Thermodynamic Properties of Normal and Deuterated Naphthalenes

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Structural and spectroscopic data and the standard enthalpy of formation at 298.15 K for $C_{10}H_8$, α-$C_{10}H_4D_4$, β-$C_{10}H_4D_4$ and $C_{10}D_8$ were reviewed. The selected values were utilized to calculate the ideal gas thermodynamic properties in the temperature range 0 to 1500 K, using the rigid rotor and harmonic oscillator model. The comparison between the third law entropies and the spectroscopically calculated entropies of $C_{10}H_8$ was studied. The agreement is satisfactory within the experimental uncertainties.

Key words: Enthalpy of formation; ideal gas thermodynamic properties; molecular structure; normal and deuterated naphthalenes; vibrational assignments.

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1. Introduction

The thermodynamic properties of naphthalene in the ideal gas state have been calculated and reported on a number of occasions [1–6].[1] However, considerable discrepancies exist in the vibrational frequencies used in the calculations and in the results obtained. The current interest in properties of aromatic compounds led us to review the available information on naphthalene and its various deuterated species and to calculate the ideal gas thermodynamic properties, using the best information available at present.

2. Molecular Structure and Moments of Inertia

Cruickshank [7] analyzed the x-ray crystal data on naphthalene measured by Abrahams et al. [8]. Bond distances and bond angles were assigned to the naphthalene rings. Later Almenningen et al. [9] obtained the molecular parameters, using electron diffraction techniques on the condensed naphthalene molecules. However, they were not sure about the accuracy of their method. In the meantime, Cruickshank and Sparks [10] reanalyzed the x-ray crystal data of Abrahams et al., [8] by means of least squares and the differential Fourier synthesis method. They concluded that the naphthalene molecule is planar with a possible out-of-plane deviation of less than 0.010 Å. The structure given by them on the assumption of the bond distance, C–H = 1.09 Å, is shown in figure 1. In this work, the deuterated species, α-$C_{10}H_4D_4$, β-$C_{10}H_4D_4$ and $C_{10}D_8$ are considered to possess the same molecular param-

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* Deceased.

[1] Figures in brackets indicate literature references.

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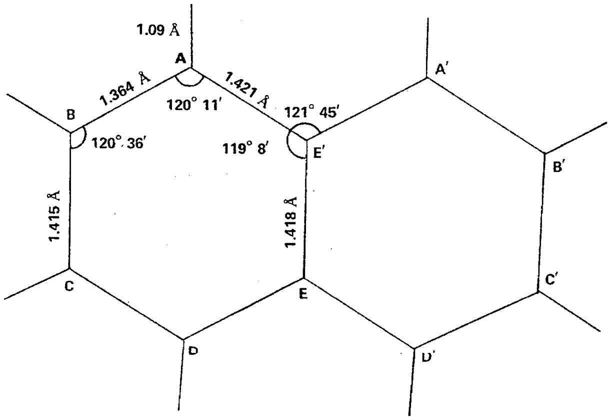
eters as $C_{10}H_8$. Using the molecular parameters given in figure 1, the moments of inertia were calculated and are presented in table 1.



AB = CD = A′B′ = C′D′
BC = B′C′
AE′ = DE = A′E′ = D′E

Figure 1. Structural parameters of naphthalene.

3. Vibrational Fundamentals

Naphthalene and its deuterated species (α-$C_{10}H_4D_4$, β-$C_{10}H_4D_4$ and $C_{10}D_8$) belong to D_{2h} point group. Each has 48 fundamental modes of vibration out of which 33 are in-plane modes and 15 are out-of-plane. They are distributed among the following symmetry species:

Planar — $9A_g + 8B_{1u} + 8B_{2u} + 8B_{3g}$
Non-planar — $4A_u + 3B_{1g} + 4B_{2g} + 4B_{3u}$

The fundamentals belonging to A_g, B_{1g} and B_{2g} are only Raman active, those belonging to B_{1u}, B_{2u} and B_{3u} are only infrared active and the A_u fundamentals are completely inactive. This is because of the mutual exclusion principle due to the center of symmetry present in the molecules.

