

LETTER TO THE EDITOR

Submillimeter Microwave Spectrum of the Hydrogen Telluride Molecule

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Hydrogen telluride (H_2Te) belongs to the H_2X ($\text{X} = \text{O}, \text{S}, \text{Se} \dots$) class of molecules, and it is of interest both for pure and applied investigations. The H_2Te spectrum has been studied earlier only in the infrared regions near 896 cm^{-1} , 2070 cm^{-1} , (1,2) and 2900 cm^{-1} (3). The present paper describes the first microwave investigation of H_2Te rotational spectrum in the ground vibrational state.

We produced hydrogen telluride electrochemically by means of electrolysis of 80% solution of orthophosphoric acid with a tellurium cathode and refined it by the fractional distillation method with removal of the head and tail fractions (4). Then H_2Te was dried by passing it through a trap containing anhydrous CaCl_2 and P_2O_5 . According to the data of mass-spectrometric analysis a sample of H_2Te contained as impurities $\text{H}_2\text{S} < 10^{-2}\%$ by volume, $\text{H}_2\text{Se} < 2 \times 10^{-2}\%$ by volume, and light hydrocarbons $< 10^{-5}\%$ by volume. Hydrogen telluride is a thermodynamically unstable substance and easily decomposes at room temperature. Therefore the sample was stored at liquid nitrogen temperature, and the temperature of the absorption cell in the experiment was between -5 and 0°C .

The H_2Te submillimeter wave spectrum was observed in the range 250-490 GHz by a microwave spectrometer RAD (5). An illustration of the spectrum recorded

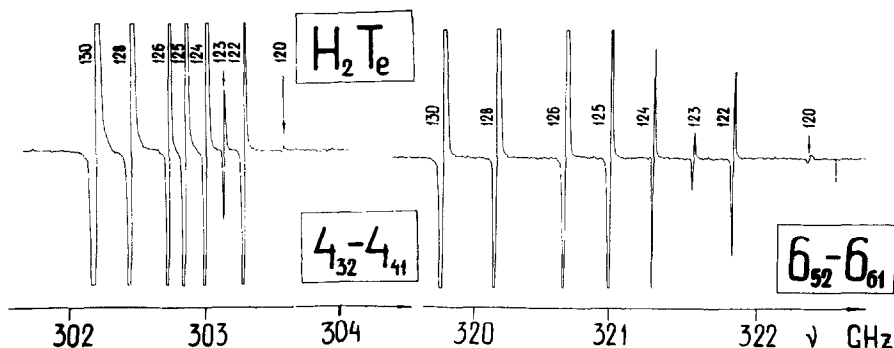


FIG. 1. A reproduction of a portion of the hydrogen telluride spectrum. The lines correspond to eight isotopic species of the molecule. The sample pressure was about 0.8 Torr.

TABLE I
Frequencies of Rotational Spectrum of H_2Te in the Ground Vibrational State

Transition	Observed frequencies, MHz									
	$\text{H}_2^{130}\text{Te}$	$\text{H}_2^{128}\text{Te}$	$\text{H}_2^{126}\text{Te}$	$\text{H}_2^{125}\text{Te}$	$\text{H}_2^{124}\text{Te}$	$\text{H}_2^{123}\text{Te}$	$\text{H}_2^{122}\text{Te}$			
7 ₅₂ → 7 ₆₁	250 478.07	250 318.01	250 156.54	250 075.65	249 994.04	249 912.39	249 829.81			
6 ₄₂ 6 ₅₁	251 571.51	251 386.22	251 196.88	251 101.06	251 004.16		250 807.67			
8 ₆₂ 8 ₇₁	254 292.44	254 205.50	254 121.72	254 080.50	254 040.23		253 962.50			
5 ₃₂ 5 ₄₁	256 023.16	255 851.06	255 674.67	255 585.02	255 494.08	255 402.13	255 308.70			
* 4 ₂₂ 4 ₃₁	262 334.95	262 202.49	262 066.53	261 997.37	261 926.78		261 782.93			
* 3 ₁₂ 3 ₂₁	269 139.58	269 059.68	268 976.94							
* 2 ₀₂ 2 ₁₁	275 288.47	275 254.97	275 225.82	275 211.02	275 195.90					
* 0 ₀₀ 1 ₁₁	278 315.13	278 370.69	278 428.21	278 457.30	278 487.12					
* 2 ₁₂ 2 ₂₁	288 657.85	288 759.75	288 864.96	288 913.64	288 973.85					
3 ₂₂ 3 ₃₁	294 682.89	294 853.33	295 029.43	295 118.89	295 210.54		295 397.88			
4 ₃₂ 4 ₄₁	302 208.09	302 469.85	302 739.87	302 877.88	303 018.60	303 160.65	303 306.18			
5 ₄₂ 5 ₅₁	310 757.99	311 133.30	311 520.30	311 719.21	311 920.95		312 334.01			
6 ₅₂ 6 ₆₁	319 701.92	320 213.13	320 739.31	321 008.26	321 282.45	321 560.85	321 843.80			
7 ₆₂ 7 ₇₁	328 257.42	328 920.38	329 604.52	329 954.18	330 310.85					
8 ₇₂ 8 ₈₁	335 493.85	336 324.18	337 180.94	337 618.83	338 065.58	338 537.70				
9 ₆₃ 9 ₇₂	413 689.36	413 405.91	413 112.01	412 961.15	412 807.28	412 650.77				
8 ₅₃ 8 ₆₂	428 474.49	428 246.11	428 008.90	427 887.09	427 762.25		427 505.67			
7 ₄₃ 7 ₅₂	441 612.12	441 460.23	441 301.90	441 220.37	441 137.11	441 051.05	440 964.64			

