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from: Robert C. Moore, Org. 6748, MS-1341, 848-0146

subject: Final Model Parameters for Deprotonation of Lactic Acid, Citric Acid, Oxalic Acid, and EDTA and Complexation of Acetate, Lactate, Citrate, Oxalate, and EDTA with NpO_2^+ , Am^{3+} , Th^{4+} , and UO_2^{2+} in NaCl media.

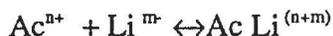
(I) Introduction

This memorandum documents final model parameters for the deprotonation of lactic acid, citric acid, oxalic acid, and EDTA in NaCl solutions, and the complexation of acetate, oxalate, citrate, lactate, and EDTA with NpO_2^+ , Am^{3+} , Th^{4+} and UO_2^{2+} . Model parameters for acetic acid deprotonation and complexation of NpO_2^+ with acetate have previously been reported by Novak (1995). The thermodynamic parameters necessary to model the equilibrium chemistry are standard chemical potentials and activity coefficients of the ions. Activity coefficients were modeled using the Pitzer equations.

Preliminary model parameters have been previously documented (Moore technical memos 10/7/95). This memorandum documents the incorporation of additional data taken at Florida State University and literature data into the model. The parameters given in this report are the final values that will be supplied to performance assessment for the 1996 compliance application to EPA. All model parameters were determined using the NONLIN computer code.

All data for actinide-ligand complexation taken at Florida State University(FSU) were obtained using solvent extraction techniques. The extraction data were used to calculate apparent stability constants for each actinide-ligand reaction. The data have been previously reported by FSU in monthly reports to the SNL WIPP program.

The general equation to represent an actinide-ligand reaction is:



where the apparent stability constant is given by:

$$\beta = [\text{AcLi}^{(n+m)}] / [\text{Ac}^{n+}] [\text{Li}^{m-}]$$

All concentrations are in molal units.

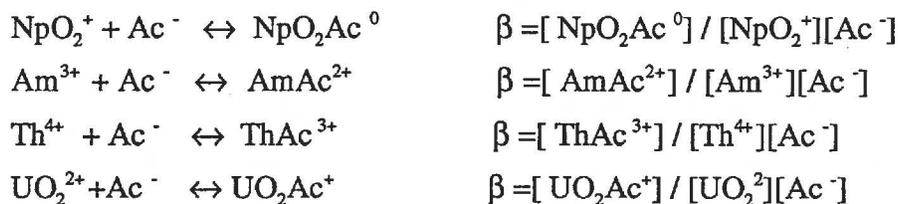
The data were all modeled using a similar procedure. Concentrations reported by FSU were converted from a molar to a molal basis using density measurements of NaCl solutions that were also taken at FSU. Concentrations of actinide, ligand, and actinide-ligand complex were calculated using the apparent stability constants. Solution pH and NaCl concentration were set according to experimental conditions. For all of the systems, the fewest number of parameters required to fit the data were used. When available, the model results were compared with literature data.

(II) Chemistry and Data Sources for Modeling Acid Deprotonation and Actinide Complexation

Acetic Acid/Acetate

Values for the deprotonation of acetic acid have been previously reported by Novak (1995).

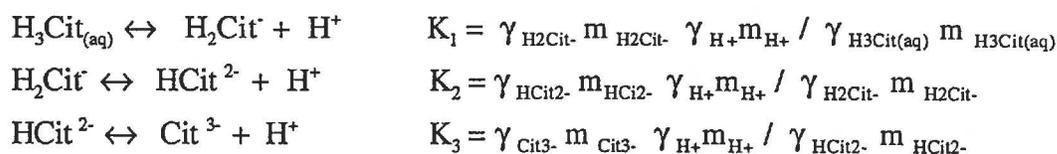
The complexation of acetate with the actinides NpO_2^+ , Am^{3+} , Th^{4+} , and UO_2^{2+} are represented by the following reactions:



where Ac⁻ represents the acetate ligand. All data for acetate complexation was determined at FSU. Martell and Smith (1977) report values for acetate at ionic strengths of 0.1 and 1.0. Although these data were collected in NaClO₄ media and were not incorporated into the model, the apparent stability constants in NaCl media should be comparable at low ionic strength. The FSU data compares favorably.

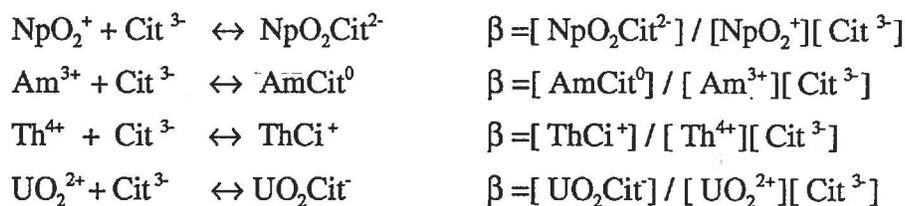
Citric Acid/Citrate

The first, second, and third deprotonation of citric acid proceeds according to the following reactions:



The data for citric acid in NaCl media were measured at FSU. The citric acid deprotonation constant at 0 ionic strength was taken from Martell and Smith, 1977.

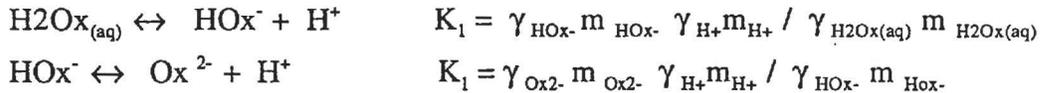
The complexation of citrate with the actinides NpO₂⁺, Am³⁺, Th⁴⁺, and UO₂²⁺ are represented by the following reactions:



where Cit³⁻ represents the citrate ligand. All data were determined at FSU. Very little data for comparison could be found in the literature. Martell and Smith report values for UO₂²⁺ and Am³⁺ complexation with citrate at ionic strengths of 0.1 and 1.0. The values are comparable with the data measured at FSU.

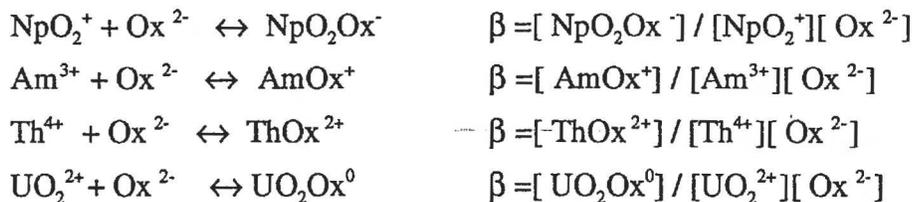
Oxalic Acid/Oxalate

The first and second deprotonation of oxalic acid proceeds according to the following reactions:



The data used for modeling the oxalate system are from Kettler et al. (1991), the FSU program, and Martell and Smith (1977). Kettler et al. gives solubility data for oxalic acid in 0 to 2 molal NaCl solutions. The Martell and Smith data are at 0 ionic strength, and the FSU data are reported in 0.3 to 5 m NaCl media.

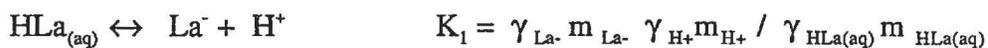
The complexation of oxalate with the actinides NpO_2^+ , Am^{3+} , Th^{4+} , and UO_2^{2+} are represented by the following reactions:



where Ox^{2-} represents the oxalate ligand. All data used in modeling complexation were measured at FSU. A value for Th^{4+} at 0 ionic strength is given by Martell and Smith. However, this value is extremely high and believed to be erroneous, so it was not used for comparison.

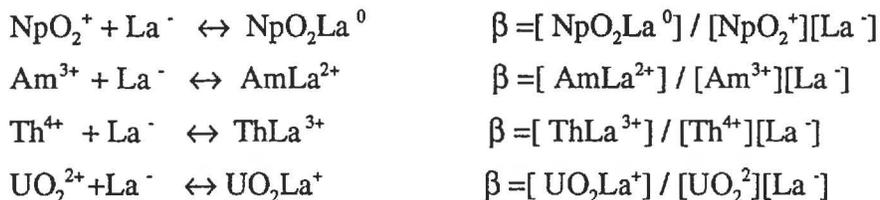
Lactic Acid/Lactate

The deprotonation of lactic acid proceeds according to the following reaction:



Data for lactic acid in NaCl media were determined by Florida State University (FSU). The lactic acid deprotonation constant at 0 ionic strength was taken from Martell and Smith.

The complexation of lactate with actinides NpO_2^+ , Am^{3+} , Th^{4+} , and UO_2^{2+} are represented by the following reactions:



where La^- represents the lactate ligand. All data were measured at FSU. A value for Th^{4+} complexation with lactate at 0 ionic strength is given Martell and Smith. Again, the value is extremely high when compared with the FSU results and was not used in the model or for comparison. A value for NpO_2^+ in 0.1 ionic strength media is reported in Martell and Smith and is consistent with the results of FSU.

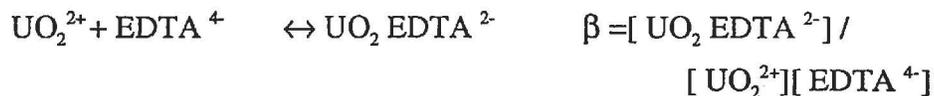
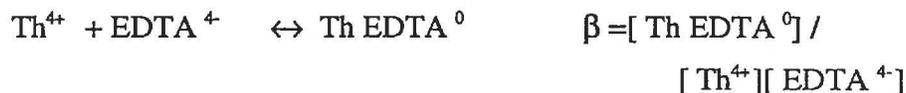
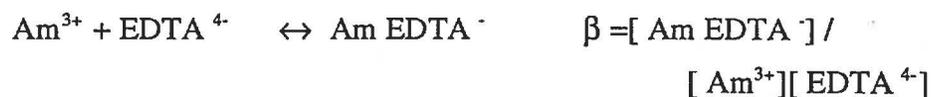
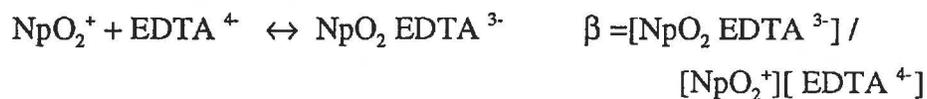
EDTA

The first, second, third and fourth deprotonation reactions for EDTA proceed according to the following reactions:



All data used for modeling EDTA deprotonation are from FSU (12/30/95 monthly report) and Martell and Smith.

The complexation of EDTA with the actinides NpO_2^+ , Am^{3+} , Th^{4+} , and UO_2^{2+} are represented by the following reactions:



All data for EDTA complexation was measured at FSU. No literature data at high ionic strength were available.

(III) MODELING RESULTS

(A) Standard Chemical Potentials

Table 1 gives standard chemical potentials for all aqueous species investigated in this work. All values were determined using the NONLIN software. For the acid deprotonation models, data were not available to determine parameters for neutral ion

interactions and standard chemical potentials so their respective values were set to 0. All other model parameters were determined on this basis. This procedure does not affect the ability or accuracy of the model to represent the data, but does assume that all ligands are present in solution (i.e.- the model does not calculate solubility of the organic acids). To include this information in the model, additional solubility data for the organic acids must be taken in NaCl media.

(B) Pitzer Parameters for Acid Deprotonation

All Pitzer parameters for the deprotonation of acetic acid, citric acid, lactic acid, oxalic acid, and EDTA are reported in table 2. Pitzer parameters for interactions between Na-Cl, H-Cl, and Na-OH are from the Harvie-Moller-Weare data base (1984).

Acetic Acid

Values for deprotonation of acetic acid have been previously reported by Novak (1995).

