Zn – O – H

(соединения)

$Zn(OH)_4$ Вр-3684-VI 1956

Venkateswarlu K;
et al.
"Z. phys. Chem"
1956, 212, N3-4, 195-8.

Potential...

$ZnO_2 \cdot 0{,}5 \cdot H_2O$ Вр-730-V 1959

Vannerberg N

(Vi; To...o) Arkiv kemi, 1959,
14, N2, 107-113

И.К. спектры...

ZnO

$Zn(OH)_4^{2-}$ (vi) Raman. 1965-

3144.vi

Fordyce J. S., Baum R. L.,

J. Chem. Phys., 1965, 43, n3, 843-846 (англ)

Vibrational spectra of solutions of zinc oxide in potassium hydroxide.

Ref Журн, 1966, 10 Б144 ю

1967

VI-4050

Vi(E-$Zn(OH)_2$, -ZnOHCl, ZnOHF,
$Zn_5(OH)_8Cl_2$, $Zn_5(OH)_8Cl_2 \cdot H_2O$)

Stivastova O.K., Secco E.A.

Canad.J.Chem, 1967, 45, N6, 585-88.

Studies on metal hydroxg compounds. II. Infrared spectra of zinc derivatives E-$Zn(OH)_2$, ZnOHCl, ZnOHF, $ZN_5(OH)_8Cl_2$ and $Zn_5(OH)_8Cl_2 \cdot H_2O$.

RX., 1967, 19Б169 J

ZnOHF.

плоск. C_i

Znопред. 1015 $см^{-1}$

Внеплоск. деф. кол.

группировок F-Zn-OH

885 $см^{-1}$

Srivastava O.K., 1967.

Secco E.A.,

Canad. J. Chem., 1967, 45,

№6, 585-588

Studies on metal hydroxy compounds.

II Infrared spectra of zinc derivatives $\alpha Zn(OH)_2$, $\beta ZnOHCl$, ZnOHF, $Zn_5(OH)_8Cl_2$, and $Zn_5(OH)_8Cl_2 \cdot H_2O$.

$Al(OH)_4^-$; $Zn(OH)_4^{2-}$; $Si(CH_3)_4$; $Ge(CH_3)_4$; $Sn(CH_3)_4$; $Pb(CH_3)_4$; $N(CH_3)_4$; $As(CH_3)_4$; $Sb(CH_3)_4$ (сил. пост.) 1969

6 14

VI 7278

Durig J.R.; Nagarajan G.,

Monatsh. Chem., 1969, 100(6), 1948-59. (нем.)

Potential energy constants and mean amplitudes of vibration in some XY_4 molecules and cons. with tetrahedral symmetry.

10 15

CA, 1970, 72, N14, 70815e

$M(H_2O)_6$ (сил. изом.)
$M = Mg, Zn, Ni, Al$ G 615 1970
VI 7290
Ananthanarayanan V.,
J. Chem. Phys., 1970, 52, № 7, 3844-5 (англ.)
Force constants of octahedral $M(H_2O)_6$ complexes: M = Mg, Zn, Ni, or Al.

10 10

CA 1970 72, N22, 116240d

Zn-OH

1972

Opitz Ch., Dünken H.H.

Энерг. связи

"Z. phys. Chem", 1972, 249, №3-4, 154-160

Природа хим. св.

(см. Cr-OH, III)

40213.1847
Ph, Ch, TE

$Zn(H_2O)_6^{2-}$

34457

1973

17222

Sanyal Nitish K., Dixit L., Subramanyam B.R. Force constants and mean amplitudes of vibration of some octahedral water complexes of Mg, Al, Ni and Zn.
"Indian J. Phys.", 1973, 47, N 10, 577-582

(см. $Mg(H_2O)_6^{3+}$ (англ.))

0044 ВМК

024 025

ВИНИТИ

$Zn(OH)_4^{2-}$

$Zn(OH)_2$

1980

8 Б46. Неэмпирическое исследование стереоэлектронных эффектов в модельных комплексах $Zn(OH)_4^{2-}$ и $Zn(OH)_2$. Lehn J. M., Wipff G., Demuynck J. An ab initio study of stereoelectronic effects in $Zn(OH)_4^{2-}$ and $Zn(OH)_2$ model complexes. «Chem. Phys. Lett.», 1980, 76, № 2, 344—346 (англ.)