	H_2 ^{130}Te	H_2 ^{128}Te	H_2 ^{126}Te	H_2 ^{125}Te	H_2 ^{124}Te	H_2 ^{123}Te	H_2 ^{122}Te
$6_{33} \rightarrow 6_{42}$	452 201.07	452 123.95	452 043.24	452 001.62	451 958.83	451 915.46	451 870.35
* 1_{11} 2_{02}	455 382.35	455 411.07	455 040.64	455 455.79	455 471.06	455 486.70	455 502.52
5_{23} 5_{32}	459 982.00	459 964.49	459 945.78	459 936.00	459 925.73		459 904.26
* 1_{01} 2_{12}	460 333.45	460 410.11	460 489.15	460 529.48			
4_{13} 4_{22}	465 185.04	465 207.35	465 230.05	465 241.46	465 253.09	465 265.02	465 276.73
3_{03} 3_{12}	468 325.85	468 370.82	468 415.91	468 439.23	468 462.99	468 487.28	468 511.53
* 3_{13} 3_{22}	470 093.31	470 153.83	470 216.32	470 248.24	470 280.82		
* 4_{23} 4_{32}	470 349.70	470 418.38	470 489.30	470 525.60	470 562.59	470 600.28	470 638.50
* 5_{33} 5_{42}	471 605.49	471 689.55	471 776.61	471 821.27	471 866.65	471 912.72	471 959.06
6_{43} 6_{52}	474 364.71	474 473.51	474 586.37	474 644.09	474 702.62	474 762.51	474 824.56
7_{53} 7_{62}	479 136.42	479 280.37	479 429.84	479 506.55	479 585.06	479 665.05	479 746.40
8_{63} 8_{72}	486 409.78	486 598.73	486 795.15	486 896.13	486 999.43	487 104.54	487 212.01

Measurement error for lines H_2 $^{130,128,126}Te$: 0.1MHz,

H_2 $^{125,124,123,122}Te$: 0.2MHz.

Number of lines: 184

TABLE II

Molecular Constants in the Kivelson-Wilson Form for H_2Te in the Ground Vibrational State, MHz

	$\text{H}_2^{130}\text{Te}$			$\text{H}_2^{128}\text{Te}$			$\text{H}_2^{126}\text{Te}$		
A'	187	341.11	± 8.74	187	385.94	± 8.74	187	432.40	± 8.74
B'	182	724.87	± 9.24	182	725.03	± 9.26	182	725.47	± 9.26
C'	91	012.730	± 0.420	91	023.564	± 0.420	91	034.820	± 0.424
τ'_{aaaa}		-93.358	± 0.186		-98.457	± 0.186		-98.693	± 0.186
τ'_{bbbb}		-85.095	± 0.226		-85.120	± 0.228		-85.376	± 0.228
τ'_{cccc}		-2.984	± 0.118		-3.072	± 0.118		-3.204	± 0.118
τ'_{aabb}		37.113	± 0.792		37.051	± 0.802		36.948	± 0.812
τ'_{aacc}		-26.75	± 18.16		-26.87	± 18.18		-27.08	± 18.20
τ'_{bbcc}		16.53	± 17.40		16.50	± 17.42		16.39	± 17.44

