

ACCURATE DISSOCIATION ENERGIES FOR THE $X^1\Sigma^+$ STATES OF KH AND CsH

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We have constructed new hybrid potential energy curves for the ground states of KH and CsH. Then for observed quasibound states ($v''=23, J''=7$ in KH; $v''=25, J''=11$ in CsH), we calculated energies and linewidths for varying dissociation energies D_e . Based on a comparison of calculated and observed linewidths, we determined improved D_e values: for KH, $D_e=14772.7 \pm 0.6$ cm^{-1} ($D_0=14282.6$ cm^{-1}); for CsH, $D_e=14791.2 \pm 2.0$ cm^{-1} ($D_0=14348.5$ cm^{-1}).

1. Introduction

Because of the ionic-covalent avoided crossing of the potential curves of the $X^1\Sigma^+$ and $A^1\Sigma^+$ states of the alkali hydrides [1,2], it is not possible to accurately estimate the dissociation energy (D_e) of the alkali hydrides by Birge-Sponer extrapolation [3,4]. Although there has been a number of earlier laser-induced fluorescence studies of the A-X system in KH [5-7], only very recently has an accurate D_e value been obtained for the $X^1\Sigma^+$ state [8]. Using high resolution Fourier transform spectroscopy, Hussein et al. [8] observed A-X system fluorescence from the $v'=7, J'=6$ level to ground state levels up to $v''=23$. From their data they were able to construct a Rydberg-Klein-Rees (RKR) potential energy curve for the X state that went $>99.9\%$ of the way to the dissociation limit.

Based on the rotationally predissociated $v''=23, J''=7$ level observed by Hussein et al. [8], we have determined a new and very precise D_e value for the $X^1\Sigma^+$ state of KH. We constructed a new hybrid potential energy curve that includes a scaled ab initio calculation at short range, RKR turning points in the potential well, and proper long range behavior. For

the observed quasibound level $E(v''=23, J''=7)$, we calculated linewidths for various dissociation energy values. The only levels affected by a variation in D_e are the uppermost $E(23, J)$ levels. Specifically for $v=20, 21$ and 22 (with $J=0$ or $J=7$), $E(v, J)$ values change by less than 0.01 cm^{-1} as the D_e value is varied from 14770 to 14777 cm^{-1} . For the same range of D_e , $E(23, 0)$ and hence its spacing with other nearby levels varies by 0.2 cm^{-1} . From a comparison with the experimental linewidth [8], we determined an improved D_e value that is 4.3 cm^{-1} lower and seven times more precise than the best previous results [8].

Encouraged by our results on KH, we used the same hybrid potential approach on the $X^1\Sigma^+$ state of CsH. Based on A-X system fluorescence studies by Crépin et al. [9], and their observed rotationally predissociated $v''=25, J''=11$ level, we determined an improved D_e value that is 15.8 cm^{-1} lower and 2.5 times more precise than (but outside the range of) the best previous result for CsH [9].

Our approach is easily described with the use of fig. 1, appropriate to the ground state of KH. The figure shows the rotationless potential $V(R)$ for $D_e=14772.7$ cm^{-1} and the effective potential