Методом ССП МО ЛКАО с использованием базиса сгруппированных гауссовых орбиталей Zn (12*s*8*p*5*d*/5*s*-4*p*2*d*), O(8*s*4*p*/3*s*2*p*) и H(4*s*/2*s*) рассчитано электронное строение модельных комплексов $Zn(OH)_4^{2-}$ (I) и $Zn(OH)_2$ (II). Комплексы I и II рассматривались в конформациях с различными, фиксированными ориентациями связей OH. Для сравнения методом ССП МО ЛКАО проведены также расчеты стерео-электронных эффектов в комплексе $Al(OH)_4^-$ и молекуле $C(OH)_4$ в той же конформации, что и I. Оптимизация длин связей в $Al(OH)_4^-$ и $C(OH)_4$ проведена в миним. базисе ОСТ—3ГФ. Вычисленная энергия стабилизации I и II по отношению к разделенным фрагментам составила 1017 и 882 ккал/моль соотв. Хелатный эффект в I (энергия, требуемая для переориентации 4 лигандов

кв. мех. расчет

Х. 1981 № 8

OH^- в правильную геометрию комплекса) составил 626 ккал/моль. Оптимизированные длины связей Zn—O в **I** и **II** показывают слабую конформац. зависимость. На основании данных проведенных расчетов сделан вывод, что стереоэлектронные эффекты, обусловленные ориентацией лигандов, слабы в соединениях $X(OH)_4^{n-}$ ($X=Zn^{2+}$, Al^{3+}), где связи являются ионными и длинными, по сравнению со стереоэлектронными эффектами в ковалентной тетраэдрич. молекуле $C(OH)_4$.

И. А. Тополь

$[Zn(H_2O)_6]^{2+}$

1980

Sano Mitsuru, et al.

Chem. Lett. 1980, (12), 1496-6.

св. мех. рас. потенц. ф-ции

см. $[Cu(H_2O)_6]^{2+}$ - III

$Zn(OH)_4$ - ион

1982

Mohan S.

Коричисов. постоян., сил. пост.

Indian J. Phys., 1982, B56, N1, 23–28.

(см. Ti Oh - ион, III)

$Zr(H_2O)^{2+}$ 1983

Sano Mitsuru,
Yamatera Hideo.
Ions and Mol. Solut Collect. Invit. Pap. Sess. Lect. and Microsymp. 6 Int. Symp. Solute-Solute-Solvent Interact. Kinoo, 4-10 July, 1982. Amsterdam e.a., 1983, 109-116.
(Ср. $Be(H_2O)^{2+}$; III)

межлиганд. расстояние.

$Zn(H_2O)_6^{2+}$ Sano Mitsuru, Yamatera Hidéo. 1983

Ions and Mol. Solut. Collect. Invit. Pap. Sess. Lect. and Microsymp. 6 Int. Symp. Solute-Solute-Solvent Interact. Minoo, 4-10 July, 1982. Amsterdam e.a., 1983, 109-116.

неэмпи-
рич.
расчёт.

(См. $Be(H_2O)^{2+}$; III)

$Zn^{n+}-OH_2 \ldots OH_2$ 1984

Тарамовский В.И.,
Сизова О.В. и др.

расчёт ж. общ. химии, 1984,
электр. 54, N 3, 507-511.
структ.

(см. $M^{n+}-OH_2 \ldots OH_2$; III)

$H_2O \cdots Zn^{2+}$ [рп. 19654] 1984

Sauer J., Hobza P.,

теор. расчёт геометр. и энергии

Theor. chim. acta, 1984, 65, N4, 291–302.

ZrOH 22327 1985

Kauffman J. W., Margrave
Mauge R. H., et al.

спектр J. Phys. Chem., 1985,
в 89, N 16, 3541-3547.
справочке

(сел. CuOH; III)

$Zn^{2+}-OH_2$

1986

11 Л224. Теоретические исследования интенсивностей ИК-полос в $Zn^{2+}OH_2$ и $Mg^{2+}OH_2$. Theoretical studies of I. R. intensities in $Zn^{2+}OH_2$ and $Mg^{2+}OH_2$. Hermansson Kersti, Lindgren Jan, Agren Hans. «Mol. Phys.», 1986, 57, № 4, 857—863 (англ.)

