show that the same number of Raman- and infrared-active internal modes of the chain are expected for both $CsNiCl_3$ and $(CH_3)_4NMnCl_3$. Further, the chain rotatory mode is now inactive. In view of the close correspondence between the Raman spectra of the two compounds we assign the 118-cm^{-1} line to the E_{1g} internal chain mode of the manganese compound.

Assuming that the corresponding bands in $CsNiCl_3$ have the same assignment as for $(CH_3)_4NMnCl_3$ the frequency differences between them are readily explained. The E_{2g} translatory mode falls (88 to 57 cm^{-1}) due to the increased mass of cesium over tetramethylammonium. The A_g mode can be taken as a measure of M–Cl bond strength because the metal atoms do not move in this vibration. The increase from 256 (Mn) to 267 (Ni) cm^{-1} can be attributed to ligand field stabilization energy, which is only operative for the nickel complex.

We conclude that all of the internal modes of the $(MnCl_3^-)_n$ chain have been observed and correctly assigned.

Acknowledgment.—We thank the Science Research Council for generous support.

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Vibrational Spectra of Lithium Tetramethylaluminate and Lithium Tetramethylzincate

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Received August 6, 1970

Infrared and Raman spectra of lithium tetramethylzincate, $Li_2Zn(CH_3)_4$, and lithium tetramethylaluminate, $LiAl(CH_3)_4$, and their isotopic analogs as solids have been measured and assigned. In both complexes, Li–C stretching modes have been observed at around 300 cm^{-1} in the ir spectra. The local symmetries of $Zn(CH_3)_4{}^{2-}$ and $Al(CH_3)_4{}^-$ ions are T_d and V_d (D_{2d}), respectively, $LiAl(CH_3)_4$ seems to form a linear chain analogous to $LiAl(C_2H_5)_4$.

Introduction

There are several reports concerned with X-ray diffraction studies of -ate complexes.[1-5] These studies have suggested that the cation–anion interaction is largely ionic. Mach[6] has reported the infrared spectra of several aluminum anions and has concluded that $LiAl(CH_3)_4$ and $NaAl(CH_3)_4$ have C_{2v} symmetry in the solid state.

This paper presents the complete infrared and Raman spectra of $LiAl(CH_3)_4$ and $Li_2Zn(CH_3)_4$. These spectra indicate T_d symmetry around both Zn and Li in $Li_2Zn(CH_3)_4$; $LiAl(CH_3)_4$ showed V_d symmetry around both Al and Li.

Results and Discussion

Lithium Tetramethylaluminate.—The ir and Raman frequencies of $^7LiAl(CH_3)_4$, $^6LiAl(CH_3)_4$, and $^6LiAl(CD_3)_4$ are given in Table I. Spectra in the pertinent region are shown in Figures 1–3.

In the C–H stretching region, four ir bands arise all of which are Raman active. Three of these are assigned to C–H stretching modes. The band at 2810 cm^{-1} (unless otherwise noted, the frequencies refer to those for $^7LiAl(CH_3)_4$) is assigned to $\nu_s(CH_3)$. The two other bands arise from the splitting of the degenerate $\nu_{as}(CH_3)$. These C–H stretching frequencies are low and comparable to those of methyl groups bonded to electropositive metals such as Li and K and suggest carbanionic character of the methyl groups in $LiAl(CH_3)_4$.[7,8] The fourth band (2894 cm^{-1}) is assigned as an overtone of the absorption at 1445 cm^{-1} in the Raman. In the ir spectrum a weak band was observed at 2166 cm^{-1}. This ir band is absent in the deuterated compound and is absent in the Raman spectrum and is probably due to an impurity.

In the C–H deformation region three ir bands arise; these are also Raman active. The ir band at 1100 cm^{-1} is split, as observed by Mach.[6] This band may be assigned to $\delta_{as}(CH_3)$.

