

Equation of State of Sodium Chloride

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BECAUSE of many requests, I wish to publish the following numerical table of results for the equation of state of NaCl as calculated in an earlier paper¹ along with a few comments on various proposed equations for NaCl. Table I gives the pressure in kilobars at the corresponding values of $\Delta a/a_0$ and temperature in the appropriate row and column. The parameter $\Delta a/a_0$ is the fractional compression of the lattice parameter where the standard value a_0 is the appropriate lattice parameter at zero pressure and 25°C. The increments between the values given in the table were chosen such that one can linearly interpolate between the tabulated values to an accuracy of better than 0.02 kbar.

In recent years several equations have been proposed to give the volume change vs pressure for NaCl at room temperature.^{2,3} A comparison of these equations and the results in Table I is given in Fig. 1 along with experimental measurements by Bridgman,⁴ Christian,⁵ and Perez-Albuérne and Drickamer.³ This figure gives the differences in $\Delta V/V_0$ of the respective equations or experimental measurements at a specified pressure to the $\Delta V/V_0$ calculated in Ref. 1, at that pressure. Experimental values of NaCl compression have been measured by Jeffery *et al.*⁶ at the pressure of the bismuth I-II phase transition. If the value of 25.4 kbar⁷ is accepted for the Bi I-II transition, then Jeffery's measurement of $\Delta V/V_0 = -0.084 \pm 0.02$ for the compression of NaCl at this transition gives one point at which both P and V are simultaneously known. This point is shown by the large square in Fig. 1. It is noted that all results agree to within the accuracy of the x-ray measurement at 25.4 kbar except Murnaghan's equation employing parameters from sound velocity measurements by Bartles and Schuele.⁸ The same Murnaghan equation definitely gives too small a compression at high pressures. If one chooses a value of $B_0' = 4.60$ rather than the 5.35 reported by Bartles and Schuele, the resulting Murnaghan equation is in good agreement

with the experimental data at low pressures. B_0' is the pressure derivative of the bulk modulus and is assumed to be independent of pressure in Murnaghan's equation. Even with the smaller choice of B_0' , the Murnaghan equation appears to become definitely less accurate at high pressures.

It is concluded that the value of B_0' given by Bartles and Schuele is probably too large and that B_0' for NaCl must vary with pressure, making the Murnaghan equation a poor equation of state at higher pressures. The experimental data is, however, too scattered to make a choice between the equations of Perez-Albuérne

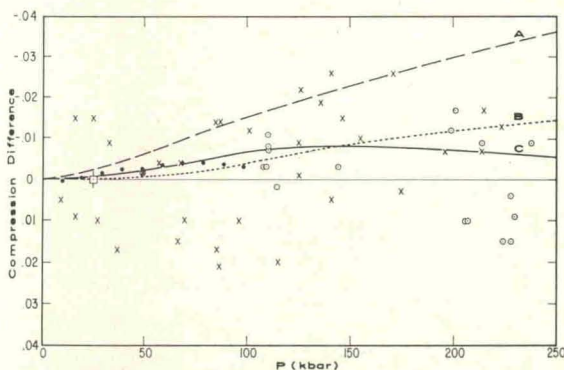


FIG. 1. Comparison of calculated and measured compressions as a function of pressure for NaCl. The ordinate is $\Delta V/V_0$ calculated by Decker minus $\Delta V/V_0$ calculated or measured by others. Curve A is Murnaghan's equation with B_0 and B_0' taken from Ref. 8. Curve B is Murnaghan's equation with B_0 as in A but $B_0' = 4.60$. Curve C is calculated by Perez-Albuérne and Drickamer, Ref. 3. ● smoothed data from Bridgman, Ref. 4. × measurements by Perez-Albuérne and Drickamer, Ref. 3. ○ dynamic measurements by Christian, Ref. 5. □ measurement by Jeffery *et al.*, Ref. 6.

TABLE I. Calculated pressure at given compressions and temperatures from 0–500 kbar and 0°C–mp for NaCl. Based on equation of state by Decker.^a

