational spectroscopic data satisfactorily for $SbCl_3$, $Ni(CO)_4$ and $Ni(CO)_3SbCl_3$. The results for the $SbCl_3$ species agreed very well with the data in the literature [13,14]. However, the situation regarding $Ni(CO)_4$ is far from certain because the force constant calculations of Jones [15,23] involved a re-assignment of the ν_9 vibration to 300 cm^{-1} from observed overtones and combination bands. Interaction constants were also chosen which were large in value, one of which matched that of the primary force constant k_ϕ. The calculations of Pistorius [24] used a different force field and assumed a value of $\nu_9 = 429$ cm^{-1}.

For $Ni(CO)_3SbCl_3$, however, although a good fit to the observed wavenumbers was generally made, the force field indicated that several frequencies had been mis-assigned. Because of the instability of the material in solution, the Raman spectra were assigned [12] without the benefit of polarization data by correlation with $SbCl_3$ and $Ni(CO)_4$. We believe that the original assignments, several of which were tentatively made on reasonable grounds, can now itself be modified in the light of our calculations.

The ν_7 mode, a NiC_3 symmetric deformation, which had originally been assigned to 119 cm^{-1} by comparison with the compound $Ni(CO)_3AsEt_3$ [25] was calculated at 48 cm^{-1}. This implies that the assignment of this mode in the spectrum of the arsenic compound is also open to question. The vibrationally inactive modes of A_2 species, ν_8 and ν_9, are calculated at 342 and 83 cm^{-1}, respectively.

Another revision of the assignment seems to be necessary for ν_{11} and ν_{12}, a NiCO asymmetric deformation and NiC asymmetric stretch, respectively, which had again been assigned on the basis of the arsenic compound. Our calculations indicate unambiguously that the assignments for ν_{11} and ν_{12} should be reversed, with ν_{11} at 376 cm^{-1} and ν_{12} at 409 cm^{-1}. Attempts to constrain the force field calculations to the observed assignment resulted in an ill-refinement of the fitting.

For the ν_{15} band, the observed and calculated frequencies do not agree very well; however, there could well be large errors in band measurements in this region of the spectrum. The E species SbCl$_3$ rocking mode, ν_{16}, was not observed in the spectrum but we predict it to be at 126 cm^{-1}; we suggest that the observed band at 119 cm^{-1} and erroneously assigned to ν_7 could well be ν_{16}. The NiCO rocking mode, ν_{17}, is predicted to lie at 358 cm^{-1} and would thus be masked by the stronger ν_{13}, SbCl asymmetric stretching mode at 351 cm^{-1}. Likewise, the ν_{18}, NiC$_3$ rocking, calculated at 82 cm^{-1} must be near-coincident with the NiC$_3$ asymmetric deformation ν_{15}, at 85 cm^{-1}. The band originally assigned to ν_{18} at 53 cm^{-1} would be better assigned to ν_7, calculated at 48 cm^{-1}. An important feature of the calculations is the unambiguous assignment of the Ni–Sb stretching frequency to the band at 232 cm^{-1}.

From our calculations the k_R (NiSb stretching) force constant has been evaluated for the first time, 1.51 mdyne Å^{-1}. It is difficult to compare the k_R (NiSb stretching) force constant directly with the k(NiP) or k(NiAs) in the monosubstituted species Ni(CO)$_3$PCl$_3$ or Ni(CO)$_3$AsCl$_3$ since complete vibrational spectroscopic data for these compounds are not available. However, following recent force constant calculations [5,7] of Ni(PX$_3$)$_4$ using similar SVFF force fields with interaction constants, it is possible to compare the k(NiSb stretching) force constant obtained here (1.51 mdyne Å^{-1}) with k(NiP stretching) in Ni(PCl$_3$)$_4$, viz. 1.67 mdyne Å^{-1}. The lower value of the NiSb stretching force constant may be attributed to the smaller donor–acceptor properties of SbCl$_3$ compared with PCl$_3$ as a ligand. It is also instructive to compare the primary force constants of the SbCl$_3$ and Ni(CO)$_3$ entities in Ni(CO)$_3$SbCl$_3$ and the parent compounds SbCl$_3$ and Ni(CO)$_4$. The k_r (SbCl stretching) force constant is increased by about 16% from the free ligand value on coordination of the SbCl$_3$ to Ni, whereas the deformation force constant k_θ is decreased by about 25% on coordination. This compares with the k(NiP) stretching force constant, which decreased by about 33% on coordination of PCl$_3$ to Ni in Ni(PCl$_3$)$_4$ and the deformation force constant which remains essentially unchanged [7]. The smaller decrease in stretching force constant for the antimony compound could result from the poor electron donation from the Sb–Cl bonds into the Ni–Sb bond compared with the phosphorus case in Ni(PCl$_3$)$_4$. The decrease in deformation force constant for the SbCl$_3$ ligand in the antimony compound probably reflects the lower steric hindrance of the SbCl$_3$ coordinated to nickel in Ni(CO)$_3$SbCl$_3$ compared with four PCl$_3$ ligands coordinated to nickel in Ni(PCl$_3$)$_4$. In all probability, the non-existence of Ni(SbCl$_3$)$_4$ and the instability of the Ni(CO)$_3$SbCl$_3$ species support the above conclusions regarding the SbCl$_3$ ligand donor and acceptor abilities, the steric problems and the lower bond strength of the Ni–Sb bond.

The k(CO) stretching force constant for free CO is 18.55 mdyne Å^{-1} [1]. In the present work, the k_d(CO) stretching force constant is 17.56 mdyne Å^{-1} for Ni(CO)$_4$ and 16.57 mdyne Å^{-1} for Ni(CO)$_3$SbCl$_3$, with the k_D(NiC) stretching force

constants being 2.14 and 2.01 mdyne $\mathring{A}^{-1}$, respectively. This decrease of about 6% is expected if the CO's are involved in donating electronic charge to the formation of the Ni–Sb bond. It is interesting to note that the effect of 6% reduction in bond force constants of the carbonyl groups is much less than that experienced by the $SbCl_3$ group (viz. 16%); it can be inferred from this that the Ni–Sb bond is more dependent on the $SbCl_3$ ligand for its electronic charge than it is upon the $Ni(CO)_3$ species.

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