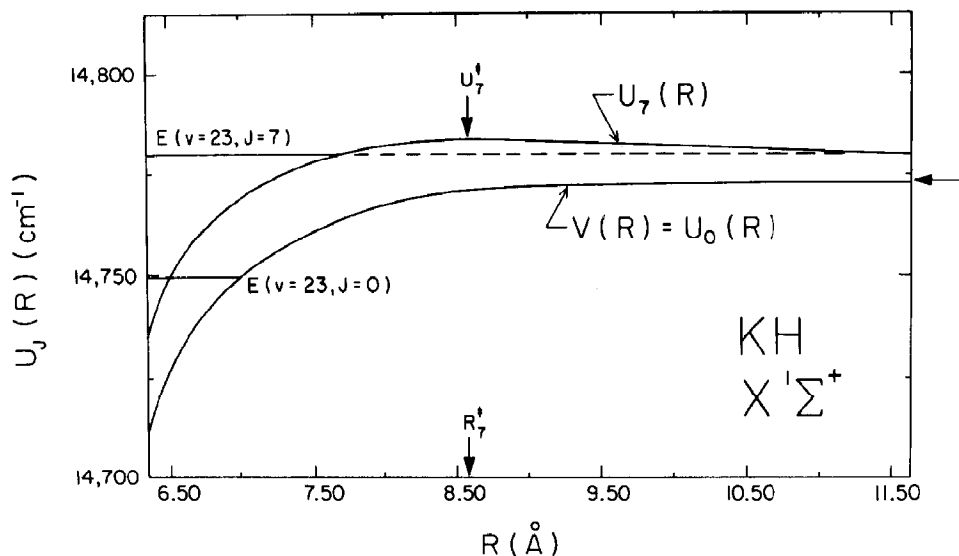


Fig. 1. The outer portion of the potential energy curve for the $X^1\Sigma^+$ state of KH. $E(v=23, J=7)$ is the quasibound level determined by the effective potential $U_7(R)$ and $E(v=23, J=0)$ is the last observed bound level determined by the true potential $V(R)=U_0(R)$. $U_7^‡$ is the barrier maximum occurring at the distance $R_7^‡$. The arrow at the far right indicates $D_e=14772.7\text{ cm}^{-1}$.

$U_J(R)=V(R)+J(J+1)\hbar^2/2\mu R^2$ in the region of the curve where the potential is dominated by the long range expansion $-C_n/R^n$ (where $n=6, 8$ and 10). In KH the quasibound level $E(v=23, J=7)$ has a width because it is above the dissociation limit of $V(R)$ and tunneling occurs. By varying the assumed depth of the potential well (i.e. varying D_e) while keeping the long-range portion of the curve unchanged, the calculated energy and width of $E_{23,7}$ change. For example, if the D_e value is decreased slightly, $E_{23,7}$ is closer to the maximum of the barrier ($U_7^‡$ at a distance of $R_7^‡$ in fig. 1) and broadens (its width Γ_{fwhm} increases). Comparison of calculated Γ_{fwhm} values with the observed value yields the accurate energy of $E_{23,7}$ with respect to the barrier maximum $U_7^‡$. Since $E_{23,7}$ is experimentally determined with respect to the minimum of the well, simple arithmetic gives us a value for D_e .

In sections 2 and 3 we present our analysis for KH and CsH, respectively. In section 4 we give our results, new dissociation energies for the ground states of KH and CsH.

2. $X^1\Sigma^+$ state of KH

The full hybrid potential energy curve for the $X^1\Sigma^+$ state consists of a spline fit of the well ($2.909200 \leq R \leq 17.0 a_0$) plus an exponential inner wall and a long range $-C_n/R^n$ expansion for $R \geq 17.0 a_0$; see table 1 and fig. 2.

The well of the curve is from the RKR turning points based on the Hussein et al. molecular constants ^{#1} from $R_{22-}=2.909200 a_0$ ^{#2} to the adjusted

^{#1} There is a mistake in the molecular constants reported in ref. [8] (personal communication from R.F. Barrow). In ref. [8], table 2 should read: $10^5 Y_{71} = -0.163822469$ (1.00 E-6), $10^7 Y_{81} = 0.633047058$ (0.64 E-7), $10^8 Y_{91} = -0.13521347$ (0.34 E-7).

^{#2} Using the corrected Y_{ij} constants of ref. [8] (see footnote 1) and the reduced mass $\mu(^{39}\text{KH})=0.982414340$ as found in Huber and Herzberg [10], we were able to reproduce $G(v)$ values to exactly the cited number of figures in ref. [8]. However our R_{v-} and R_{v+} turning points were systematically all 0.0001–0.0004 Å larger than those of ref. [8]. Our $R_e=2.240316$ Å, while $R_e=2.2401$ Å in ref. [8]. We are unable to identify the source of this small difference. Also, the innermost turning point R_{23-} is out of line with the rest of the adjoining inner turning points and was not included in the final potential $V(R)$.