Citric Acid

For the first, second and third deprotonation reactions of citric acid in NaCl media, binary parameters β^0 and β^1 were determined for the $\text{Na}^+ - \text{H}_2\text{Cit}^-$, $\text{Na}^+ - \text{HCit}^{2-}$, and $\text{Na}^+ - \text{Cit}^{3-}$ ion pairs respectively. No additional parameters were needed to represent the data in NaCl media. The data and model are given in figure 1.

Oxalic Acid

The first deprotonation reaction of oxalic acid required a single parameter, β^0 , for the $\text{Na}^+ - \text{HOx}^-$ ion pair to fit the data. FSU data taken at an ionic strength lower than 1.0 were not used in the model. FSU reports significant uncertainty in these values, and excessively high Pitzer parameters resulted when they were included. However, the largest deviation between the model and these points is < 0.2 log units. For the second deprotonation, much more data were available and the parameters β^0 , β^1 , and c^ϕ for the

Na^+ - Ox^{2-} ion pair were determined. The model for oxalic acid in NaCl is presented graphically in figure 2.

Lactic Acid

For the deprotonation reaction of lactic acid in NaCl media, binary parameters β^0 and β^1 were determined for the Na^+ - La^- ion pair. No additional parameters were needed to represent the data. The model is presented graphically in figure 3.

EDTA

For the first, second, third, and fourth deprotonation of EDTA in NaCl media, binary parameters β^0 and β^1 were determined for the Na^+ - H_3EDTA^- , Na^+ - $\text{H}_2\text{EDTA}^{2-}$, Na^+ - HEDTA^{3-} and Na^+ - EDTA^{4-} ion pairs. No additional parameters were needed to represent the data in NaCl media. The model is presented graphically in figure 4.

(C) Pitzer Parameters for Organic Ligand Complexation

Pitzer parameters for organic ligand complexation are given in table 3. All systems were modeled using binary and neutral-ion parameters only. No ternary parameters were required.

Acetate

The results for acetate complexation with Am^{3+} , Th^{4+} , and UO_2^{2+} are presented in figures 1-3. Values for neptunium acetate complexation have previously been reported by Novak (1995). For americium complexation with acetate it was necessary to fit three parameters, β^0 , β^1 , and c^ϕ to the data. For thorium acetate complexation, the parameters β^0 and β^1 were needed to fit the data. The model provides an excellent representation of the data with the largest deviation of .2 log units occurring at the 1 and 3 m NaCl data points. A single parameter, β^0 , was required to fit the uranyl acetate complexation data.

The model deviates from the data by approximately 0.2 log units at low ionic strength, but the addition of a second parameter to increase the accuracy of the uranyl model was not helpful. More data at low ionic strength is needed.

Citrate

Figures 8-11 give the experimental data and model fits for citrate complexation with NpO_2^+ , Am^{3+} , Th^{4+} , and UO_2^{2+} . Americium-citrate is a neutral species and a single parameter, λ , was required to fit the data. The value at 4 molal NaCl taken at FSU was extremely high and was discarded. It is not shown on the plot. The largest deviation between the model and data occurs at the lowest ionic strength point of .1 m NaCl. The difference between the model and data is approximately 0.5 log units. Two parameters, β^0 and β^1 , were required to fit the thorium citrate data. Overall the fit of the data is good with the exception of the point at 3 molal NaCl. The difference between the model and data at this point is approximately 0.25 log units. For neptunyl citrate complexation, it was necessary to use three parameters, β^0 , β^1 , and c^ϕ , to fit the data. This system exhibited atypical behavior when compared to the other systems in this work. The apparent stability constant rapidly increases then decreases with increasing ionic strength. A good fit of the data for uranyl citrate was obtained using only a single β^0 parameter.

Lactate

Figures 12 through 15 give the results for lactate complexation with NpO_2^+ , Am^{3+} , Th^{4+} , and UO_2^{2+} , respectively. For the americium, thorium, and uranyl systems two binary parameters, β^0 and β^1 , were required to fit the data. Neptunyl lactate is a neutral species and two parameters were required to fit the data. A neutral ion parameter for the $\text{NpO}_2\text{Lac-Cl}^-$ neutral ion pair and a higher order neutral ion parameter, ζ , to account for the $\text{NpO}_2\text{Lac-Cl}^- \text{-Na}^+$ interactions. All four models fit the data to within 0.1 log units with the exception of the data points at 4 and 5 m NaCl for americium acetate. The differences between these points and the model are approximately 0.25 log units. The value of 6.331 for β^1 for the $\text{AmLac}^{2+} \text{-Cl}^-$ interaction is high for this type of interaction but not unacceptable.

Oxalate

Oxalate results are given in figures 16-19. The americium oxalate and neptunyl oxalate systems required only a single β^0 parameter to represent the data. For the neptunyl oxalate system no data was reported below 1 m NaCl. Two parameters β^0 and β^1 , were used to represent the thorium oxalate data. An excellent fit of the data for this system was obtained. The data for the uranyl oxalate system was fit using β^0 and β^1 parameters. The data for this system does have some scatter. FSU data for uranyl oxalate at 5 m NaCl was considered to be in error and was not used in modeling.

EDTA

Results for EDTA are presented in figures 20 through 23. The americium EDTA system was fit using a single parameter while the neptunyl and uranium oxalate systems required 2 parameters. For americium and uranyl excellent fits of the data were obtained. For neptunyl EDTA complexation, the data are well represented except at the 4m NaCl point. The difference between the data and model at this point is approximately 0.15 log units. The thorium EDTA complex is a neutral species and a single neutral ion parameter, λ , was used to fit the data. The value of -.832 is high for a neutral ion parameter but not unacceptable.

List of Symbols

β = Apparent stability constant

K = Equilibrium constant

m = Concentration in molality

γ = Activity coefficient

β^0 = Binary interaction Pitzer parameter for representing high ionic strength region

β^1 = Binary interaction Pitzer parameter for representing low ionic strength region

β^2 = Binary interaction Pitzer parameter for representing middle ionic strength region

c^ϕ = Binary interaction Pitzer parameter independent of ionic strength

λ = Neutral-ion interaction Pitzer parameter

ξ = Higher order neutral-ion interaction Pitzer parameter

R = Ideal gas constant

T = Temperature

References

Novak, C.F., "A preliminary model for the deprotonation of acetic acid in NaCl media.", SNL Technical memo, 1995.

Novak, C.F., M. Borkowski and G.R. Choppin, Thermodynamic Modeling of Neptunium(V)-Acetate Complexation in Concentrated NaCl Media.", 1995, In preparation.

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Martell, A.E. and R.M. Smith. "Critical Stability Constants: Volume 3: Other Organic Ligands." Plenum Press: New York 1977

Harvie, C.E., N. Møller, and J.H. Weare. 1984. "The Prediction of Mineral Solubilities in Natural Waters: The Na-K-Mg-Ca-H-Cl-SO₄-OH-HCO₃-CO₃-CO₂-H₂O System to High Ionic Strength at 25°C." *Geochimica et Cosmochimica Acta* vol. 48: 723-751.

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Table 1. Standard state chemical potentials for actinide complexation in NaCl media. Values determined using NONLIN software.

Species	μ° / RT	reference
H ₂ O	-95.6635	HMW 1984
Na ⁺	-105.651	HMW 1984
Cl ⁻	-52.955	HMW 1984
H ⁺	0	HMW 1984
OH ⁻	-63.435	HMW 1984
HA _{C₆₀}	-158.3	Novak, 1995
Ac ⁻	-147.347	Novak, 1995
H ₂ Ox _(aq)	0	this work
HOx ⁻	3.05233	this work
Ox ²⁻	12.7901	this work
H ₃ Cit _(aq)	0	this work
H ₂ Cit ⁻	7.245	this work
HCit ²⁻	18.3	this work
Cit ³⁻	33.068	this work
HL _{2(aq)}	0	this work
La ⁻	9.002	this work
H ₄ EDTA _(aq)	0	this work
H ₃ EDTA ⁻	5.3601	this work
H ₂ EDTA ²⁻	11.6586	this work
HEDTA ³⁻	26.6997	this work
EDTA ⁴⁻	52.1088	this work
Th ⁴⁺	-284.227	Roy et al 1992
Am ³⁺	-241.694	Fuger and Oetting 1976
NpO ₂ ⁺	-369.1	Fuger and Oetting 1976
UO ₂ ²⁺	-384.258	Fuger and Oetting 1976
NpO ₂ -Ac ⁺	-519.809	Novak, 1995
NpO ₂ -Ox ⁻	-366.443	this work
NpO ₂ -Cit ²⁻	-343.057	this work
NpO ₂ -La ⁰	-364.257	this work
NpO ₂ -EDTA ³⁻	-328.425	this work
Am-Ac ²⁺	-395.358	this work
Am-Ox ⁺	-243.483	this work
Am-Cit ⁺	-228.687	this work
Am-La ³⁺	-242.339	this work
Am-EDTA ⁻	-232.977	this work
Th-Ac ³⁺	-448.639	this work
Th-Ox ²⁺	-297.076	this work
Th-Cit ⁺	-285.706	this work
Th-La ³⁺	-291.182	this work
Th-EDTA ⁰	-285.817	this work
UO ₂ -Ac ⁺	-538.492	this work
UO ₂ -Ox ⁺	-387.845	this work
UO ₂ -Cit ⁺	-366.897	this work
UO ₂ -La ⁺	-382.999	this work
UO ₂ -EDTA ²⁻	-352.299	this work

Table 2. Pitzer parameters for organic acid deprotonation

Binary Pitzer Parameters

Species i	Species j	β^0_{ij}	β^1_{ij}	β^2_{ij}	c^*_ij	reference
Na ⁺	Cl ⁻	0.0765	0.2664	0	0.00127	HMW 1984
H ⁺	Cl ⁻	0.1775	0.2945	0	0.008	HMW 1984
Na ⁺	OH ⁻	0.0864	0.253	0	0.0044	HMW 1984
Na ⁺	Ac ⁻	0.1426	0.22	0	-0.00629	Novak, 1995
Na ⁺	HOx ⁻	-0.0307	0	0	0	this work
Na ⁺	Ox ²⁻	0.0028	1.661	0	0.027	this work
Na ⁺	H ₂ Cit ⁻	-0.0613	0.5548	0	0	this work
Na ⁺	HCit ²⁻	-0.0014	2.339	0	0	this work
Na ⁺	Cit ³⁻	0.2823	5.411	0	0	this work
Na ⁺	La ⁻	0.1349	-0.7242	0	0	this work
Na ⁺	H ₅ EDTA ⁻	-0.0908	0.0825	0	0	this work
Na ⁺	H ₂ EDTA ²⁻	-0.1272	2.863	0	0	this work
Na ⁺	HEDTA ³⁻	0.2619	8.325	0	0	this work
Na ⁺	EDTA ⁴⁻	1.034	11.34	0	0	this work

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Table 3. Pitzer parameters for organic ligand interactions with actinides.