Various workers have studied the infrared and Raman spectra of $C_{10}H_8$ [11–26], α-$C_{10}H_4D_4$ [17, 18, 27], β-$C_{10}H_4D_4$ [18, 27], and $C_{10}D_8$ [12, 13, 15, 17, 18, 19, 23, 28, 29]. The electronic-vibrational spectra of $C_{10}H_8$ and $C_{10}D_8$ have been investigated [30–33]. Since naphthalene is the simplest member of the polycyclic aromatic ring compounds, many studies of the vibrational spectra of naphthalene and its deutero derivatives have been carried out. However, despite the abundant experimental data, the various interpretations have differed substantially from one another. The difficulties encountered in making a complete vibrational assignment arise from the fact that many of the fundamentals are weak, in fact often much less intense than some combination tones and overtones. In addition the proper interpretation of the spectra has been hampered because of accidental resonance, strong shadows of the Raman exciting lines and the large number of active fundamentals. On the basis of theoretical relations like the sum rule, the product rule, normal coordinate analysis etc., the interpretation of the spectra has been made by various workers [34–39]. The most reliable assignments seem to be those reported by Krainov [37], except for two frequencies. Taking into consideration the assignments reported by various workers, we have evaluated the best sets of fundamentals for $C_{10}H_8$, α-$C_{10}H_4$, β-$C_{10}H_4D_4$ and $C_{10}D_{10}$. We have preferred the vapor phase values whenever available. The adopted fundamentals are presented in table 2. As seen from table 3, the comparison of the theoretical and experimental values of the sum and difference rules [40–42] is satisfactory. The vibrational fundamentals in the A_u species are more uncertain than those in the other species as they are inactive in the IR and Raman spectra. For B_{1u} and B_{2g} species we have adopted the assignment of Scully and Whiffen [34] for $C_{10}H_8$.

4. Standard Enthalpies of Formation

Much work has been done on the enthalpy of combustion of normal naphthalene [43–51]. Cox and Pilcher [52] have critically reviewed the enthalpy of combustion and obtained values of the enthalpy of formation for solid naphthalene ranging from 64.85–82.01 kJ mol^{-1}. Adopting $\Delta H_f°$ (c, 298.15) = 77.95 ± 0.92 kJ mol^{-1} and $\Delta H_{sub}°$ = 72.89 ± 0.29 kJ mol^{-1} [53] they obtained $\Delta H_f°$ (g, 298.15) = 150.83 ± 1.05 kJ mol^{-1}. It is found that $\Delta H_{sub}°$ reported by various workers vary from 71.4–73.6 kJ mol^{-1} [49, 53–58]. The most recent calorimetric value, $\Delta H_{sub}°$ = 72.05 ± 0.25 kJ mol^{-1}, reported by Morawetz [55] seems to be the best value, and it was selected in this work. Irving [56] made 13 determinations and the $\Delta H_{sub}°$ fluctuated as much as 1.7 kJ mol^{-1}. The average value 73.00 ± 0.25 kJ mol^{-1} does not seem to be very accurate.

Regarding the enthalpy of combustion, we have selected the value ($\Delta H_c°$ = 5165.95 ± 1.6 kJ mol^{-1}) reported by Speros and Rossini [49] on the basis of purity of the sample and the accuracy of the experiment. We obtained $\Delta H_f°$ (c, 298.15) = 78.53 ± 1.59 kJ mol^{-1} using $\Delta H_f°$ (H_2O, 1, 298.15) =—285.830 kJ mol^{-1} and $\Delta H_f°$ (CO_2, g, 298.15) = 393.509 kJ mol^{-1}. Using our selected values of $\Delta H_f°$ (c, 298.15) and $\Delta H_{sub}°$ we obtained $\Delta H_f°$ (g, 298.15) = 150.58 ± 1.61 kJ mol^{-1}, which is adopted in this work.

No experimental standard enthalpies of formation are available for the deuterated species α-$C_{10}H_4D_4$, β-$C_{10}H_4D_4$, and $C_{10}D_8$. We estimated $\Delta H_f°$ at 0 K from the corresponding calculated zero point energies and in turn obtained $\Delta H_f°$ (g, 298.15) = 134.10, 134,44, and 118.05 kJ mol^{-1} for α-$C_{10}H_4D_4$, β-$C_{10}H_4D_4$ and $C_{10}D_8$, respectively.