Table I

Potential energy curves (in au with respect to the dissociation limit) for $X^1\Sigma^+$ states of KH and CsH. $V(R)$ and dV/dR are continuous

State	Region	Range of R (a_0) ^{a)}	Function ^{a)}
KH $X^1\Sigma^+$	I	$R \leq 2.909200$	$(1.46589) \exp(-0.372253R^2) - 0.063415627$
	II	$2.909200 \leq R \leq 17.0$	tensioned cubic spline fit of RKR turning points ^{b)} and the long range point at $17.0 a_0$
	III	$17.0 \leq R$	$-105.7/R^6 - 7076/R^8 - 642800/R^{10}$
CsH $X^1\Sigma^+$	I	$R \leq 3.402405$	$(57.34445) \exp(-2.07000R) - 0.067401380$
	II	$3.402405 \leq R \leq 18.0$	tensioned cubic spline fit of RKR turning points ^{b)} and the long range point at $18.0 a_0$
	III	$18.0 \leq R$	$-132.9R^6 - 10690/R^8 - 1143000/R^{10}$

^{a)} $1a_0 = 0.5291770 \text{ \AA}$; $1 \text{ au} = 1 \text{ hartree} = 219474.6 \text{ cm}^{-1}$.^{b)} See text for details of specific points.

$R_{23+} = 13.215548 a_0$ ^{#3}. The inner wall of the curve consists of an exponential function of the form $A \exp(BR^2) - C$ and is based on the Langhoff et al. points [12] at 2.50, 2.75 and $3.00 a_0$ and shifted to fit smoothly onto the innermost R_{22-} turning point. The long range expansion $V_{LR}(R) = -C_6/R^6 - C_8/R^8 - C_{10}/R^{10}$ is well defined. The C_6 , C_8 and C_{10} coefficients are directly from Proctor and Stwalley

^{#3} Although the R_{23-} value was discarded, the difference $R_{23+} - R_{23-}$ should be preserved. This difference is the RKR $f_{v=23}$ integral and its uncertainty is related to the uncertainty in the $G(v=23)$ value. The value of R_{23-} was estimated to be too small by $0.0188540 a_0$, so the associated R_{23+} was shifted to a larger value by precisely that amount to preserve $R_{23+} - R_{23-}$. Thus the final adjusted $R_{23+} = 13.196694 + 0.018854 = 13.215548 a_0$. See the papers by Yang [11] and LeRoy [4] where this approach and a more complete rationale are given.