Методами одно- и многоконфигурационного самосогласованных полей рассчитаны интенсивности ИК-полос валентных колебаний связей O—H в комплексах $Mg^{2+}OH_2$ и $Zn^{2+}OH_2$, а также в изолированных молекулах H_2O. В гармонич. приближении определены силовые постоянные связей и ф-ции дипольного момента в гидратированных ионах. Обнаружено увеличение равновесной длины связи O—H молекул H_2O при их координации с ионами Mg^{2+} и Zn^{2+}. Изложена модель гидратирования этих ионов. Показано, что в комплексах Mg^{2+} орбитали иона и молекул H_2O не перекрываются, тогда как в комплексах Zn^{2+} обобщенные орбитали приобретают характер $3d$-σ. Сделан вывод о возможности образования водородных связей с участием этих комплексов и 2 молекул H_2O в жидкой фазе. Библ. 21.

И. В. А.

(М.П.)

Ф (+)

Ф. 1986, 18, N 11

Zr(OH)Ht [от. 31286] 1988

Zr(OH)$_2$Ht Tran Q., Kabellas N.S., et al.,

присут-
ствие
в
пламени,
масс-
спектр.

Can. J. Chem. 1988, 66, N 9,
2216–2218.

Ion chemistry of transition
metals in hydrocarbon
flates. I Cations of Fe,

Co, Ni, Cu and Zn.

ZnOH+ [ОИ. 31286] 1988

Tran Q., Kabellas N.S., et al.,

присут-
ствие в
пламени,
масс-
спектр.

Can. J. Chem. 1988, 66, N 9,
2216-2218.

Ion chemistry of transition metals in flates. I hydrocarbon cations of Fe, Co,

Ni, Cu and Zn.

$Zn(H_2O)_n^+$ (OM 33941) 1990

Rosi M., Bauschlicher Ch.W.,

Do, J. Chem. Phys., 1990, 92, Fr.

4 Hf. N3, 1876-1878.

The binding energies of one and two water molecules to the first transi-

tion row metal positive ions

II.

$[Zn(H_2O)_6]^{2+}$

1992

Aakesson R., Peterson L.F.M. et al.,

D(Zn-O), ab initio' расчет

J. Phys. Chem. 1992, 96 (26), 10773-9

(см. $[Ca(H_2O)_6]^{2+}$, III)

$[Zn(H_2O)_6]^{2+}$ 1992

Waizumi Kenji, и Ohtaki Hitoshi et al.

Chem. Lett. 1992, (8), 1489-92.

структ. энергия связи, теор. расчёт.

(см. $[Cr(H_2O)_6]^{2+}$; III)

$Zn^{2+}-OH_2$

$Zn^{2+}-OH^-$

1992

10 Д118. Параметризация полуэмпирического квантовохимического метода MINDO/3 для цинксодержащих соединений / Жанпеисов Н. У., Жидомиров Г. М. // Ж. структур. химии.— 1992.— 33, № 1.— С. 151—153

Предложена параметризация метода МЧПДП/3 для изучения геометрии и энергетики Zn-содержащих молекул. Получены значения энтальпии образования и потенциалы ионизации. Рассмотрена реакция образования комплексов катиона Zn^{2+} с рядом электронодонорных молекул и оценена энергия связи в комплексах $Zn^{2+}—X$, где $X=OH_2$, CO_2, SH_2, OH^-, SH^-.

($\Delta_f H$, м.п.)

Ф (+3)

Ф. 1992, N 10

Zn-H-OH

1993

119: 234388k **Nascent rotational and vibrational distributions in both products of the reaction zinc + water → zinc hydride + hydroxyl ($Zn(4\ ^1P_1) + H_2O \rightarrow ZnH(X\ ^2\Sigma^+) + OH(X\ ^2\Pi)$).** Kuwahara, Kazuya; Ikeda, Hiroyuki; Misaizu, Fuminori; Fuke, Kiyokazu (Dep. Energy Sci., Tokyo Inst. Technol., Tokyo, Japan 152). *J. Chem. Phys.* 1993, 99(4), 2715–22 (Eng). The reaction $Zn(4\ ^1P_1)+H_2O \rightarrow ZnH\ (X\ ^2\Sigma^+) + OH(X\ ^2\Pi)$ was studied under thermal equil. conditions at 700 K. The nascent internal state distributions of both products ZnH and OH were detd. by using a pump-and-probe technique. The rotational distributions of ZnH and OH were both Boltzamnn-like for their $v'' = 0$ vibrational levels. However, the rotational temperautres were significantly different–12,000 K for ZnH and 900 K for OH. ZnH was also vibrationally excited. The nascent vibrational distribution of ZnH was detd. to be obsd. such a nonstatistical energy partitioning is explained by consideringa short-lived Zn-H-OH. intermediate in a nonlinear geometry.