5. Thermodynamic Properties

Using the data given in tables 1 and 2 for naphthalene and its three deuterated species, the ideal gas thermodynamic properties, $C_p°$, $S°$, $-(G° - H_0°)/T$, $H° - H_0°$, $\Delta H_f°$, $\Delta G_f°$ and log K_f were calculated, assuming rigid-rotor and harmonic oscillator approximations. The most recent fundamental constants [59] and atomic weights [60] were used. To obtain enthalpy ($\Delta H_f°$), Gibbs energy ($\Delta G_f°$) and logarithmic equilibrium constant (log K_f), the enthalpy and the Gibbs energy function for C [61] and H_2 [62] in their reference states were used. The ideal gas thermodynamic properties are presented in tables 4, 5, 6 and 7.

6. Comparison and Uncertainties

The reliability of the calculated thermodynamic properties is determined by comparing the vapor heat capacities or the third law entropies with the spectroscopically calculated values. For normal naphthalene we have vapor heat capacities as well as the third law entropies for comparison. The vapor heat capacities are those of Barrow and McClellan [1]. We have obtained the third law entropies in this work by using the more reliable relevant data [58, 63] than used by Barrow and McClellan [1, 64, 65]. The details of the calculations of the third law entropy are given in table 8. The comparison of the experimental and calculated values is presented in table 9. It is seen that the agreement is quite satisfactory. In table 10 the heat capacities and the entropies at various temperatures calculated by different workers are compared. As we have used more reliable input data in our calculations, our calculated thermodynamic properties are believed to be the most reliable.

The uncertainties given in table 11 were obtained by calculating the thermodynamic properties after increasing, and then decreasing, all fundamental assignments by 10 cm^{-1}. Since it is unlikely that all frequency assignments are in error by this amount in the same direction, the errors due to uncertainty in the fundamental frequencies are probably much less than the values in table 11. Uncertainties due to errors in molecular geometry are smaller still.

Errors due to deviation from the rigid rotor-harmonic oscillator model are probably small compared to the values in table 11 up to 800 K. However, such error may increase significantly at higher temperatures. We have no way of giving quantitative estimates of these effects however.

TABLE 1. Molecular constants of naphthalene and deuterated naphthalenes

	$C_{10}H_8$	α-$C_{10}H_4D_4$	β-$C_{10}H_4D_4$	$C_{10}D_8$
Molecular weight, $g \cdot mol^{-1}$	128.1732	132.1980	132.1980	136.2228
Symmetry number	4	4	4	4
I_a, $\mu Å^2$	161.7238	186.7147	167.8671	192.8580
I_b, $\mu Å^2$	406.0319	412.2270	451.6953	457.8904
I_c, $\mu Å^2$	567.7557	598.9417	619.5624	650.7484
ΔH_f^0 (g, 298.15), kJ mol^{-1}	150.58	134.10	134.44	118.05

TABLE 2. Vibrational fundamentals (cm^{-1}) of naphthalene and deuterated naphthalenes

	$C_{10}H_8$	α-$C_{10}H_4D_4$	β-$C_{10}H_4D_4$	$C_{10}D_8$
A_g	3060	3045	3048	2272
	3030	2276	2294	2257
	1577	1569	1565	1553
	1463	1397	1413	1386
	1380	1355	1378	1298
	1145	1095	1030	863
	1025	864	853	835
	761	710	738	692
	512	505	501	495
B_{1g}	950	871	905	785
	725	639	590	545
	386	350	376	346
B_{2g}	980	958	900	875
	876	871	853	760
	778	673	732	663
	466	456	415	410
B_{3g}	3092	3063	3070	2302
	3060	2276	2277	2275
	1628	1610	1621	1604
	1443	1410	1398	1330
	1242	1140	1220	1030
	1168	958	974	929
	936	844	900	830
	506	500	495	490
A_u	970	966	873	800
	841	682	768	653
	581	557	531	507
	191	183	181	177
B_{1u}	3065	3046	3046	2286
	3058	2278	2263	2258
	1595	1581	1564	1545
	1389	1362	1278	1258
	1265	1199	1256	1050
	1125	929	948	889
	877	775	696	715
	359	338	343	328
B_{2u}	3090	3076	3046	2289
	3027	2260	2278	2258
	1509	1480	1524	1439
	1361	1318	1359	1316
	1209	1199	1173	1082
	1144	1098	998	880
	1008	823	849	825
	617	602	595	593
B_{3u}	958	874	921	791
	782	729	635	628
	472	407	470	404
	176	172	165	163