In the region 500–800 cm^{-1}, four ir bands are observed. The two at 632 and 567 cm^{-1} are also Raman active and shift to 619 and 526 cm^{-1}, respectively, on substitution of protium with deuterium. The isotopic frequency ratios, ν_H/ν_D, of these bands are 1.02 and 1.08, respectively; these are comparable to 1.06 calculated for Al–CH$_3$, using a diatomic harmonic oscillator approximation, considering CH$_3$ as an atom. These are assigned to the Al–C stretching modes in accord with Mach.[6] The band at 526 cm^{-1} in the ir spectrum of $^6LiAl(CD_3)_4$ shows a splitting in the Raman spectrum (498 and 518 cm^{-1}) possibly due to a crystal field effect. In the Raman spectrum an intense line appears at 493 cm^{-1} which shifts to 441 cm^{-1} ($\nu_H/\nu_D = 1.12$) in $LiAl(CD_3)_4$ and may be assigned to an Al–C stretching mode.

Mach suggested C_{2v} symmetry for $LiAl(CH_3)_4$,[6] *i.e.*

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TABLE I

INFRARED (4000–100 CM^{-1}) AND RAMAN FREQUENCIES OF LITHIUM TETRAMETHYLALUMINATE AND THE ASSIGNMENTS[a]

$^7LiAl(CH_3)_4$		$^6LiAl(CH_3)_4$		$^6LiAl(CD_3)_4$		
Ir	Raman	Ir	Raman	Ir	Raman	Assignment
	108 m		108 m		91 m	$\delta(Al–C_4)$
	140 vw		140 vw		121 vw	?
	185 s		186 s		157 s	$\delta(Al–C_4)$
214 w	215 m	214 w	216 m	184 w	186 m	$\delta(Al–C_4)$
251 w	272 m	252 w	271 m	222 vw	233 m	$\delta(Al–C_4)$
					291 vw	?
284 vs		295 vs		288 vs		$\nu(Li–C_4)$
320 vs		348 vs		344 vs		$\nu(Li–C_4)$
	493 vs		494 vs		441 vs	$\nu(Al–C_4)$ (A_1)
				470 w		?
567 vs	571 s	567 vs	570 s	526 s	498 w	$\nu(Al–C_4)$ (E)
					518 w, b	
632 vs	646 m	632 vs	646 m			$\nu(Al–C_4)$ (B_1)
739 vs	735 m	739 vs	736 m	619 vs, b	612 s	$\rho(CH_3)$
766 s, sh	766 w, sh	766 s, sh	766 w, sh			$\rho(CH_3)$
1100 vs	1100 w, sh	1100 vs	1100 w, sh	869 vs	872 w, sh	$\delta(CH_3)$
1111 m, sh	1109 s	1111 m, sh	1109 s	875 sh	875 s	
1204 s	1202 m	1204 s	1202 m	933 vs	929 s	$\delta(CH_3)$
1450 vw	1445 w	1450 vw	1445 w	1045 m	1049 vw	$\delta(CH_3)$
2166 w		2166 w				Impurity
2810 s	2812 s	2810 s	2812 s	2052 s	2054 s	$\nu(CH_3)$
2863 w, sh	2863 s	2863 w, sh	2863 s	2193 m, sh	2194 m	$\nu(CH_3)$
2897 vw, sh	2894 vw, sh	2897 vw, sh	2893 vw, sh	2090 w	2088 m, b	2 × 1445
2911 vs	2911 s	2911 vs	2911 s	2168 vs	2169 vs	$\nu(CH_3)$

[a] Abbreviations: v, very; s, strong; w, weak; sh, shoulder; m, medium.

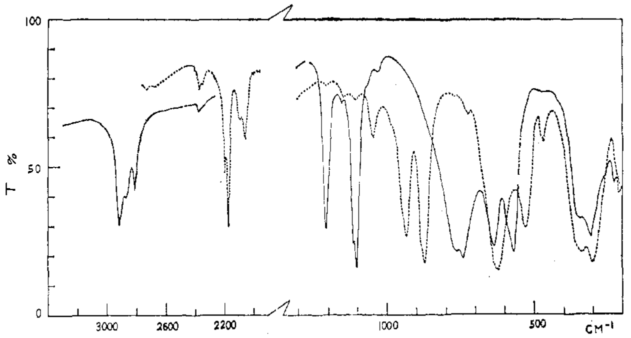


Figure 1.—Infrared spectra of $^7LiAl(CH_3)_4$ (——) and $^6LiAl(CD_3)_4$ (· · ·).