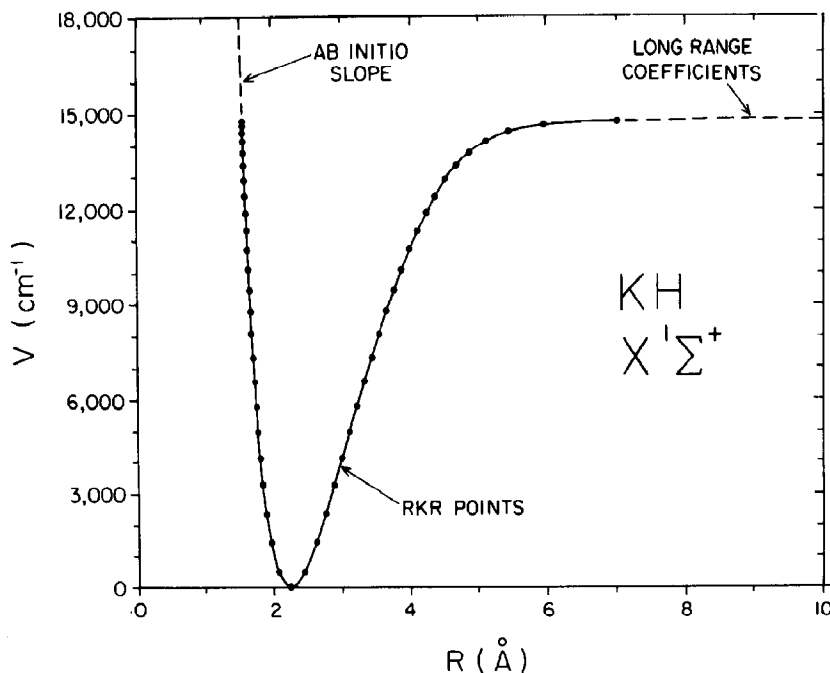


Fig. 2. Hybrid potential energy curve for the $X^1\Sigma^+$ state of KH. The inner dashed portion of the curve is based on the slope found in the calculations of Langhoff et al. [12]. The solid line is a spline fit through the RKR turning points R_{22-} to R_{23+} . The outer dashed portion of the curve is a spline fit from the last turning point ($R_{23+} = 7.0 \text{ \AA}$) through the long range portion of the curve $V_{LR}(R)$ defined by the C_6 , C_8 and C_{10} long range coefficients. The analytical form $V_{LR}(R) = -\sum_{n=6,8,10} (C_n/R^n)$ holds for $R \geq 9.0 \text{ \AA}$.

[13]. The LeRoy criterion [14] for the onset of the breakdown of the long range expansion occurs at $\approx 14 a_0$, so we take $V_{LR}(R)$ as valid for $R \geq 17.0 a_0$.

With a complete potential energy curve, energies and widths for the quasibound level $E_{23,7}$ were computed as the assumed depth D_e was varied. Plotted in fig. 3 are linewidths as a function of the energy level $E_{23,7}$ below the barrier maximum U_7^\ddagger . The intercept of the smooth near-linear curve with the observed Γ_{fwhm} value ($0.40 \pm 0.05 \text{ cm}^{-1}$ [8]) yields the

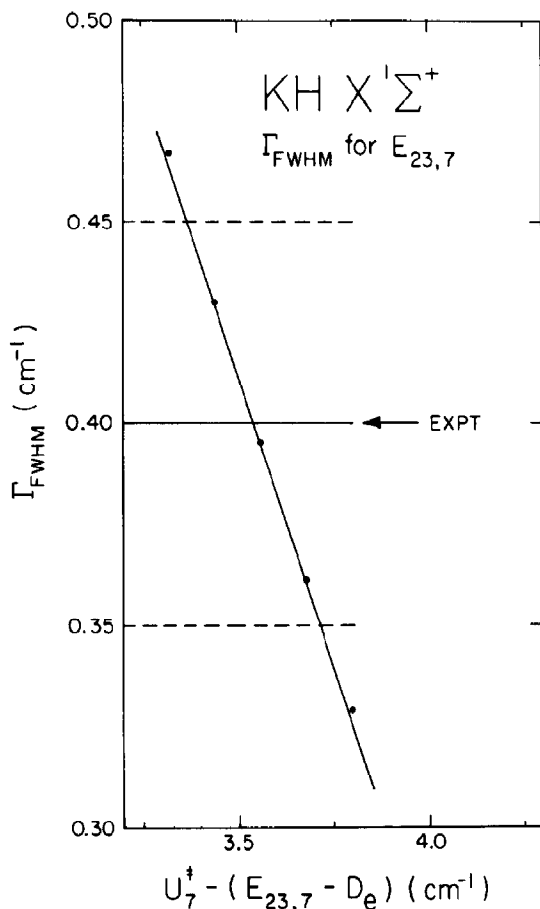


Fig. 3. The linewidth Γ_{fwhm} of the quasibound level $E_{23,7}$ for the $X^1\Sigma^+$ state of KH for various D_e values. The barrier U_7^\ddagger is defined with respect to the dissociation limit; $E_{23,7}$ is determined with respect to the minimum of the well. Thus the quantity $U_7^\ddagger - (E_{23,7} - D_e)$ measures the energy difference between the top of the barrier and the quasibound level. The experimental Γ_{fwhm} of 0.40 cm^{-1} (solid horizontal line) is from ref. [8]; the $\pm 0.05 \text{ cm}^{-1}$ uncertainty (estimated by us) is indicated by the dashed horizontal lines.

value $3.5 \pm 0.2 \text{ cm}^{-1}$ below the barrier maximum for $E_{23,7}$.