TARLE 3. Comparison of theoretical and experimental values of sum and difference rules

	Theoretical	$\frac{\Sigma\nu_i(\alpha\text{-d}_4) + \Sigma\nu_i(\beta\text{-d}_4)}{\Sigma\nu_i(\text{d}_0) + \Sigma\nu_i(\text{d}_8)}$	$\frac{\Sigma\nu_i^2(\alpha\text{-d}_4) + \Sigma\nu_i^2(\beta\text{-d}_4)}{\Sigma\nu_i^2(\text{d}_0) + \Sigma\nu_i^2(\text{d}_8)}$	$\frac{\Sigma\nu_i^2(\text{d}_0) - \Sigma\nu_i^2(\alpha\text{-d}_4)}{\Sigma\nu_i^2(\beta\text{-d}_4) - \Sigma\nu_i^2(\text{d}_8)}$
A_g	1.0	1.0012	1.0036	0.9664
B_{1g}	1.0	0.9984	0.9983	1.0158
B_{2g}	1.0	0.9969	0.9938	1.0971
B_{3g}	1.0	0.9954	0.9921	1.0716
A_u	1.0	1.0044	1.0094	0.8984
B_{1u}	1.0	0.9972	0.9946	1.0496
B_{2u}	1.0	1.0013	1.0031	0.9722
B_{3u}	1.0	0.9998	0.9991	1.0093

TABLE 4. Ideal gas thermodynamic properties of naphthalene, $C_{10}H_8$

$\frac{T}{\text{K}}$	$C_p°$	$S°$	$-(G°-H°_0)/T$	$H°-H°_0$	$\Delta H_f°$	$\Delta G_f°$	$\log K_f$
		J K^{-1} mol^{-1}			kJ mol^{-1}		
0	0	0	0	0	174.25	174.25	$-\infty$
50	35.71	219.91	186.19	1.686	167.44	174.02	−181.80
100	46.94	247.82	210.51	3.731	164.67	181.65	−94.88
150	63.35	269.79	226.67	6.467	161.39	190.83	−66.45
200	84.22	290.78	240.08	10.141	157.73	201.22	−52.55
273.15	119.46	322.15	257.83	17.570	152.34	218.10	−41.71
298.15	131.92	333.15	263.68	20.713	150.58	224.10	−39.26
300	132.84	333.97	264.11	20.957	150.45	224.56	−39.10
400	180.07	378.80	287.17	36.653	144.19	250.27	−32.68
500	219.74	423.40	309.97	56.713	139.22	277.34	−28.97
600	251.53	466.38	332.49	80.337	135.35	305.33	−26.58
700	277.01	507.14	354.55	106.81	132.33	333.95	−24.92
800	297.73	545.52	376.05	135.58	130.05	362.92	−23.70
900	314.85	581.61	396.91	166.24	128.43	392.15	−22.76
1000	329.17	615.55	417.09	198.46	127.51	421.70	−22.03
1100	341.24	647.50	436.60	231.99	127.10	450.63	−21.40
1200	351.50	677.65	455.44	266.65	126.96	480.45	−20.91
1300	360.26	706.13	473.64	302.24	127.06	509.77	−20.48
1400	367.78	733.11	491.22	338.65	127.39	539.74	−20.14
1500	374.27	758.72	508.21	375.76	127.92	568.94	−19.81

TABLE 5. Ideal gas thermodynamic properties of naphthalene-α-d$_4$, $C_{10}H_4D_4$

