The bond parameters made available in this study should prove useful in ascertaining the magnitude of steric and electronic effects for new members as well as an aid in calibrating theoretical investigations. Future papers[34] take advantage of this feature.

Acknowledgment. The support of this research by the National Science Foundation (Grant CHE85-04737) is gratefully acknowledged. We also thank the University of Massachusetts Computing Center for generous allocation of computer time.

Registry No. 1, 106568-07-4; **2**, 106568-09-6; [PhMeSiF$_3$][Et$_4$N], 106568-10-9; Ph$_2$(1-Np)SiOMe, 106543-90-2; 1-NpPh$_2$SiH, 100447-84-5; Ph$_2$(1-Np)SiNMe$_2$, 106543-91-3; MePhSiF$_2$, 328-57-4; 1-bromonaphthalene, 90-11-9; dimethoxydiphenylsilane, 6843-66-9; methylphenyldimethoxysilane, 3027-21-2.

Supplementary Material Available: For **1** and **2**, respectively, anisotropic thermal parameters (Tables S1 and S4), fixed hydrogen atom parameters (Tables S2 and S5), additional bond lengths and angles (Tables S3 and S6), and deviations from selected least-squares mean planes (Tables S7 and S8) (13 pages); tables of calculated and observed structure factors (14 pages). Ordering information is given on any current masthead page.

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Synthesis and Characterization of *tert*-Butyl(*tert*-butyltellurio)mercury(II)

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The compound (t-Bu)HgTe(t-Bu) was prepared by the reaction of (t-Bu)HgCl with (t-Bu)TeLi in tetrahydrofuran solution at −5 °C. The yellow crystalline light-sensitive solid is stable in an inert atmosphere but decomposes in solution at 20 °C. It gives a strong $(M + 1)^+$ peak in the methane chemical ionization mass spectrum. ^{1}H, ^{13}C, ^{125}Te, and ^{199}Hg NMR spectra (toluene, −15 °C) show two distinct *tert*-butyl groups, one type on mercury ($\delta_{Hg} = -883$ vs. dimethylmercury) and one type on tellurium ($\delta_{Te} = 339$ vs. dimethyl telluride), with couplings $^1J_{Te-C} = 390$, $^1J_{Hg-C} = 1285$, $^2J_{Hg-C} = 17$, $^3J_{Te-C-C-H} = 20$, and $^3J_{Hg-C-C-H} = 196$ Hz. The far-infrared spectrum is interpreted in terms of Hg–Te stretching at 151 cm^{-1}, C–Hg–Te and C–Te–Hg bending at 239 and 224 cm^{-1}, and Te–C and Hg–C stretching at 491 and 511 (shoulder) cm^{-1}. The ultraviolet spectrum (pentane solution) exhibits bands at 365 (shoulder, log ϵ = 2.6), 295 (shoulder, log ϵ = 3.6), and 227 nm (log ϵ = 4.7). Nuclear magnetic resonance, far-infrared, and ultraviolet spectra are also reported for (t-Bu)$_2$Hg and (n-Bu)$_2$Te.

Introduction

Mercury cadmium telluride is an important semiconductor with applications in infrared detection.[1-3] Photolysis of a mixture of the organometallic compounds RHgTeR and RCdTeR could produce mercury cadmium telluride. As an initial test of this idea, we prepared (t-Bu)HgTe(t-Bu), the first compound of the type RHgTeR, and demonstrated[4] that it produces a film of mercury telluride upon photolysis in the gas phase. We report here the synthesis and characterization of the title compound, *tert*-butyl(*tert*-butyltellurio)mercury(II).

Experimental Section

General Procedures. Unless otherwise noted, all reactions were carried out under Ar atmosphere in a fume hood by using Schlenk techniques.[5] Sample preparation for spectroscopy was done in a Vacuum Atmospheres drybox. Tetrahydrofuran and toluene were distilled from sodium and benzophenone. Pentane was distilled from sodium. Melting points were measured with sealed capillaries and are uncorrected. Infrared spectra were recorded with a Nicolet 60SX Fourier transform infrared spectrophotometer. Solids were examined by diffuse reflectance. Liquid samples for mid-infrared spectra were thin films on CsBr plates. For far-infrared spectra, neat liquids in polyethylene cells with 0.2-mm path length were used. Ultraviolet–visible spectra were measured with a Cary 17D spectrophotometer using Teflon-stoppered cuvettes. To measure the spectrum of (t-Bu)HgTe(t-Bu), the sample compartment was purged with Ar and cooled to 0 °C.