Сущ. конф-ции с нели-нейн. структ.

C. A. 1993, 119, N 22

$[Zn(H_2O)_6]^{2+}$

1993

Waizumi K., Ohtaki H. et al.

теория
расчеты
структуры
Do

Comput. Aide d Innovation New. Mater. 2 Proc. Int. Conf. Exib. Comput. Appl. Mater. Mol. Sci. Eng, 2nd 1992 (Pub. 1993), Pt 1, 861-4.

(ссс. $[Cr(H_2O)_6]^{2+}$; III)

$Zn(H_2O)_n^{2+}$ 1994

$n = 1, 2$

Åkesson, Ralf; Petterson, Lars G.M.;

спектр. парам., жидкие сверх., теорет. расчет.

Chem. Phys., 1994, 184 (1-3), 85–95

(см. $Ca(H_2O)_n^{2+}$, $n = 1, 2$; III)

MZnOH | Om. 38046. | 1995

Green T.M., Andrews L., et al;
J. Am. Chem. Soc., 1995,
117, 8180-8187.

ik

в

матрице

$Zn(H_2O)_n^{2+}$
$n = 1 \div 6$

1996

125: 151552g **Ab Initio Study of the Structures, Energetics, and Spectra of Aquazinc(II).** Lee, Sik; Kim, Jongseob; Park, Jong Keun; Kim, Kwang S. (Department of Chemistry and Center for Biofunctional Molecules, Pohang University of Science and Technology, Pohang, 790-784 S. Korea). *J. Phys. Chem.* 1996, 100(34), 14329-14338 (Eng). Using extensive ab initio calcns. including electron correlation, the authors have studied the structures, thermodn. quantities, and spectra of hydrated zinc ions [$Zn(H_2O)_n^{2+}$ (n = 1-6)]. Various conformers for $n = n_1 + n_2$ (where n_1 and n_2 are the nos. of water mols. in the first and second hydration shells, resp.) were investigated along with their thermodn. quantities. The entropy effect was found to be important for the stabilities. At 0 K, the most stable structures for n = 5 and 6 are 5 + 0 and 6 + 0, resp. However, at room temp., both 4 + 1 and 5 + 0 seem to be almost equally populated in the case of n = 5, while 6 + 0 is the most populated in the case of n = 6. The predicted successive binding energies for the addn. of each water mol. to the zinc ion are reported. The vibrational frequency shifts, depending on the no. of water mols., were investigated along with the frequency characteristics, depending on the presence/absence of outer-shell water mols.

структ., термодин. характ., спектр., колеб. част.

С. А. 1996, 125, N 12

1999

VF: ZnOH
P: 3
131:149998 Thermochemistry of ZnCl(g). Hildenbrand, D. L.; Lau, K. H.; Ro J. W. (SRI International, Menlo Park, CA 94025, USA). J. Chem. Phys., 11 1337-1338 (English) 1999 The gaseous species Zn, ZnCl, and ZnCl2 were generated in an effusion ce by reaction of Cl2(g) with ZnO(s) near 1400 K, and were identified and mo by mass spectrometry. Equil. consts. were evaluated for the gaseous reac + ZnCl2 = 2ZnCl from ion intensities measured over the

range 1336-1436 K used to derive the third law enthalpy change .DELTA.H298.degree. = 176 .+ mol-1 and the dissocn. energy D0.degree.(ZnCl) = 229 .+-. 8 kJ mol-1. Th result is in good agreement with an earlier value derived from equil. measurements made by monitoring the electronic spectrum of ZnCl(g) in equ with gaseous Zn and ZnCl2. The results are useful in estg. the thermoche properties of gaseous ZnOH and Zn(OH)2 for chem. modeling applications.

