Thermochimica Acta, 25 (1978) 21–33

THERMODYNAMIC FUNCTIONS FOR 1,4-DICHLORONAPHTHALENE, 1,4-DIBROMONAPHTHALENE AND 2,3-DIBROMONAPHTHALENE FROM 0.25 TO 16 ATMOSPHERES

D. G. McFEE* AND J. LIELMEZS

Chemical Engineering Department, The University of British Columbia, Vancouver, B.C. (Canada)

(Received 8 August 1977)

ABSTRACT

Real gas thermodynamic functions, C_p, S, $(H - H_0)/T$, and $-(F - H_0)/T$, have been calculated for dihalonaphthalenes (1,4-dichloronaphthalene, 1,4-dibromonaphthalene and 2,3-dibromonaphthalene) from 0.25 atm to 16 atm within the temperature range of 273.15–1200 K, correcting the thermodynamic property ideal gas values by means of the Berthelot equation of state.

INTRODUCTION

McFee and Lielmezs[1–3] have calculated the ideal gas state thermodynamic functions at 1 atm for naphthalene and 11 halogenated naphthalenes[1], and the real gas state thermodynamic functions from 0.25 atm to 16 atm for α- and β-halonaphthalenes[2, 3], all calculations having been kept within the temperature range 273.15–1200 K. In this work, additionally, real gas thermodynamic functions have been calculated for dihalogenated naphthalenes (1.4-dichloronaphthalene, 1,4-dibromonaphthalene and 2,3-dibromonaphthalene), again from 0.25 to 16 atm and within the temperature range 273.15–1200 K. The calculated results are presented in Table 1. These results have also been fitted to a five-constant polynomial of the form

$$A = a + bT + cT^2 + dT^3 + eT^4 \quad (1)$$

where A is the real gas thermodynamic function in question at temperature T(K). The constants a, b, c, d and e in eqn. (1) have been obtained using linear least-squares curve fitting methods[4] and are found in Table 2. The molecular structural data needed for thermodynamic function calculations are presented in Table 3.

DISCUSSION

The real gas state thermodynamic properties of dihalogenated naphthalenes

* Northwood Pulp, Prince George, British Columbia, Canada.

TABLE I

HEAT CAPACITY [C_p^0], ENTHALPY [$(H^0 - H_0^0)/T$], FREE ENERGY FUNCTIONS [$(F^0 - H_0^0)/T$] AND ENTROPY [S^0], ALL IN UNITS OF CAL MOL^{-1} K^{-1}

Temperature (K)	*1,4-Dichloronaphthalene*				*1,4-Dibromonaphthalene*				*2,3-Dibromonaphthalene*			
	C_p	$(H - H_0)/T$	$-(F - H_0)/T$	S	C_p	$(H - H_0)/T$	$-(F - H_0)/T$	S	C_p	$(H - H_0)/T$	$-(F - H_0)/T$	S
P = 0.25 atm												
451.00	55.93	30.78	86.36	117.14	56.60	31.83	90.95	122.77	56.50	31.63	91.81	123.43
522.70	61.59	34.63	91.18	125.81	62.13	35.61	95.92	131.53	62.07	35.43	96.75	132.18
273.15	38.02	19.98	73.79	93.76	39.29	21.11	77.82	98.93	39.02	20.90	78.78	99.68
298.15	40.77	21.60	75.61	97.21	41.91	22.74	79.74	102.48	41.66	22.53	80.68	103.21
300.00	40.97	21.72	75.74	97.46	42.10	22.86	79.88	102.74	41.85	22.65	80.82	103.47
350.00	46.32	24.86	79.33	104.19	47.26	25.98	83.64	109.62	47.06	25.77	84.55	110.32
400.00	51.31	27.86	82.84	110.70	52.10	28.95	87.30	116.25	51.96	28.74	88.19	116.92
450.00	55.84	30.72	86.29	117.01	56.51	31.77	90.88	122.65	56.41	31.57	91.74	123.31
500.00	59.90	33.44	89.67	123.11	60.48	34.45	94.37	128.81	60.41	34.26	95.20	129.46
550.00	63.50	36.01	92.98	128.99	64.01	36.98	97.77	134.75	63.96	36.80	98.59	135.39
600.00	66.70	38.44	96.22	134.66	67.15	39.36	101.09	140.45	67.12	39.20	101.89	141.09
650.00	69.56	40.72	99.38	140.11	69.95	41.61	104.33	145.94	69.94	41.46	105.12	146.58
700.00	72.10	42.88	102.48	145.36	72.46	43.73	107.49	151.22	72.45	43.58	108.27	151.85
750.00	74.39	44.90	105.51	150.41	74.71	45.72	110.58	156.29	74.71	45.58	111.35	156.93
800.00	76.45	46.81	108.47	155.28	76.73	47.59	113.59	161.18	76.74	47.47	114.35	161.82
850.00	78.31	48.61	111.36	159.97	78.57	49.36	116.53	165.89	78.58	49.24	117.28	166.53
900.00	80.00	50.31	114.19	164.50	80.23	51.03	119.40	170.43	80.24	50.92	120.14	171.07
950.00	81.53	51.91	116.95	168.86	81.75	52.61	122.20	174.81	81.76	52.50	122.94	175.45
1000.00	82.94	53.43	119.65	173.08	83.13	54.10	124.93	179.04	83.14	54.00	125.67	179.68
1050.00	84.22	54.86	122.30	177.16	84.40	55.51	127.61	183.12	84.41	55.42	128.34	183.76
1100.00	85.39	56.23	124.88	181.11	85.56	56.85	130.22	187.08	85.57	56.77	130.95	187.72
1150.00	86.47	57.52	127.41	184.93	86.62	58.12	132.78	190.90	86.64	58.04	133.50	191.54
1200.00	87.46	58.74	129.88	188.63	87.60	59.33	135.28	194.61	87.62	59.25	136.00	195.25