We examined the effect an adjustment of the outermost RKR turning point would have on $E_{23,7}$ and its width. Shifting R_{23+} inwards by $\approx 0.01 \text{ \AA}$ ($\approx 0.02 a_0$; see footnote 3) resulted in an increase in $E_{23,7}$ by 0.17 cm^{-1} and a decrease in its Γ_{fwhm} by 0.04 cm^{-1} (as the barrier got thicker). This is within the uncertainty already noted. Moreover, trial and error adjustments in R_{23+} and D_e left the value of U_7^\ddagger unchanged to within $\pm 0.1 \text{ cm}^{-1}$. Clearly, the shape and height of the rotational barrier, and in turn the quasibound level, are strongly determined by the long range portion of the curve, $V_{LR}(R)$. This is not surprising since the barrier maximum (see fig. 1) occurs at $R_7^\ddagger = 16.2 a_0$ (8.6 \AA), very near the $17 a_0$ threshold for the $V_{LR}(R)$ expansion. Based on the reported uncertainty in the C_6 long range coefficient [13], we generously assign an uncertainty in U_7^\ddagger of 0.4 cm^{-1} . Thus the energy of the quasibound level above the dissociation limit is determined to be $(E_{23,7} - D_e) = (11.0 \pm 0.4) - (3.5 \pm 0.2) = 7.5 \pm 0.6 \text{ cm}^{-1}$.

3. $X^1\Sigma^+$ state of CsH

The full hybrid potential energy curve for the X state of CsH was constructed in a fashion similar to that for the X state of KH; see table 1 and fig. 4. The inner wall of the potential consists of an exponential function of the form $A \exp(-BR) - C$, based on the work of Yang et al. [15]. Similar to the case with KH, there are theoretical calculations for short, inner wall distances [16,17]. However, the theoretical inner wall slopes did not match the innermost RKR curve of Crépin et al. [9]. The A and B constants are taken directly from Yang et al.; the C constant differs since the scaling here is to the Crépin et al. RKR curve instead of the Hsieh et al. [18] RKR curve.

The well of the curve is from the RKR turning points based on the Crépin et al. molecular constants from $R_{15-} = 3.402405 a_0$ to $R_{15+} = 8.427850 a_0$. The RKR points at Hsieh et al. agree well with these points, but only up to $v=14$. Although Yang [11] obtains a potential up to $v=24$, his inner wall shows a ripple above $v=15$ and we did not use his inner $V(R)$ points. However, we did use his points for the