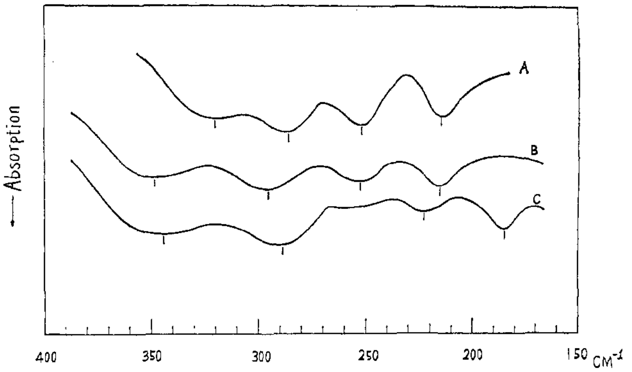


Figure 2.—Far-infrared spectra of $^7LiAl(CH_3)_4$ (A), $^6LiAl(CH_3)_4$ (B), and $^6LiAl(CD_3)_4$ (C).

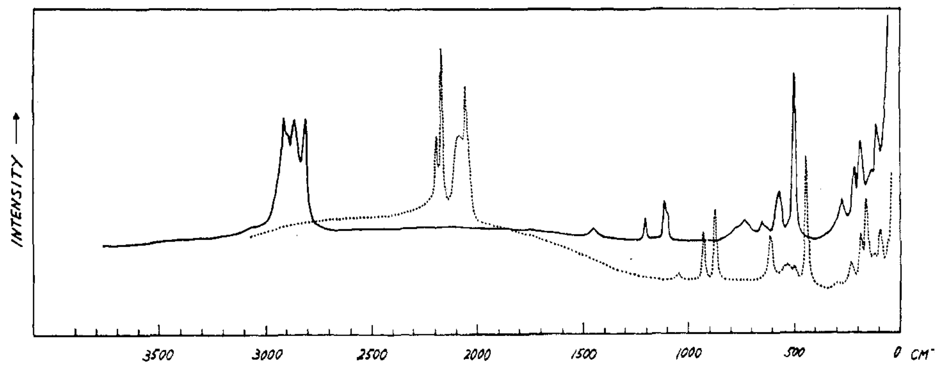
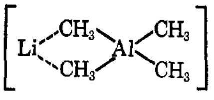


Figure 3.—Laser Raman spectra of $^6LiAl(CH_3)_4$ (——) and $^6LiAl(CD_3)_4$ (· · ·). The spectrum of $^7LiAl(CH_3)_4$ is identical with that of $^6LiAl(CH_3)_4$.



C_{2v} symmetry predicts four stretching modes of species A_1, A_2, B_1, and B_2 (for selection rules see Table II) all of which should be active in both the ir and Raman spectra. Mach argued that the two Al–C stretching bands in the ir spectra are due to the overlap of two modes of species A_1 and A_2 with those of species B_1 and B_2 and concluded C_{2v} symmetry for the anion. If this is so, one expects only two lines in the Raman spectrum coinciding with the ir bands. The observation of a Raman line at 493 cm^{-1} which is absent in the ir spectrum does not support Mach's argument. The present data can be satisfactorily accounted for by assuming that $LiAl(CH_3)_4$ forms a linear chain analogous to

TABLE II

SELECTION RULES[a] FOR M SKELETAL VIBRATIONS OF $M(CH_3)_4$

Point group	Str modes	Bending modes
T_d	$A_1(R) + T_2(I, R)$	$E(R) + T_2(I, R)$
$V_d\ (=D_{2d})$	$A_1(R) + B_2(I, R) + E(I, R)$	$A_1(R) + B_1(R) + B_2(I, R) + E(I, R)$
C_{3v}	$2A_1(I, R) + E(I, R)$	$A_1(I, R) + 2E(I, R)$
C_{2v}	$2A_1(I, R) + B_1(I, R) + B_2(I, R)$	$2A_1(I, R) + A_2(R) + B_1(I, R) + B_2(I, R)$

[a] I, ir active; R, Raman active.