P = 0.50 atm

451.00	56.15	30.67	85.02	115.68	56.85	31.70	89.61	121.31	56.75	31.50	90.47	121.97
522.70	61.73	34.55	89.83	124.38	62.29	35.53	94.57	130.10	62.24	35.35	95.40	130.75
273.15	39.04	19.47	72.58	92.05	40.43	20.54	76.63	97.17	40.17	20.33	77.59	97.92
298.15	41.55	21.22	74.36	95.57	42.79	22.31	78.50	100.81	42.54	22.09	79.45	101.54
300.00	41.74	21.34	74.49	95.83	42.96	22.44	78.64	101.08	42.72	22.22	79.59	101.80
350.00	46.81	24.62	78.03	102.65	47.80	25.71	82.35	108.07	47.61	25.49	83.26	108.76
400.00	51.64	27.70	81.52	109.22	52.46	28.77	85.99	114.76	52.32	28.56	86.87	115.43
450.00	56.07	30.61	84.95	115.56	56.77	31.65	89.54	121.19	56.67	31.44	90.40	121.84
500.00	60.06	33.36	88.32	121.68	60.66	34.36	93.02	127.37	60.59	34.17	93.85	128.02
550.00	63.63	35.95	91.62	127.57	64.15	36.91	96.41	133.32	64.10	36.73	97.23	133.96
600.00	66.80	38.39	94.85	133.25	67.26	39.31	99.73	139.04	67.23	39.14	100.53	139.68
650.00	69.63	40.69	98.02	138.71	70.04	41.57	102.97	144.53	70.02	41.41	103.76	145.17
700.00	72.17	42.85	101.11	143.96	72.52	43.69	106.12	149.82	72.52	43.55	106.90	150.45
750.00	74.44	44.88	104.14	149.02	74.76	45.69	109.21	154.90	74.76	45.56	109.98	155.53
800.00	76.49	46.79	107.10	153.89	76.78	47.57	112.22	159.79	76.78	47.45	112.98	160.43
850.00	78.34	48.59	109.99	158.58	78.60	49.34	115.15	164.50	78.61	49.23	115.91	165.14
900.00	80.03	50.29	112.82	163.11	80.26	51.02	118.02	169.04	80.28	50.91	118.77	169.68
950.00	81.56	51.90	115.58	167.48	81.77	52.60	120.82	173.42	81.79	52.49	121.57	174.06
1000.00	82.96	53.42	118.28	171.70	83.15	54.09	123.56	177.65	83.17	53.99	124.30	178.29
1050.00	84.24	54.86	120.92	175.78	84.42	55.50	126.23	181.74	84.43	55.41	126.97	182.38
1100.00	85.41	56.22	123.50	179.72	85.57	56.85	128.85	185.69	85.59	56.76	129.58	186.33
1150.00	86.48	57.51	126.03	183.54	86.64	58.12	131.40	189.52	86.65	58.03	132.13	190.16
1200.00	87.47	58.74	128.51	187.25	87.62	59.33	133.90	193.23	87.63	59.25	134.62	193.87