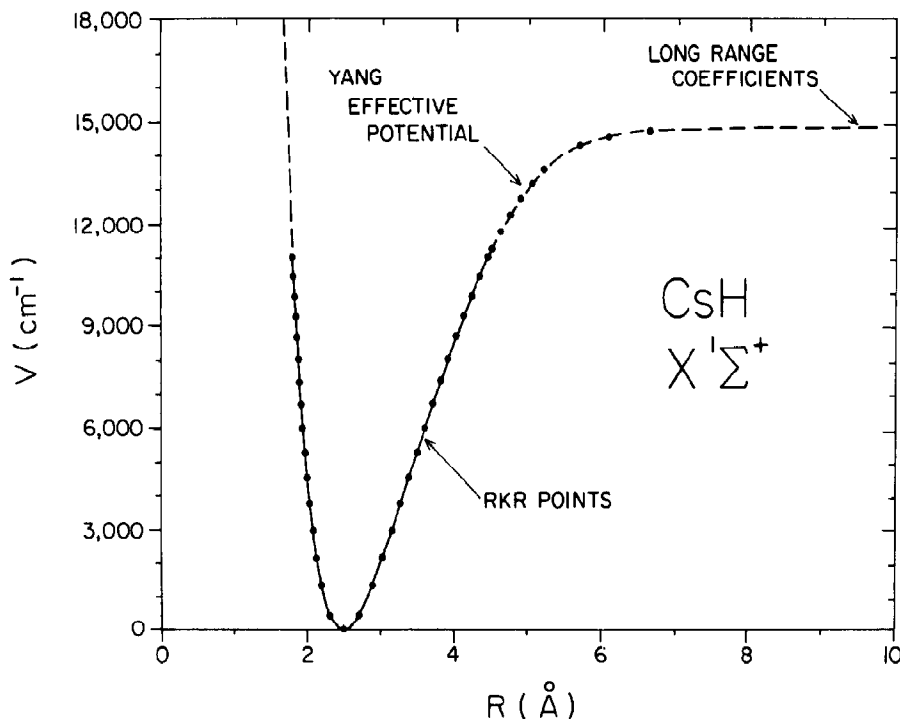


Fig. 4. Hybrid potential energy curve for the $X^1\Sigma^+$ curve of CsH. The inner dashed portion of the curve is based on the earlier curve of Yang et al. [15]. The solid line is a spline fit through the RKR [9] turning points R_{15-} to R_{15+} . The scaled Yang effective potential at intermediate distances 4.5–6.6 Å [11] fits smoothly onto the RKR curve and is shown as a dashed line through solid points. The outer dashed portion of the curve is a spline fit from the last Yang point through the long range portion of the curve $V_{LR}(R)$ which holds for $R \geq 9.5$ Å.

outer portion of the well beyond the range of the Crépin et al. points.

The Yang points are based on a $U_{15}(R)$ effective potential obtained from $B^1\Sigma^+ - X^1\Sigma^+$ laser-induced fluorescence measurements. To obtain rotationless potential points, the proper centrifugal term is subtracted from $U_{15}(R)$ at each R value. We scaled the rotationless Yang points to match smoothly onto the R_{15+} outermost Crépin et al. point and extended the well out to $12.561015 a_0$ ^{#4}.

^{#4} Our scaling factor is 1.015497; multiplying nine points from table V of Yang [11] by this factor gave the following lowered energies: -0.01652328 au at 4.501 Å; -0.01412328 au at 4.626 Å; -0.01184035 au at 4.756 Å; -0.00967864 au at 4.895 Å; -0.00764186 au at 5.048 Å; -0.00573463 au at 5.211 Å; -0.00248559 au at 5.692 Å; -0.00132007 au at 6.084 Å; and -0.00046084 au at 6.647 Å. These energies are with respect to a dissociation limit of 0.0 au. The point at 5.386 Å causes tension in the spline fit and was not included in the final potential $V(R)$.

With a complete potential energy curve, energies and widths for the quasibound level $E_{25,11}$ were computed as the assumed well depth D_e was varied. Plotted in fig. 5 are linewidths as a function of the level $E_{25,11}$ below the barrier maximum U_{11}^{\dagger} . The intercept of the smooth near-linear curve with the observed Γ_{fwhm} value ($0.6 \pm 0.1 \text{ cm}^{-1}$ [9]) yields the value $5.3 \pm 0.3 \text{ cm}^{-1}$ below the barrier maximum for $E_{25,11}$.

Because the location of the barrier maximum ($R_{11}^{\dagger} \approx 15.3 a_0$) is midway between the last Yang RKR point and the threshold for the $V_{LR}(R)$ expansion, the value of U_{11}^{\dagger} is not as strongly dominated by the long range expansion as was the case for KH. We examined the effect an adjustment of this outermost RKR point would have on U_{11}^{\dagger} . A shift of ± 0.10 Å ($\approx 0.2 a_0$), about six times the shift in R noted by Yang [11], caused U_{11}^{\dagger} to vary as much as the uncertainty in the long range coefficients. Thus we conservatively assign an uncertainty in U_{11}^{\dagger} twice