Binary Pitzer Parameters

Species i	Species j	β^0_{ij}	β^1_{ij}	β^2_{ij}	c^4_{ij}	reference
Am ³⁺	Cl ⁻	0.6117	5.403	0	-0.0284	Felmy et al. 1995
NpO ₂ ²⁺	Cl ⁻	0.1415	0.281	0	0	Fanghanel et al. 1991
UO ₂ ²⁺	Cl ⁻	0.4274	1.644	0	-0.0184	Pitzer, 1991
Th ⁴⁺	Cl ⁻	1.092	13.7	-160	-0.122	Roy et al. 1992
AmAc ²⁺	Cl ⁻	0.227	2.154	0	-0.102	this work
ThAc ³⁺	Cl ⁻	1.239	4.934	0	0	this work
UO ₂ Ac ⁺	Cl ⁻	0.0473	0	0	0	this work
Na ⁺	NpO ₂ Ox ⁻	-0.1893	0	0	0	this work
AmOx ⁺	Cl ⁻	-0.3219	0	0	0	this work
ThOx ³⁺	Cl ⁻	-0.2061	-0.525	0	0	this work
ThCit ⁺	Cl ⁻	-0.604	-1.607	0	0	this work
Na ⁺	UO ₂ Cit ⁻	-0.5817	0	0	0	this work
Na ⁺	NpO ₂ Cit ²⁻	-0.4092	1.221	0	0.213	this work
AmLa ²⁺	Cl ⁻	-0.0572	6.331	0	0	this work
UO ₂ La ⁺	Cl ⁻	0.1809	0.7125	0	0	this work
ThLa ³⁺	Cl ⁻	0.2138	5.371	0	0	this work
Na ⁺	NpO ₂ EDTA ³⁻	0.3469	0	0	0	this work
Na ⁺	AmEDTA ⁻	-0.2307	0	0	0	this work
Na ⁺	UO ₂ EDTA ²⁻	-0.1687	-0.4847	0	0	this work

Neutral-ion Pitzer Parameters

Species i	Species j	Species k	λ_{ij}	ξ_{ijk}	reference
NpO ₂ Ac ⁰	Cl ⁻	-	0	0	Novak, 1995
UO ₂ Ox ⁰	Cl ⁻	-	-0.347	0	this work
NpO ₂ La ⁰	Cl ⁻	Na ⁺	-0.1853	0.059	this work
ThEDTA ⁰	Cl ⁻	-	-0.832	0	this work
AmCit ⁰	Cl ⁻	-	-0.2731	0	this work

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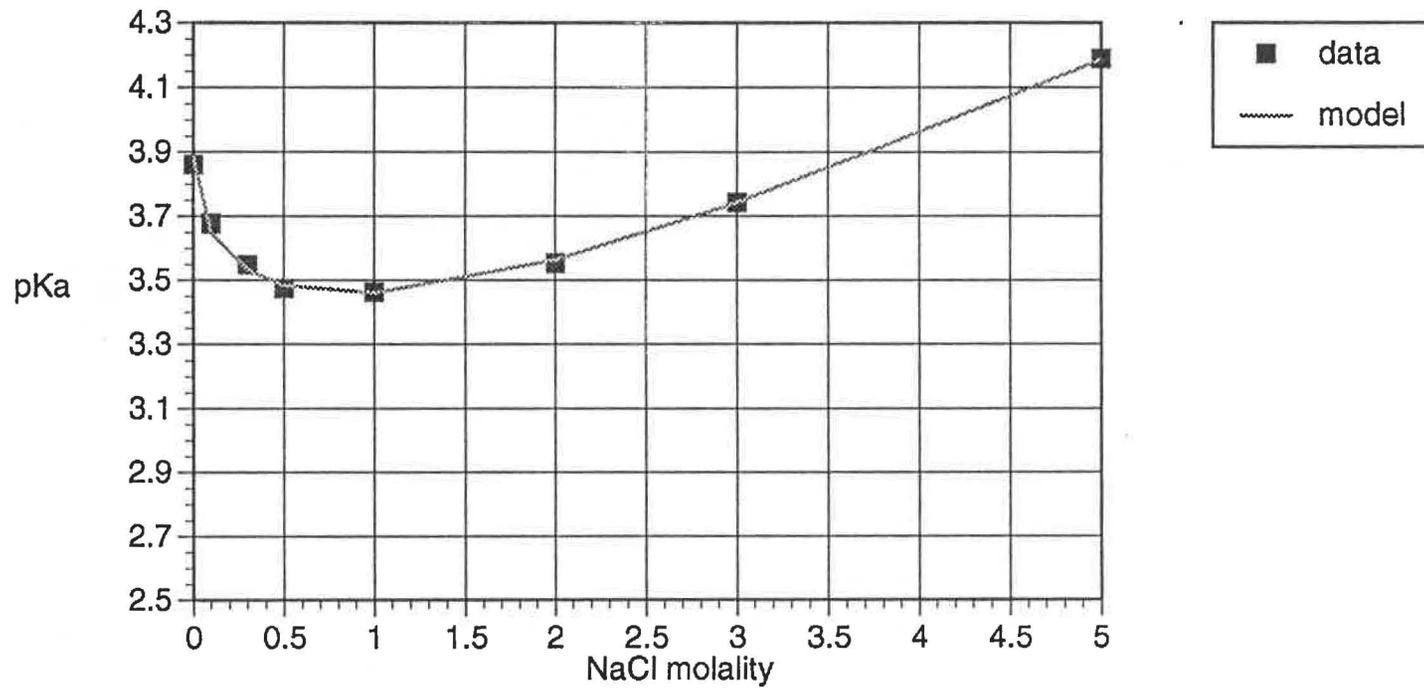


Figure 1. Lactic acid deprotonation as a function of NaCl molality.

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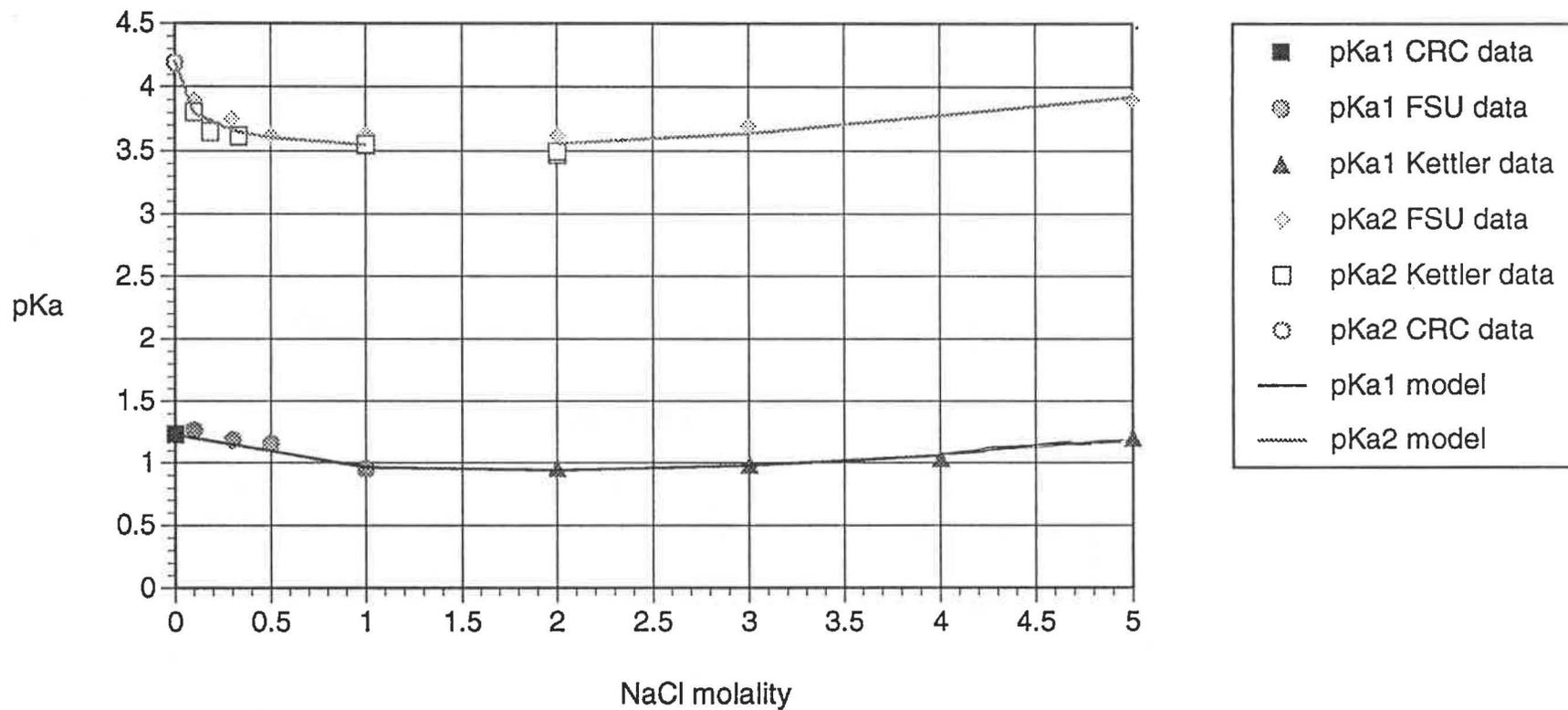


Figure 2. Oxalic acid deprotonation as a function of NaCl molality.

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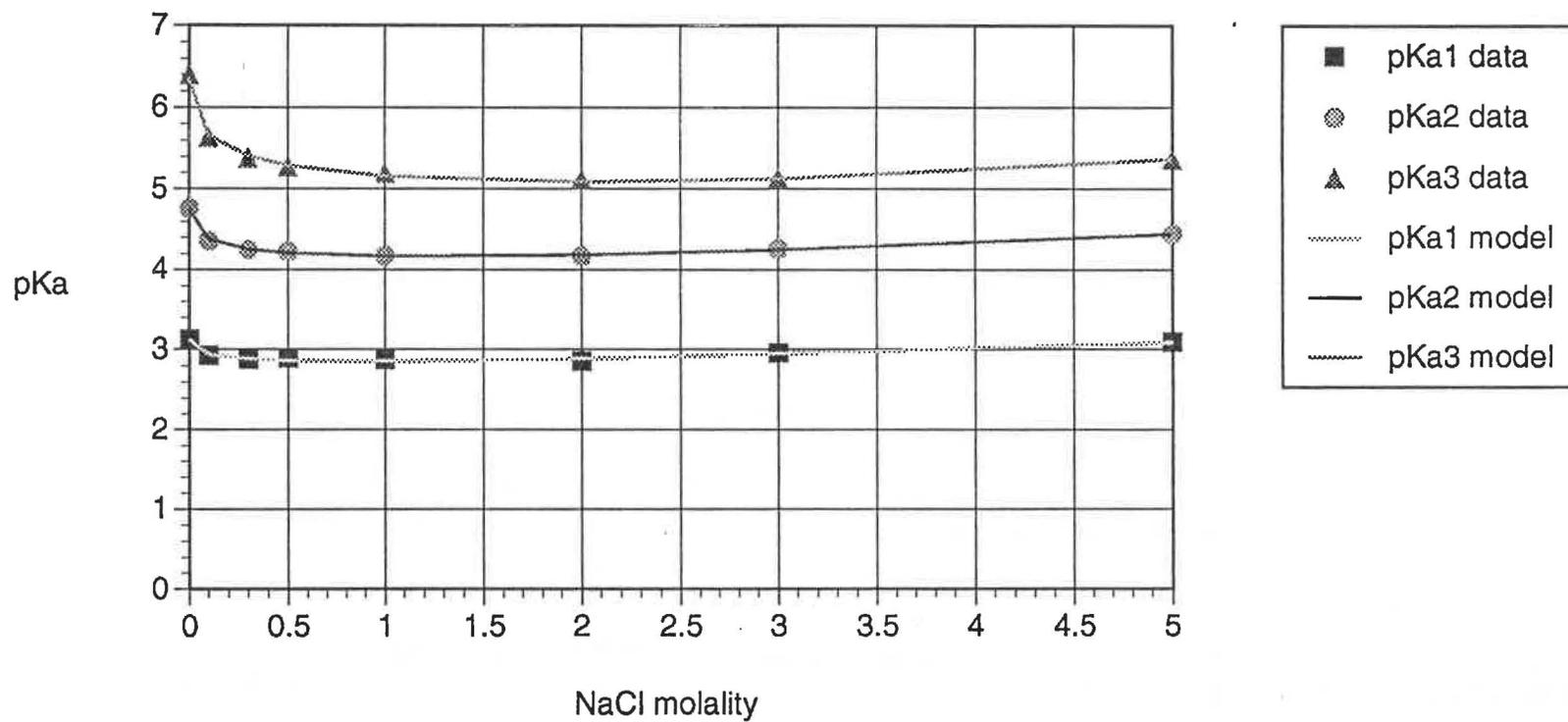


Figure 3 . Citric acid deprotonation as a function of NaCl molality.