TABLE 1 *(continued)*

Temperature (K)	1,4-Dichloronaphthalene				1,4-Dibromonaphthalene				2,3-Dibromonaphthalene			
	C_p	$(H-H_0)/T$	$-(F-H_0)/T$	S	C_p	$(H-H_0)/T$	$-(F-H_0)/T$	S	C_p	$(H-H_0)/T$	$-(F-H_0)/T$	S
P = 1.00 atm												
451.00	56.61	30.44	83.71	114.15	57.36	31.45	88.32	119.77	57.27	31.25	89.17	120.42
522.70	62.02	34.41	88.49	122.91	62.62	35.37	93.24	128.62	62.57	35.19	94.07	129.26
273.15	41.07	18.46	71.53	89.99	42.71	19.41	75.62	95.03	42.47	19.18	76.59	95.77
298.15	43.11	20.44	73.23	93.68	44.54	21.44	77.41	98.85	44.32	21.21	78.36	99.57
300.00	43.27	20.58	73.36	93.94	44.68	21.58	77.55	99.13	44.46	21.35	78.49	99.85
350.00	47.77	24.14	76.81	100.95	48.88	25.18	81.15	106.33	48.71	24.95	82.06	107.01
400.00	52.29	27.38	80.24	107.62	53.19	28.41	84.72	113.14	53.06	28.19	85.61	113.80
450.00	56.53	30.39	83.64	114.03	57.28	31.39	88.25	119.64	57.19	31.19	89.10	120.29
500.00	60.39	33.20	86.99	120.19	61.03	34.17	91.70	125.87	60.97	33.98	92.54	126.52
550.00	63.87	35.83	90.28	126.11	64.43	36.77	95.08	131.85	64.39	36.59	95.90	132.49
600.00	66.99	38.30	93.51	131.80	67.47	39.21	98.38	137.59	67.45	39.04	99.19	138.23
650.00	69.78	40.62	96.66	137.28	70.20	41.49	101.61	143.10	70.19	41.33	102.41	143.74
700.00	72.29	42.79	99.75	142.54	72.66	43.63	104.77	148.39	72.66	43.48	105.55	149.03
750.00	74.54	44.83	102.78	147.61	74.87	45.64	107.85	153.48	74.87	45.50	108.62	154.12
800.00	76.57	46.75	105.73	152.49	76.87	47.53	110.85	158.38	76.88	47.40	111.62	159.02
850.00	78.41	48.56	108.62	157.18	78.68	49.31	113.79	163.10	78.69	49.19	114.54	163.73
900.00	80.08	50.27	111.45	161.71	80.33	50.99	116.65	167.64	80.34	50.88	117.40	168.28
950.00	81.61	51.88	114.21	166.09	81.83	52.57	119.45	172.02	81.84	52.47	120.20	172.66
1000.00	83.00	53.40	116.91	170.31	83.20	54.07	122.19	176.26	83.21	53.97	122.93	176.90
1050.00	84.27	54.84	119.55	174.39	84.46	55.49	124.86	180.35	84.47	55.39	125.59	180.99
1100.00	85.44	56.20	122.13	178.34	85.61	56.83	127.47	184.30	85.62	56.74	128.20	184.94
1150.00	86.51	57.50	124.66	182.16	86.67	58.10	130.03	188.13	86.68	58.02	130.75	188.77
1200.00	87.50	58.73	127.13	185.86	87.64	59.31	132.53	191.84	87.66	59.24	133.25	192.48

P = 2.00 atm

451.00	57.51	30.00	82.48	112.48	58.37	30.95	87.10	118.05	58.29	30.74	87.96	118.70
522.70	62.60	34.13	87.21	121.33	63.27	35.06	91.97	127.02	63.22	34.87	92.80	127.66
273.15	45.14	16.44	70.82	87.26	47.27	17.15	74.99	92.14	47.09	16.89	75.97	92.86
298.15	46.24	18.89	72.37	91.26	48.04	19.70	76.61	96.31	47.86	19.45	77.57	97.01
300.00	46.34	19.06	72.48	91.54	48.12	19.87	76.73	96.60	47.94	19.62	77.69	97.31
350.00	49.71	23.18	75.74	98.93	51.05	24.11	80.12	104.23	50.90	23.87	81.04	104.91
400.00	53.58	26.74	79.07	105.81	54.64	27.69	83.58	111.28	54.53	27.47	84.47	111.94
450.00	57.43	29.94	82.41	112.35	58.30	30.89	87.03	117.92	58.22	30.68	87.89	118.57
500.00	61.06	32.87	85.72	118.59	61.78	33.81	90.44	124.25	61.72	33.61	91.28	124.89
550.00	64.37	35.59	88.98	124.57	64.98	36.50	93.79	130.29	64.95	36.32	94.61	130.93
600.00	67.38	38.11	92.19	130.30	67.90	39.00	97.07	136.07	67.88	38.83	97.88	136.71
650.00	70.08	40.47	95.33	135.80	70.54	41.32	100.29	141.61	70.54	41.17	101.08	142.25
700.00	72.53	42.67	98.41	141.09	72.93	43.50	103.43	146.93	72.93	43.35	104.21	147.56
750.00	74.73	44.74	101.43	146.17	75.09	45.53	106.50	152.03	75.10	45.40	107.27	152.67
800.00	76.73	46.68	104.38	151.05	77.05	47.44	109.50	156.94	77.06	47.31	110.26	157.58
850.00	78.55	48.50	107.26	155.76	78.83	49.24	112.43	161.67	78.84	49.12	113.19	162.31
900.00	80.20	50.21	110.88	160.30	80.45	50.93	115.29	166.22	80.47	50.81	116.04	166.86
950.00	81.70	51.83	112.84	164.68	81.94	52.52	118.09	170.61	81.95	52.42	118.83	171.25
1000.00	83.08	53.36	115.54	168.90	83.29	54.03	120.82	174.85	83.31	53.93	121.56	175.49
1050.00	84.34	54.81	118.18	172.99	84.54	55.45	123.49	178.94	84.55	55.36	124.23	179.58
1100.00	85.50	56.18	120.76	176.94	85.68	56.80	126.11	182.90	85.69	56.71	126.83	183.54
1150.00	86.57	57.47	123.29	180.76	86.73	58.08	128.66	186.73	86.74	57.99	129.38	187.38
1200.00	87.55	58.71	125.76	184.47	87.70	59.29	131.16	190.45	87.71	59.21	131.88	191.09