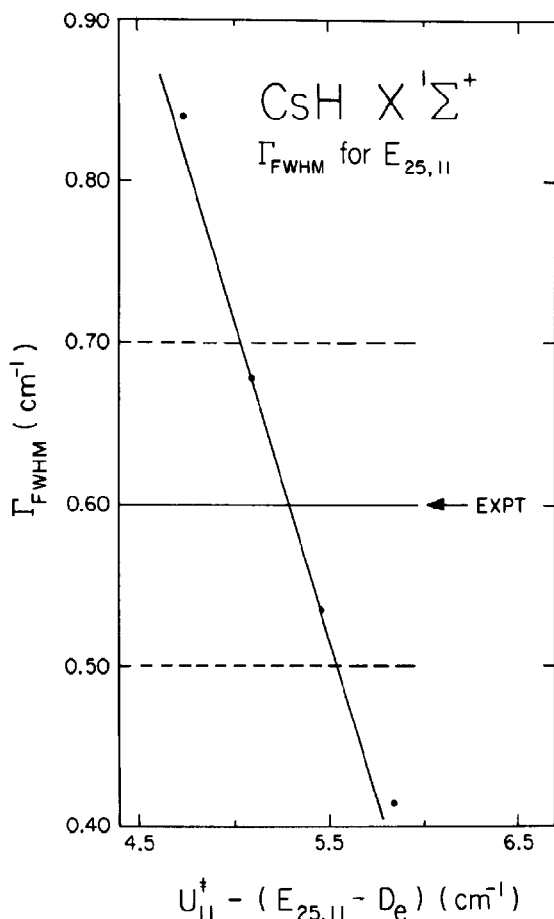


Fig. 5. The linewidth Γ_{fwhm} of the quasibound level $E_{25,11}$ for the $X^1\Sigma^+$ state of CSH for various D_e values. The barrier maximum U_{11}^\dagger is defined with respect to the dissociation limit; $E_{25,11}$ is determined with respect to the minimum of the well. Thus the quantity $U_{11}^\dagger - (E_{25,11} - D_e)$ measures the energy difference between the top of the barrier and the quasibound level. The experimental Γ_{fwhm} of 0.6 cm^{-1} (solid horizontal line) is estimated from fig. 3 of ref. [9]; the $\pm 0.1 \text{ cm}^{-1}$ uncertainty (estimated by us) is indicated by the dashed horizontal lines.

as large as that due to the long range coefficients (0.74 cm^{-1} [13]). Consequently the energy of the quasibound level above the dissociation limit is determined to be $(E_{25,11} - D_e) = (26.1 \pm 1.5) - (5.3 \pm 0.3) = 20.8 \pm 1.8 \text{ cm}^{-1}$.

4. Results and conclusions

In the $X^1\Sigma^+$ state of KH, the rotational predis-

Table 2

Dissociation energies (D_e) for the $X^1\Sigma^+$ state of ^{39}KH

Ref.	$D_e \text{ (cm}^{-1}\text{)}$
[10]	15000
[16] ^{a)}	14490
[2]	14500 ± 500
[4]	15020 ± 400
[12] ^{a)}	14500
[8]	14777 ± 4
this work	14772.7 ± 0.6

^{a)} Ab initio calculations with no error bounds cited.

sociated level $E_{23,7}$ is observed [8] to be 14780.18 cm^{-1} above the minimum of the potential well. In section 2 we determined $E_{23,7}$ to be $7.5 \pm 0.6 \text{ cm}^{-1}$ above the dissociation limit. Therefore we calculate $D_e(\text{KH}(X^1\Sigma^+)) = 14772.7 \pm 0.6 \text{ cm}^{-1}$ ($D_0 = 14282.6 \text{ cm}^{-1}$). This value agrees well with the best previous value [8], $D_e = 14777 \pm 4 \text{ cm}^{-1}$. Table 2 contains a list of the most recent determinations of the dissociation energy, both experimental and theoretical. They converge very nicely to the most precise value, that of this work.

