

LiF and LiH. Haven showed that lattice energy considerations accounted for the lack of solubility in the case of LiF, but the data on LiH for the same type of calculation are lacking.

The larger distance $d_{\text{Ca}-\text{H}} = 2.35 \text{ \AA}$ (mean) (5, 15) would be expected to be much less favorable to solid solubility of CaH₂ in LiH. However, Grube and Rüdel (6) report limited solid solutions in the system LiCl-CaCl₂.

Direct calorimetric eutectic latent heats of fusion would be preferable to the corrected eutectic half times used here, since the heat transfer characteristics of the apparatus might simulate solid solubility of a fraction of 1%.

ACKNOWLEDGMENT

W.T. Grimes of Oak Ridge National Laboratory supervised the mass spectrographic analysis of the lithium.

LITERATURE CITED

- (1) Douglas, T.B., Dever, J.L., *J. Am. Chem. Soc.* **76**, 4826 (1954).
- (2) Dworkin, A.S., Bredig, M.A., *J. Phys. Chem.* **64**, 269 (1960).
- (3) Edwards, R.K., Levesque, P., Cubiciotti, D., *J. Am. Chem. Soc.* **77**, 1307 (1955).
- (4) Gibb, T.R.P., Jr., McSharry, J.J., Bragdon, R.W., *Ibid.* **73**, 1751 (1951).
- (5) Gibb, T.R.P., Jr., Schumacher, D.P., *J. Phys. Chem.* **64**, 1407 (1960).
- (6) Grube, G., Rüdel, W., *Z. anorg. allgem. Chem.* **133**, 375 (1924).
- (7) Haven, Y., *Rec. trav. chim.* **69**, 1505 (1950).
- (8) Libowitz, G.G., Gibb, T.R.P., Jr., *J. Phys. Chem.* **60**, 510 (1956).
- (9) McQuillan, A.D., *Proc. Roy. Soc. (London)* **204**, 309 (1950).
- (10) Messer, C.E., Damon, E.B., Maybury, P.C., Mellor, J., Seales, R.A., *J. Phys. Chem.* **62**, 220 (1958).
- (11) Messer, C.E., Mellor, J., *Ibid.* **64**, 503 (1960).
- (12) Pauling, L., "Nature of the Chemical Bond," 3rd ed., pp. 526-36, Cornell University Press, Ithaca, N.Y., 1960.
- (13) Roake, W.E., *J. Electrochem. Soc.* **104**, 661 (1957).
- (14) Staritzsky, E., Walker, D.J., *Anal. Chem.* **28**, 1055 (1956).
- (15) Zintl, E., Harder, A., *Z. Elektrochem.* **41**, 33 (1935).

RECEIVED for review July 27, 1960. Accepted January 10, 1961. Research sponsored by U.S. At. Energy Comm., Contract AT(30-1)1410.

Thermodynamic Functions for Nitryl Chloride

JOHN P. LARMANN, DANIEL E. MARTIRE, and L.Z. POLLARA, Stevens Institute of Technology, Hoboken, N. J.

RYASON and Wilson (6) have investigated the infrared spectrum of gaseous NO₂Cl and the Raman spectrum of liquid NO₂Cl and assigned the fundamental frequencies; however, they were unable to establish definitely whether the molecule was planar or pyramidal. Millen and Sinnott (3) established the planar structure of the molecule. More recently (4), they assigned rotational transitions in the microwave spectra of NO₂³⁵Cl and NO₂³⁷Cl, and evaluated the molecular rotational constants. Clayton, Williams, and Weatherly (1) reported microwave data and rotational constants in agreement with the values of Millen and Sinnott.

These data permit calculation of thermodynamic functions for the isotopic NO₂Cl mixture. Using the rigid rotator-harmonic oscillator approximation, we have calculated C_p° , $(H^\circ - E_0^\circ/T)$, $-(F^\circ - E_0^\circ/T)$, and S° for nitryl chloride (Table I). The constants used are: $h = 6.62377 \times 10^{-27}$ erg-sec., $k = 1.380257 \times 10^{16}$ ergs per degree, $N_0 = 6.02380 \times 10^{23}$ and $R = 1.98719$ cal. per mole-degree, selected by Rossini and others (5).