TABLE 1 *(continued)*

Temperature (K)	1,4-Dichloronaphthalene				1,4-Dibromonaphthalene				2,3-Dibromonaphthalene			
	C_p	$(H-H_0)/T$	$-(F-H_0)/T$	S	C_p	$(H-H_0)/T$	$-(F-H_0)/T$	S	C_p	$(H-H_0)/T$	$-(F-H_0)/T$	S
P = 4.00 atm												
451.00	59.32	29.11	81.39	110.50	60.39	29.96	86.04	116.00	60.34	29.73	86.91	116.64
522.70	63.76	33.56	86.01	119.57	64.57	34.42	90.79	125.21	64.54	34.22	91.63	125.85
273.15	53.27	12.40	70.77	83.17	56.38	12.62	75.11	87.72	56.31	12.30	76.11	88.41
298.15	52.49	15.78	72.01	87.79	55.05	16.22	76.37	92.59	54.95	15.92	77.35	93.27
300.00	52.48	16.01	72.11	88.12	55.00	16.46	76.48	92.93	54.91	16.16	77.45	93.61
350.00	53.57	21.27	74.99	96.26	55.38	21.96	79.45	101.41	55.28	21.69	80.37	102.07
400.00	56.17	25.46	78.11	103.57	57.54	26.26	82.67	108.93	57.46	26.02	83.56	109.58
450.00	59.25	29.04	81.32	110.36	60.34	29.89	85.98	115.87	60.28	29.66	86.84	116.51
500.00	62.38	32.22	84.55	116.77	63.26	33.08	89.29	122.37	63.23	32.87	90.14	123.01
550.00	65.37	35.10	87.76	122.86	66.10	35.95	92.58	128.54	66.08	35.76	93.14	129.17
600.00	68.14	37.74	90.93	128.67	68.76	38.58	95.83	134.41	68.75	38.40	96.63	135.04
650.00	70.69	40.18	94.04	134.22	71.22	41.00	99.01	140.01	71.22	40.83	99.81	140.64
700.00	73.01	42.44	97.11	139.55	73.47	43.24	102.13	145.37	73.48	43.09	102.92	146.00
750.00	75.13	44.55	100.11	144.66	75.53	45.32	105.19	150.51	75.54	45.18	105.96	151.14
800.00	77.06	46.52	103.05	149.57	77.41	47.27	108.18	155.44	77.43	47.14	108.94	156.08
850.00	78.82	48.37	105.92	154.29	79.13	49.09	111.10	160.19	79.15	48.97	111.85	160.83
900.00	80.42	50.11	108.74	158.85	80.71	50.81	113.95	164.76	80.73	50.69	114.70	165.40
950.00	81.90	51.74	111.49	163.23	82.15	52.42	116.74	169.16	82.17	52.31	117.49	169.80
1000.00	83.25	53.29	114.18	167.47	83.48	53.94	119.47	173.41	83.50	53.84	120.21	174.05
1050.00	84.49	54.74	116.62	171.56	84.70	55.38	122.14	177.51	84.71	55.28	122.87	178.15
1100.00	85.63	56.12	119.40	175.52	85.82	56.73	124.74	181.48	85.84	56.64	125.47	182.12
1150.00	86.67	57.43	121.92	179.35	86.85	58.02	127.30	185.32	86.87	57.94	128.02	185.96
1200.00	87.64	58.67	124.39	183.06	87.80	59.24	129.79	189.03	87.82	59.16	130.51	189.68