NMR Measurements. Spectra of (t-Bu)HgTe(t-Bu) were recorded on a Nicolet NT-200-WB spectrometer. Saturated samples were prepared with toluene/toluene-d_8 (2:1) in serum-capped 12-mm tubes and run at −15 °C. ^{199}Hg spectra were recorded at 35.84 MHz and referenced to an external solution of HgCl$_2$ (1.0 M in dimethyl sulfoxide), whose chemical shift was taken to be −1501.6 ppm relative to neat dimethylmercury at 0 ppm.[6,7] Positive chemical shifts are downfield of the reference. A 45° pulse and 1.5-s recycle time were employed. ^{125}Te spectra were recorded at 63.20 MHz by using a 45° pulse and 3.6-s recycle time. The reference was 1.0 M TeCl$_4$ in tetrahydrofuran, with a chemical shift taken to be 1725 ppm relative to neat dimethyl telluride at 0 ppm.[7] Chemical shifts in ^{13}C spectra were referenced to the center of the deuteriated methyl carbon atom of toluene at 20.4 ppm (relative to tetramethylsilane at 0 ppm). ^{1}H spectra were referenced to the CHD$_2$ multiplet of deuteriotoluene at 2.09 ppm. Spectra of other compounds in toluene-d_8 were run on an IBM NR-80 spectrometer whose probe temperature was ~39 °C.

***tert*-Butylmercuric Chloride.** To 29 g (107 mmol) of mercuric chloride dissolved in 180 mL of tetrahydrofuran at 0 °C was added 55 mL (88 mmol) of *tert*-butyllithium in pentane (1.6 M from Aldrich), dropwise with stirring over 25 min. After 1 h of additional stirring at 0 °C, the mixture of liquid plus gray solid was treated with 5 mL of water, allowed to settle for 1 h, and decanted in the air through a medium-porosity fritted-glass filter with suction. The filtrate, including solid that precipitated during filtration, was concentrated to dryness under vacuum. The solid residue was fractionated between 300 mL of benzene and 200 mL of water in a separatory funnel. The organic phase was extracted five times with 150-mL portions of water, dried over calcium chloride, filtered, and concentrated to dryness under vacuum. The white residue was crystallized (in the air under dim light) by dissolution in 150 mL of refluxing methanol and slow cooling to −40 °C to give 6.2 g (24%) of white needles. The crude product was crystallized a second time to give material used for further synthesis. An analytical sample was crystallized four times; mp 105.5–108 °C (lit.[8] mp 117–119 °C dec). Anal. Calcd for C$_4$H$_9$HgCl: C, 16.39; H, 3.09; Hg, 68.42; Cl, 12.09. Found: C, 16.42; H, 3.00; Hg, 68.49; Cl, 11.28. The ^{13}C and ^{199}Hg NMR spectra were in good agreement with those in the literature,[9] with the previously unreported coupling, $^3J_{^{199}Hg-^1H} = 256$ Hz.

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(*t*-Bu)TeLi.[10] A solution of this compound was prepared by dropwise addition of 1.6 M *tert*-butyllithium (in pentane) to 0.84 g of Te (6.6 mmol, freshly ground in a glovebox) in 16 mL of tetrahydrofuran with stirring at −5 °C. About 90% of the theoretical amount of *tert*-butyllithium was required to turn the suspension from dark red to light green. No further *tert*-butyllithium was added, as the remaining Te was unreactive. (We believe that the red species formed prior to the end point of the reaction is a polytelluride of the type (t-Bu)Te$_n$Li, where $n \geq 2$.) The mixture was stirred for 10 min at −5 °C, centrifuged in graduated centrifuge tubes, and stored at −20 °C for use within 20 min. The concentration of (t-Bu)TeLi was estimated from the volume of *tert*-butyllithium used and the volume of the final solution.

