COMPONENTS:	EVALUATOR:
(1) Sodium dihydrogenphosphate; NaH_2PO_4; [7558-80-7]	J. Eysseltová and J. Makovička Charles University Prague, Czechoslovakia
(2) Water; H_2O; [7732-18-5]	May 1985

CRITICAL EVALUATION:

THE BINARY SYSTEM

The isothermal method has been used to determine the solubility of sodium dihydrogenphosphate in water (1, 2). The solubility has also been reported as a limiting condition in the study of several multicomponent systems (3-12). The nature of the equilibrium solid phases was studied in detail by Imadsu (2). He reported the existence of the following solid phases: NaH_2PO_4 [7558-80-7]; $NaH_2PO_4 \cdot H_2O$ [10049-21-5]; $NaH_2PO_4 \cdot 2H_2O$ [13472-35-0]; and $NaH_2PO_4 \cdot 4H_2O$ [101056-45-5]. The transition temperature of the anhydrous salt to the monohydrate was estimated to be 330.5 K while that of the monohydrate to the dihydrate was estimated to be 313.9 K. The transition between the dihydrate and the tetrahydrate was not determined but was considered to be below 273 K (2).

Evaluation Procedure. All the data were examined and evaluated by using the method described by Cohen-Adad (13). Only experimentally obtained data were evaluated. Data obtained from smoothing equations or by extrapolation were excluded from consideration. The data calculated on the basis of sodium determination (1) and the 298 K values reported by others (3, 4) are clearly incorrect and were not included. Some data (4) were reported as mol dm^{-3} and could not be used here because no density information was given and the values could not be recalculated in terms of mole fraction. All the other data are consistent with each other and were evaluated together.

The data were fitted to equation [1], suggested by Cohen-Adad (13).

$$\ln(x/x_o) = A\cdot(1/T-1/T_o) + B\cdot\ln(T/T_o) + C\cdot(T-T_o) \qquad [1]$$

A, B and C are adjustable parameters. No attempt was made to give a physical meaning to them. The system is too complex for that, as is shown by reported activity coefficient data (14, 15). x_o is a reference mole fraction at temperature T_o. Its choice is arbitrary. The evaluators used the following two criteria for making their selection.

1. x_o was chosen as the mean value of the experimental data of more than one study. Furthermore, the standard deviation did not exceed the experimental uncertainty in obtaining the data.
2. T_o was chosen near the middle of the temperature range in which the hydrate exists rather than at or near a transition point of one hydrate into another.

Each datum selected was given a weight equal to the number of independent determinations of the value. In some reports (5, 7, 10, 12) a given value appears to be reported more than once. In such cases the value was given a weight of one. Then an iterative method analagous to that described by others (16) was used. It was necessary to know the experimental uncertainty of the values before the next iteration could be made. However, such information was included in only two reports (2, 4). Therefore, the evaluators tried to estimate the experimental uncertainty on the basis of the data that were included in the report. It appears that for the isothermal studies (1-4, 6-9, 11, 12) the precision is 0.1 to 0.5% while for data derived from polythermal studies (5, 10) it is about 1%. The selection conditions that were used are given in equation [2]. x_j and T_j are the coordinates of the experimental point j in terms of mole fraction and

$$\left|\frac{x_j - x(T_j)}{x(T_j)}\right| \leq 0.015 \qquad [2]$$

temperature. $x(T_j)$ is the calculated mole fraction. Data points that did not meet the conditions of equation [2] were eliminated before the next iteration.

The value of coefficients A, B and C of equation [1] were determined by using a non-linear regression with the experimental points selected as described above. For the regression, equation [1] was put in the form of equation [3]. The calculation was stopped

$$x = x_o\cdot\exp[A(1/T - 1/T_o) + B\cdot\ln(T/T_o) + C\cdot(T-T_o)] \qquad [3]$$

when steady values were obtained for A, B and C.

The solubility results are summarized in Table I. During the iteration procedure all the data in refs (6-8, 12) and most of the data in ref (1) were eliminated. Table II

(continued next page)

COMPONENTS:	EVALUATOR:
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CRITICAL EVALUATION: (cont'd)

Table I. Solubility of NaH_2PO_4 in water.