P = 8.00 atm

451.00	62.93	27.33	80.58	107.91	64.44	27.96	85.31	113.27	64.44	27.71	86.18	113.90
522.70	66.08	32.43	84.99	117.42	67.17	33.15	89.82	122.97	67.17	32.93	90.66	123.59
273.15	69.54	4.31	72.06	76.37	74.60	3.56	76.72	80.27	74.76	3.13	77.75	80.88
298.15	65.00	9.58	72.67	82.25	69.06	9.26	77.29	86.55	69.14	8.88	78.29	87.17
300.00	64.76	9.92	72.73	82.65	68.75	9.63	77.34	86.97	68.83	9.25	78.34	87.59
350.00	61.30	17.44	74.86	92.30	64.04	17.67	79.47	97.14	64.05	17.35	80.42	97.77
400.00	61.35	22.91	77.56	100.47	63.34	23.40	82.22	105.62	63.34	23.11	83.13	106.24
450.00	62.89	27.25	80.52	107.77	64.41	27.88	85.25	113.13	64.41	27.63	86.12	113.75
500.00	65.03	30.92	83.59	114.51	66.23	31.62	88.38	120.01	66.23	31.40	89.23	120.63
550.00	67.36	34.13	86.69	120.82	68.33	34.86	91.55	126.42	68.34	34.66	92.38	127.04
600.00	69.68	37.00	89.78	126.78	70.48	37.74	94.71	132.45	70.50	37.56	95.52	133.08
650.00	71.90	39.60	92.85	132.44	72.57	40.34	97.84	138.18	72.59	40.17	98.64	138.81
700.00	73.98	41.98	95.87	137.85	74.55	42.72	100.92	143.63	74.58	42.56	101.70	144.26
750.00	75.91	44.18	98.84	143.02	76.41	44.90	103.94	148.84	76.43	44.76	104.71	149.47
800.00	77.70	46.22	101.76	147.98	78.14	46.92	106.90	153.83	78.16	46.79	107.67	154.46
850.00	79.36	48.12	104.62	152.74	79.74	48.81	109.80	158.61	79.76	48.68	110.56	159.24
900.00	80.88	49.90	107.42	157.32	81.22	50.57	112.64	163.21	81.24	50.45	113.39	163.85
950.00	82.28	51.56	110.16	161.73	82.59	52.22	115.42	167.64	82.61	52.11	116.17	168.28
1000.00	83.58	53.13	112.85	165.98	83.85	53.77	118.14	171.91	83.87	53.67	118.88	172.55
1050.00	84.77	54.61	115.48	170.09	85.02	55.23	120.80	176.03	85.04	55.13	121.53	176.67
1100.00	85.87	56.01	118.05	174.06	86.10	56.61	123.40	180.01	86.12	56.52	124.13	180.65
1150.00	86.89	57.33	120.57	177.90	87.10	57.91	125.95	183.86	87.12	57.83	126.67	184.50
1200.00	87.83	58.58	123.04	181.62	88.02	59.15	128.44	187.58	88.04	59.07	129.16	188.23

TABLE I *(continued)*

Temperature	*1,4-Dichloronaphthalene*				*1,4-Dibromonaphthalene*				*2,3-Dibromonaphthalene*			
(K)	C_p	$(H-H_0)/T$	$-(F-H_0)/T$	S	C_p	$(H-H_0)/T$	$-(F-H_0)/T$	S	C_p	$(H-H_0)/T$	$-(F-H_0)/T$	S
P = 16.00 atm												
451.00	70.16	23.78	80.35	104.13	72.54	23.98	85.22	109.20	72.63	23.68	86.11	109.79
522.70	70.73	30.16	84.34	114.49	72.37	30.60	89.26	119.86	72.44	30.35	90.11	120.46
273.15	102.08	−11.85	76.00	64.15	111.04	−14.56	81.31	66.75	111.65	−15.22	82.42	67.21
298.15	90.02	−2.84	75.37	72.53	97.08	−4.66	80.49	75.83	97.51	−5.21	81.54	76.33
300.00	89.32	−2.27	75.36	73.08	96.26	−4.03	80.46	76.43	96.68	−4.58	81.51	76.93
350.00	76.77	9.79	75.98	85.77	81.37	9.09	80.90	89.99	81.59	8.66	81.88	90.54
400.00	71.71	17.79	77.85	95.64	74.95	17.66	82.71	100.37	75.09	17.31	83.64	100.95
450.00	70.17	23.68	80.30	103.97	72.56	23.87	85.17	109.04	72.66	23.57	86.06	109.63
500.00	70.34	28.32	83.04	111.36	72.17	28.71	87.94	116.65	72.25	28.45	88.80	117.25
550.00	71.35	32.19	85.92	118.11	72.80	32.68	90.87	123.55	72.86	32.45	91.71	124.16
600.00	72.75	35.51	88.87	124.38	73.92	36.07	93.86	129.93	73.98	35.86	94.68	130.54
650.00	74.31	38.43	91.83	130.26	75.28	39.03	96.87	135.90	75.33	38.84	97.67	136.52
700.00	75.91	41.05	94.78	135.83	76.72	41.67	99.86	141.53	76.77	41.50	100.65	142.15
750.00	77.48	43.43	97.69	141.12	78.17	44.06	102.82	146.87	78.22	43.90	103.60	147.50
800.00	79.00	45.60	100.56	146.17	79.59	46.23	105.73	151.96	79.63	46.09	106.50	152.59
850.00	80.44	47.61	103.39	151.00	80.95	48.24	108.59	156.83	80.99	48.10	109.36	157.46
900.00	81.79	49.47	106.16	155.64	82.24	50.09	111.40	161.49	82.27	49.97	112.16	162.12
950.00	83.06	51.21	108.89	160.09	83.45	51.81	114.16	165.97	83.49	51.70	114.91	166.61
1000.00	84.24	52.83	111.55	164.38	84.59	53.42	116.86	170.28	84.62	53.32	117.60	170.92
1050.00	85.35	54.35	114.17	168.52	85.66	54.93	119.50	174.44	85.69	54.83	120.24	175.07
1100.00	86.37	55.78	116.73	172.51	86.65	56.35	122.09	178.45	86.68	56.26	122.82	179.08
1150.00	87.33	57.13	119.24	176.38	87.58	57.69	124.63	182.32	87.61	57.60	126.35	182.96
1200.00	88.22	58.41	121.70	180.11	88.45	58.96	127.11	186.06	88.47	58.87	127.83	186.70

