NUMERICAL PROCEDURES FOR THE CALCULATIONS OF INORGANIC SOLUBILITY AND COHESIVE PARAMETERS

DANIEL D. I, AWSON

Jet Propul sionLaborat

The basic equation for the Hildebrand parameter is:

$$\delta = (\Delta H - RT)^{1/2} / V^{1/2} \quad (I)$$

Where AH is the change in enthalpy, R is the gas constant-, T is the temperature (K) , and V is the molar volume . The controlling term is ΔH , which hastwo (liquid and crystal) states. From t_he first law of thermodynamics it is evident that heats of vaporization (AH,) and sublimation(ΔH_s) can be calculated for liquid or crystalline phases . 'l'he equations are :

$$\Delta H_v^\circ = \Delta H_f^\circ(\text{ideal gas}) - \Delta H_f^\circ(l) \quad \text{(II) liquid state}$$

$$\Delta H_s^\circ = \Delta H_f^\circ(\text{ideal gas}) - \Delta H_f^\circ(c) \quad \text{(III) crystal] ine state}$$

When the reaction or process evolves heat , the sign of the change in enthalpy is negative. Conversely, when the react, ion or process absorbs heat, the sign of the change in ent hal py is positive .

Density Data

To prepare tables of the parameters it is requi red to have density data as a functi on of temperature , Two types of data are needed : densi ty of SO I j d materials and density of me] t phase materials . Toulourian et. al (Ref . 1) havegenerated large numbers of therms l 1 i near expansion data for so] i ds . These can be used to estimate densi ty by means of : (10)

$$D_T = \frac{D_0}{1 + (0.03\,\overline{\Delta \ell} / \overline{\ell_0})} \quad \text{(III)}$$

Where D_t and D_o are the densities at temperature T_k and T_o respectively, and $\Delta\ell/\ell_0$ is the relative change in linear dimension. The reference temperature for D_o of the solid at a temperature T/K of the solid material is 20'c. It is also necessary to have density data for the same material in the melt phase (Ref . 2) .

Tabl e I Cal cul ati on of Inorganic Solubility and Cohesive Parameters for Lithium Chloride

LITHIUM CHLORIDE			COHESION PARAMETERS		
	T, K	V, cm^3/mol	AH, kcal/mole	δ, $cal^{1/2}cm^{-3/2}$	δ, $MPa^{1/2}$
SOLID	298	20. s?	50.81	49.46	101.17
	300	20.52	50.79	49.46	101.46
	400	20.81	50.42	48.84	99.91
	500	21.11	50.03	48.19	98.58
	600	21.45	49.61	47. 51	97.58
	700	21.81	49.12	46.78	95.71
	800	22.07	48. 59	46.14	94.39
	883	22.22	48.03	45.64	93.36
	883	28. 22	43.37	38.41	78.55
	900	28.37	44.26	38.69	79.15
	1100	30.11	41.99	36 .36	74.37
	1200	31.07	41.39	35.43	72.48
			SOLUBITY PARAMETERS		
LIQUID	298	20.53	46.62	47.34	96.84
	300	20.52	46.61	47.35	96.86
	400	20.81	46.24	46.74	95.61
	500	21.11	45.84	46.09	94.27
	600	21.45	45.36	45.38	92.82
	700	21.81	44.62	44.53	91.88
	800	22.07	43.92	43. 79	89.58
	883	26.21	43.71	42.91	78.88
	883	28.21	43.37	38.01	78.66
	900	28.37	43.24	38.23	78.21
	1000	29.21	42.61	37, 29	76.27
	1100	30.11	41.92	36.33	74.31
	1200	31.07	41.39	35.43	72.48