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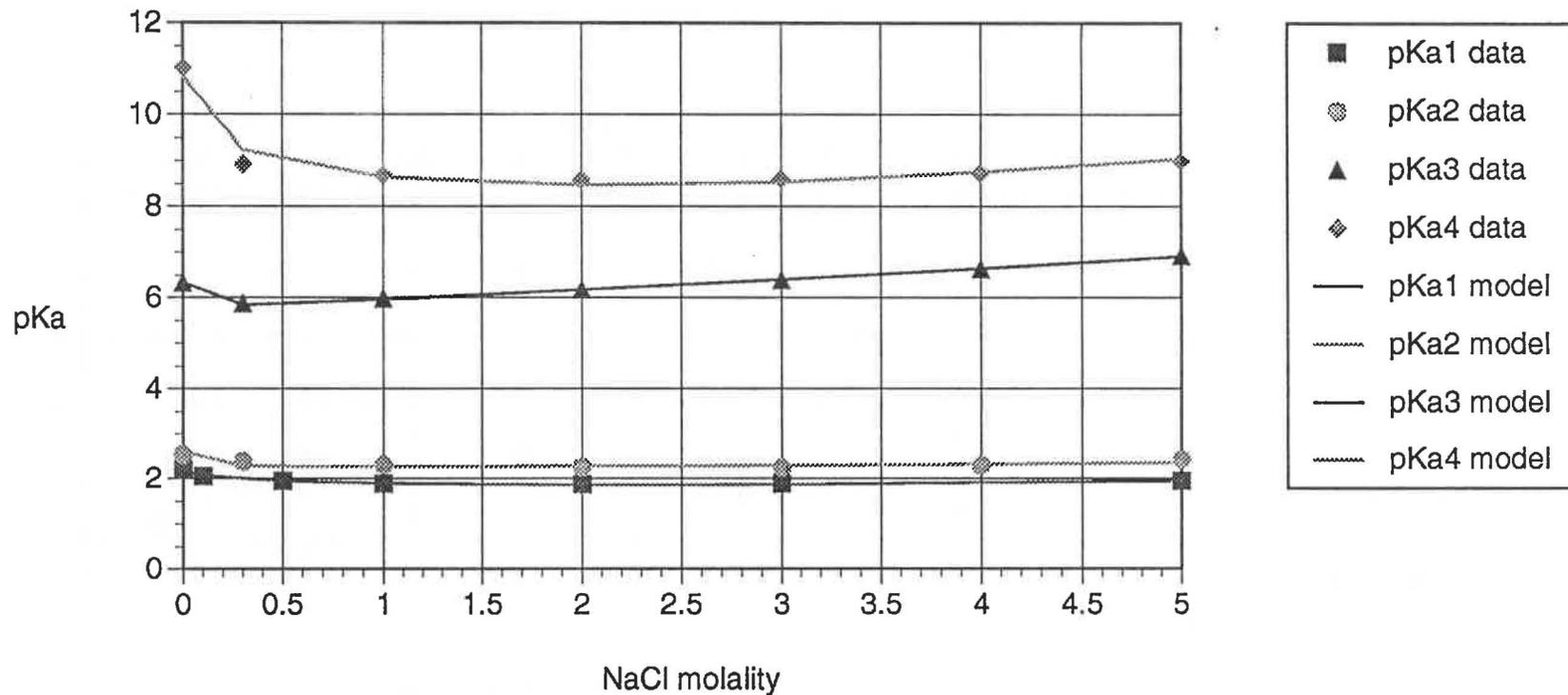


Figure 4. EDTA deprotonation as a function of NaCl molality.

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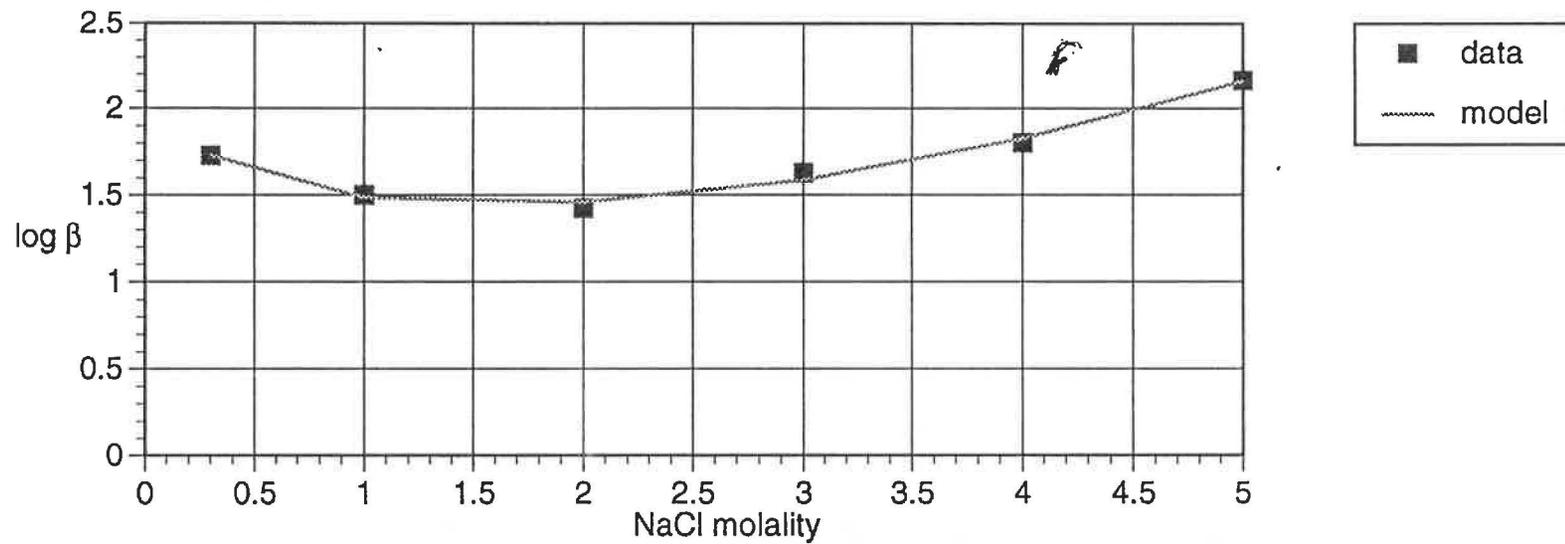


Figure 5. Apparent stability constant for acetate complexation with americium in NaCl media.

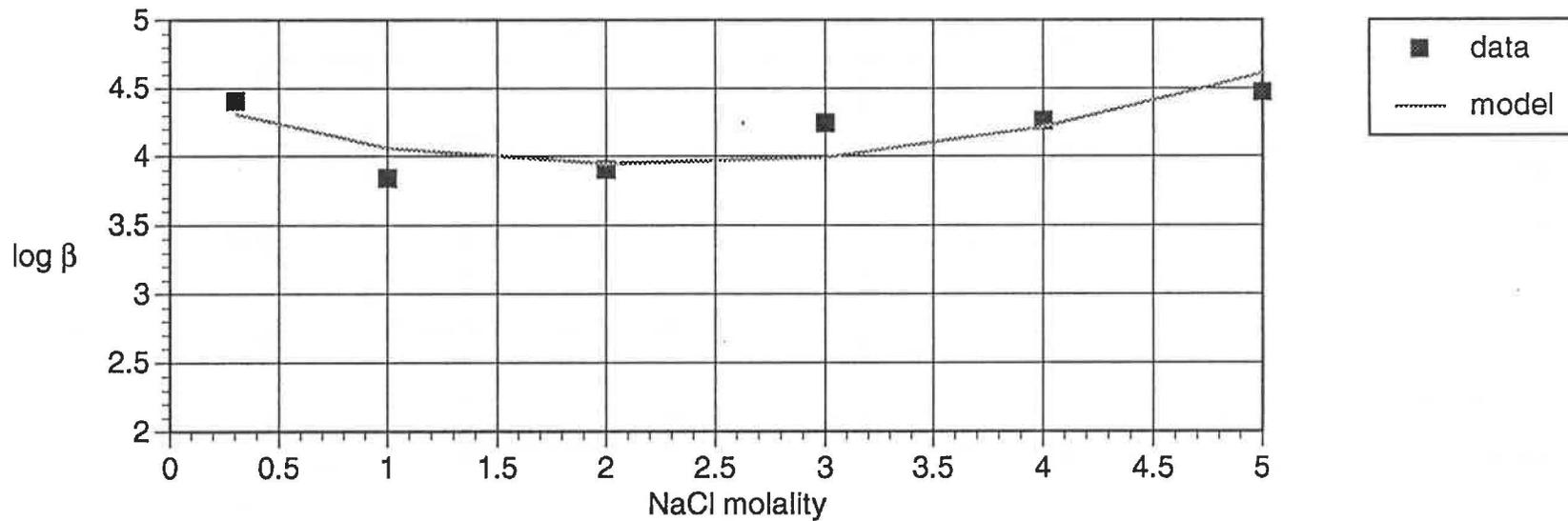


Figure 6. Apparent stability constant for acetate complexation with thorium in NaCl media.

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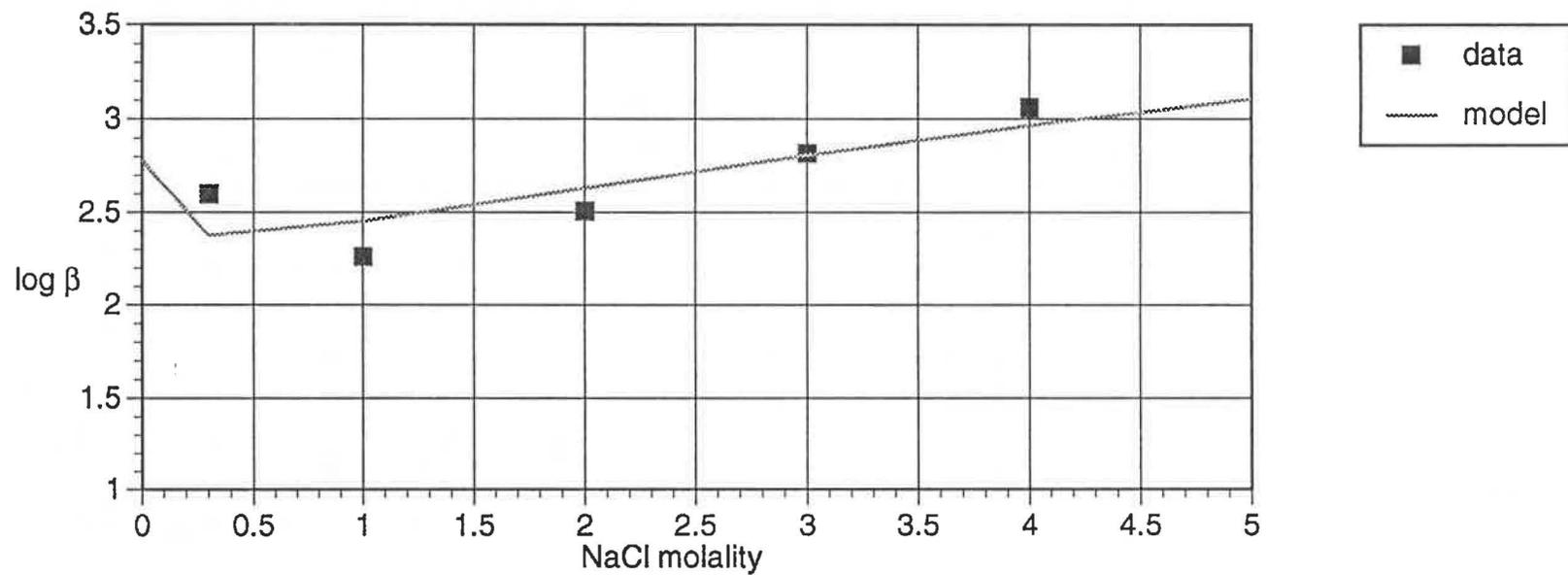


Figure 7: Apparent stability constant for acetate complexation with uranyl in NaCl media.