TABLE 2

CALCULATED CONSTANTS a, b, c, d AND e IN EQN. (1)

Pressure (atm)					
A. 1,4-Dichloronaphthalene					
	Cp				
	a	*b*	$c \times 10^3$	$d \times 10^7$	$e \times 10^{11}$
0.25	−5.06558	0.19826	−0.16811	0.57045	−0.92124
0.50	−0.26267	0.17478	−0.12506	0.32499	0.09599
1.00	9.34374	0.12783	−0.03893	−0.36605	2.13090
2.00	28.55632	0.03393	0.13332	−1.74805	6.20036
4.00	66.98050	−0.15387	0.47780	−4.51189	14.33874
8.00	143.8327	−0.52949	1.16683	−10.04033	30.61833
16.00	247.5320	−1.28070	2.54481	−21.09631	63.17413
$-(F - H_0)/T$					
	a	$b \times 10$	$c \times 10^2$	$d \times 10^6$	$e \times 10^{11}$
0.25	52.87711	0.79790	−0.10948	−0.37749	0.17104
0.50	52.29250	0.75903	−0.03813	−0.95018	0.33971
1.00	52.50105	0.68128	0.10465	−2.09640	0.67735
2.00	54.29585	0.52576	0.39023	−4.38884	1.35260
4.00	59.26212	0.21470	0.96126	−8.97258	2.70270
8.00	70.57228	−0.40725	2.10338	−18.14066	5.40316
16.00	94.56909	−1.65119	4.38742	−36.47466	10.80318
$(H - H_0)/T$					
	a	$b \times 10$	$c \times 10^1$	$d \times 10^5$	$e \times 10^{11}$
0.25	−0.34884	0.82461	−0.28825	−0.39783	0.41174
0.50	−2.74291	0.94174	−0.50319	1.32696	−0.09620
1.00	−7.53073	1.17598	−0.93300	4.77601	−1.11191
2.00	−17.10756	1.64454	−1.79293	11.67612	−3.14402
4.00	−36.25911	2.58150	−3.51206	25.47184	−7.20656
8.00	−74.56635	4.45575	−6.95136	53.07234	−15.33507
16.00	−151.1715	8.20356	−13.82821	108.255	−31.58549
S					
	a	*b*	$c \times 10^1$	$d \times 10^5$	$e \times 10^{11}$
0.25	52.52809	0.16225	−0.39775	−0.77521	0.58276
0.50	49.54965	0.17008	−0.54129	0.37654	0.24360
1.00	44.97041	0.18572	−0 82832	2.67927	−0.43441
2.00	37.18875	0.21703	−1.40250	7.28617	−1.79099
4.00	23.00304	0.27963	−2.55081	16.49953	−4.50401
8.00	−3.99098	0.40483	−4.84743	34.92626	−9.93007
16.00	−56.60272	0.65524	−9.44085	71.78111	−20.78253
B. 1,4,-Dibromonaphthalene					
	Cp				
	a	*b*	$c \times 10^3$	$d \times 10_1$	$e \times 10^{11}$
0.25	−1.60320	0.18593	−0.14904	0.53215	−0.53961
0.50	3.77721	0.15963	−0.10081	0.14514	0.59998
1.00	14.53819	0.10704	−0.00433	−0.62894	2.87935
2.00	36.06052	0.00185	0.18863	−2.17715	7.43834
4.00	79.10579	−0.20854	0.57456	−5.27360	16.55631
8.00	165.1921	−0.62928	1.34635	−11.46590	34.79035
16.00	337.3684	−1.47080	2.88999	−23.85109	71.26033

TABLE 2 *(continued)*

Pressure (atm)

$-(F - H_o)/T$

	a	*b* × 10	*c* × 10^4	*d* × 10^8	*e* × 10^{11}
0.25	0.58102	0.84589	−0.35196	0.17880	0.23378
0.50	−2.10156	0.97712	−0.39277	2.11122	−0.33531
1.00	−7.46619	1.23956	−1.07430	5.97516	−1.47317
2.00	−18.19701	1.76454	−2.03764	13.70589	−3.74992
4.00	−39.65651	2.81434	−3.96388	29.16278	−8.30166
8.00	−82.57599	4.91400	−7.81655	60.07901	−17.40627
16.00	−168.4168	9.11341	−15.52207	121.9119	−35.61540

$(H - H_o)/T$

	a	*b* × 10	*c* × 10^5	*d* × 10^8	*e* × 10^{13}
0.25	55.26588	0.88277	−0.21727	0.31924	−0.72692
0.50	54.7774	0.83920	−0.13729	−0.32273	18.17952
1.00	55.17790	0.75207	0.02269	−1.60690	56.00358
2.00	57.35649	0.57777	0.34270	−4.17563	131.6639
4.00	63.09090	0.22921	0.98268	−9.31264	282.9693
8.00	75.93867	−0.46904	2.26291	−19.58954	585.6822
16.00	103.0089	−1.86234	4.92284	−40.13748	1190.884