$\frac{T}{\mathrm{K}}$	C_p°	S°	$-(G^\circ - H_0^\circ)/T$	$H^\circ - H_0^\circ$	ΔH_f°	ΔG_f°	$\log K_f$
	$\mathrm{J\ K^{-1}\ mol^{-1}}$			$\mathrm{kJ\ mol^{-1}}$			
0	0	0	0	0	156.48	156.48	$-\infty$
50	36.02	221.27	187.48	1.689	151.25	158.34	−165.42
100	48.63	249.75	211.95	3.780	147.79	166.72	−87.08
150	67.62	272.85	228.45	6.660	144.09	176.98	−61.63
200	91.82	295.52	242.37	10.630	140.44	188.45	−49.22
273.15	130.90	329.89	261.17	18.769	135.59	206.97	−39.58
298.15	144.15	341.92	267.44	22.208	134.10	213.53	−37.41
300	145.12	342.82	267.90	22.475	134.00	214.03	−37.26
400	193.53	391.40	292.70	39.477	129.01	241.39	−31.52
500	233.12	439.00	317.23	60.883	125.37	270.03	−28.21
600	264.68	484.40	341.34	85.832	122.79	299.22	−26.05
700	289.94	527.17	364.87	113.61	120.99	328.81	−24.54
800	310.35	567.26	387.69	143.66	119.83	358.55	−23.41
900	327.04	604.81	409.75	175.56	119.25	388.50	−22.55
1000	340.79	640.00	431.03	208.97	119.26	418.62	−21.87
1100	352.23	673.04	451.55	243.64	119.69	448.01	−21.27
1200	361.81	704.11	471.31	279.35	120.30	478.12	−20.81
1300	369.88	733.39	490.36	315.95	121.05	507.91	−20.41
1400	376.73	761.06	508.71	353.29	121.94	538.16	−20.08
1500	382.57	787.26	526.42	391.26	122.93	542.47	−18.89

TABLE 6. Ideal gas thermodynamic properties of naphthalene-β-d$_4$, $C_{10}H_4D_4$

$\frac{T}{\mathrm{K}}$	C_p°	S°	$-(G^\circ - H_0^\circ)/T$	$H^\circ - H_0^\circ$	ΔH_f°	ΔG_f°	$\log K_f$
	$\mathrm{J\ K^{-1}\ mol^{-1}}$			$\mathrm{kJ\ mol^{-1}}$			
0	0	0	0	0	156.85	156.85	$-\infty$
50	36.23	221.42	187.57	1.692	151.62	158.71	−165.80
100	48.52	249.98	212.11	3.787	148.17	167.07	−87.27
150	67.37	273.00	228.61	6.657	144.46	177.32	−61.75
200	91.54	295.59	242.53	10.614	140.80	188.80	−49.31
273.15	130.64	329.87	261.29	18.733	135.93	207.31	−39.64
298.15	143.90	341.89	267.55	22.165	134.44	213.87	−37.47
300	144.87	342.78	268.01	22.432	134.33	214.37	−37.32
400	193.31	391.29	292.76	39.411	129.32	241.74	−31.57
500	232.90	438.84	317.25	60.795	125.66	270.39	−28.25
600	264.47	483.21	341.33	85.723	123.06	299.59	−26.08
700	289.74	526.94	364.83	113.48	121.23	329.21	−24.57
800	310.18	567.01	387.63	143.51	120.06	358.97	−23.44
900	326.88	604.54	409.67	175.39	119.45	388.95	−22.57
1000	340.66	639.72	430.93	208.79	119.46	419.09	−21.89
1100	352.11	672.74	451.43	243.44	119.87	448.51	−21.30
1200	361.70	703.80	471.18	279.15	120.47	478.66	−20.84
1300	369.79	733.08	490.21	315.73	121.21	508.47	−20.43
1400	376.65	760.74	508.55	353.07	122.09	538.75	−20.10
1500	382.50	786.94	526.25	391.03	123.08	543.10	−18.91