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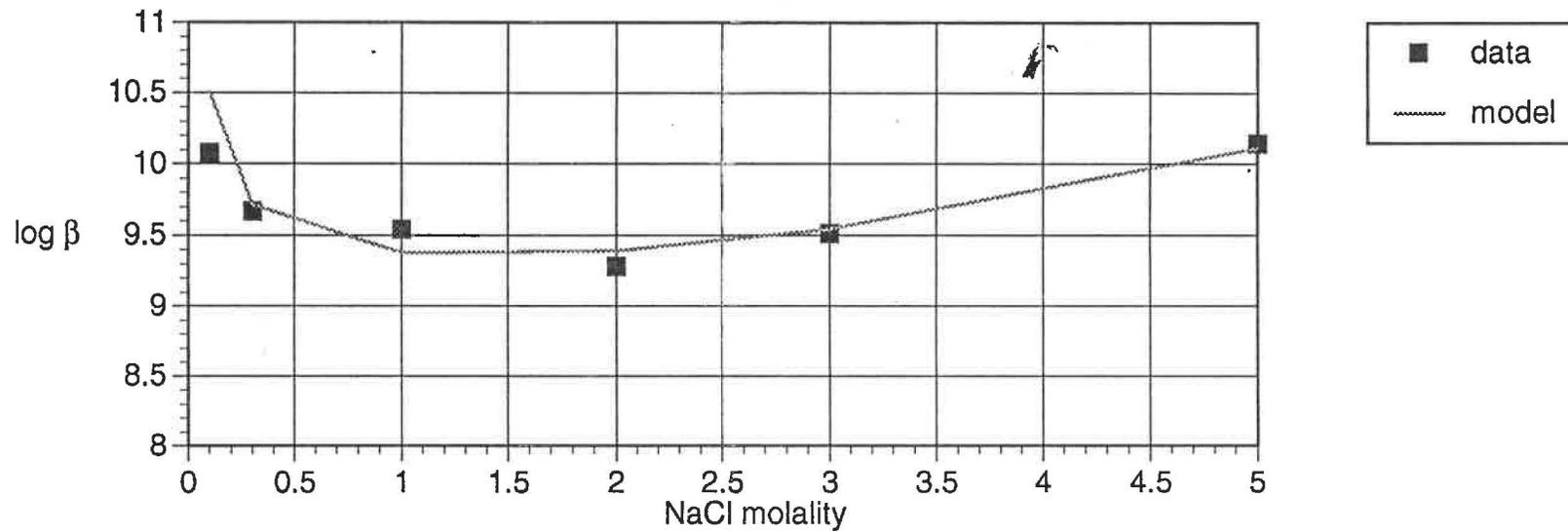


Figure 8. Apparent stability constant for citrate complexation with americium in NaCl media.

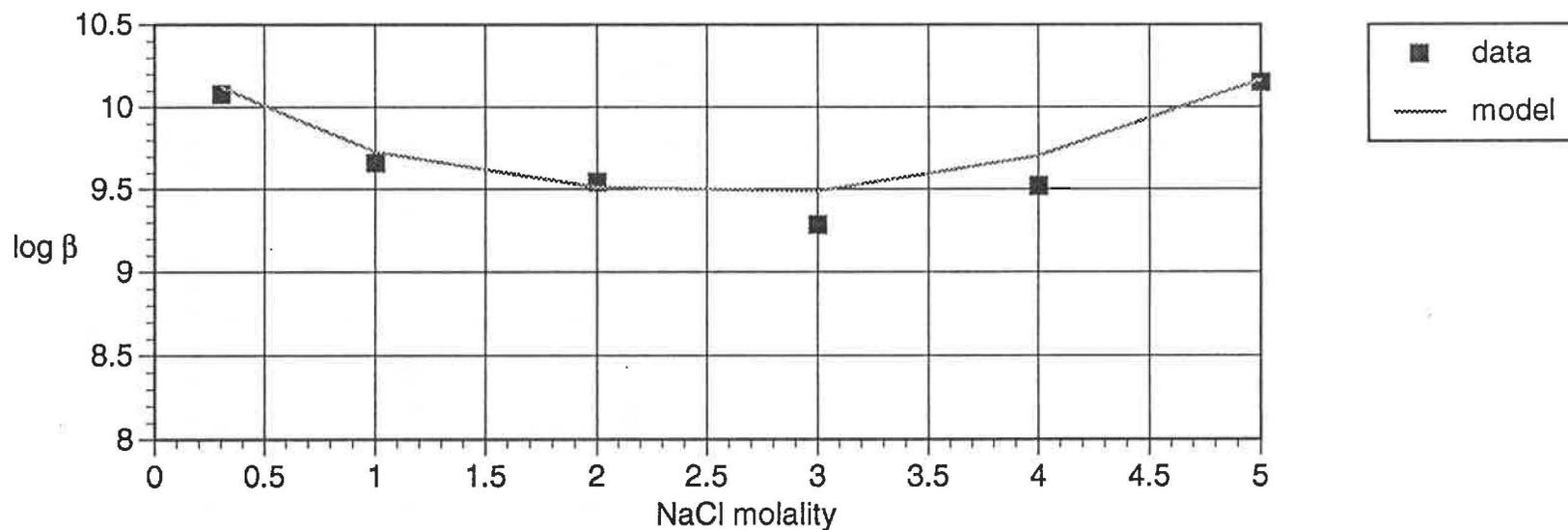


Figure 9. Apparent stability constant for citrate complexation with thorium in NaCl media.

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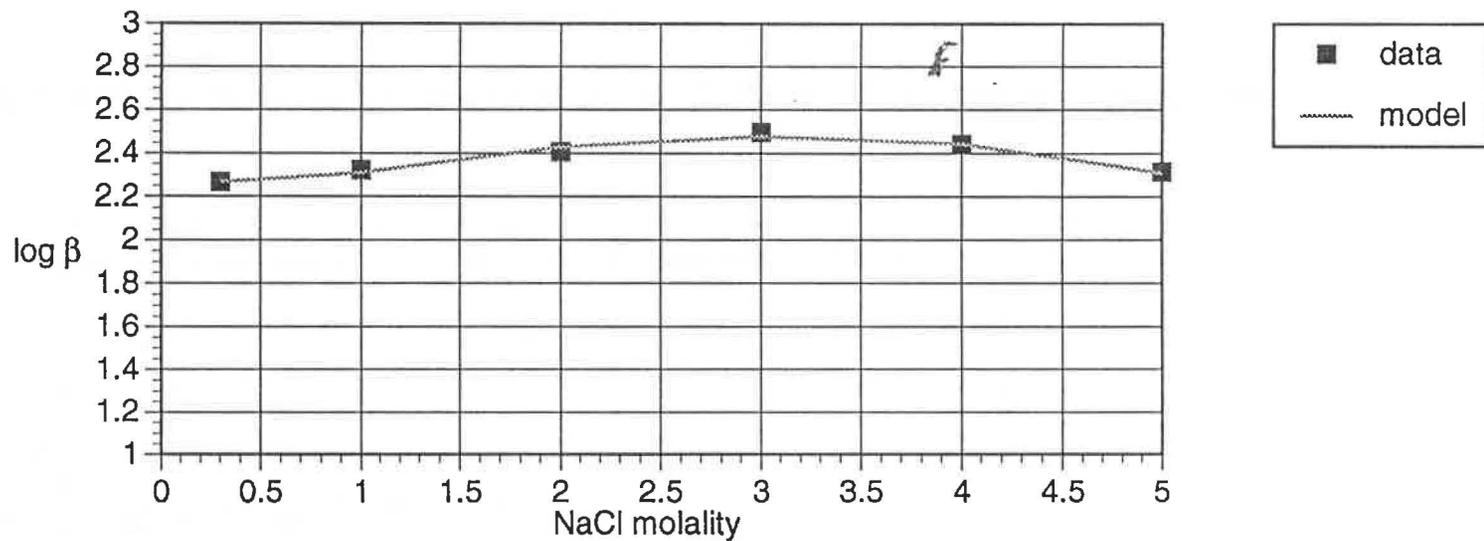


Figure 10. Apparent stability constant for citrate complexation with neptunyl in NaCl media.

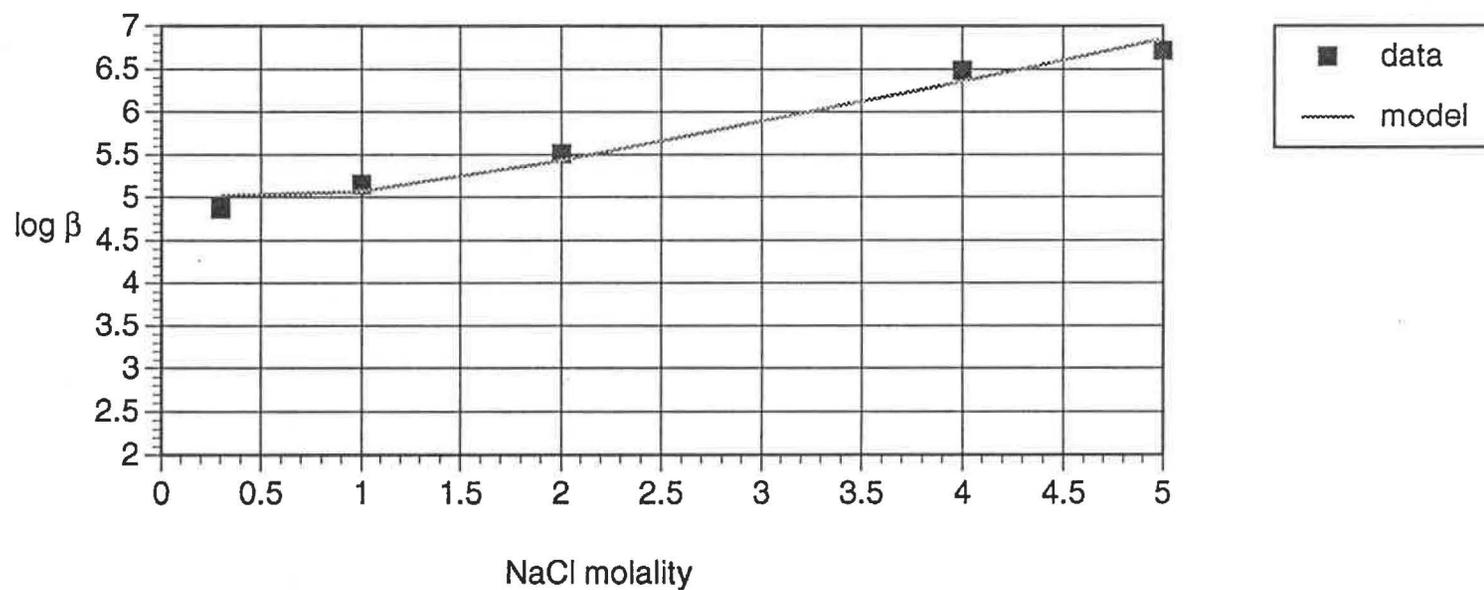


Figure 11. Apparent stability constant for citrate complexation with uranyl in NaCl media.