S

	a	*b* × 10	*c* × 10^4	*d* × 10^8	*e* × 10^{13}
0.25	55.26588	0.88277	−0.21727	0.31924	−0.72692
0.50	52.67624	1.81630	−0.72999	1.78775	−15.32358
1.00	47.71114	1.99167	−1.05171	4.36931	−91.35060
2.00	39.15916	2.34234	−1.69499	9.53081	−243.3435
4.00	23.43484	3.04351	−2.98112	19.84449	−547.1784
8.00	−6.63981	4.44613	−5.55407	40.49389	−1155.105
16.00	−65.4109	7.25128	−10.69973	81.77953	−2370.819

C. 2,3-Dibromonaphthalene

	Cp				
	a	*b*	*c* × 10^3	*d* × 10^7	*e* × 10^{11}
0.25	−2.483980	0.1890391	−0.1530041	0.5538795	−0.5622517
0.50	2.962775	0.1624179	−0.1041716	0.1620785	0.5714625
1.00	13.85629	0.1091756	−0.0065063	0.6215271	2.878904
2.00	35.64401	0.0026856	0.1888381	−2.188885	7.494336
4.00	79.21877	−0.2102894	0.5795124	−5.323444	16.72456
8.00	166.3656	−0.6362184	1.360807	−11.59196	35.1829
16.00	340.6704	−1.488164	2.92363	−24.13157	72.10914

$-(F - H_o)/T$

	a	*b* × 10	*c* × 10^4	*d* × 10^8	*e* × 10^{12}
0.25	56.54803	0.8663541	−0.1966534	0.1916614	0.2383302
0.50	56.07050	0.8222568	−0.1156993	−0.458048	2.151901
1.00	56.49339	0.7340217	0.0462995	−1.758424	5.981887
2.00	58.71620	0.5575763	0.3702517	−4.358732	13.64078
4.00	64.53960	0.2046604	1.018211	−9.559864	28.96033
8.00	77.56296	−0.5011096	2.313966	−19.96039	59.59294
16.00	104.9895	−1.912822	4.905909	−40.76595	120.8743

TABLE 2 *(continued)*

Pressure (atm)

	$(H - H_0)/T$				
	a	$b \times 10$	$c \times 10^5$	$d \times 10^9$	$e \times 10^{11}$
0.25	0.5262215	0.8336449	−0.3215286	−0.8931202	0.3156192
0.50	−2.189636	0.9665096	−0.565331	18.67157	−0.2605558
1.00	−7.620900	1.232204	−1.052851	57.79253	−1.412622
2.00	−18.48347	1.763598	−2.027895	136.0345	−3.716744
4.00	−40.20947	2.826445	−3.978116	292.5313	−8.325361
8.00	−83.55006	4.952063	−7.878472	605.5255	−17.54304
16.00	−170.5600	9.203175	−15.67872	1231.448	−35.97547
	S				
	a	*b*	$c \times 10^4$	$d \times 10^8$	$e \times 10^{11}$
0.25	57.07390	0.1700024	−0.5182411	0.1029281	0.3392538
0.50	53.88126	0.1788733	−0.6809413	1.408112	−0.0450000
1.00	48.87277	0.1966203	−1.006487	4.020139	−0.814167
2.00	40.23260	0.232118	−1.657655	9.244786	−2.352651
4.00	24.32994	0.3031125	−2.959988	19.69445	−5.429883
8.00	−6.096951	0.4450924	−5.56438	40.59023	−11.58285
16.00	−65.57256	−0.1912822	−4.905909	−40.76595	12.08743

were calculated in the same way as those for α- and β-halonaphthalenes[2, 3], that is, the already calculated ideal gas state thermodynamic function values for dihalogenated naphthalenes[1] were corrected by means of the second virial coefficient expansion of the Berthelot equation of state[2, 3]. The resulting equations, given as the real gas deviations from the ideal gas state (at one atmosphere pressure) are[2, 5]

$$(H - H_0)/T = \frac{9}{128}\frac{RT_c}{P_c}\left[1 - 18\left(\frac{T_c}{T}\right)^2\right]P \tag{2}$$

$$(C_p - C_p^0) = \frac{81}{32}\left(\frac{RT_c^3}{P_cT^3}\right)P \tag{3}$$

$$(S^0 - S) = \frac{27}{32}\left(\frac{RT_c^3}{P_cT^3}\right)P + R\ln P \tag{4}$$

The term $R\ln P$ [eqn. (4)] is a correction factor which must be included to obtain the ideal gas entropy at pressure P, provided that this correction term has not already been included in the ideal gas S^0-expression. The free energy function (Table 1) however is found by subtracting eqn. (4) from eqn. (2). The applicability of the second virial coefficient-truncated Berthelot state equation [eqns. (2–4)] has been discussed in detail by Butler and Lielmezs[5] for fluorobenzene, and by McFee and Lielmezs[2, 3] for α- and β-halonaphthalenes. The critical point properties (T_c, P_c) needed for 1,4-dichloronaphthalene were estimated by means of the Lydersen