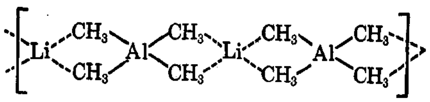
TABLE III

FREQUENCIES AND ASSIGNMENTS OF THE INFRARED (4000–100 CM^{-1}) AND RAMAN SPECTRA OF LITHIUM TETRAMETHYLZINCATE[a]

$^7Li_2Zn(CH_3)_4$		$^6Li_2Zn(CH_3)_4$		$^7Li_2Zn(CD_3)_4$		
Ir	Raman	Ir	Raman	Ir	Raman	Assignment
	204 vs		204 vs		173 s	$\delta(Zn–C_4)$
	300 vw		300 vw		260 vw	$\delta(Zn–C_4)$
302 vs, b		321 vs, b		289 vs, b		$\nu(Li–C_4)$
	416 vs		416 vs		381 s	$\nu_s(Zn–C_4)$
				416 m, sh		$\rho(CH_3)$
569 vs		569 vs		459 s, b		
				520 m		$\nu_{as}(Zn–C_4)$
	599 w		599 w			Impurity
				829 w		?
1063		1063		1011		Dec
1185 w	1185 w	1185 w	1185 w	908 s	910 m	$\delta_s(CH_3)$
1201 w	1201 w	1201 w	1201 w	1139		Dec
1477 w	1468 w	1477 w	1467 w	1072 m	1067 w	$\delta_{as}(CH_3)$
2807 vs	2805 vs	2807 vs	2804 vs	2055 s	2052 vs	$\nu_s(CH_3)$
2869 s	2870 s	2869 s	2870 s	2160 s	2161	
2907 m	2907 m	2907 m	2907 m	2124 w	2120 m	$\nu_{as}(CH_3)$

[a] Abbreviations: v, very; s, strong; w, weak; sh, shoulder; m, medium.

$LiAl(C_2H_5)_4$, *i.e.*



In this structure, the local symmetry of $Al(CH_3)_4^-$ is V_d. For this model one predicts three Al–C stretching modes of species A_1, B_2, and E in the Raman spectrum, two of these should also be ir active (B_2 and E). The spectrum is consistent with this prediction.

The two ir absorptions at 766 and 739 cm^{-1} shift and overlap at 619 cm^{-1} on substitution of H with D. The isotropic frequency ratios of these bands, 1.24 and 1.19, are significantly lower than those (ν_H/ν_D = 1.31–1.37) for the C–H vibrations in methyl chloride[9] but are assigned to methyl rocking modes, $\rho_r(CH_3)$, in accord with Mach.[6] The weak band at 470 cm^{-1} in the ir spectrum of $^6LiAl(CH_3)_4$ which is absent in the Raman spectrum cannot be explained satisfactorily and may be due to some impurity.

In the far-infrared spectrum four bands are observed between 400 and 100 cm^{-1}. V_d symmetry predicts two Li–C stretching modes and two Al–C bending modes in this region. The absorptions at 320 and 248 cm^{-1} in the spectrum of $^7LiAl(CH_3)_4$ move to 348 and 295 cm^{-1}, respectively, in $^6LiAl(CH_3)_4$. For $^6LiAl(CD_3)_4$ detectable shifts are also observed, to 344 and 288 cm^{-1}, respectively. These must involve the motion of Li and a methyl group and may be assigned as the two Li–CH_3 stretching modes.[10] The bands at 251 and 214 cm^{-1} show no lithium isotope effect but do shift on substitution of D for H. These are assigned to the two predicted Al–C bending modes.

The Raman spectrum in this region should contain three Li–C stretching frequencies and four Al–C bending modes. The Li–C modes are not observed, consistent with a substantially ionic Li–C bond.[11] Four Raman absorptions at 272, 215, 185, and 108 cm^{-1} are observed. These are all affected by deuterium substitution and are assigned to the predicted Al–C bending modes.