TABLE 7. Ideal gas thermodynamic properties of naphthalene-d$_8$, $C_{10}D_8$

$\frac{T}{K}$	C_p°	S°	$-(G^\circ-H_0^\circ)/T$	$H^\circ-H_0^\circ$	ΔH_f°	ΔG_f°	log K_f
	J K^{-1} mol^{-1}			kJ mol^{-1}			
0	0	0	0	0	139.19	139.19	—∞
50	36.43	222.03	188.14	1.695	135.52	143.16	—149.56
100	50.04	251.04	212.78	3.826	131.38	152.32	—79.56
150	71.60	275.14	229.58	6.834	127.24	163.70	—57.00
200	99.18	299.43	243.99	11.088	123.59	176.39	—46.07
273.15	142.08	336.71	263.79	19.918	119.26	196.51	—37.58
298.15	156.12	349.76	270.45	23.647	118.05	203.65	—35.68
300	157.13	350.73	270.94	23.937	117.96	204.19	—35.55
400	206.73	402.98	297.43	42.218	114.22	233.44	—30.48
500	246.26	453.53	323.64	64.945	111.89	263.62	—27.54
600	277.63	501.31	349.31	91.200	110.58	294.11	—25.60
700	302.69	546.06	374.26	120.26	109.98	324.80	—24.24
800	322.81	587.84	398.37	151.57	109.92	355.49	—23.21
900	339.06	626.83	421.62	184.69	110.35	386.20	—22.42
1000	352.27	663.26	443.98	219.28	111.29	417.01	—21.78
1100	363.08	697.36	465.48	255.07	112.54	446.97	—21.22
1200	371.99	729.35	486.15	291.84	113.89	477.70	—20.79
1300	379.38	759.42	506.03	329.42	115.28	507.88	—20.41
1400	385.56	787.77	525.15	367.67	116.72	538.52	—20.09
1500	390.78	814.56	543.56	406.50	118.16	518.10	—18.04

TABLE 8. The third law entropies (J K^{-1} mol^{-1}) at 298.15 and 353.43 K for naphthalene

	S° at 298.15 K	
		Reference
S_{solid}	167.40	[63]
$\frac{\Delta H_{sub}}{T}$	241.66	[55]
$R \ln P$	—75.71	[58]
Gas imperfection correction	0.	[57, 58]
$S^\circ_{298.15}$	333.35 ± 0.53	
	S° at 353.43 K	
		Reference
S_{solid}	198.95	[63]
$\frac{\Delta H_{sub}}{T}$	197.30	[58]
$R \ln P$	—38.40	[58]
Gas imperfection correction	0.02	[58; Berthelot eq]
$S^\circ_{353.43}$	357.87 ± 0.37	

TABLE 9. Comparison of experimental and spectroscopic heat capacities and entropies (J K^{-1} mol^{-1}) for naphthalene

T/K	C_p°		S°	
	Exp.[a]	Cal.	Exp.[b]	Cal.
298.15			333.35	333.15 ± 1.11
353.43			357.87	357.84 ± 1.42
451.0	201.59	201.36 ± 0.98		
522.7	226.65	227.60 ± 0.91		

[a] Ref. [1].

[b] See table 8.

TABLE 10. Comparison of C_p° and S° (J K^{-1} mol^{1-}) calculated by various workers

Year	Ref.	298.15 K		700 K		1000 K	
		C_p°	S°	C_p°	S°	C_p°	S°
1951	[1]	129.83	335.98	277.44	509.40	329.99	618.06
1955	[2]	134.22	336.52	276.19	510.74	328.82	618.95
1957	[4]			270.91		325.26	
1969	[5]	132.55	335.64	275.18	508.73	327.94	616.55
1974	[6]	133.39	334.64				
1977	This work	131.92	333.15	277.01	507.14	329.17	615.55

TABLE 11. Effect of uncertainties in the vibrational fundamentals on the calculated thermodynamic properties properties

$\frac{T}{\mathrm{K}}$	C_p°	S°	$-(G^\circ - H_0^\circ)/T$	$H^\circ - H_0^\circ$
	J K^{-1} mol^{-1}			kJ mol^{-1}
		$C_{10}H_8$		
200	0.81	0.75	0.32	0.08
298.15	0.96	1.11	0.52	0.18
400	1.00	1.40	0.71	0.28
700	0.71	1.89	1.19	0.54
1000	0.49	2.10	1.39	0.71
1500	0.28	2.26	1.66	0.90
		$C_{10}H_4D_4$-α		
200	0.50	0.67	0.32	0.07
298.15	0.65	0.90	0.47	0.13
400	0.70	1.09	0.61	0.20
700	0.56	1.46	0.90	0.39
1000	0.39	1.63	1.10	0.53
1500	0.23	1.76	1.30	0.68
		$C_{10}H_4D_4$-β		
200	0.93	0.86	0.36	0.10
298.15	1.07	1.26	0.60	0.20
400	1.03	1.57	0.81	0.31
700	0.71	2.07	1.26	0.56
1000	0.48	2.28	1.54	0.74
1500	0.28	2.44	1.82	0.92
		$C_{10}D_{10}$		
200	1.05	0.95	0.40	0.11
298.15	1.18	1.41	0.66	0.22
400	1.10	1.74	0.90	0.34
700	0.73	2.26	1.39	0.61
1000	0.49	2.47	1.69	0.79
1500	0.27	2.63	1.98	0.97

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8. References

[1] Barrow, G. M., and McClellan, A. L., J. Am. Chem. Soc. **73**, 573 (1951).