(*t*-Bu)HgTe(*t*-Bu). The reaction and all handling of the product were carried out in dim light. To 1.07 g of *tert*-butylmercuric chloride (3.65 mmol) in 11 mL of tetrahydrofuran was added 11.8 mL of (t-Bu)TeLi solution (~3.7 mmol) with stirring at −5 °C. After 10 min the green-yellow solution was placed in a CCl_4/dry ice slush bath (−23 °C) and kept at this temperature while being concentrated to dryness under vacuum. The yellow residue was extracted for 3 min with 30 mL of toluene at −5 °C and centrifuged, after which the solid was discarded. The yellow liquid was diluted with 15 mL of pentane and left to crystallize at −78 °C. The resultant yellow solid was washed twice with pentane at −78 °C and dried under a stream of Ar for 7 h in the dark at 20 °C. The mother liquor was concentrated to 5 mL under vacuum at −23 °C, warmed to room temperature for less than 1 min to dissolve the solid, and diluted with 5 mL of pentane, and a second crop of crystals was collected at −78 °C. Combined yield of yellow powder = 1.19 g (74%). Recrystallization from toluene–pentane or from neat pentane gave fine yellow prisms with irreproducible *partial* melting in the 80–90 °C range and gradual darkening above 110 °C. Anal. Calcd for $C_8H_{18}HgTe$: C, 21.72; H, 4.10; Hg, 45.34; Te, 28.84. Found: C, 20.71; H, 3.91; Hg, 44.17, 45.32; Te, 30.00. Ultraviolet spectrum (pentane solution): 365 nm (shoulder, log ϵ = 2.6), 295 nm (shoulder, log ϵ = 3.6), 227 nm (log ϵ = 4.7).

Solid (t-Bu)HgTe(t-Bu) was briefly exposed to air as it was introduced with a direct-insertion probe into the mass spectrometer of a Hewlett-Packard 5985 gas chromatograph/mass spectrometer. Mass spectra were recorded with electron-impact (70 eV) or chemical ionization (173 eV) using methane as the reagent gas. The chemical ionization mass spectrum had a strong isotopic multiplet at 443 mass units, corresponding to $[(t\text{-Bu})HgTe(t\text{-Bu})]H^+$. Other strong multiplets were observed at 387, 370, 315, 244, 203, and 187 mass units. The electron-impact mass spectrum showed almost exclusively t-Bu$^+$, with very weak signals at the positions of Te$^+$ and Hg$^+$.

Di-*tert*-butylmercury. To 15 g (55 mmol) of mercuric chloride dissolved in 185 mL of tetrahydrofuran at 0 °C was added 80 mL (128 mmol) of *tert*-butyllithium in pentane, dropwise with stirring over 15 min. After 1 h of stirring at 0 °C, the mixture was treated with 2 mL of water, filtered through a frit under Ar, and concentrated to dryness under vacuum. The yellow solid was extracted at 20 °C with 100 mL of pentane under Ar, and the extract was centrifuged. The pale yellow supernate deposited white prisms at −78 °C. The product was washed with pentane at −78 °C and dried in a stream of Ar in the dark. The supernate from the crystallization was concentrated to 6 mL and cooled to give a second crop of product. Combined yield = 5.0 g (29%). The volatile white solid was crystallized twice more from pentane; mp 63–64 °C (lit.[11] mp 58–60 °C). Anal. Calcd for $C_8H_{18}Hg$: C, 30.52; H, 5.76; Hg, 63.72. Found: C, 30.41; H, 5.88; Hg, 62.90. Ultraviolet spectrum (pentane solution): 300 nm (shoulder, log ϵ = 2.6), 275 nm (shoulder, log ϵ = 2.9), 245 nm (shoulder, log ϵ = 3.7), 217 nm (log ϵ = 4.4).

Di-*n*-butyl Telluride. This pale yellow liquid was isolated in 48% yield after one spinning band distillation (bp 72–76 °C (~4 Torr)) by using the synthesis described by Balfe et al.[12] All steps were carried out under Ar, and petroleum ether (bp 30–60 °C) was used instead of diethyl ether for extraction. The product was distilled twice more through Vigreux columns and was not decolorized by passage through charcoal or alumina. Anal. Calcd for $C_8H_{18}Te$: C, 39.73; H, 7.50; Te, 52.76. Found: C, 40.14; H, 7.39; Te, 52.48. Ultraviolet spectrum (pentane solution): 356 nm (log ϵ = 2.0), 288 nm (log ϵ = 2.2), 257 nm (shoulder, log ϵ = 2.5), 235 nm (log ϵ = 3.8), 220 nm (shoulder, log ϵ = 3.7).

