

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-Albuerne 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-Albuerne

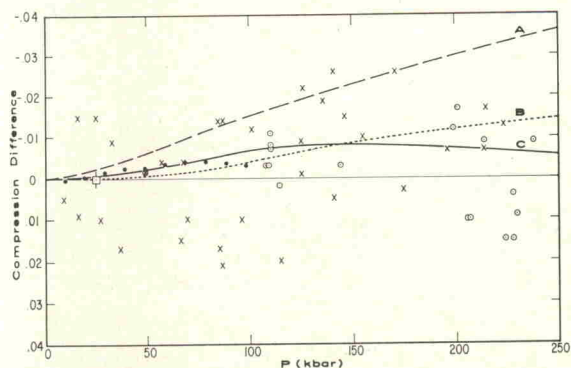


FIG. 1. Comparison of calculated and measured compressions as a function of pressure for NaCl. The ordinate is $\Delta V/V_0$ calculated by Decker minus $\Delta V/V_0$ calculated or measured by others. Curve A is Murnaghan's equation with B_0 and B_0' taken from Ref. 8. Curve B is Murnaghan's equation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

$\frac{\Delta s}{s_0}$	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										2.94	5.74						
0.032									0.15	1.03	3.83	6.63					
0.030									1.94	4.75	7.55	10.36					
0.028								0.07	2.88	5.69	8.51	11.32					
0.026								1.03	3.85	6.67	9.49	12.31					
0.024								2.02	4.83	7.67	10.50	13.30					
0.022								3.01	5.87	8.71	11.55	14.39					
0.020							0.21	1.25	4.10	6.93	9.78	12.62	15.47				
0.018							2.33	5.18	8.03	10.88	13.74	16.59					
0.016						0.60	3.45	6.30	9.16	12.02	14.88	17.74	23.47				
0.014						1.74	4.56	7.46	10.32	13.19	16.06	18.93	24.67				
0.012					0.06	2.92	5.78	8.65	11.52	14.40	17.28	20.15	25.91				
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				0.92	2.24	5.11	8.00	10.90	13.80	16.70	19.61	22.52	25.43	31.25			
0.002			0.73	3.59	6.47	9.37	12.27	15.18	18.09	21.01	23.92	26.84	32.68				
0.000		0.00	2.12	4.99	7.88	10.78	13.69	16.61	19.53	22.45	25.38	28.03	34.16	40.02			
-0.002	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			
-0.004	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			
-0.006	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			
-0.008	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			
-0.010	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			
-0.012	8.55	9.26	11.40	14.38	17.24	20.19	23.15	26.11	29.07	32.05	35.02	37.99	43.95	49.90			
-0.014	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			
-0.016	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			
-0.018	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		
-0.020	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		
-0.022	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		
-0.024	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		
-0.026	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		
-0.028	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		
-0.030	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		
-0.032	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		
-0.034	30.36	31.08	32.27	35.25	39.26	42.30	45.34	48.39	51.45	54.51	57.48	60.66	66.78	72.92	79.06	85.20	
-0.036	32.71	33.43	34.62	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	
-0.038	35.12	35.84	37.04	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	
-0.040	37.60	38.32	39.53	43.52	46.56	49.61	52.68	55.76	58.84	61.93	64.99	68.11	74.30	80.48	86.68	92.88	
-0.042	40.15	40.87	42.08	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
-0.044	42.78	43.50	44.71	48.72	51.77	54.84	57.93	61.02	64.12	67.22	70.33	73.42	79.61	85.88	92.11	98.34	104.58
-0.046	45.47	46.20	47.41	51.43	54.49	57.57	60.66	63.75	66.86	69.96	73.10	76.21	82.45	88.69	94.94	101.19	107.44
-0.048	48.25	48.97	50.19	54.22	57.28	60.37	63.47	66.57	69.69	72.81	75.94	79.08	85.32	91.57	97.84	104.11	110.37
-0.050	51.10	51.82	53.05	57.08	60.15	63.24	66.35	69.47	72.59	75.72	78.86	82.01	88.26	94.54	100.82	107.10	113.39
-0.052	54.03	54.78	56.00	60.02	63.10	66.20	69.32	72.44	75.57	78.71	81.86	85.00	91.29	97.58	103.88	110.18	116.49
-0.054	57.04	57.80	60.00	63.05	66.13	69.24	72.36	75.50	78.64	81.78	84.94	88.09	94.35	100.70	107.02	113.34	119.66
-0.056	60.14	60.87	63.10	66.15	69.25	72.36	75.50	78.64	81.78	84.94	88.11	91.27	97.59	103.91	110.25	116.59	122.92
-0.058	63.32	64.05	66.29	69.35	72.45	75.57	78.71	81.86	85.02	88.18	91.36	94.54	100.87	107.27	113.56	119.92	126.27
-0.060	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	116.96	123.33	129.71
-0.062	69.95	70.68	72.93	76.00	79.12	82.26	85.41	88.58	91.75	94.91	98.13	101.31	107.69	114.06	120.45	126.84	133.24
-0.064	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
-0.066	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
-0.068	80.60	81.34	83.59	86.68	89.82	92.98	96.16	99.35	102.55	105.76	108.98	112.19	118.60	125.05	131.49	137.94	144.38
-0.070	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
-0.072	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	132.77	139.25	145.73	152.21
-0.074	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	136.83	143.31	149.80	156.29
-0.076	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	141.01	147.52	154.04	160.56
-0.078	100.38	101.12	103.39	106.51	109.68	112.89	116.11	119.34	122.58	125.83	129.08	132.36	138.88	145.39	151.92	158.46	165.00
-0.080	104.66	105.40	107.68	110.80	113.98	117.19	120.42	123.67	126.92	130.17	133.45	136.72	143.26	149.79	156.34	162.89	169.45
-0.082	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
-0.084	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
-0.086	118.22	118.96	121.24	124.39	127.58	130.82	133.99	137.35	140.62	143.91	147.19	150.50	157.10	163.68	170.29	176.90	183.51
-0.088	122.98	123.72	126.01	129.16	132.37	135.61	138.89	142.15	145.44	148.73	152.04	155.34	161.95	168.56	175.18	181.81	188.44
-0.090	127.87	128.61	130.91	134.06	137.28	140.52	143.81	147.08	150.38	153.68	156.98	160.31	166.94	173.58	180.20	186.85	193.50
-0.092	132.89	133.63	135.93	139.09	142.32	145.57	148.86	152.14	155.45	158.76	162.09	165.40	172.06	178.70	185.36	192.02	198.69
-0.094	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
-0.096	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	189.37	196.07	202.77	209.48
-0.098	148.78	149.52	151.82	155.00	158.24	161.52	164.83	168.15	171.48	174.82	178.15	181.52	188.25	194.94	201.66	208.38	215.10
-0.100	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
-0.102	160.05	160.80	163.10	166.28	169.51	172.74	176.00	179.29	182.58	185.89	189.19	192.57	199.30	206.03	212.76	219.51	226.27
-0.104	165.88	1															