F: Zn(OH)2
P: 3
131:149998 Thermochemistry of ZnCl(g). Hildenbrand, D. L.; Lau, K. H.; Ro J. W. (SRI International, Menlo Park, CA 94025, USA). J. Chem. Phys., 11 1337-1338 (English) 1999 The gaseous species Zn, ZnCl, and ZnCl2 were generated in an effusion ce by reaction of Cl2(g) with ZnO(s) near 1400 K, and were identified and mo by mass spectrometry. Equil. consts. were evaluated for the gaseous reac +

ZnCl2 = 2ZnCl from ion intensities measured over the range 1336-1436 K used to derive the third law enthalpy change .DELTA.H298.degree. = 176 .+ mol-1 and the dissocn. energy D0.degree.(ZnCl) = 229 .+-. 8 kJ mol-1. Th result is in good agreement with an earlier value derived from equil. measurements made by monitoring the electronic spectrum of ZnCl(g) in equ with gaseous Zn and ZnCl2. The results are useful in estg. the thermoche properties of gaseous ZnOH and Zn(OH)2 for chem. modeling applications.

Zn - H_2O (OM · 40830) 2001

комплекс, ридберг свеч. Grant D. Smith+, Richard Bell et al.; J. Phys. Chem. 2001, A105, 6506 - 6512.

A Density Functional

Theory Study of the Structure and Energetics of Zincate Complexes.

135: 171003p **A Density Functional Theory Study of the Structure and Energetics of Zincate Complexes.** Smith, Grant D.; Bell, Richard; Borodin, Oleg; Jaffe, Richard L. (Department of Materials Science and Engineering and Department of Chemical and Fuels Engineering, University of Utah, Salt Lake City, UT 84112 USA). *J. Phys. Chem. A* 2001, 105(26), 6506–6512 (Eng), American Chemical Society. The accuracy of the DFT/B3LYP method and the adequacy of the at. basis sets employed were established through investigation of the ionization potentials of Zn, the geometry and bond energy of ZnO, and the geometries and energies of selected Zn–OH and Zn–H_2O complexes. Our investigation revealed that the $[Zn(OH)]^+$, $Zn(OH)_2$, and $[Zn(OH)_3]^-$ zincate complexes are stable in the gas phase. However, we found that dissocd. $[Zn(OH)_3]^- + OH^-$ is more stable than $[Zn(OH)_4]^{2-}$ in the gas phase and that the gas–phase geometry of $[Zn(OH)_4]^{2-}$ differs significantly from that gleaned from exptl. studies of aq. KOH/zincate solns. We also investigated zincate complexes involving mol. water and K^+

$[Zn(OH)]^+$ iso-1

(стр-ра и энергетика)

cations in order to better understand the influence of condensed phase effects in aq. KOH solns. on the stability and geometry of the zincate complexes. We found that water does not significantly influence complex binding energies or the geometries of the underlying $[Zn(OH)_n]^{2-n}$ complexes for n = 1, 2, and 3. In contrast, for $[Zn(OH)_4]^{2-}$ the introduction of water strongly stabilizes the complex relative to the gas phase and results in a structure close to that obsd. exptl. We were unable to find a stable $[Zn(OH)_4(H_2O)_2]^{2-}$ complex with a planar $Zn(OH)_4$ arrangement and close $Zn-H_2O$ coordination, corresponding to a Zn–O coordination of no. of six, as has been suggested in some interpretations of expts. We found through investigation of the $K_2Zn(OH)_4$ complex that K^+ cations are also effective in engendering a structure that is very close to expt. and that K^+ ions are even more strongly bound to the $[Zn(OH)_4]^{2-}$ complex than water. Finally, we detd. the structure and stability of $[ZnO(OH)_2]^{2-}$(oxodihydroxozincate), a species that has been hypothesized to be important in water–poor zincates solns.

$[Zn(OH)_3]^-$ $[Zn(OH)]^+$, $Zn(OH)_2$, 2001

135: 171003p **A Density Functional Theory Study of the Structure and Energetics of Zincate Complexes.** Smith, Grant D.; Bell, Richard; Borodin, Oleg; Jaffe, Richard L. (Department of Materials Science and Engineering and Department of Chemical and Fuels Engineering, University of Utah, Salt Lake City, UT 84112 USA). *J. Phys. Chem. A* 2001, 105(26), 6506–6512 (Eng), American Chemical Society. The accuracy of the DFT/B3LYP method and the adequacy of the at. basis sets employed were established through investigation of the ionization potentials of Zn, the geometry and bond energy of ZnO, and the geometries and energies of selected Zn–OH and Zn–H_2O complexes. Our investigation revealed that the $[Zn(OH)]^+$, $Zn(OH)_2$, and $[Zn(OH)_3]^-$ zincate complexes are stable in the gas phase. However, we found that dissocd. $[Zn(OH)_3]^- + OH^-$ is more stable than $[Zn(OH)_4]^{2-}$ in the gas phase and that the gas–phase geometry of $[Zn(OH)_4]^{2-}$ differs significantly from that gleaned from exptl. studies of aq. KOH/zincate solns. We also investigated zincate complexes involving mol. water and K^+