$\Delta \epsilon / \epsilon_0$	0 c	25 c	100 c	200 c	300 c	400 c	500 c	600 c	700 c	800 c	900 c	1000 c	1200 c	1400 c	1600 c	1800 c	2000 c
0.040										0.45							
0.038										1.25	4.03						
0.036										2.09	4.87						
0.034										1.03	3.83	6.63					
0.032										1.94	4.75	7.55	10.36				
0.030										2.88	5.69	8.51	11.32				
0.028									0.07	3.85	6.67	9.49	12.31				
0.026									2.02	4.83	7.67	10.50	13.33				
0.024									3.04	5.87	8.71	11.55	14.39				
0.022							0.21	1.25	4.10	6.93	9.78	12.62	15.47				
0.020							2.33	5.18	8.03	10.88	13.74	16.59					
0.018							3.45	6.30	9.16	12.02	14.88	17.74	23.47				
0.016						0.60	4.56	7.46	10.32	13.19	16.06	18.93	24.67				
0.014						1.74	5.78	8.65	11.52	14.40	17.28	20.15	25.91				
0.012					0.06	2.92	5.38	8.26	11.15	14.03	16.93	19.82	22.71	28.50			
0.010					1.26	4.13	7.00	9.88	12.76	15.64	18.53	21.41	27.19				
0.008					2.50	5.38	8.26	11.15	14.03	16.93	19.82	22.71	28.50				
0.006					3.79	6.67	9.56	12.45	15.35	18.25	21.15	24.05	29.86				
0.004					5.11	8.00	10.90	13.80	16.70	19.61	22.52	25.43	31.25				
0.002				0.92	3.79	6.67	9.56	12.45	15.35	18.25	21.15	24.05	29.86				
0.000			0.73	3.59	6.47	9.37	12.27	15.18	18.09	21.01	23.92	26.84	32.68				
-0.002		0.00	2.12	4.99	7.88	10.78	13.69	16.61	19.53	22.45	25.38	28.30	34.16	40.02			
-0.004	0.74	1.43	3.56	6.43	9.33	12.24	15.16	18.08	21.01	23.94	26.87	29.80	35.68	41.56			
-0.006	2.21	2.91	5.03	7.91	10.82	13.74	16.66	19.59	22.53	25.47	28.41	31.34	37.24	43.13			
-0.008	3.72	4.42	6.56	9.44	12.35	15.28	18.21	21.15	24.10	27.04	29.99	32.94	38.84	44.75			
-0.010	5.28	5.99	8.12	11.02	13.93	16.87	19.81	22.76	25.71	28.66	31.62	34.58	40.50	46.42			
-0.012	6.89	7.60	9.74	12.64	15.56	18.50	21.45	24.41	27.37	30.33	33.30	36.26	42.20	48.14			
-0.014	8.55	9.26	11.40	14.38	17.24	20.19	23.15	26.11	29.07	32.03	35.02	37.99	43.95	49.90			
-0.016	10.26	10.97	13.12	16.03	18.97	21.92	24.89	27.86	30.84	33.81	36.80	39.78	45.75	51.72			
-0.018	12.02	12.73	14.88	17.80	20.75	23.71	26.68	29.66	32.65	35.63	38.62	41.62	47.60	53.59			
-0.020	13.83	14.54	16.70	19.62	22.58	25.55	28.53	31.51	34.51	37.50	40.50	43.50	49.50	55.51	61.52		
-0.022	15.69	16.40	18.56	21.50	24.46	27.44	30.43	33.42	36.42	39.43	42.39	45.45	51.46	57.48	63.51		
-0.024	17.61	18.32	20.49	23.43	26.40	29.39	32.38	35.38	38.39	41.40	44.43	47.44	53.48	59.51	65.55		
-0.026	19.59	20.30	22.47	25.42	28.40	31.39	34.39	37.40	40.42	43.44	46.46	49.49	55.54	61.59	67.65		
-0.028	21.62	22.33	24.51	27.46	30.45	33.45	36.46	39.48	42.50	45.53	48.57	51.60	57.67	63.74	69.81		
-0.030	23.71	24.43	26.61	29.57	32.56	35.57	38.59	41.62	44.65	47.68	50.71	53.77	59.86	65.94	72.03		
-0.032	25.87	26.58	28.77	31.73	34.73	37.75	40.78	43.81	46.85	49.90	52.95	56.00	62.10	68.20	74.31		
-0.034	28.08	28.80	30.00	33.66	36.97	39.99	43.03	46.07	49.12	52.17	55.24	58.29	64.41	70.53	76.65		
-0.036	30.36	31.08	33.27	36.25	39.26	42.30	45.34	48.39	51.45	54.51	57.58	60.66	66.78	72.92	79.06	85.20	
-0.038	32.71	33.43	35.62	38.61	41.63	44.67	47.72	50.78	53.85	56.91	60.00	63.08	69.22	75.37	81.53	87.69	
-0.040	35.12	35.84	38.04	41.03	44.06	47.11	50.17	53.23	56.31	59.39	62.48	65.56	71.74	77.89	84.07	90.25	
-0.042	37.60	38.32	40.53	43.52	46.56	49.61	52.68	55.76	58.84	61.93	65.00	68.11	74.30	80.48	86.68	92.88	
-0.044	40.15	40.87	43.08	46.09	49.13	52.19	55.27	58.35	61.44	64.54	67.65	70.74	76.95	83.15	89.36	95.57	101.79
-0.046	42.78	43.50	45.71	48.72	51.77	54.84	57.93	61.02	64.12	67.22	70.33	73.42	79.63	85.84	92.05	98.26	104.48
