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A computational study of the hydride affinities of Group I and Group II metals

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Abstract

A computational study of the hydride affinities of Group I and Group II metals is described. Hydride affinities are reported for MH and M (M = Li, Na) and MH_2 and MH (M = Be, Mg). Calculated hydride affinities range from ~35 kcal mol^{-1} for Na to ~67 kcal/mol for BeH. The unusually high hydride affinity for BeH is shown to reflect the high Be–H bond energy in BeH_2. Where comparisons are possible, the results obtained using the MP2, MP4, BLYP, and B3LYP methods with a 6-311++G(3*df*,3*pd*) basis set are in good agreement with experimental or high level theoretical values. Hydride affinities calculated using the G2 approach are too high because of the G2 energy for hydride ion. More reasonable values are obtained from the G2 calculations using the exact energy for the hydride ion. (Int J Mass Spectrom 195/196 (2000) 319–325) © 2000 Elsevier Science B.V.

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1. Introduction

Metal hydride ions are commonly used in chemical synthesis for the reduction of a wide variety of functional groups. For example, March [1] lists 39 different functional groups that can be reduced using lithium aluminum hydride. Although many of these contain carbonyl or other π bonds, ethers and alkyl and aryl halides also react with these types of reagents. The reactions generally proceed via a transfer of hydride ion from the metal hydride ion to the substrate.

Although metal hydride reductions are commonly utilized in chemical synthesis, little is known about the thermochemical properties of these reactions. In select cases (MBH_4, $LiAlH_4$) the enthalpies of formation for the metal hydride salts have been measured [2], but the thermochemistry of a metal hydride reduction reaction ultimately depends on the hydride binding energy of the ion, or, conversely, the hydride affinity (HA) [3] of the neutral metal hydride [Eq. (1)]

$$MH_{n+1}^{-} \rightarrow MH_n + H^{-} \qquad -\Delta H = HA \tag{1}$$

The only metal hydride ions for which the hydride binding energies are known are gas-phase BH_4^- and SiH_5^- ions [4–6]. Studies such as these carried out by Squires and co-workers provided important insight into the nature of metal hydride reduction reactions. For example, in the study of borohydride ion, Workman and Squires showed that the hydride affinity of BH_3 in the gas phase was much larger than that of

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Dedicated to the memory of Professor Robert R. Squires.

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ketones or aldehydes [4]. Therefore, borohydride reductions of carbonyl compounds in solution are driven by factors beyond the thermochemistry of the isolated reactants, such as solvent and/or counter-ion effects. In a later article that was described as "a landmark publication" by one reviewer, Ho and Squires reported, for the first time, the stereoselectivities of cyclohexananone in the gas phase [7]. In this work, they demonstrated that the stereochemical outcomes of reduction reactions in solution were the same as those in the gas phase, such that the chemical models used to account for the observations did *not* need to include solvent and/or counter-ion effects.

Future studies of gaseous metal hydride ions will require accurate values for the hydride affinities in order to be interpreted properly. Small metal hydride ions have previously been the subjects of computational studies [8], but generally the emphasis has been on determining whether the ions are stable with respect to electron detachment. In this work, calculations of the hydride affinities of metal hydrides MH_x (M = Li, Be, Na, Mg) are described. It is found that all of the species examined in this study have very high hydride affinities (>35 kcal mol^{-1}) with the highest values obtained for BeH_2, BeH, and MgH_2, which add hydride to form BeH_3^-, BeH_2^-, and MgH_3^-, respectively.

2. Computational methods

Geometries, energies, and frequencies were calculated at the MP2, MP4, BLYP, and Becke3LYP levels of theory. All calculations were carried using the 6-311++G(3*df*,3*pd*) basis set, which includes three sets of *d* functions and one set of *f* functions on heavy atoms, three sets of *p* functions and one set of *d* functions on hydrogens, and diffuse functions on all atoms. Calculations were carried out using the GAUSSIAN 94 [9] program using default convergence criteria.

3. Results and discussion

This section describes the results of the calculations of the hydride affinities of the Group I and Group II metals at the MP2, MP4, BLYP, and B3LYP levels of theory. Geometries, energies, and frequencies are reported for all species involved. The discussion begins with the results for the lithium and sodium system, followed by the results for berylium and magnesium.