Information Only

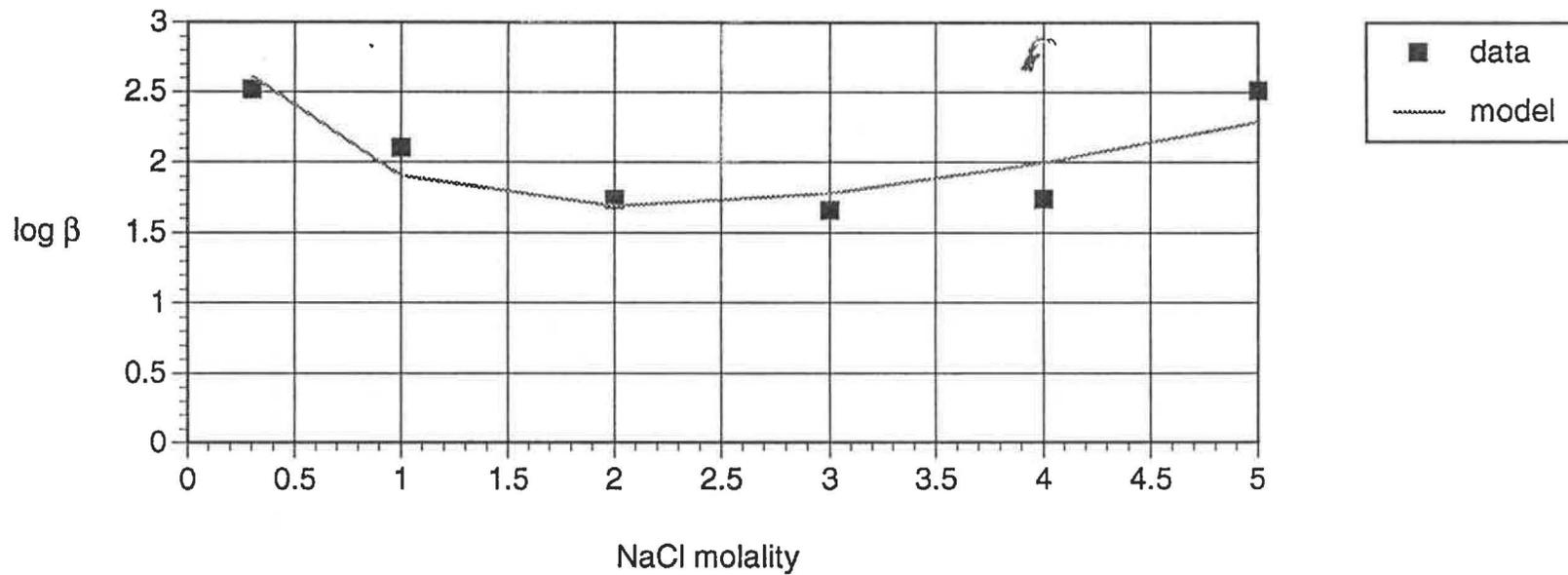


Figure 12. Apparent stability constant for lactate complexation with americium in NaCl media.

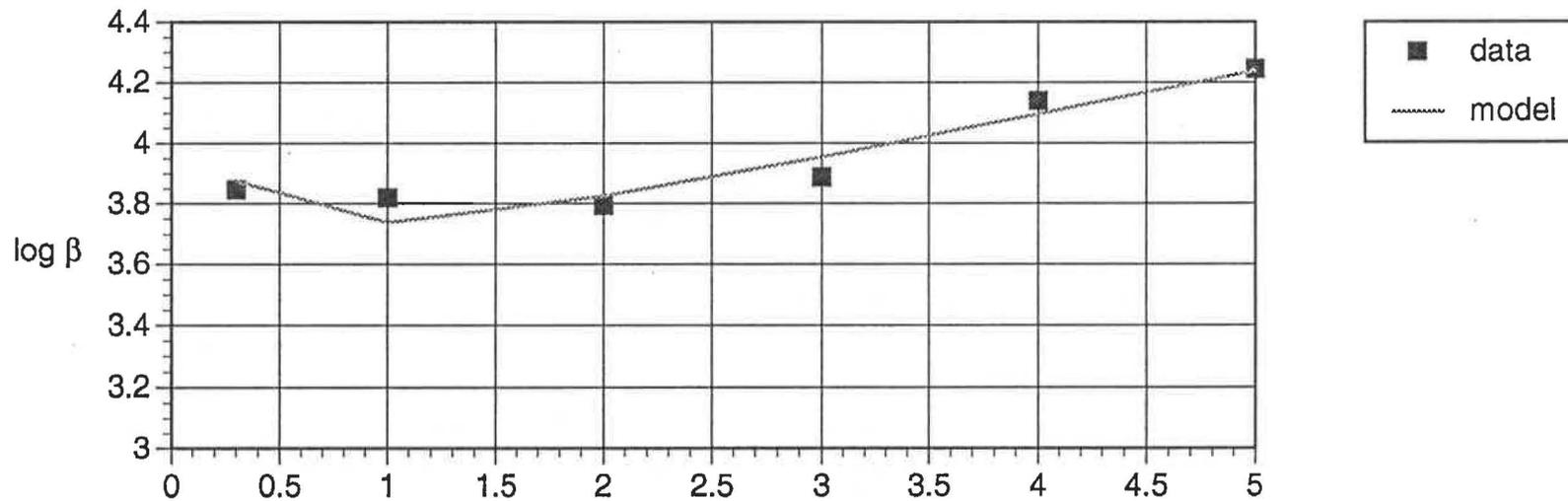


Figure 13. Apparent stability constant for lactate complexation with thorium in NaCl media.

Information Only

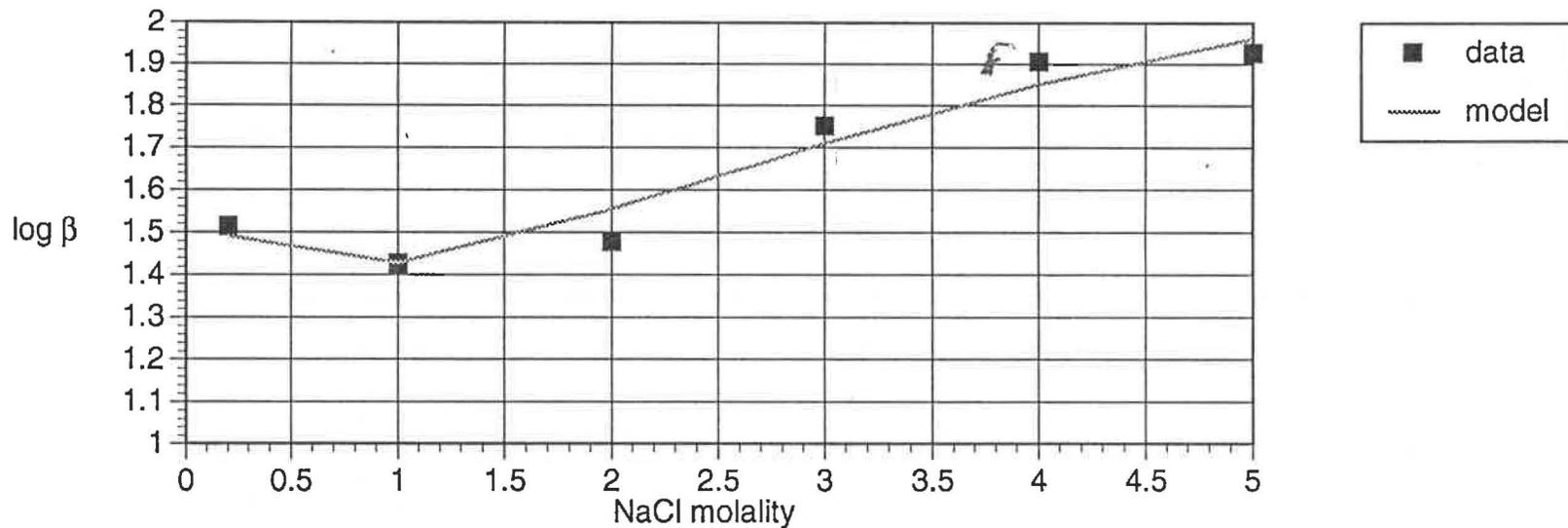


Figure 14. Apparent stability constant for lactate complexation with neptunyl in NaCl media.

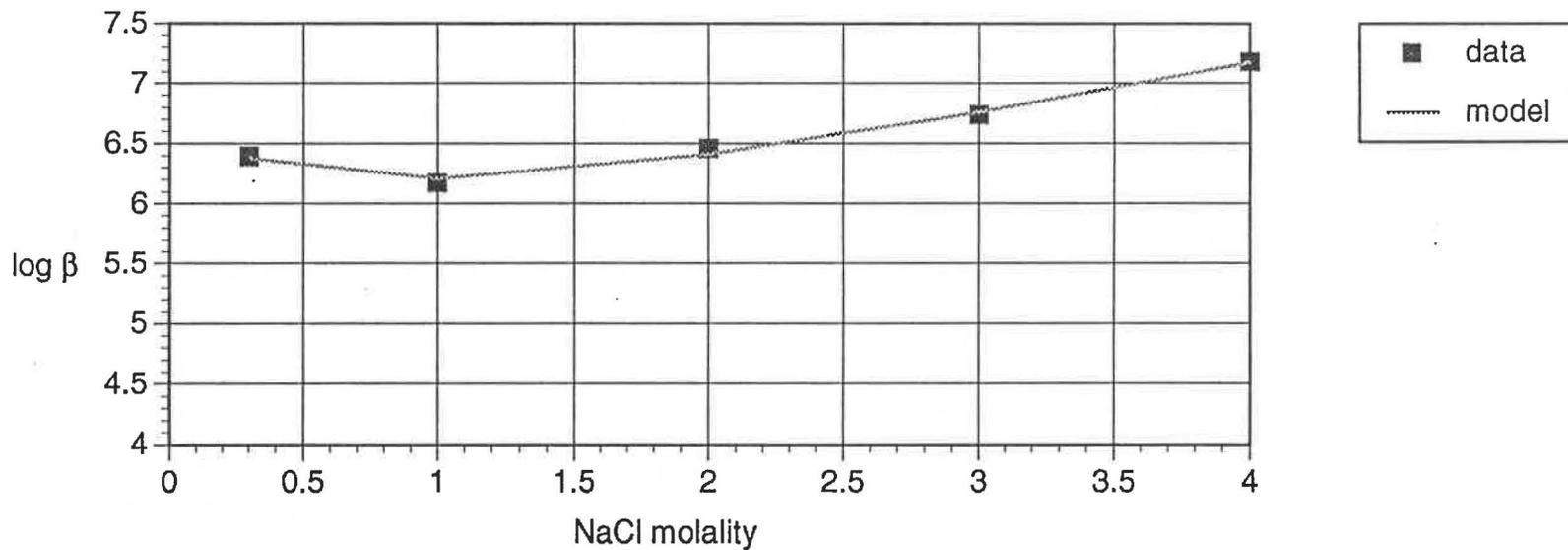


Figure 15. Apparent stability constant for lactate complexation with uranyl in NaCl media.