(структура и строение)

cations in order to better understand the influence of condensed phase effects in aq. KOH solns. on the stability and geometry of the zincate complexes. We found that water does not significantly influence complex binding energies or the geometries of the underlying $[Zn(OH)_n]^{2-n}$ complexes for n = 1, 2, and 3. In contrast, for $[Zn(OH)_4]^{2-}$ the introduction of water strongly stabilizes the complex relative to the gas phase and results in a structure close to that obsd. exptl. We were unable to find a stable $[Zn(OH)_4(H_2O)_2]^{2-}$ complex with a planar $Zn(OH)_4$ arrangement and close $Zn-H_2O$ coordination, corresponding to a Zn–O coordination of no. of six, as has been suggested in some interpretations of expts. We found through investigation of the $K_2Zn(OH)_4$ complex that K^+ cations are also effective in engendering a structure that is very close to expt. and that K^+ ions are even more strongly bound to the $[Zn(OH)_4]^{2-}$ complex than water. Finally, we detd. the structure and stability of $[ZnO(OH)_2]^{2-}$(oxodihydroxozincate), a species that has been hypothesized to be important in water–poor zincates solns.

$Zn^{2+}(OH^-)$

2001

135: 247458p Interactions of Metal Ions with Water: Ab Initio Molecular Orbital Studies of Structure, Vibrational Frequencies, Charge Distributions, Bonding Enthalpies, and Deprotonation Enthalpies. 2. Monohydroxides. Trachtman, Mendel; Markham, George D.; Glusker, Jenny P.; George, Philip; Bock, Charles W. (Department of Chemistry, Philadelphia University, Philadelphia, PA 19144 USA). *Inorg. Chem.* 2001, 40(17), 4230–4241 (Eng), American Chemical Society. The formation and properties of a wide range of metal ion monohydroxides, $M^{n+}[OH^-]$, where n = 1 and 2, have been studied by ab initio MO calcns. at the MP2(FULL)/6–311++G**//MP2(FULL)/6–311++G** and CCSD(T)(FULL)/6–311++G**//MP2(FULL)/6–311++G** computational levels. The ions M^{n+} are from groups 1A, 2A, 3A, and 4A in the second, third, and fourth periods of the Periodic Table and from the first transition series. Geometrical parameters, vibrational frequencies, at. charge distributions, orbital occupancies, and bonding enthalpies are reported. The M^{n+}–O distances are shorter in the hydroxides than in the corresponding hydrates (published previously as Part 1, Inorg. Chem. 1998, 37, 4421–4431) due to a greater electrostatic interac-

α-ba, спрукт, Di, ΔH_{298}, теор. расчет

(F7)

tion in the hydroxides. The natural bond orbitals for most of the first-row transition metal ion hydroxides do not contain a formal metal–oxygen bonding orbital; nevertheless the at. charge distributions show that for both n = 1 and 2 a significant amt. of electron d. is consistently transferred from the hydroxide ion to the bound metal ion. Deprotonation enthalpies for the hydrates have been evaluated according to the simple dissocn. process, $M^{n+}[OH_2] \rightarrow M^{n+}[OH^-] + H^+$, and also via proton transfer to another water mol., $M^{n+}[OH_2] + H_2O \rightarrow M^{n+}[OH^-] + H_3O^+$. The drastic redn. in these deprotonation enthalpies as H_2O mols. are sequentially bonded in the first coordination shell of the metal ion (amounting to 71, 64, 85, and 91 kcal/mol for the bonding of six water mols. to Mg^{2+}, Ca^{2+}, Mn^{2+}, and Zn^{2+}, resp.) is found to be due to the greater decrease in the bonding enthalpies for the hydroxides relative to the hydrates. Proton transfer to bases other than water, for example side chain groups of certain amino acids, could more than offset the decrease in deprotonation energy due to the filling of the first coordination shell. Linear relationships have been found between the pK_a values for ionization of the Mg^{2+}, Ca^{2+}, Mn^{2+}, Fe^{2+}, Co^{2+}, Ni^{2+}, Cu^{2+}, and Zn^{2+}