Table 1
Calculated bond lengths in lithium and sodium hydrides and hydride ions[a]

	MP2	MP4	BLYP	B3LYP
LiH_2^-	1.753	1.754	1.736	1.731
LiH^-	1.677	1.683	1.668	1.664
LiH	1.605	1.607	1.595	1.589
NaH_2^-	2.093	2.099	2.072	2.062
NaH^-	2.023	2.031	2.004	1.997
NaH	1.910	1.915	1.884	1.876

[a] Bond lengths in angstroms.

3.1. Lithium and sodium

The hydride affinities considered for lithium and sodium correspond to the enthalpy changes for the reaction shown in Eq. (1), where M = Li or Na and $n = 0$ and 1. The hydride ions are the $D_{\infty h}$ MH_2^- and $C_{\infty v}$ MH^- ions, and the corresponding neutrals are MH and M. The optimized bond lengths for the hydrides and the hydride ions are shown in Table 1. The bond lengths obtained for LiH and NaH are 1.59–1.60 Å and 1.88–1.91 Å, respectively. Experimental values are 1.5957 Å and 1.8874 Å, respectively [10], falling within the ranges of the calculated values. The bond lengths calculated for the MH_2^- ions are 1.73–1.75 Å and 2.06–2.09 Å for M = Li and Na, respectively. Experimental comparisons are not available for these ions, but the values agree with previously reported computational results. Senekowitsch and Rosmus [11] obtained a bond length of 1.741 Å from CEPA calculations, whereas Boldyrev and Simons [12] found a bond length of 1.735 Å using MP2(full)/6-311++G** calculations.

The bond lengths calculated in this work for LiH^- and NaH^- are 1.66–1.68 Å and 2.00–2.02 Å, respectively. The results for LiH^- are slightly shorter than the experimental value of 1.724 ± 0.025 Å obtained

Table 2
Calculated energies for lithium and sodium hydrides and hydride ions[a]

	MP2	MP4	BLYP	B3LYP	G2[b]
LiH_2^-	−8.61266	−8.63082	−8.68270	−8.70798	−8.63243
LiH^-	−8.02424	−8.03247	−8.08291	−8.10250	−8.03090
LiH	−8.01221	−8.02117	−8.07058	−8.08669	−8.01916
Li	−7.43203	−7.43203	−7.48044	−7.49133	−7.43222
NaH_2^-	−162.99759	−163.01381	−163.44439	−163.47023	−163.01548
NaH^-	−162.41974	−162.42825	−162.85797	−162.87808	−162.43040
NaH	−162.40776	−162.41530	−162.84612	−162.86194	−162.41792
Na	−161.84617	−161.84598	−162.27499	−162.28684	−161.84598
H^-	−0.51214	−0.52250	−0.52668	−0.53416	−0.49883

[a] Electronic energies, unless otherwise noted; values in Hartrees.
[b] G2 energies correspond to E (0 K).

from the photoelectron spectrum [13], but agrees with previously reported computational results [14–17]. The results for NaH^- are also consistent with previous theoretical predictions [15–17].

The calculated energies of all the species described above as well as the metal atoms and the hydride ion are listed in Table 2. Also shown in Table 2 are the energies for each obtained using the G2 procedure [18]. The G2 results listed correspond to 0 K energies, whereas those from the other levels of theory are electronic energies and are not corrected for zero-point vibrational energy (ZPE). The hydride affinities of the Li and Na species listed in Table 3 correspond to the 298 K enthalpies for the reaction $MH_{n+1}^- \rightarrow MH_n + H^-$. The zero-point energies and temperature corrections were computed from the calculated vibrational frequencies at each level of theory. Representative vibrational frequencies calculated at the BLYP/6-311++G(3*df*,3*pd*) level of theory are listed in Table 4. Calculated frequencies are the B3LYP and MP2 levels of theory are generally 1–3% higher. The ZPE and temperature corrections for the MP4 results were calculated using the MP2 frequencies.

In general, the hydride ions of lithium and sodium are strongly bound with respect to dissociation, with the hydride affinities ranging from ∼1.5–2.4 eV. The hydride affinity of LiH is calculated to be 52.7–54.4 kcal mol^{-1}. These agree with the previously reported values of 54.0, 54.1, and 52.8 kcal mol^{-1} obtained at the QCISD(T)/6-311++G**, CEPA, and CCSD(T) levels of theory, respectively [11,12,19]. The hydride affinity of Li is calculated to be 46.8–48.3 kcal mol^{-1}. Experimentally, the dissociation energy (0 K) of HLi^- can be derived using the electron affinity of HLi, 0.342 ± 0.012 eV [13], and is found to be 46.5 ± 0.5 kcal mol^{-1}. Using the BLYP results to