The red liquid (bp 85–88 °C (~10^{-1} Torr)) remaining after the first distillation of dibutyl telluride is *dibutyl ditelluride* and represents most of the remaining Te in the reaction. The ultraviolet–visible spectrum is very similar to one already published,[13] and the infrared spectrum exhibits one band in the region 100–200 cm^{-1} at 192 cm^{-1}, assigned to ν(Te–Te).

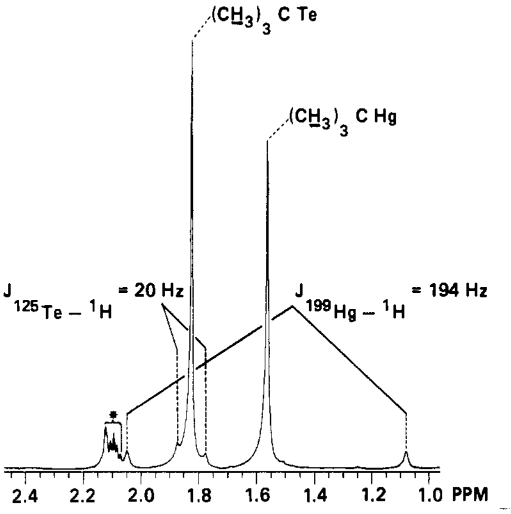

Figure 1. ^{1}H NMR spectrum of (t-Bu)HgTe(t-Bu). Peaks marked by an asterisk are due to the solvent.

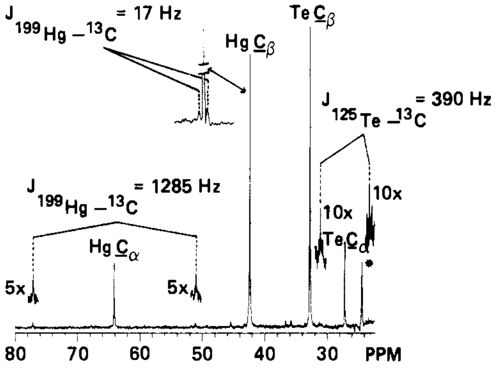

Figure 2. ^{13}C NMR spectrum of (t-Bu)HgTe(t-Bu). ^{199}Hg satellites of HgC$_\beta$ shown in the inset were brought out by Gaussian resolution enhancement. The peak marked by an asterisk is a solvent sideband.

Results and Discussion

Preparation and Properties. (t-Bu)HgTe(t-Bu) was produced by the reaction

$$RHgCl + RTeLi \rightarrow RHgTeR + LiCl \qquad R = t\text{-Bu}$$

The yellow light-sensitive solid is stable for at least 8 h at 20 °C under Ar in the dark. It sublimes at 10^{-4} Torr at 70 °C, and the soluble sublimate gave the same ^{13}C NMR spectrum as unsublimed material. Solutions in toluene or tetrahydrofuran are stable for ~3 days at −78 °C but deposit an unidentified green solid in a period of hours at 0 °C.

NMR Spectra. The spectra in Figures 1 and 2 and chemical shifts reported in Table I are consistent with a structure containing two distinct *tert*-butyl groups, one type on a mercury atom and one type on a tellurium atom. The tertiary carbon atom attached to Te is shifted upfield of the methyl carbons. This Te-induced shift of an α-carbon atom is consistent with that observed for (n-Bu)$_2$Te and (n-Bu)$_2$Te$_2$ in Table I and with the shifts seen in (t-Bu)$_2$Te$_2$ (α-^{13}C at 24 ppm, ^{13}CH$_3$ at 36 ppm).[14] Attachment of the other *tert*-butyl group of (t-Bu)HgTe(t-Bu) to Hg is confirmed by the large (1285 Hz) ^{13}C–^{199}Hg coupling constant, which is in the range observed for alkylmercuric halides.[9] We were unable to observe ^{199}Hg–^{125}Te coupling in either the ^{199}Hg spectrum or the ^{125}Te spectrum. The coupling is either >3800 Hz or buried within the line width of the central peak ($\lesssim$30 Hz).