Lithium Tetramethylzincate.—The observed frequencies of $^7Li_2Zn(CH_3)_4$, $^6Li_2Zn(CH_3)_4$, and $^7Li_2Zn(CD_3)_4$ are given in Table III. Infrared and Raman spectra are shown in Figures 4–6. In the C–H stretching region, there are three ir bands which are also Raman active. The ir band at 2807 cm^{-1} (unless otherwise noted, the frequencies refer to those for $^7Li_2Zn(CH_3)_4$) is assigned to the C–H symmetric stretching mode. The two bands at 2869 and 2907

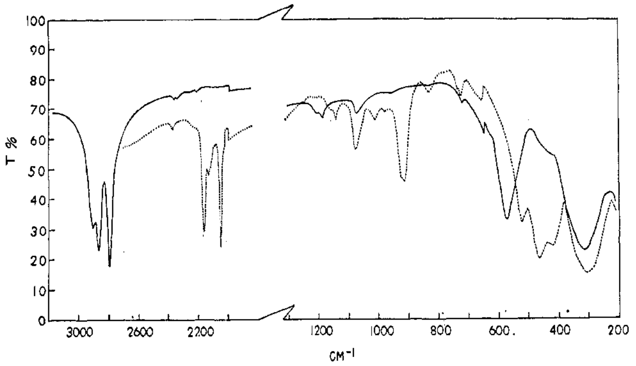


Figure 4.—Infrared spectra of $^7Li_2Zn(CH_3)_4$ (——) and $^7Li_2Zn(CD_3)_4$ (· · ·).

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(9) G. Herzberg, "Infrared and Raman Spectra of Polyatomic Molecules," Van Nostrand, New York, N. Y., 1945, p 315.

(10) The diatomic harmonic oscillator approximation, considering CH_3 as an atom, for a Li–CH_3 vibration predicts a shift of about 18 cm^{-1} for an absorption around 300 cm^{-1} upon substitution of ^6Li and ^7Li.

(11) J. H. B. George, J. A. Rolfe, and L. A. Woodward, *Trans. Faraday Soc.*, **49**, 375 (1953).

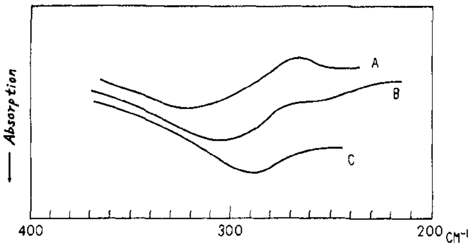

Figure 5.—Far-infrared spectra of $^6Li_2Zn(CH_3)_4$ (A), $^7Li_2Zn(CH_3)_4$ (B), and $^7Li_2Zn(CD_3)_4$ (C).

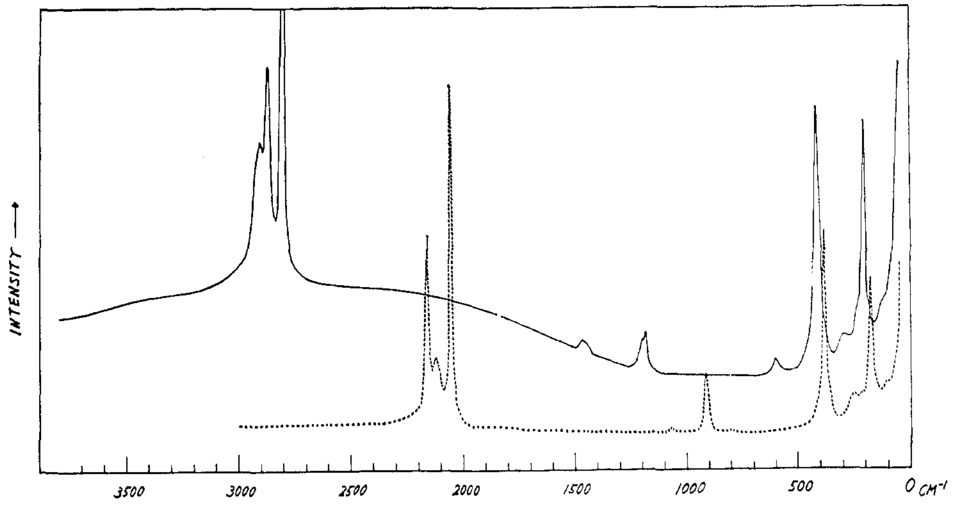

Figure 6.—Laser Raman spectra of $^7Li_2Zn(CH_3)_4$ (——) and $^7Li_2Zn(CD_3)_4$ (···). The spectrum of $^6Li_2Zn(CH_3)_4$ is identical with that of $^7Li_2Zn(CH_3)_4$.