Information Only

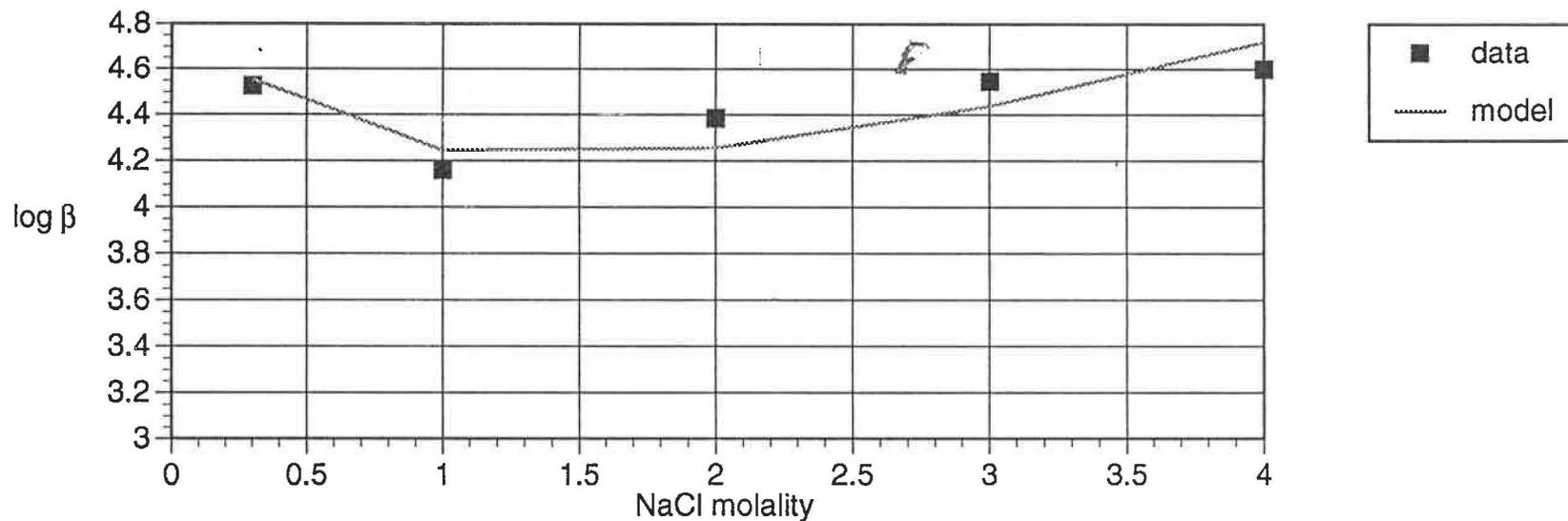


Figure 16. Apparent stability constant for oxalate complexation with americium in NaCl media.

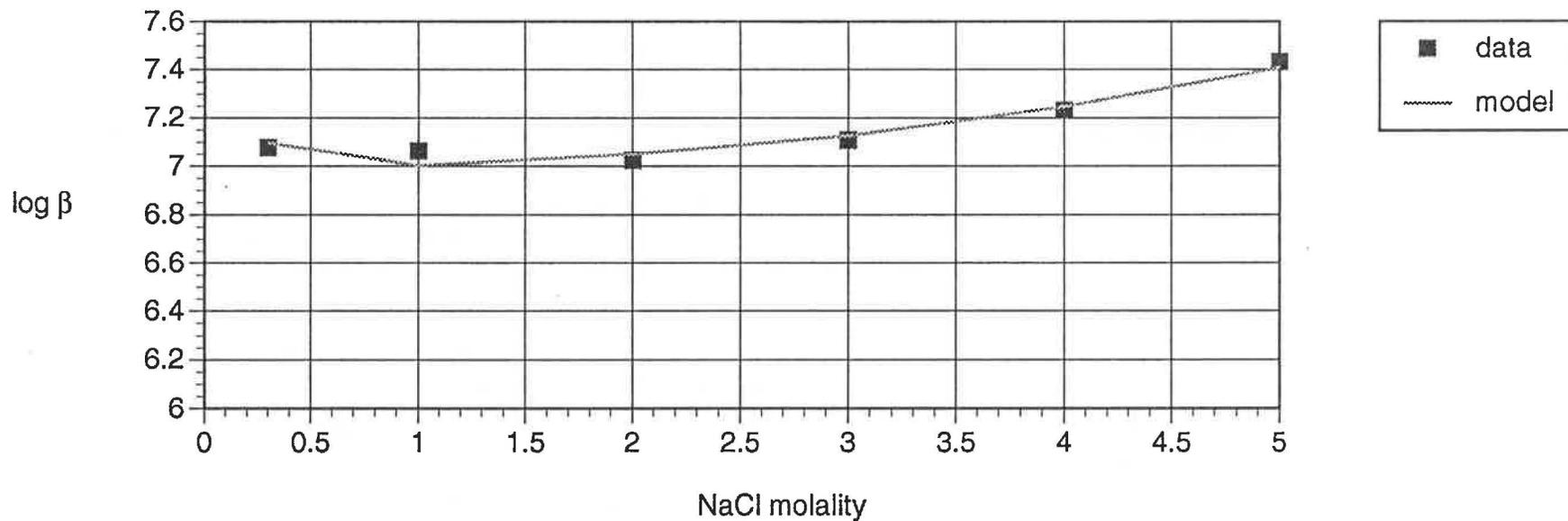


Figure 17. Apparent stability constant for oxalate complexation with thorium in NaCl media.

Information Only

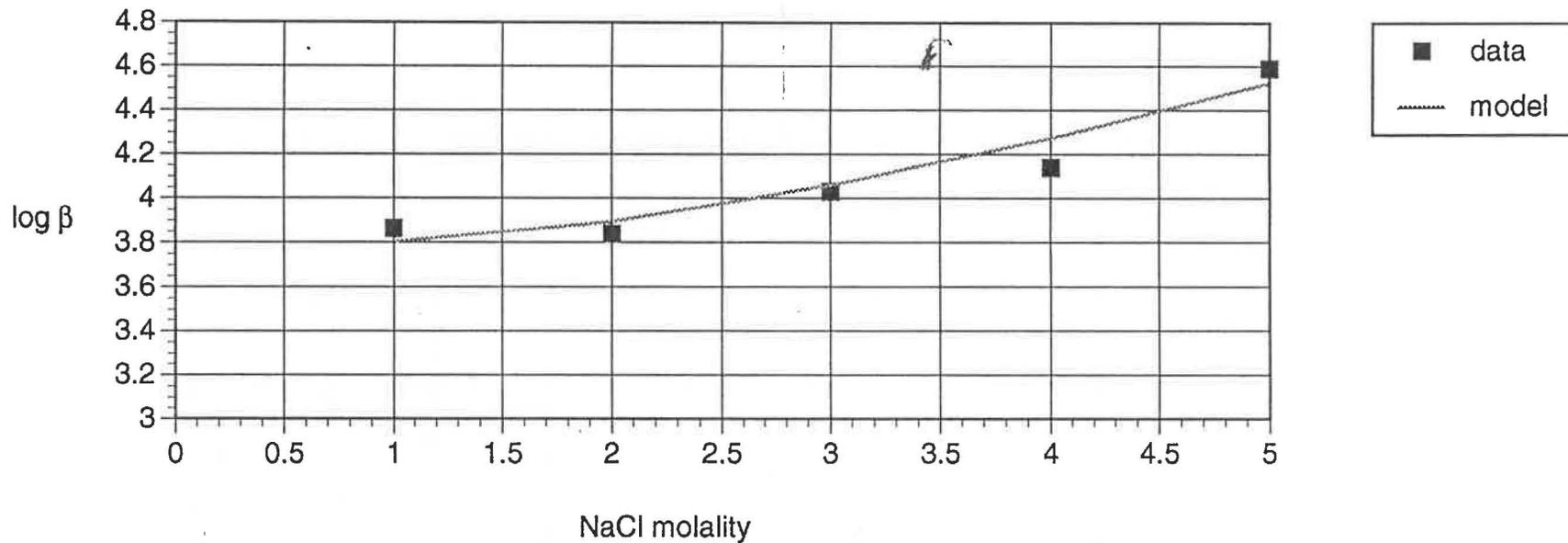


Figure 18. Apparent stability constant for oxalate complexation with neptunyl in NaCl media.

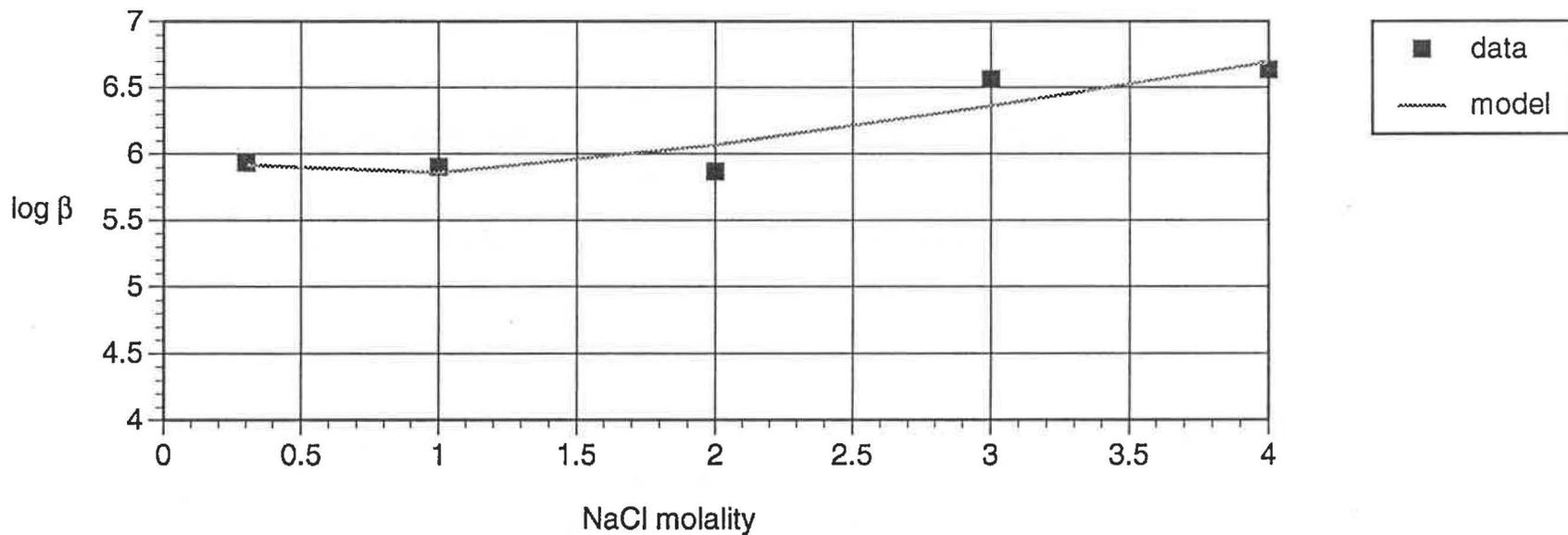


Figure 19. Apparent stability constant for oxalate complexation with uranyl in NaCl media.

Information Only

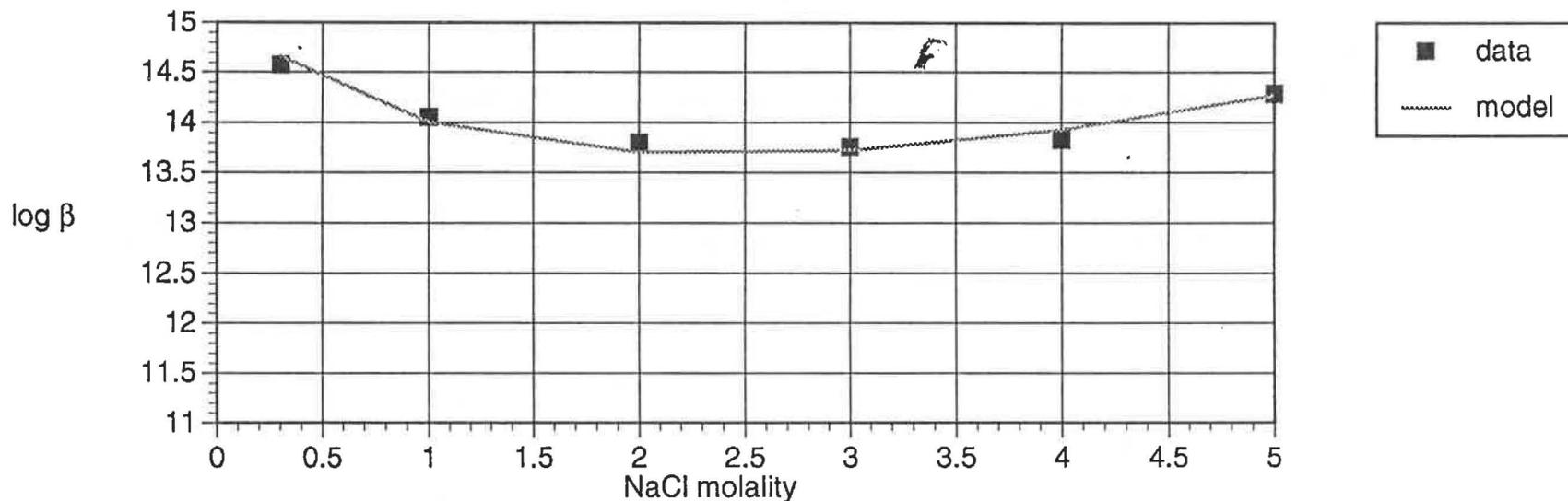


Figure 20. Apparent stability constant for EDTA complexation with americium in NaCl media.