Far-Infrared Spectra. Table II gives an interpretation of the spectrum of (t-Bu)HgTe(t-Bu) in Figure 3, which is facilitated

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Table I. NMR Shifts and Couplings

spectrum		chem shift, ppm[a]	coupling, Hz
		(*t*-Bu)HgTe(*t*-Bu)	
^{13}C	TeC_α	27.1	$^1J_{TeC} = 390$
	TeC_β	32.7	
	HgC_α	64.0	$^1J_{HgC} = 1285$
	HgC_β	42.4	$^2J_{HgC} = 17$
^1H	$TeC_\beta H$	1.82	$^3J_{TeCCH} = 20$
	$HgC_\beta H$	1.56	$^3J_{HgCCH} = 194$
^{125}Te		338.8[b]	
^{199}Hg		−882.7[c]	$^3J_{HgCCH} = 198$
		(*t*-Bu)$_2$Hg	
^{13}C	C_α	60.5	$^1J_{HgC} = 628$
	C_β	31.2	$^2J_{HgC} = 30$
^1H		1.18	$^3J_{HgCCH} = 103$
^{199}Hg		−838[d]	
		(*t*-Bu)$_2$Te	
^{125}Te		992[e]	
		(*t*-Bu)$_2$Te$_2$	
^{125}Te		499[e]	
		(*n*-Bu)$_2$Te	
^{13}C	C_α	1.8	$^1J_{TeC} = 156$
	C_β	34.7	$^2J_{TeC} = 11$
	C_γ	25.2	$^3J_{TeC} = 11$
	C_δ	13.4	
^1H	H_α	2.51	$^3J_{HH} = 7$
	H_β	~1.6	complex multiplet
	H_γ	~1.3	
	H_δ	0.84	$^3J_{HH} = 7$
^{125}Te		224[f]	$^2J_{TeCH} = 24$ (4 H coupling) $^3J_{TeCCH} = 12$ (4 H coupling)
		(*n*-Bu)$_2$Te$_2$	
^{13}C	C_α	3.9	$^1J_{TeC} = 170$, $^2J_{TeC} = 15$
	C_β	36.1	$^2J_{TeC} = 6$
	C_γ	24.7	$^3J_{TeC} = 6$
	C_δ	13.3	
^1H	H_α	2.94	$^3J_{HH} = 6$
	H_β	~1.6	complex multiplet
	H_γ	~1.2	
	H_δ	0.83	$^3J_{HH} = 7$
^{125}Te		98[g]	$^2J_{TeCH} = 32$ (2 H coupling) $^3J_{TeCCH} = 12$ (2 H coupling)

[a] ^{125}Te and ^{199}Hg chemical shifts are with respect to $(CH_3)_2Te$ and $(CH_3)_2Hg$, as described in the Experimental Section. [b] Line width = 16 Hz. [c] Line width = 26 Hz. [d] Reference 9. [e] Reference 14. [f] Symmetric 13-line multiplet with peaks evenly spaced at 12 Hz. [g] Triplet of triplets.

Table II. Far-Infrared Spectral Assignments (cm^{-1})

(*t*-Bu)HgTe(*t*-Bu)	(*t*-Bu)$_2$Hg	(*n*-Bu)$_2$Te	assignment
511 sh			Hg–C and Te–C str
491	524	505	
385	391	407	alkyl skeletal vib
239	~250	250	C–Hg–X and X–Te–C bending
224			
151			Hg–Te str

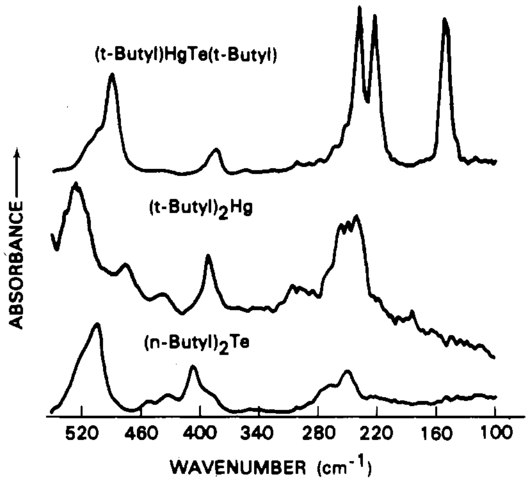

Figure 3. Far-infrared spectra of neat solids and liquids.