T/K	mass%	ref.	weight init/final	T/K	mass%	ref.	weight init/final
			$NaH_2PO_4 \cdot 2H_2O$				
263.3	32.4	5	1/1	298.2	48.97	1	1/1
263.3	30.4	10	1/0	298.2	48.62	2	2/2
266.2	33.6	10	1/1	298.2	48.69	9	1/1
268.2	35.4	12	1/0	298.2	48.03	8	1/0
268.9	34.6	10	1/1	298.2	48.47	11	1/0
273.2	36.1	1	1/0	299.2	49.16	2	1/1
273.2	36.4	5	1/1	299.2	49.17	2	1/1
273.2	36.25	11	1/1	300.2	49.80	2	2/2
273.2	37.6	12	1/0	301.2	50.43	2	1/1
273.3	36.64	2	1/1	301.2	50.41	2	1/1
274.2	37.13	2	1/1	303.2	51.55	2	1/1
274.2	37.15	2	1/1	303.2	51.57	2	1/1
276.2	38.06	2	1/1	303.2	51.2	5	1/1
276.2	38.08	2	1/1	306.2	52.15	2	1/1
278.2	38.95	2	1/1	306.2	52.12	2	1/1
278.2	38.96	2	1/1	307.2	53.93	2	1/1
283.2	41.12	2	1/1	307.2	53.96	2	1/1
283.2	41.14	2	1/1	308.2	54.63	2	1/1
283.2	40.5	5	1/0	308.2	54.64	2	1/1
283.2	42.2	12	1/0	308.2	54.79	3	1/1
288.2	43.42	2	1/1	308.7	53.65	1	1/0
288.2	43.41	2	1/1	313.2	56.41	1	1/0
293.2	46.01	2	1/1	313.2	58.02	2	1/0
293.2	46.00	2	1/1	313.2	58.00	2	1/0
293.2	45.30	5	1/0	313.2	56.31	7	1/0
293.2	46.60	12	1/0				
			$NaH_2PO_4 \cdot H_2O$				
314.2	58.76	2	1/1	323.2	61.16	6	1/0
314.2	58.78	2	1/1	323.2	60.58	8	1/0
315.2	58.98	2	1/1	325.2	62.11	2	1/1
315.2	58.99	2	1/1	325.2	62.09	2	1/0
317.2	57.97	1	1/0	328.2	63.85	1	1/0
318.2	59.71	2	2/2	328.2	63.09	2	1/1
323.2	61.81	1	1/1	328.2	63.07	2	1/1
323.2	61.32	2	1/1	329.2	63.41	2	1/1
323.2	61.34	2	1/1	329.2	63.39	2	1/1
			NaH_2PO_4				
331.2	65.53	1	1/0	338.2	65.89	1	1/0
331.2	63.94	2	1/0	342.2	65.54	2	1/1
331.2	63.92	2	1/0	342.2	65.55	2	1/1
333.2	64.20	2	2/2	343.2	66.25	1	1/0
334.2	65.77	1	1/0	348.2	67.21	1	1/0
335.2	64.44	2	1/1	348.2	66.57	11	1/1
335.2	64.48	2	1/1	353.2	67.44	2	1/0
338.2	64.92	2	1/1	353.2	67.48	2	1/1
338.2	64.90	2	1/1	356.2	69.13	1	1/1

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CRITICAL EVALUATION: (cont'd)

Table II. Values for the parameters in equation [1].

	dihydrate		monohydrate		anhydrous	
Parameter	value	σ^a	value	σ^a	value	σ^a
A	-3.52×10^4	100	1.596×10^6	5000	-6.29×10^5	3000
B	-253	1	9940	40	-3700	10
C	0.472	0.002	-15.47	0.07	5.45	0.02
x_o	0.12454		0.19467		0.21720	
T_o	298.2		323.2		338.2	

[a] These are the standard deviations for the respective parameter.

Table III. Solubility data calculated by equation [1].

T/K	mol fraction	mol/kg	mass%
	$NaH_2PO_4 \cdot 2H_2O$		
273.2	0.079491	4.80	36.54
278.2	0.086735	5.28	38.77
283.2	0.094636	5.81	41.07
288.2	0.10340	6.41	43.47
293.2	0.11327	7.10	46.00
298.2	0.12454	7.90	48.68
303.2	0.13759	8.86	51.54
308.2	0.15287	10.02	54.61
313.2[a]	0.17095	11.46	57.89
313.7[a]	0.17299	11.62	58.24
	$NaH_2PO_4 \cdot H_2O$		
313.7	0.17299	11.62	58.24
315.2	0.17505	11.79	58.59
317.2	0.17893	12.11	59.23
319.2	0.18376	12.51	60.02
321.2	0.18915	12.96	60.87
323.2	0.19467	13.43	61.71
325.2	0.19981	13.87	62.48
327.2	0.20412	14.25	63.10
329.2[b]	0.20707	14.51	63.52
331.2	0.20815	14.60	63.67
	NaH_2PO_4		
333.2	0.19865	13.77	62.30
338.2	0.21720	14.72	63.85
343.2	0.22437	16.07	65.86
348.2	0.23358	16.93	67.02
353.2	0.24767	18.29	68.70
358.2	0.27010	20.56	71.16

[a] The dihydrate to monohydrate transition temperature.

[b] The monohydrate to anhydrous salt transition temperature.

The above transition temperature values were determined graphically by the evaluators.

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CRITICAL EVALUATION: (cont'd)

gives a summary of the values for the parameters of equation [1]. In Table III are given some solubility values obtained by the use of equation [1] and the parameters given in Table II. In Table III, the values for $NaH_2PO_4 \cdot 2H_2O$ are recommended values. For the dihydrate and the anhydrous salt the values given are tentative values because only the data of Imadsu (2) survived the iteration procedure.

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