TABLE III

Matrices of Correlation Coefficients for A' , B' , C' , and τ 's Constants

	A'	B'	C'	τ'_{aaaa}	τ'_{aabb}	τ'_{bbbb}	τ'_{aacc}	τ'_{bbcc}	τ'_{cccc}
A'	+1.000								
B'	-0.999	+1.000							
C'	+0.827	-0.818	+1.000						
τ'_{aaaa}	-0.201	+0.182	-0.226	+1.000					
τ'_{aabb}	+0.991	-0.993	+0.774	-0.229	+1.000				
τ'_{bbbb}	+0.672	-0.689	+0.383	+0.489	+0.664	+1.000			
τ'_{aacc}	-1.000	+1.000	-0.832	+0.190	-0.991	-0.675	+1.000		
τ'_{bbcc}	+1.000	-1.000	+0.828	-0.187	+0.991	+0.678	-1.000	+1.000	
τ'_{cccc}	+0.089	-0.103	-0.466	+0.168	+0.171	+0.380	-0.081	+0.088	+1.000
A'	+1.000								
B'	-0.999	+1.000							
C'	+0.830	-0.822	+1.000						
τ'_{aaaa}	-0.202	+0.184	-0.228	+1.000					
τ'_{aabb}	+0.991	-0.993	+0.778	-0.230	+1.000				
τ'_{bbbb}	+0.672	-0.689	+0.387	+0.488	+0.664	+1.000			
τ'_{aacc}	-1.000	+1.000	-0.836	+0.192	-0.991	-0.675	+1.000		
τ'_{bbcc}	+1.000	-1.000	+0.832	-0.189	+0.992	+0.678	-1.000	+1.000	
τ'_{cccc}	+0.093	-0.103	-0.460	+0.168	+0.171	+0.380	-0.081	+0.088	+1.000
A'	+1.000								
B'	-0.999	+1.000							
C'	+0.833	-0.825	+1.000						
τ'_{aaaa}	-0.205	+0.186	-0.230	+1.000					
τ'_{aabb}	+0.991	-0.993	+0.782	-0.232	+1.000				
τ'_{bbbb}	+0.672	-0.689	+0.391	+0.486	+0.664	+1.000			
τ'_{aacc}	-1.000	+1.000	-0.839	+0.194	-0.991	-0.675	+1.000		
τ'_{bbcc}	+1.000	-1.000	+0.835	-0.192	+0.992	+0.678	-1.000	+1.000	
τ'_{cccc}	+0.090	-0.104	-0.4555	+0.167	+0.171	+0.380	-0.082	+0.089	+1.000

is presented in Fig. 1. The lines corresponding to eight isotopic species of this molecule of the form H_2^XTe are seen ($X = 130$ (34.5%), 128 (31.8%), 126 (18.7%), 125 (6.99%), 124 (4.61%), 123 (0.875%), 122 (2.46%), and 120 (0.09%)). In parentheses the natural abundance for each molecular species is given. The measurements of spectral line frequencies were made at a pressure ~ 0.8 Torr in the absorption cell with an accuracy of 0.1–0.2 MHz. Experimental values of the line frequencies for the seven most abundant isotopic species of the molecule and assignments of the transitions are given in Table I.

A theoretical description of the rotational spectrum of H_2X -type molecules ($X = O, S, Se, \dots$) meets significant difficulties connected with their nonrigidity. A preliminary processing of the data was made by using the rotational Hamiltonian in the Kivelson–Wilson form (6):

$$H_2 + H_4 = A'P_a^2 + B'P_b^2 + C'P_c^2 + \frac{1}{4} \sum_{\alpha, \beta} \tau'_{\alpha\alpha\beta\beta} P_\alpha^2 P_\beta^2 \quad (1)$$

where $\alpha, \beta = a, b$, and c , and P_α^2 is the square of the angular momentum component operator along the main axis "a" in the molecule. The processing was made for three species of the molecule $H_2^{130,128,126}Te$ using only frequencies of 10 transitions with lowest centrifugal shifts (< 0.5 GHz). These transitions are marked in Table I with an asterisk. The Hamiltonian parameters with the matrix of correlation coefficients are given in Tables II and III. The mean difference between the measured and calculated frequencies for these selected transitions is 0.17 MHz.

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