[2] McClellan, A. L., and Pimentel, G. C., J. Chem. Phys. **23**, 245 (1955).

[3] Miller, G. A., J. Chem. Eng. Data **8**, 69 (1963).

[4] Vvedneskii, A. A., and Maiorov, D. M., J. Gen. Chem. USSR (Eng. Translation) **27**, 2106 (1957).

[5] Stull, D. R., Westrum, E. F., and Sinke, G. C., *The Chemical Thermodynamics of Organic Compounds*, John Wiley and Sons, Inc., New York (1969).

[6] Sinke, G. C., J. Chem. Thermodyn. **6**, 311 (1974).

[7] Cruickshank, D. W. J., Acta Crystallogr. **10**, 504 (1957).

[8] Abrahams, S. C., Robertson, J. M., and White, J. G., Acta Crystallogr. **2**, 233 (1949); **2**, 238 (1949).

[9] Almenningen, A., Bastiansen, O., and Dyvik, F., Acta Crystallogr. **14**, 1056 (1961).

[10] Cruickshank, D. W. J., and Sparks, R. A., Proc. R. Soc. London A **258**, 270 (1961).

[11] Luther, H., Feldman, K., and Hampel, B., Z. Elektrochem. **59**, 1008 (1955).

[12] Person, W. B., Pimentel, G. C., and Schnepp, O., J. Chem. Phys. **23**, 230 (1955).

[13] Pimentel, G. C., McClellan, A. L., Person, W. B., and Schnepp, O., J. Chem. Phys. **23**, 234 (1955).

[14] Luther, H., Brandes, G., Gunzler, H., and Hampel, B., Z. Elektrochem. **59**, 1012 (1955).

[15] Lippincott, E. R., and O'Reilly, E. J., Jr., J. Chem. Phys. **23**, 238 (1955).

[16] Bruhn, W., and Mecke, R., Z. Elektrochem. **62**, 441 (1958).

[17] Mitra, S. S., and Bernstein, H. J., Can. J. Chem. **37**, 553 (1959).

[18] Peregudov, G. V., Opt. Spectrosc., USSR **11**, 397 (1961).

[19] Chantry, G. W., Anderson, A., and Gebbie, H. A., Spectrochim. Acta A **20**, 1465 (1964).

[20] Friedman, H. M., Spectrochim. Acta A **22**, 1465 (1966).

[21] Suzuki, M., Yokoyama, T., and Ito, M., Spectrochim. Acta Part A **24**, 1091 (1968).

[22] Hanson, D. M., and Gee, A. E., J. Chem. Phys. **51**, 5052 (1969).

[23] Bree, A., and Kydd, R. A., Spectrochim. Acta A **26**, 1791 (1970).

[24] Stenman, F., J. Chem. Phys. **54**, 4217 (1971).

[25] Dodson, C. L., and Graham, J. F., J. Phys. Chem. **77**, 2903 (1973).

[26] Broude, V. L., and Umarov, L. M., Opt. Spectrosc. USSR **39**, 39 (1975).

[27] Shatenshtein, A. I., Peregudov, G. V., Izrailevich, E. A., and Kalinachenko, V. R., Zh. Fiz. Khim. **32**, 553 (1959).

[28] Goubeau, J., Luther, H., Feldmann, K., and Brandes, G., Chem. Ber. **86**, 214 (1953).

[29] Person, W. B., and Pimentel, G. C., J. Chem. Phys. **20**, 1913 (1952).

[30] Bolotnikova, T. N., Opt. Spectrosc. USSR **7**, 24 (1959).

[31] Craig, D. R., Hollas, J. M., Redies, M. F., and Wait, S.C., Proc. Chem. Soc. London 361, (1959).

[32] Hollas, J. M., J. Mol. Spectrosc. **9**, 138 (1962).