Table 3
Hydride affinities of lithium and sodium atoms and hydrides[a]

	LiH	Li	NaH	Na
MP2[b]	54.4	48.3	47.4	37.6
MP4[b]	53.9	47.3	45.9	36.1
BLYP[b]	52.5	46.8	44.1	35.0
B3LYP[b]	53.5	47.5	45.7	35.4
G2[b,c]	52.7	47.5	47.4	38.4
QCISD(T)[d]	54.0		46.9	
CEPA[e]	54.1			
CCSD(T)[f]	52.8			
HF-EOM[g]		44.7		38.0
MCSCF[h]		40.0		31.1
PNO-CI[i]		44.3		33.5
CEPA[i]		45.2		33.7
expt[j]		46.5 ± 0.5		

[a] Values in kcal/mol.
[b] This work; values correspond to the −ΔH for Eq. (1) at 298 K.
[c] Using $H_{298}(H^-) = -0.52536$ Hartree.
[d] [12].
[e] [11].
[f] [19].
[g] Hartree–Fock equation-of-motion method [15].
[h] [16].
[i] [17].
[j] [13]. Corresponds to ΔE at 0 K.

Table 4
Vibrational frequencies for lithium and sodium hydrides calculated at the BLYP/6-311++G(3*df*,2*dp*) level of theory[a]

	$D_{\infty h}$ LiH_2^-	$D_{\infty h}$ NaH_2^-
π_u	431.7	299.8
σ_g	996.3	827.6
σ_u	1070.3	873.7
	$C_{\infty v}$ LiH^-	$C_{\infty v}$ NaH^-
σ_g	1171.6	897.4
	$C_{\infty v}$ LiH	$C_{\infty v}$ NaH
σ_g	1390.2	1138.5

[a] Values in cm^{-1}.

convert this value to ΔH at 298 K gives a value of 47.4 kcal mol^{-1}, in excellent agreement with the theoretical predictions. These results indicate that the theoretical methods employed in this work provide accurate values for the hydride affinities in these types of systems.

The hydride affinities of the sodium species are smaller than the corresponding lithium hydrides. The hydride affinity of NaH is found to be 44.1–47.4 kcal mol^{-1}, similar to the value of 46.9 kcal mol^{-1} reported by Boldyrev and Simons [12]. Interestingly, although the NaH_2^- ion is strongly bound with respect to hydride loss, it is not expected to be a stable ion in the gas phase. Boldyrev and Simons [12] have calculated the energy change for the reaction $NaH_2^- \rightarrow Na + H_2 + e^-$ and obtained a value of −0.12 eV. Therefore, NaH_2^- is calculated to be unstable with respect to electron detachment accompanied by dissociation. However, NaH_2^- is still likely to be kinetically stable. Like BH_2^+ [20,21], BeH_2 [22], and LiH_2^- [19], NaH_2^- should have a large barrier for dissociation into $Na^- + H_2$. Moreover, the *vertical* electron detachment energy is calculated to be 3.12 eV [12], which means the $HNaH^-$ ion is stable with respect to vertical electron detachment. The net result is that there is a barrier for the dissociation of NaH_2^- into $Na + H_2 + e^-$. This is similar to the situation with the hydridosilconate ion, SiH_5^- [23], which is thermodynamically unstable but kinetically stable with respect to dissociation to $SiH_3^- + H_2$ [5]. The NaH^- ion is calculated to be bound to about the same extent as LiH^- (0.342 ± 0.012 eV) [13], in agreement with previous calculations [15–17,24–26].

The hydride affinities calculated using the G2 approach deserve some comment. As indicated in Table 2, the energy calculated for the hydride ion with the G2 method is −0.49883 Hartree. The actual energy of hydride ion should be lower than that of the hydrogen atom (−0.5000 Hartree) by the electron affinity, 0.75419 eV [27], giving a total absolute energy of H^- of −0.52772 Hartree, 18.1 kcal mol^{-1} lower than that obtained for the 0 K value from the G2 calculation. Not coincidentally, the hydride affinity values calculated using the G2 energy for hydride are ∼18 kcal mol^{-1} higher than those obtained from the other levels of theory. Therefore, the G2 hydride affinities listed in Table 3 were calculated using the G2 energies for MH_{n+1}^- and MH_n, but with the experimental energy for hydride ion. The hydride affinities obtained in this fashion are in excellent agreement with those found using the other methods, and, moreover, do not show a systematic bias toward higher or lower values. The energies of hydride calculated at the BLYP, MP2, and MP4 levels of theory are higher than the experimental value by 0.7, 9.8, and 3.3 kcal mol^{-1}, respectively, whereas the B3LYP energy is 4.0 kcal mol^{-1} lower than the experimental value. Therefore, only the BLYP results would not change significantly if the experimental energy of hydride were used for the calculation.