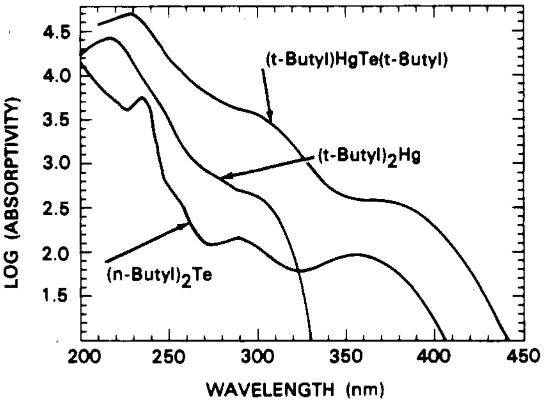

Figure 4. Ultraviolet–visible spectra of pentane solutions. Units of absorptivity are M^{-1} cm^{-1}.

by comparison with the spectra of $(t\text{-}Bu)_2Hg$ and $(n\text{-}Bu)_2Te$. The band at 151 cm^{-1} is assigned to ν(Hg–Te) because it has no corresponding band in the reference compounds, which have no Hg–Te linkage. This value can be compared to ν_s(Hg–Te–Hg) = 156 and ν_{as}(Hg–Te–Hg) = 165 cm^{-1} in $(CH_3Hg)_2Te$[15] and to ν(Hg–Se) = 194 cm^{-1} in $CH_3HgSe(t\text{-}Bu)$.[16] In the compounds $(C_6H_5)_2TeHgX^+X^-$ (X = Cl, Br, I), ν(Hg–Te) is observed in the range 133–118 cm^{-1}.[17] Bands for ν(Hg–C) and ν(Te–C) are assigned near 500 cm^{-1} by analogy to many alkylmercury[18] and alkyltellurium compounds.[19] For example, ν(Hg–C) = 521 cm^{-1} in $CH_3HgSe(t\text{-}Bu)$,[16] and ν_{as}(C–Hg–C) = 542 cm^{-1} in $(CH_3)_2Hg$ and 535 cm^{-1} in $(C_2H_5)_2Hg$.[18] A band at 516 cm^{-1} is assigned to ν(Te–C) in CH_3TeH,[20] while ν_{as}(C–Te–C) is assigned at 507 cm^{-1} in $(CH_3)_2Te_2$[21] and a band is observed at 503 cm^{-1} in $(C_2H_5)_2Te$.[22] The *tert*-butyl group has a skeletal vibration near 415 cm^{-1} in hydrocarbons.[23] While this is not directly transferable to non-hydrocarbons, both of the *tert*-butyl compounds in Figure 3 have bands near this position, which we assign as alkyl group skeletal vibrations. Normal alkanes also have weak absorptions in this region,[24] so we assign the spectrum of $(n\text{-}Bu)_2Te$ in a similar manner. The remaining vibrations near 250 cm^{-1} are logically assigned to carbon–heavy-atom bending vibrations. The two bands in (*t*-Bu)HgTe(*t*-Bu) arise from δ(C–Hg–Te) and δ(Hg–Te–C). These may be compared to δ(Te–Te–C) = 170 cm^{-1} in $(CH_3)_2Te_2$.[21]

Ultraviolet–Visible Spectra. The spectra in Figure 4 were obtained in an attempt to identify absorptions associated with the Hg–Te chromophore. Unfortunately, bands from $(t\text{-}Bu)_2Hg$ and/or $(n\text{-}Bu)_2Te$ are at energies similar to that of each band in (*t*-Bu)HgTe(*t*-Bu), so bands unique to (*t*-Bu)HgTe(*t*-Bu) cannot be distinguished. The pale yellow color of $(n\text{-}Bu)_2Te$ is not due to contamination by $(n\text{-}Bu)_2Te_2$ because the long-wavelength

