

## SCDbase

17.02.09 JJ

Stepwise complex formation

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## Ligand

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Stepwise complex formation

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## Metal ion

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Stepwise complex formation

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## References

Full Display of Data for Experiments in List

Step Size: New, Mid, Far | Exp to Clipboard | Temp. Dependence

Previous Exp | Next Exp | Experiment no. 23678 | No. 133 of 241 in list | Specification | Ionic Strength De

Method: Reference and Legend (continued)

Stepwise complex formation - 1003904 - 1976 in origin seen for data

P. Pascoe, Pure & Appl Chem, 36, 491 (1964)

$C_2H_5N_2$  Ethylenediamine L CAS: 107-15-7

1,2-Diaminoethane

$H_2NCH_2CH_2NH_2$

Logarithmic primary amines

Data: K1=0.12[M], K2=0.12[M], Beta2=0.12[M], F2

Method: Glass Electrode Medium: KCl

Temperature: 25°C Ionic Strength: 1.0M Calibration: Concentration

Constants (log values): NIPAC Recommended  $R_2 = 13.94$

$\log K_1 = 7.554$   $R_1 = 6.40$   $\log K_2 = 17.941 = 43.04$   $\log K_3 = 19.401 = 36.53$   $\log \beta_2 = 13.941 = 79.97$

$R_3 = 18.39$

NIPAC evaluation:  $\Delta H K_1 = -37.7$ ,  $\Delta H K_2 = -38.5$ ,  $\Delta H K_3 = -48.5 \text{ kJ mol}^{-1}$

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## Speciation

Speciation - Calculation and Display

File Output Precision/Speed Help

1,2-Diaminoethane H2N OH CH3 OH NH3

Reactants Constants Solubility Data

Reactant	Amount	Initial	Final
H2N	1.00000	1.00000	0.00000
OH	0.00000	0.00000	0.00000

Calculate as a function of: pH, pI, Reactant conc. Show additional data

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## Add constant

Speciation - Calculation and Display

File Output Precision/Speed Help

1,2-Diaminoethane H2N OH CH3 OH NH3

Reactants Constants Solubility Data

Add Constant Remove Constant

log beta	pKa	log beta	log beta
1	1	0	
11.94	1	2	0
10.65	0	1	1
10.69	0	1	2

NIPAC evaluation:  $\Delta H K_1 = -37.7$ ,  $\Delta H K_2 = -38.5$ ,  $\Delta H K_3 = -48.5 \text{ kJ mol}^{-1}$

$R_2 = 13.94$

NIPAC evaluation:  $\log \beta_1 = 7.554$ ,  $\log \beta_2 = 13.941$ ,  $\log \beta_3 = 19.401$

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## Calculate

File Output Precision/Speed Help

File: 1,2-Diaminoethane HON,CH2,CH2,NH2

Reactants: Constants Solubility Data

Eq. No.	Species	Equation	Equilibrium
1	H <sup>+</sup>	1	0
2	H <sub>2</sub> O	1	2
3	H <sub>2</sub> O	0	1
4	H <sub>2</sub> O	0	1
5	H <sub>2</sub> O	0	1
6	H <sub>2</sub> O	0	1
7	H <sub>2</sub> O	0	1
8	H <sub>2</sub> O	0	1
9	H <sub>2</sub> O	0	1
10	H <sub>2</sub> O	0	1
11	H <sub>2</sub> O	0	1
12	H <sub>2</sub> O	0	1
13	H <sub>2</sub> O	0	1
14	H <sub>2</sub> O	0	1
15	H <sub>2</sub> O	0	1
16	H <sub>2</sub> O	0	1
17	H <sub>2</sub> O	0	1
18	H <sub>2</sub> O	0	1
19	H <sub>2</sub> O	0	1
20	H <sub>2</sub> O	0	1
21	H <sub>2</sub> O	0	1
22	H <sub>2</sub> O	0	1
23	H <sub>2</sub> O	0	1
24	H <sub>2</sub> O	0	1
25	H <sub>2</sub> O	0	1
26	H <sub>2</sub> O	0	1
27	H <sub>2</sub> O	0	1
28	H <sub>2</sub> O	0	1
29	H <sub>2</sub> O	0	1
30	H <sub>2</sub> O	0	1
31	H <sub>2</sub> O	0	1
32	H <sub>2</sub> O	0	1
33	H <sub>2</sub> O	0	1
34	H <sub>2</sub> O	0	1
35	H <sub>2</sub> O	0	1
36	H <sub>2</sub> O	0	1
37	H <sub>2</sub> O	0	1
38	H <sub>2</sub> O	0	1
39	H <sub>2</sub> O	0	1
40	H <sub>2</sub> O	0	1
41	H <sub>2</sub> O	0	1
42	H <sub>2</sub> O	0	1
43	H <sub>2</sub> O	0	1
44	H <sub>2</sub> O	0	1
45	H <sub>2</sub> O	0	1
46	H <sub>2</sub> O	0	1
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48	H <sub>2</sub> O	0	1
49	H <sub>2</sub> O	0	1
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60	H <sub>2</sub> O	0	1
61	H <sub>2</sub> O	0	1
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64	H <sub>2</sub> O	0	1
65	H <sub>2</sub> O	0	1
66	H <sub>2</sub> O	0	1
67	H <sub>2</sub> O	0	1
68	H <sub>2</sub> O	0	1
69	H <sub>2</sub> O	0	1
70	H <sub>2</sub> O	0	1
71	H <sub>2</sub> O	0	1
72	H <sub>2</sub> O	0	1
73	H <sub>2</sub> O	0	1
74	H <sub>2</sub> O	0	1
75	H <sub>2</sub> O	0	1
76	H <sub>2</sub> O	0	1
77	H <sub>2</sub> O	0	1
78	H <sub>2</sub> O	0	1
79	H <sub>2</sub> O	0	1
80	H <sub>2</sub> O	0	1
81	H <sub>2</sub> O	0	1
82	H <sub>2</sub> O	0	1
83	H <sub>2</sub> O	0	1
84	H <sub>2</sub> O	0	1
85	H <sub>2</sub> O	0	1
86	H <sub>2</sub> O	0	1
87	H <sub>2</sub> O	0	1
88	H <sub>2</sub> O	0	1
89	H <sub>2</sub> O	0	1
90	H <sub>2</sub> O	0	1
91	H <sub>2</sub> O	0	1
92	H <sub>2</sub> O	0	1
93	H <sub>2</sub> O	0	1
94	H <sub>2</sub> O	0	1
95	H <sub>2</sub> O	0	1
96	H <sub>2</sub> O	0	1
97	H <sub>2</sub> O	0	1
98	H <sub>2</sub> O	0	1
99	H <sub>2</sub> O	0	1
100	H <sub>2</sub> O	0	1

Calculate as a function of: pH, pI, or Reactant conc. Show additional data

pH range from pH: 10.0 to pH: 11.0 Calculate

Reactant to Plot: H<sub>2</sub>O 1.00 Cancel

Display Graphs

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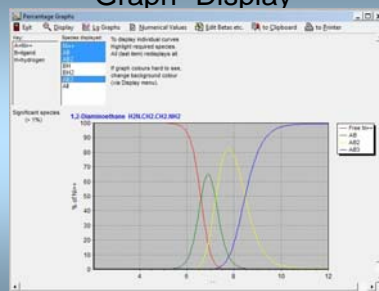


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## Graph- Display



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