cm^{-1} may be due to the splitting of the antisymmetric C–H stretching mode.

A very weak ir band appearing at 1477 cm^{-1} may be assigned to the antisymmetric methyl deformation mode. The symmetric deformation of the CH_3 group occurs at 1185 cm^{-1}. The two ir bands at 1201 and 1063 cm^{-1} vary in their intensities from sample to sample, and the intensities increase upon exposure of the sample to the air. These two bands are probably due to decomposition of the sample by oxidation or hydrolysis. These decomposition bands occur at 1139 and 1011 cm^{-1} in the ir spectrum of the deuterated compound and are probably due to CH_3–O vibrations.

In the region of 500–700 cm^{-1}, one expects ir absorptions due to CH_3 rocking and C–Zn stretching modes.[12–14] Only one absorption is observed, at 569 cm^{-1}. This band is actually an overlap of three bands as can be seen from the ir spectrum of $^7Li_2Zn(CD_3)_4$ which shows three bands at 520, 459, and 416 cm^{-1}. The 520-cm^{-1} band shows a small isotopic frequency ratio, $\nu_H/\nu_D = 1.08$, and is assigned to the C–Zn stretching mode. The two other bands having $\nu_H/\nu_D =$ 1.26 and 1.37 are assigned to the methyl rocking modes. The observation of only one Zn–C mode in the infrared spectrum seems to point toward T_d symmetry and the assignments have been made on this basis. The X-ray study showing approximately equivalent Zn–C bond lengths shows two C–Zn–C bond angles; nonetheless, tetrahedral symmetry seems best to describe the spectral results. Unexpectedly, the C–Zn stretching mode (T_2) and methyl rocking modes are absent in the Raman spectrum. The Raman line at 599 cm^{-1} shows no corresponding line in the Raman spectrum of the deuterated compound and is possibly due to some impurity. The intense Raman line at 416 cm^{-1} may be assigned to the symmetric C–Zn stretching mode of the species A_1 in accord with a T_d symmetry of $Zn(CH_3)_4{}^{2-}$.

Only one band is observed in the far-infrared spectrum (400–100 cm^{-1}). This band occurs at 302 cm^{-1} in $^7Li_2Zn(CH_3)_4$ moving to 321 cm^{-1} in $^6Li_2Zn(CH_3)_4$ and 289 cm^{-1} in $^7Li_2Zn(CD_3)_4$. These large isotope effects indicate the involvement of Li and CH_3 in the vibration and lead to the assignment as the Li–CH_3 stretching mode. The observation of only one infrared line suggests T_d symmetry around Li, since this predicts one ir and two Raman lines. The Raman lines are not observed, indicating a substantially ionic Li–C bond. Two low-frequency Raman lines are observed at 300 and 204 cm^{-1}. These show only a deuterium isotope effect and may be assigned as the two predicted Zn–C bending modes. The infrared-active bending mode is not seen.

Both compounds show Li–C stretching modes in the infrared spectra only. The average of the two Li–C modes in $LiAl(CH_3)_4$ is exactly the frequency observed in $Li_2Zn(CH_3)_4$. The C–H stretching frequencies are also fairly similar and are low. The proton chemical shifts in ether are also similar (both 1.1 ppm above TMS) and $J_{^{13}C-^{1}H}$ seems to be relatively low (we observe 109 cps in $Li_2Zn(CH_3)_4$). All these observations indicate that the methyl groups are similarly carbanionic and support a largely ionic Li–C bond.