[33] Hanson, D. M., J. Chem. Phys. **51**, 5063 (1969).

[34] Scully, D. B., and Whiffen, D. H., Spectrochim. Acta **16**, 1409 (1960).

[35] Freeman, D. E., and Ross, I. G., Spectrochim. Acta **16**, 1393 (1960).

[36] Scherer, J. R., J. Chem. Phys. **36**, 3308 (1962).

[37] Krainov, E. P., Opt. Spectrosc. USSR **16**, 415 (1964).

[38] Neto, N., Scrocco, M., and Califano, S., Spectrochim. Acta **22**, 1981 (1966).

[39] Hagen, G., and Cyvin, S. J., J. Phys. Chem. **72**, 1446 (1968).

[40] Decius, J. C., and Wilson, E. B., J. Chem. Phys. **19**, 1409 (1951).

[41] Sverdlov, L. M., Dokl. Akad. Nauk. SSSR **78**, 1115 (1951).

[42] Zhirnov, N. I., Opt. Spectrosc. USSR **14**, 306 (1963).

[43] Keffler, L. J. P., J. Chim. Phys. **28**, 457 (1931).

[44] Beckers, M., Bull. Soc. Chim. Belg. **40**, 518 (1931).

[45] Milone, M., and Rossignoli, P., Gass. Chim. Ital. **62**, 644 (1932).

[46] Huffman, H. M., and Ellis, E. L., J. Am. Chem. Soc. **57**, 41 (1935).

[47] Matsui, M., and Abe, T., Bull. Tokyo Univ. Eng. **8**, 339 (1939); Chem. Zent. I, 804 (1941).

[48] Bender, P., and Farber, J., J. Am. Chem. Soc. **74**, 1450 (1952).

[49] Speros, D. M., and Rossini, F. D., J. Phys. Chem. **64**, 1723 (1960).

[50] Mackle, H., and O'Hare, P. A. G., Trans. Faraday Soc. **59**, 2693 (1963).

[51] Coleman, D. J., and Pilcher, G., Trans. Faraday Soc. **62**, 821 (1966).

[52] Cox, J. D., and Pilcher, G., *Thermochemistry of Organic and Organometallic Compounds*, Academic Press, London and New York (1970).

[53] Miller, G. A., J. Chem. Eng. Data **8**, 69 (1963).

[54] Bradley, R. S., and Cleasby, T. G., J. Chem. Soc., 1690 (1953).

[55] Morawetz, E. J., J. Chem. Thermodyn. **4**, 455 (1972).

[56] Irving, R. J., J. Chem. Thermodyn. **4**, 793 (1972).

[57] Sinke, G. C., J. Chem. Thermodyn. **6**, 311 (1974).

[58] Ambrose, D., Lawrenson, I. J., and Sparke, C. H. S., J. Chem. Thermodyn. **7**, 1173 (1975).

[59] The ICSU Committee on Data for Science and Technology, CODATA Bull. No. 11 (December 1973).

[60] Commission on Atomic Weights, Greenwood, N. N., Chairman, International Union of Pure and Applied Chemistry, Pure Appl. Chem. **30**, 639 (1972); **37**, 4 (1974).

[61] Evans, W. H., National Bureau of Standards report 6928, Table 13–39 (1960); West, E. D., and Ishihara, S., "Advances in Thermophysical Properties at Extreme Temperatures and Pressures," A.S.T.M. (1965); "JANAF Thermochemical Tables," 2nd Edition, NSRDS–NBS–37.

[62] Zwolinski, B. J. et al., "Selected Values of Properties of Hydrocarbons and Related Compounds," American Petroleum Institute Research Project 44, Thermodynamics Research Center, Texas A&M University, College Station, Texas, Tables 1–s, 2–s, 1–u, 2–u (1968).

[63] McCullough, J. P., Finke, H. L., Messerly, J. F., Todd, S. S., Kincheloe, T. C., and Waddington, G., J. Phys. Chem. **61**, 1105 (1957).

[64] Huffman, H. M., Parks, G. S., and Daniels, A. C., J. Am. Chem. Soc. **52**, 1547 (1930).

[65] Southard, J. C., and Brickwedde, F. G., J. Am. Chem. Soc. **55**, 4378 (1933).