In the $X^1\Sigma^+$ state of CSH, the rotationally predissociated level $E_{25,11}$ is observed ^{#5} to be $14812.0 \pm 0.2 \text{ cm}^{-1}$ above the minimum of the potential well. In section 3 we determined $E_{25,11}$ to be $20.8 \pm 1.8 \text{ cm}^{-1}$ above the dissociation limit. Therefore we calculate $D_e(\text{CSH}(X^1\Sigma^+)) = 14791.2 \pm 2.0 \text{ cm}^{-1}$ ($D_0 = 14348.5 \text{ cm}^{-1}$).

Table 3 contains a list of the most recent determinations of the dissociation energy, both spectroscopic and theoretical. They bracket the very precise

^{#5} In the experiments of Crépin et al. [9], they pumped from the $v''=0, J''=9$ level of the $X^1\Sigma^+$ state with the 457.9 nm line of the Ar^+ laser to reach the $v'=19, J'=10$ level of the $A^1\Sigma^+$ state. Then they measured fluorescence into numerous high-lying vibrational-rotational levels of the X state, including the predissociated $E_{25,11}$ level. A mistake was made in their statement (in ref. [9]) of the $E(v''=0, J''=9)$ level energy and thus their subsequent value of $E_{25,11}$ should be decreased by 1.3 cm^{-1} (personal communication from C. Amiot). In addition, they did not include the zero-point correction Y_{00} (which equals 0.18 cm^{-1}) in the determination of $E(v''=0, J''=9)$. So, contrary to their value of $E_{25,11} = 14813.1 \text{ cm}^{-1}$, the value of the quasibound level should be 1.1 cm^{-1} lower than reported: $E_{25,11} = (14813.1 \pm 0.1) - 1.3 + Y_{00} = (14811.8 \pm 0.1) + (0.2 \pm 0.1) = 14812.0 \pm 0.2 \text{ cm}^{-1}$.

Table 3

Dissociation energies (D_e) for the $X^1\Sigma^+$ state of ^{133}CsH

Ref.	D_e (cm^{-1})
[10]	14600
[19]	15000 \pm 500
[16] ^{a)}	15384
[17] ^{a)}	14900
[2]	14500 \pm 500
[11]	14805 \pm 30
[4]	14910 \pm 400
[20] ^{a)}	14500
[9]	14807 \pm 5
[12] ^{a)}	14500
this work	14791.2 \pm 2.0

^{a)} Ab initio calculations with no error bounds cited.

value reported in this work, except for the value of Crépin et al. [9]. The disagreement arises because of the way Crépin et al. determined D_e . In their fluorescence measurements they observed a noticeably broadened line, associated with the quasibound level $E_{25,11}$ which they correctly assigned as an upper bound to D_e . The next line associated with the level $E_{25,10}$ was assumed to be a lower bound because the line was not perceptively broadened. Thus they reported a D_e bounded by the last sharp level and the first broadened level: $E_{25,10}(\text{sharp}) \leq D_e \leq E_{25,11}(\text{broad})$, or $14801.7 \leq D_e \leq 14812.0 \text{ cm}^{-1}$.

Clearly the $E_{25,11}$ level is broadened due to rotational predissociation and becomes a valid upper bound to D_e . However, the inability to observe broadening in the "last sharp level" does not mean $E_{25,11}$ is not quasibound. Our calculations show that $E_{25,10}$ is quasibound like $E_{25,11}$ (but with $\Gamma_{\text{fwhm}} < 0.1 \text{ cm}^{-1}$, the uncertainty in the width of the observed quasibound $E_{25,11}$ level). Thus the Crépin et al. contention that $E_{25,10} \leq D_e$ is not valid and their D_e value of 14807 cm^{-1} should be lowered, closer to the value $D_e = 14791.2 \text{ cm}^{-1}$ determined in this work.

Based on an analysis of the binding energy of the last vibrational levels near dissociation, similar to that presented earlier by Stwalley [21], we predict there may be a $v=24$ level in the ground state of KH, but definitely no $v=25$. Finally, the present status of the alkali hydrides is that the ground state dissociation energies for LiH [22], KH and CsH are known to within 2 cm^{-1} . Further experimental investigation is underway on NaH and RbH at the University of Iowa.

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