The agreement between the observed structure for $LiAl(C_2H_5)_4$ and these results for $LiAl(CH_3)_4$ is very good; for $Li_2Zn(CH_3)_4$ the agreement is not so good as these results fail to show the deviation from T_d symmetry as was observed crystallographically.[2]

Experimental Section

All preparations of air-sensitive compounds were performed by high-vacuum techniques. The handling of the products was carried out in a nitrogen-filled drybox where the atmosphere was equilibrated with an Na–K alloy. Analyses were performed by Schwarzkopf Microanalytical Laboratories, Woodside, N. Y. ($Li_2Zn(CH_3)_4$), and Alfred Bernhardt Microanalytisches Labora-

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[12] H. S. Gutowsky, *J. Chem. Phys.*, **17**, 128 (1949).

[13] G. E. Goates and D. Ridley, *J. Chem. Soc.*, 1870 (1965).

[14] D. E. Evans and I. Wharf, *ibid.*, *A*, 783 (1968).

torium, 5251 Elbach über Engelskirchen, West Germany (LiAl(CH_3)$_4$).

Reagents.—The ^{7}Li (1% Na) and ^{6}Li were obtained from Lithium Corp. of America and Oak Ridge National Laboratory, respectively. CH_3I and CD_3I (99.5% D) were obtained from Aldrich Chemical Co. and Stohler Isotope Chemicals, respectively. Al(CH_3)$_3$ was purchased from the Ethyl Corp. Diethyl ether and cyclopentane were dried by refluxing over the Na–K alloy and were stored on a vacuum line. Hg(CH_3)$_2$ and Hg(CD_3)$_2$ were synthesized by the method of Gilman and Brown.[15] Zn(CH_3)$_2$ and Zn(CD_3)$_2$ were prepared by the reaction of Hg(CH_3)$_2$ or Hg(CD_3)$_2$ with Zn powder (Matheson Coleman and Bell) at 90° in the presence of a catalytic amount of $HgCl_2$. Al(CD_3)$_3$ was synthesized by refluxing Hg(CD_3)$_2$ with Al dust (Baker and Adamson) at 90°.[9] CH_3Li and CD_3Li were synthesized by the reaction of ^{6}Li or ^{7}Li (washed in cyclohexane, fivefold excess) with Hg(CH_3)$_2$ or Hg(CD_3)$_2$ in ether. The ether solutions of methyllithium (*ca.* 0.5 *M*) were filtered and used directly.

Preparation of Lithium Tetramethylzincate.—The ^{6}Li$_2$Zn(CH_3)$_4$, ^{7}Li$_2$Zn(CH_3)$_4$, and ^{7}Li$_2$Zn(CD_3)$_4$ were synthesized by adding Zn(CH_3)$_2$ or Zn(CD_3)$_2$ (*ca.* 20% excess) to the ether solution of ^{6}LiCH_3 or ^{7}LiCD_3.[2,10] The solution was allowed to stand at room temperature overnight. The excess dimethylzinc and ether were removed under vacuum and the residue was evacuated at 50° for 2 hr under high vacuum.[2] *Anal.* Calcd for ^{6}Li$_2$ZnC_4H_{12}: C, 34.94; H, 8.80; Zn, 47.54. Found: C, 34.94; H, 8.66; Zn, 47.76.

Preparation of Lithium Tetramethylaluminate.—The ^{7}LiAl(CH_3)$_4$, ^{6}LiAl(CH_3)$_4$, and ^{6}LiAl(CD_3)$_4$ were synthesized by the reaction of Al(CH_3)$_3$ or Al(CD_3)$_3$ (*ca.* 50% excess) with ^{6}LiCH_3, ^{7}LiCH_3, or ^{6}LiCD_3 in ether.[16] The mixture was allowed to stand at room temperature for 5 hr. The ether and excess trimethylaluminum were removed and the residue was evacuated at 80–90° for 5 hr under high vacuum, mp 273° dec (lit.[11] mp 260° dec). *Anal.* Calcd for ^{7}LiAlC_4H_{12}: C, 51.10; H, 12.87; Al, 28.69. Found: C, 50.46; H, 12.52; Al, 27.29.