TABLE 3

MOLECULAR PARAMETERS

1,4-Dichloronaphthalene	*1,4-Dibromonaphthalene*	*2,3-Dibromonaphthalene*
Fundamental frequencies[a] (ν, cm^{-1})		
188 150 224 371 411	185 140 215 371 409	174 139 249 357 406
494 517 530 597 676	470 517 527 560 662	481 574 593 607 635
755 745 826 790 816	753 745 823 791 814	758 745 784 814 862
328 900 824 926 120	289 905 823 927 95	132 878 890 957 294
956 987 987 1023 224	956 963 963 1021 174	890 947 961 1019 139
1146 1163 443 1205 1184	1142 1161 377 1207 1187	1136 1148 357 1192 1198
1260 1371 1363 1371 1415	1256 1368 1352 1368 1410	1262 1338 1301 1418 1428
1450 1502 1560 1589 1624	1450 1494 1556 1566 243	1476 1576 1556 1383 1624
3076 328 517 3027 3031	377 3027 3031 3060 3060	3076 279 357 3027 3031
3060 3060 3076	3076 1624 3076	3060 3060 3076
Product of the principal moment of inertia[b] (gm^3 cm^6)		
$2{,}398{,}517 \times 10^{-117}$	$10{,}377{,}640 \times 10^{-117}$	$9{,}213{,}850 \times 10^{-117}$
Normal boiling point (K)		
563.15	560.00	584.15
Critical temperature[c] (K)		
823.80	859.50	868.00
Critical pressure[c] (atm)		
33.93	34.00	35.00
Symmetry number (σ)		
2	2	
Molecular weight		
197.07	285.97	285.97

[a] Frequencies selected by McFee and Lielmezs[1].
[b] Principal moments of inertia calculated by McFee and Lielmezs[1].
[c] Estimated, this work.

method[6] using the experimentally-known boiling point[7] corrected to one atm pressure. However, the critical properties of 1,4-dibromonaphthalene and 2,3-dibromonaphthalene were estimated by analogy with 1,4-dichloronaphthalene as well as with the chlorinated naphthalenes[2, 3] and benzenes[8]. The error introduced in the critical parameter values will not exceed $\pm$ 2.0% since the molecular weights of 1,4-dibromonaphthalene and 2,3-dibromonaphthalene are the same; the critical parameters of 1,4-dichloronaphthalene were estimated on the basis of an experimentally-available boiling point temperature value.

The accuracy of the results presented in Tables 1 and 2, and the range of applicability of eqns. (2–4), however, must be inferred from previously discussed[2] general considerations. Using the error estimation methods already introduced[1–3,5] it is found that the calculated ideal gas state thermodynamic functions for dihalogenated naphthalenes should be reliable within the 400–1000 K temperature range 400–1000 K, with the expected error ranging from $\pm$ 0.5% to $\pm$ 2%.

Indeed, following the error analysis as outlined by McFee and Lielmezs[2, 3] for real gas thermodynamic function values of α- and β-halonaphthalenes, it is suggested that the calculated real gas thermodynamic function values for dihalogenated naphthalenes (Tables 1 and 2) should not exceed the overall error estimate of $\pm$ 1% to $\pm$ 2.5%. This error is expected to hold for all pressures between temperatures of 500 and 1100 K. However, it should be noted that thermodynamic properties of any dihalogenated naphthalene gas are determined from their boiling points up. Hence, calculated thermodynamic property values (Tables 1 and 2) should be used noting this limitation. If, however, any thermodynamic property value is used below the boiling point, then such a value would refer to a hypothetical vapor of the dihalogenated naphthalene. This effect starts to become noticeable at pressures higher than 4 atm (Table 1).

ACKNOWLEDGEMENTS

The financial assistance of the National Research Council of Canada and the President's Research Grant, University of British Columbia, Vancouver, B.C., Canada, is gratefully acknowledged.

REFERENCES

1 D. G. McFee and J. Lielmezs, unpublished material.
2 D. G. McFee and J. Lielmezs, *Thermochim. Acta*, 24 (1978) 39.
3 D. G. McFee and J. Lielmezs, *Thermochim. Acta*, 24 (1978) 55.
4 J. Streal and L. C. Moore, *Curve Fitting Methods*, Computer Centre, The University of British Columbia, 1976.
5 J. B. Butler and J. Lielmezs, *Thermochim. Acta*, 9 (1974) 359.
6 R. C. Reid, J. M. Prausnitz and J. K. Sherwood, *The Properties of Gases and Liquids*, 3rd. edn., McGraw-Hill, 1977.
7 R. C. Weast, (Ed.), *Handbook of Chemistry and Physics*, 56th ed. The Chemical Rubber Co., Cleveland, Ohio, 1975.
8 J. B. Butler and J. Lielmezs, *J. Chem. Eng. Data*, 14 (1969) 335.