3.2. Berylium and magnesium

The calculated bond lengths for these and all the berylium and magnesium species are shown in Table 5. The bond lengths for these systems are generally shorter than those for the corresponding Li or Na species. The bond lengths calculated for the D_{3h}, BeH_3^-, and MgH_3^- ions are ∼1.42 Å and ∼1.81 Å, which agree with the values reported previously [12,28–30]. The experimental bond lengths in BeH and MgH are 1.3426 Å and 1.7297 Å, respectively, which agree very well with the values of 1.339–1.346 Å and 1.729–1.756 Å obtained in this work.

The calculated energies for BeH_n and MgH_n ions and neutrals, including those calculated using the G2

Table 5
Calculated bond lengths for beryllium and magnesium hydrides and hydride ions[a]

	MP2	MP4	BLYP	B3LYP
BeH_3^- [b]	1.421	1.422	1.420	1.415
BeH_2^-	1.371	1.377	1.367	1.363
angle[c]	136.5	135.4	142.5	140.4
BeH_2	1.329	1.330	1.329	1.325
BeH	1.339	1.344	1.346	1.341
MgH_3^- [b]	1.809	1.813	1.814	1.805
MgH_2^-	1.783	1.790	1.791	1.781
angle[c]	124.7	124.4	126.1	125.5
MgH_2	1.704	1.708	1.710	1.700
MgH	1.729	1.736	1.756	1.742

[a] Bond lengths in angstroms.
[b] Corresponds to a D_{3h} geometry.
[c] Bond angle for the C_{2v} molecule, in degrees.

Table 7
Hydride affinities for beryllium and magnesium hydrides[a]

	BeH_2	BeH	MgH_2	MgH
MP2[b]	60.9	69.5	61.0	58.2
MP4[b]	60.1	68.0	53.2	54.4
BLYP[b]	57.1	67.3	55.6	52.2
B3LYP[b]	58.7	68.4	57.6	54.0
G2[b,c]	59.2	67.2	58.5	56.0
QCISD(T)[d]	60.1		59.9	
MP2[e]	55.5			

[a] Values in kcal/mol.
[b] This work; values correspond to the $-\Delta H$ for Eq. (1) at 298 K.
[c] Calculated using $H_{298}(H^-) = -0.52536$ Hartree.
[d] [12].
[e] [30].

procedure, are listed in Table 6. As above, the G2 energies correspond to the 0 K values, whereas the energies listed for the other theoretical methods are electronic energies and are not ZPE corrected. The 298 K hydride affinities are listed in Table 7. Representative frequencies, calculated at the BLYP/6-311++G(3*df*,3*pd*) level of theory, are listed in Table 8. The frequencies calculated at the MP2 and B3LYP levels of theory are generally 2–5% higher. Again, the MP2 ZPE and temperature correction was also used with the MP4 results. The G2 hydride affinities were calculated using $E(H^-) = -0.52772$ Hartree and H_{298} $(H^-) = 0.52536$ Hartree, as described above.

The hydride affinities for Be and Mg species are higher than those obtained for the alkali metals, Li and Na. Moreover, for a given neutral type, the hydride affinities for the first row species are slightly higher than those for the second row. The hydride affinities calculated at the QCSID(T)/6-311++G(2*df*,2*pd*) level of theory are 60.1 kcal mol^{-1} for BeH_2 and 56.0 kcal mol^{-1} for MgH_2 [12]. The QCISD(T) value for BeH_2 is slightly higher than that obtained in this work, whereas the result for MgH_2 is within the 53.2–61.0 kcal mol^{-1} range of values obtained here.