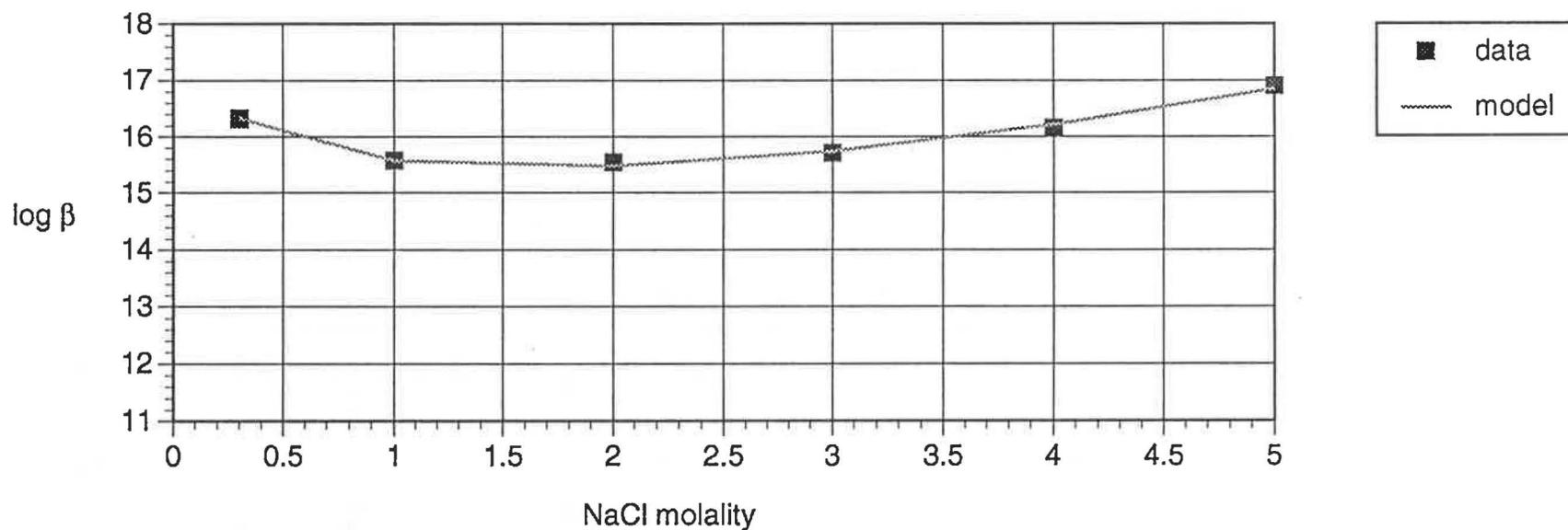


Figure 21. Apparent stability constant for EDTA complexation with thorium in NaCl media.

Information Only

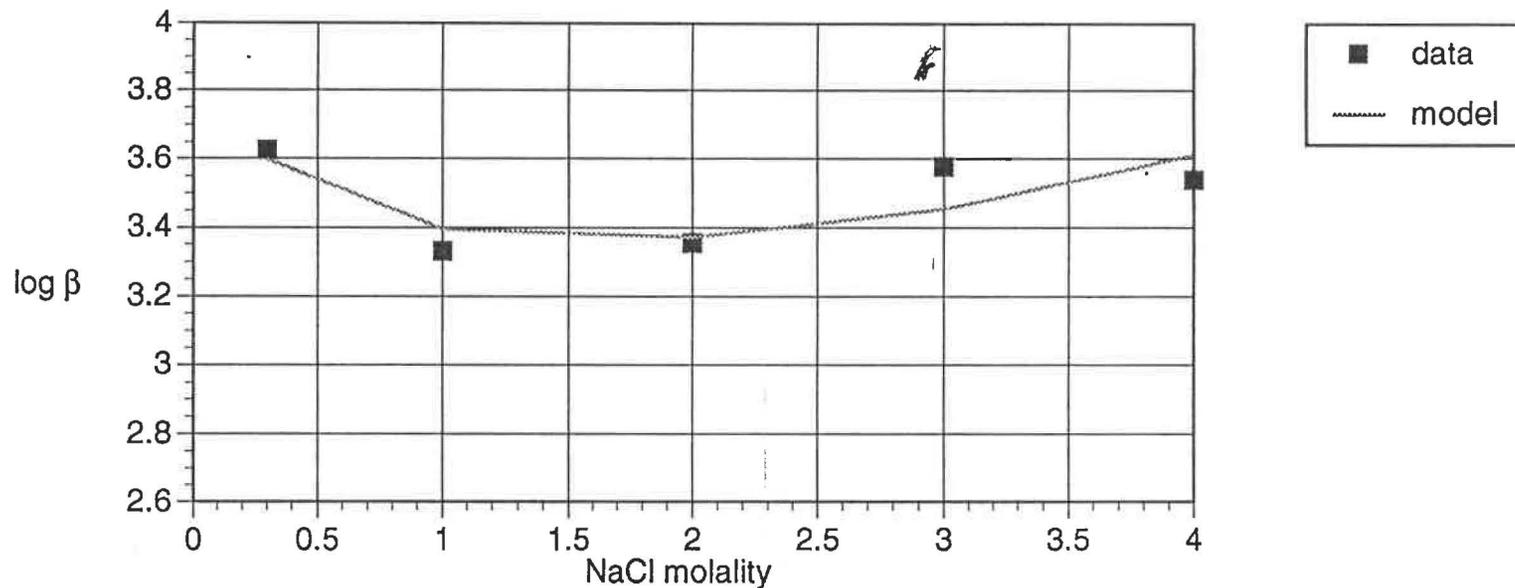


Figure 22. Apparent stability constant for EDTA complexation with neptunyl NaCl media.

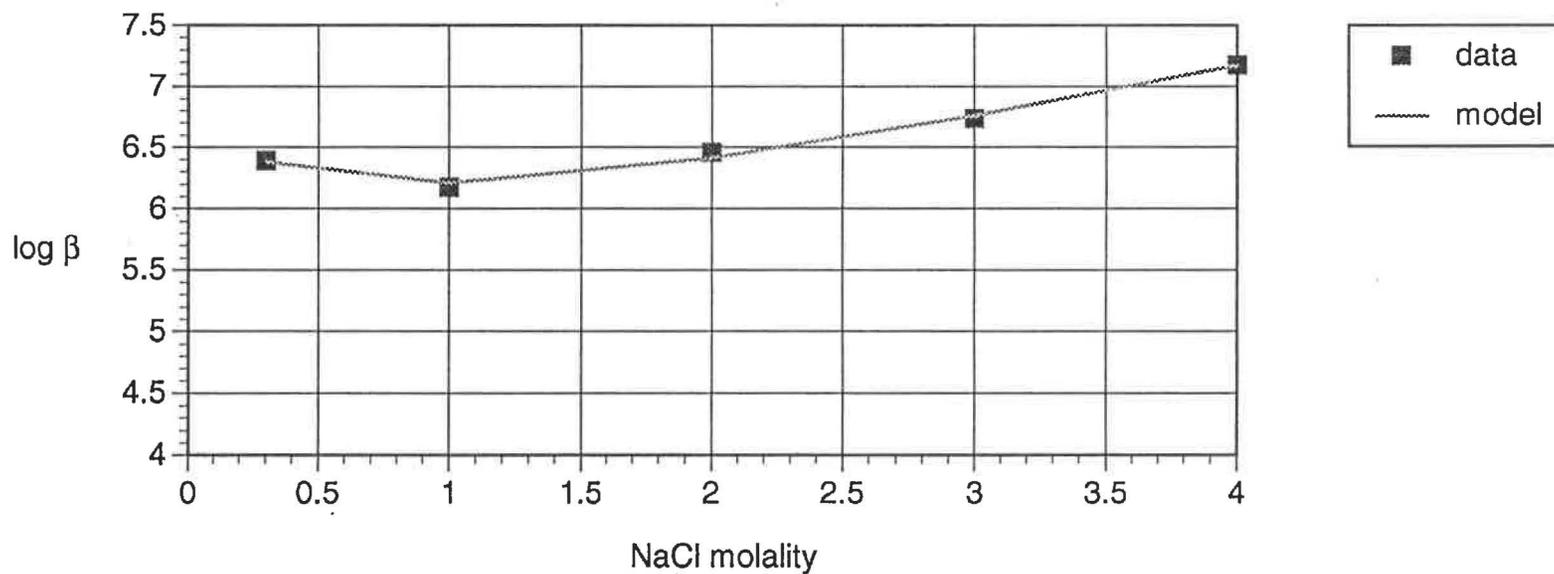


Figure 23. Apparent stability constant for EDTA complexation with uranyl NaCl media.

Information Only

File=FMT_ERDA6_NESQ_970407.IN

'Actinides in ERDA6 Saturated with NaCl,CaSO4,Brucite,Nesquehonite'

'CHEMFILE'

'BATCH' 'EXPLICIT'

'nMOLES' 'nEXACT'

1.13289995E+02	Hydrogen
6.57555273E+01	Oxygen
7.19980915E+00	Sodium
1.10087747E-01	Potassium
2.04429362E+00	Magnesium
1.01344192E+00	Calcium
6.96738842E+00	Chlorine
1.19112712E+00	Sulfur
1.00103149E+00	Carbon
0.00000000E+00	PosIon:EL
0.00000000E+00	NegIon:EL
0.00000000E+00	Oxalate:EL
7.08491570E-02	Boron
1.23704871E-02	Bromine
0.00000000E+00	Acetate:EL
11.00000678E-03	Th(IV)
1.00041150E-03	Am(III)
0.00000000E+00	Pu(III)
1.00253377E-03	Np(V)
0.00000000E+00	ClO4:EL
0.00000000E+00	Phosphorus
0.00000000E+00	U(IV)
0.00000000E+00	Lactate:EL
0.00000000E+00	EDTA:EL
0.00000000E+00	Citrate:EL
0.00000000E+00	Electron:E
0.0	Charge

Information Only

File=FMT_SPC_HMAG4323_970407.IN

'Actinides in SPC Saturated with NaCl,CaSO4,Brucite,Hydromagnesite4232'
'CHEMFILE'
'BATCH' 'EXPLICIT'

'nMOLES' 'nEXACT'
1.36767180E+02 Hydrogen
7.99098638E+01 Oxygen
5.69295395E+00 Sodium
1.04775026E+00 Potassium
6.80724482E+00 Magnesium
1.03305403E+00 Calcium
9.81438839E+00 Chlorine
1.06024227E+00 Sulfur
1.00104081E+00 Carbon
0.00000000E+00 PosIon:EL
0.00000000E+00 NegIon:EL
0.00000000E+00 Oxalate:EL
2.71882500E-02 Boron
1.35941250E-02 Bromine
0.00000000E+00 Acetate:EL
1.00497956E-03 Th(IV)
1.00438590E-03 Am(III)
0.00000000E+00 Pu(III)
1.00263669E-03 Np(V)
0.00000000E+00 ClO4:EL
0.00000000E+00 Phosphorus
0.00000000E+00 U(IV)
0.00000000E+00 Lactate:EL
0.00000000E+00 EDTA:EL
0.00000000E+00 Citrate:EL
0.00000000E+00 Electron:E
0.0 Charge:EL

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