-0.048	45.47	46.20	48.41	51.43	54.49	57.57	60.66	63.76	66.86	69.96	73.07	76.17	82.38	88.59	94.80	101.01	107.24
-0.050	48.25	48.97	51.19	54.22	57.28	60.37	63.47	66.57	69.67	72.78	75.88	79.00	85.21	91.42	97.63	103.84	110.07
-0.052	51.10	51.82	54.05	57.08	60.15	63.24	66.35	69.47	72.59	75.72	78.86	82.01	88.22	94.43	100.64	106.85	113.09
-0.054	54.03	54.78	56.98	60.02	63.10	66.20	69.32	72.44	75.57	78.71	81.86	85.00	91.21	97.42	103.63	109.84	116.09
-0.056	57.04	57.80	60.00	63.05	66.13	69.24	72.36	75.50	78.64	81.78	84.94	88.09	94.30	100.51	106.72	112.93	119.16
-0.058	60.14	60.87	63.10	66.15	69.25	72.36	75.50	78.64	81.78	84.94	88.11	91.27	97.49	103.71	109.93	116.15	122.38
-0.060	63.32	64.05	66.29	69.35	72.45	75.57	78.71	81.86	85.02	88.18	91.36	94.54	100.77	106.99	113.21	119.44	125.67
-0.062	66.59	67.32	69.57	72.63	75.74	78.87	82.02	85.17	88.34	91.51	94.70	97.88	104.24	110.59	116.94	123.30	129.71
-0.064	69.95	70.68	72.93	76.00	79.12	82.25	85.41	88.58	91.75	94.91	98.13	101.31	107.69	114.06	120.45	126.84	133.24
-0.066	73.41	74.14	76.39	79.47	82.59	85.74	88.90	92.08	95.26	98.44	101.66	104.84	111.24	117.63	124.04	130.45	136.86
-0.068	76.96	77.69	79.94	83.03	86.15	89.31	92.48	95.67	98.86	102.05	105.27	108.47	114.88	121.29	127.72	134.14	140.57
-0.070	80.60	81.34	83.59	86.68	89.82	92.98	96.16	99.35	102.55	105.76	108.98	112.19	118.62	125.05	131.49	137.94	144.38
-0.072	84.35	85.08	87.34	90.44	93.58	96.75	99.94	103.14	106.35	109.56	112.79	116.07	122.47	128.91	135.37	141.83	148.30
-0.074	88.20	88.93	91.20	94.30	97.45	100.63	103.82	107.03	110.25	113.47	116.71	119.93	126.31	132.75	139.20	145.65	152.11
-0.076	92.15	92.88	95.15	98.26	101.43	104.61	107.81	111.03	114.25	117.48	120.73	123.97	130.36	136.81	143.26	149.73	156.20
-0.078	96.21	96.95	99.22	102.33	105.50	108.69	111.90	115.13	118.36	121.60	124.86	128.11	134.51	141.00	147.50	154.00	160.50
-0.080	100.38	101.12	103.39	106.51	109.68	112.89	116.11	119.34	122.58	125.83	129.08	132.36	138.81	145.35	151.92	158.46	165.00
-0.082	104.66	105.40	107.68	110.80	113.98	117.19	120.42	123.67	126.92	130.17	133.45	136.72	143.20	149.75	156.34	162.93	169.53
-0.084	109.06	109.80	112.08	115.21	118.40	121.62	124.86	128.11	131.37	134.63	137.90	141.19	147.75	154.30	160.87	167.44	174.02
-0.086	113.58	114.32	116.60	119.74	122.93	126.16	129.41	132.67	135.93	139.21	142.50	145.79	152.36	158.93	165.52	172.11	178.70
-0.088	118.22	118.96	121.24	124.39	127.58	130.82	134.09	137.35	140.62	143.91	147.19	150.50	157.10	163.68	170.29	176.90	183.51
-0.090	122.98	123.72	126.01	129.16	132.37	135.61	138.89	142.15	145.44	148.73	152.04	155.34	162.00	168.65	175.31	181.98	188.64
-0.092	127.87	128.61	130.91	134.06	137.28	140.52	143.78	147.08	150.38	153.68	156.98	160.31	167.05	173.76	180.48	187.20	193.90
-0.094	132.89	133.63	135.93	139.09	142.32	145.57	148.86	152.14	155.45	158.76	162.09	165.40	172.15	178.87	185.56	192.26	198.99
-0.096	138.05	138.79	141.09	144.26	147.49	150.75	154.05	157.34	160.65	163.97	167.29	170.64	177.31	183.97	190.64	197.33	204.02
-0.098	143.34	144.08	146.39	149.56	152.81	156.06	159.38	162.67	166.00	169.32	172.67	176.01	182.75	189.49	196.26	203.03	209.80
-0.100	148.78	149.52	151.82	155.00	158.24	161.52	164.85	168.15	171.48	174.82	178.15	181.52	188.23	194.94	201.66	208.38	215.10
-0.102	154.35	155.10	157.41	160.59	163.86	167.12	170.46	173.77	177.11	180.45	183.82	187.18	193.90	200.63	207.36	214.11	220.90
-0.104	160.05	160.80	163.11	166.29	169.50	172.71	175.97	179.28	182.59	185.9							