The highest hydride affinity is found to be about 68 kcal mol^{-1} for BeH. The hydride affinity of BeH is higher even than the hydride affinity of BeH_2, which is somewhat surprising. In all the other cases the open-shell radical hydride affinity is lower than that of the closed-shell hydride, including the case where M = Mg. This suggests that there is some fundamental difference between BeH/BeH_2^- and MgH/MgH_2^-

Table 6
Calculated energies for berylium and magnesium hydrides and hydride ions[a]

	MP2	MP4	BLYP	B3LYP	G2[b]
BeH_3^-	−16.44057	−16.46774	−16.51861	−16.55368	−16.46367
BeH_2^-	−15.81274	−15.82958	−15.88494	−15.91278	−15.82784
BeH_2	−15.82937	−15.84732	−15.89862	−15.92363	−15.84348
BeH	−15.18541	−15.19420	−15.24764	−15.26599	−15.19486
MgH_3^-	−201.40132	−201.42435	−201.85827	−201.89373	−201.42237
MgH_2^-	−200.78893	−200.80578	−201.24267	−201.27143	−200.80701
MgH_2	−200.78942	−200.80455	−201.24140	−201.26600	−200.80426
MgH	−200.18150	−200.18972	−200.63089	−200.64896	−200.19177

[a] Electronic energies, except where noted; values in Hartrees.
[b] Corresponds to 0 K energy.

Table 8
Frequencies for beryllium and magnesium hydrides and hydride ions calculated at the BLYP/6-311++G(3*df*,2*pd*) level of theory[a]

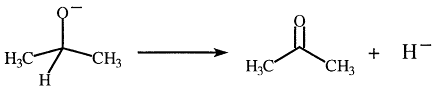
	D_{3h} BeH_3^-	D_{3h} MgH_3^-
a_2''	829.1	537.2
e'	844.1	595.8
e'	1659.6	1247.7
a_1'	1667.5	1322.9
	C_{2v} BeH_2^-	C_{2v} MgH_2^-
a_1	508.0	515.8
b_2	1823.2	1292.4
a_1	1971.3	1311.2
	$D_{\infty h}$ BeH_2	$D_{\infty h}$ MgH_2
π_u	715.4	411.7
σ_g	2021.7	1575.1
σ_u	2232.2	1601.5
	$C_{\infty v}$ BeH	$C_{\infty v}$ MgH
σ_g	2025.9	1397.6

[a] Values in cm^{-1}.

that leads to an unusually high hydride affinity for BeH. Additional insight into the difference between BeH_2^- and MgH_2^- is obtained examining their electron binding energies. Zero-point corrected electron affinities of BeH_2 and MgH_2 at the BLYP/6-311++G(3*df*,3*pd*) level of theory are -6.6 and $+2.1$ kcal mol^{-1}, respectively, and so it seems by this measure that MgH_2^- is more stable than BeH_2^-. Ultimately, the hydride affinity and electron affinities for these species are related according to the thermochemical cycle shown in Eq. (2), where $HA(MH_n)$ is the hydride affinity, $D(H_nM–H)$ is the homolytic bond dissociation energy in MH_{n+1}, and $EA(MH_{n+1})$ and EA(H) are the electron affinities of the metal hydride and hydrogen atom, respectively

$$HA(MH_n) = D(H_nM\text{–}H) + EA(MH_{n+1}) - EA(H) \tag{2}$$

This relationship shows that the hydride affinity depends on the electron affinity and the M–H bond energy of the neutral metal hydride. The calculated M–H bond energies in BeH_2 and MgH_2 are ~95 kcal mol^{-1} and ~70 kcal mol^{-1}, respectively. Therefore, the high hydride affinity for BeH can be attributed to the exceptionally high bond energy in BeH_2, which, by virtue of its smaller atomic radius, can accommodate a significantly shorter M–H bond distance.



(3)

4. Conclusion

In order to put the hydride affinities in perspective, it is useful to compare them to values obtained for other systems. For example, an important use for metal hydride ions in solution is for the reduction of carbonyl compounds. Therefore, it is instructive to compare the hydride affinities of metals with those of carbonyl compounds. The hydride affinity of acetone [Eq. (3)] is calculated from the enthalpies of formation of acetone [2], iso-propoxide ion [27], and hydride ion [27] to be 36.5 ± 2.2 kcal mol^{-1}. The only metal hydride ion that may be capable of transferring a hydride ion to acetone in the gas phase is NaH^-, whereas the hydride affinities of the remaining species examined in this work are too large to reduce carbonyl compounds in the gas phase. However, this does not preclude the possibility that these ions will reduce carbonyl groups in solution, where solvent and/or counter-ion effects can promote the reaction.

In almost all cases, the hydride affinities calculated in this work agree very well with those reported previously by Boldyrev and Simons [12], calculated at the QCISD(T)/6-311++G(2*df*,2*pd*) level of theory. Therefore, density functional and perturbation theory calculations with large basis sets give hydride affinities that agree well with those obtained using much more expensive computational methods, which provide the benchmark until experimental values are available. Experimental measurements of these hydride affinities are currently underway.

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