Infrared Spectra.—Infrared spectra in the range 4000–100 cm^{-1} were measured on a Beckman IR-12 (4000–200 cm^{-1}) and a Hitachi Perkin-Elmer FIS-3 (400–33 cm^{-1}) spectrophotometer. The IR-12 was calibrated with polystyrene; the FIS-3, with Teflon. The frequencies below 400 cm^{-1} reported in this study are those recorded on the far-infrared spectrophotometer. The Nujol technique with CsI plates (4000–200 cm^{-1}) or polyethylene plates (400–100 cm^{-1}) was employed for all compounds. In addition, the $Li_2Zn(CH_3)_4$ and $LiAl(CH_3)_4$ samples were studied as mulls in perfluorokerosene in the region 1300–4000 cm^{-1} to eliminate complications for C–H bands in the mulling agent.

The ir samples were prepared and loaded into cells in a drybox. In spite of these precautions some bands observed in the range 1000–1200 cm^{-1} varied in relative intensity in successive runs. These were most prominent for $Li_2Zn(CH_3)_4$ and are probably from hydrolysis or oxidation occurring during sample preparation or spectral determination. To minimize this difficulty, spectra were run several times on different preparations. Additionally, the samples were exposed to the air for 2–4 sec and the spectra were recorded again to observe the behavior of each band.[6] The bands associated with decomposition became very intense but the bands not due to decomposition became weaker and broader. Compared to lithium tetramethylzincate, lithium tetramethylaluminate was more stable to the air. The far-infrared spectra were all measured under vacuum.

To determine the frequencies, the infrared spectra were run on an expanded frequency scale with a scanning speed of 2–3 cm^{-1}/min. Reproducibility of the spectra was checked by multiple scans over the desired frequency range. The average error in frequency reading was ±0.5 cm^{-1}.

Raman Spectra.—Raman spectra of solid samples were measured on a Spex Ramalog Model 1401 with a Coherent Radiation Model 54 argon ion laser source. The spectrometer was calibrated with CCl_4.

The capillary tube for the Raman measurement was evacuated, placed in a drybox, and filled with a suitable amount of the sample (fine powder). The open end of the tube was closed with grease. The tube was removed from the drybox and immediately sealed with a small flame.

To determine the frequencies, the Raman spectra were run on an expanded frequency scale with a scanning speed of 10–20 cm^{-1}/min. The average error in frequency reading was ±1 cm^{-1}.

Nmr Spectra.—Nmr spectra were obtained on a Varian A-60-A spectrometer.

Acknowledgment.—The partial support of the Marquette University Committee on Research is gratefully acknowledged.

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[15] H. Gilman and R. E. Brown, *J. Amer. Chem. Soc.*, **52**, 3314 (1930).

[16] D. T. Hurd, *J. Org. Chem.*, **13**, 711 (1948).

CONTRIBUTION FROM THE DEPARTMENT OF CHEMISTRY, UNIVERSITY OF KENTUCKY, LEXINGTON, KENTUCKY,
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THE SHIONOGI RESEARCH LABORATORY, SHIONOGI AND COMPANY, LTD., FUKUSHIMA-KU, OSAKA, JAPAN

Vibrational Spectra of *B*-Trihaloborazines

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Received August 24, 1970

The vibrational spectra of *B*-trihaloborazines, (–BX–NH–)$_3$, with X = Cl or Br, have been examined and an assignment of the fundamentals is proposed. The data are supported by data obtained from isotopically labeled derivatives and a normal-coordinate treatment.

Introduction

Recently[2] the vibrational spectrum of borazine, (–BH–NH–)$_3$, has been reexamined utilizing data from isotopically labeled derivatives. This study resulted in the revision of assignments for some of the fundamental vibrations of borazine. Based on these data, a valence force field has been calculated; the resultant information confirms the suggested reassignments and the calculated force constants agree with recent considerations on the strength of the bonds in the borazine molecule.[3] The potential energy distribution of the isotopically labeled derivatives indicated that the character of several fundamentals is substantially altered by deuteration at either the boron or the nitrogen

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