A summary of data used in the calculation follows. The fundamental frequencies in reciprocal centimeters are 1293, 794, 651, 1685, 367, and 411. None are degenerate. The molecular weight of the isotopic mixture is 81.465. The molecule has type C_{2v} symmetry. The moments of inertia in a.m.u. sq. Å. are $I_A = 38.1822$, $I_B = 97.710$, and $I_C = 135.845$. Vibrational contributions were calculated using the Einstein tables of Johnston, Savedoff, and Belzer (2).

LITERATURE CITED

- (1) Clayton, L., Williams, Q., Weatherly, T.L., *J. Chem. Phys.* **30**, 1328 (1959).
- (2) Johnston, H.L., Savedoff, L., "Contributions to the Thermodynamic Functions of a Planck-Einstein Oscillator in One Degree of Freedom," Office of Naval Research Rept. NAVEXOS p-646, U. S. Government Printing Office, Washington, D. C., 1949.
- (3) Millen, D.J., Sinnott, K.M., *Chem. & Ind. (London)* **1955**, 538.
- (4) Millen, D.J., Sinnott, K.M., *J. Chem. Soc.* **1958**, 350.
- (5) Rossini, F.D., Gucker, F.T., Johnston, H.L., Pauling, L., Vinal, G.W., *J. Am. Chem. Soc.* **74**, 2699 (1952).
- (6) Ryason, R., Wilson, M.K., *J. Chem. Phys.* **22**, 2200 (1954).

Thermodynamic Functions for Nitryl Chloride

T, °K.	C_p°	$H^\circ - E_0^\circ$	$-(F^\circ - E_0^\circ)$	S° Cal./Mole °K.
		T	T	
150	9.56	8.35	49.07	57.42
175	10.16	8.57	50.39	58.95
200	10.74	8.80	51.54	60.34
225	11.30	9.05	52.59	61.64
250	11.82	9.30	53.55	62.85
273.15	12.26	9.53	54.39	63.92
275	12.30	9.55	54.45	64.00
298.15	12.71	9.78	55.23	65.01
300	12.74	9.80	55.29	65.09
325	13.16	10.04	56.09	66.13
350	13.55	10.28	56.84	67.12
375	13.92	10.51	57.56	68.07
400	14.26	10.73	58.24	68.97
425	14.57	10.95	58.90	69.85
450	14.87	11.16	59.53	70.69
475	15.15	11.36	60.14	71.50
500	15.41	11.56	60.73	72.28
525	15.65	11.75	61.30	73.04
550	15.88	11.93	61.85	73.77
575	16.09	12.10	62.38	74.49
600	16.29	12.28	62.90	75.17
625	16.48	12.44	63.40	75.84
650	16.65	12.60	63.89	76.49
675	16.81	12.75	64.37	77.12
700	16.97	12.90	64.84	77.74
750	17.24	13.18	65.74	78.92
800	17.49	13.44	66.60	80.04
850	17.70	13.69	67.42	81.11
900	17.89	13.91	68.21	82.12
950	18.05	14.13	68.97	83.09
1000	18.20	14.33	69.70	84.02
1050	18.33	14.52	70.40	84.92
1100	18.45	14.69	71.08	85.77
1150	18.55	14.86	71.74	86.59
1200	18.65	15.01	72.37	87.39
1250	18.73	15.16	72.99	88.15
1300	18.81	15.30	73.59	88.88
1350	18.88	15.43	74.17	89.60
1400	18.94	15.56	74.73	90.28
1450	19.00	15.67	75.28	90.95
1500	19.05	15.78	75.81	91.59

RECEIVED for review December 9, 1960. Accepted March 27, 1961.