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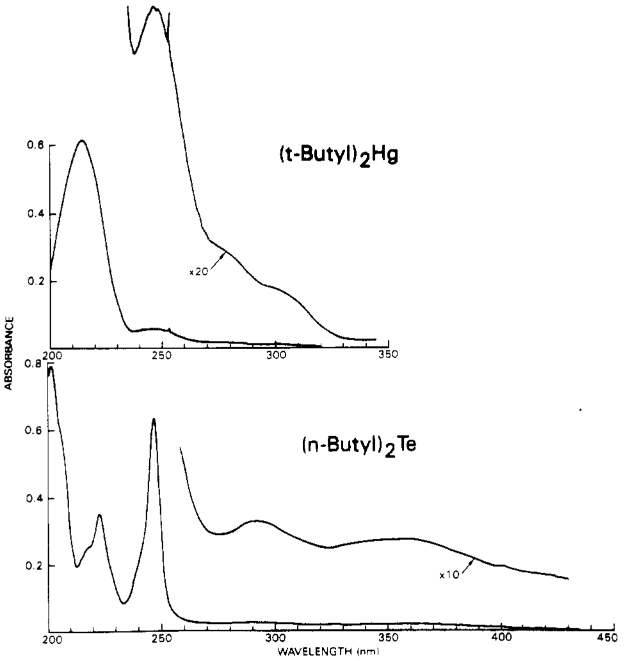

Figure 5. Ultraviolet–visible spectra of gas-phase samples. The atmosphere was saturated at 30 °C. Dibutyl telluride path length = 10 cm. Di-*tert*-butylmercury path length = 0.50 cm.

absorption of $(n\text{-Bu})_2Te_2$ at 395 nm ($\log \epsilon = 2.7$) is missing in the spectrum of $(n\text{-Bu})_2Te$ in Figure 4.

Our spectrum of $(t\text{-Bu})_2Hg$ is consistent with the brief description of the spectrum in the literature,[25] with the lowest energy absorption near 300 nm. In contrast, the published gas-phase spectrum of $(CH_3)_2Hg$ has almost no long-wave absorption[26,27] ($\lambda_{max} \approx 200$ nm, $\epsilon_{193} = 6480$ M^{-1} cm^{-1}, $\epsilon_{248} = 85$ M^{-1} cm^{-1}). To see if this could be an effect of solvent vs. gas phase, the gas-phase spectrum in Figure 5 was recorded. The spectrum of $(t\text{-Bu})_2Hg$ is qualitatively the same in pentane solution as in the gas phase.

In the gas-phase spectrum of $(t\text{-Bu})_2Hg$ in Figure 5, there is a small spike at 254 nm. This absorption is from atomic Hg that is presumably formed by irradiation of the sample in the spectrophotometer. Comparison with the spectrum of pure Hg suggests that the cuvette containing $(t\text{-Bu})_2Hg$ is saturated with Hg vapor.

In contrast to the low-energy bands of dibutyl telluride at 356 and 288 nm in Figure 4, the longest wavelength absorptions of diethyl telluride and dimethyl telluride are reported at 249[28] and 258 nm,[29] respectively. The gas-phase spectrum of dibutyl telluride in Figure 5 does exhibit the long-wavelength bands seen in solution. There is an absorption maximum at 247 nm, with two much weaker bands at 297 and 359 nm. Very careful inspection of Figure 2 of ref 29 shows that these weak bands are present in the spectrum of diethyl telluride as well.

Summary

Multinuclear magnetic resonance spectroscopic results are consistent with the structure $(t\text{-Bu})HgTe(t\text{-Bu})$. The α-carbon atom attached to Te is shifted characteristically upfield, and the α-carbon attached to Hg exhibits a large nuclear coupling constant. The far-infrared spectrum is interpreted in terms of stretching (C–Te, C–Hg, Hg–Te) and bending (C–Hg–Te, Hg–Te–C) vibrations appropriate for this structure. A unique ultraviolet absorption for the Hg–Te moiety could not be assigned because each band in the spectrum of $(t\text{-Bu})HgTe(t\text{-Bu})$ has an approximately corresponding band in $(t\text{-Bu})_2Hg$ and/or $(n\text{-Bu})_2Te$. Long-wavelength ultraviolet absorptions of $(t\text{-Bu})_2Hg$ and $(n\text{-Bu})_2Te$ seen in solution are also present in the gas phase, in contrast to inferences drawn from the literature.

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