

**A DPF Analysis Yields Improved  
Dissociation Energies and Potential Functions  
for the  $X^1\Sigma^+$  and  $A^1\Sigma^+$  States of NaH**

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# The past 82 years has seen a considerable amount of work on NaH.

Table 1: Summary of experimental data used in the present work.

Isotop.	Type	Unc.(cm <sup>-1</sup> )	$v(A^1\Sigma^+)$	$v(X^1\Sigma^+)$	#data	source
NaH	Ultraviolet	0.3	3-20	0-3	1884	Hori (1930, 1931)
	Ultraviolet	0.3	4-13	0-1	524	Olsson (1935)
	Ultraviolet	0.1	1-20	0-8	27	Pankhurst (1949)
	Ultraviolet	0.1	0-1	6-8	261	Orth <i>et al.</i> (1980)
	Ultraviolet	0.03	8-15	0	298	Lochbrunner <i>et al.</i> (1996)
	Ultraviolet	0.15	13-25	0-1	27	Rafi <i>et al.</i> (1993)
	Ultraviolet	0.3	0-10, 12	0-1	137	Stwalley, Zemke & Yang (1991)
	Ultraviolet	0.001 – 0.022	2-8	6-9	280	Pesl, Lutz & Bergmann (2000)
	Ultraviolet	1.033	7-8, 10-12	0	41	Huang (2010)
	Ultraviolet	1.033	7-8, 10-11	9-21	286	Huang (2010)
	Microwave	0.1	—	3-8	146	from Pankhurst (1949)
	Microwave	0.1	1-7	—	183	from Pankhurst (1949)
	Microwave	0.000007	—	0-3	4	Sastry, Herbst & De Lucia (1981)
	Microwave	0.000003 – 0.000015	—	0-3	21	Leopold <i>et al.</i> (1987)
	Infrared	0.001	—	0-2	25	Magg & Jones (1988)
	Infrared	0.001 – 0.002	—	0-3	58	Maki & Olson (1989)
	Infrared	1.033	—	9-21	286	from Huang (2010)
NaD	Ultraviolet	0.2	7-17	0-1	604	Olsson (1935)
	Microwave	0.000007	—	0-3	5	Sastry, Herbst & De Lucia (1981)
Overall			0-1,3-20	0-3,6-21	4631	

**However,** prior to 2010, the data range for the  $X^1\Sigma^+$  state was only  $v = 0-9$ , spanning only 60% of its potential well, and the  $v = 0-25$  range for the  $A^1\Sigma^+$  state spanned only 86% of its well. This left the ground-state dissociation energy *a very uncertain property!*

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THE JOURNAL OF CHEMICAL PHYSICS **133**, 044301 (2010)

### **Dissociation energy of the ground state of NaH**

Hsien-Yu Huang,<sup>1</sup> Tsai-Lien Lu,<sup>1</sup> Thou-Jen Whang,<sup>1,a)</sup> Yung-Yung Chang,<sup>2</sup> and Chin-Chun Tsai<sup>2</sup>

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Their Stimulated Emission Pumping and Fluorescence Depletion spectroscopy measurements allowed them access to levels  $v(X) = 9-21$ , the highest of which is bound by only ca.  $38\text{ cm}^{-1}$ .

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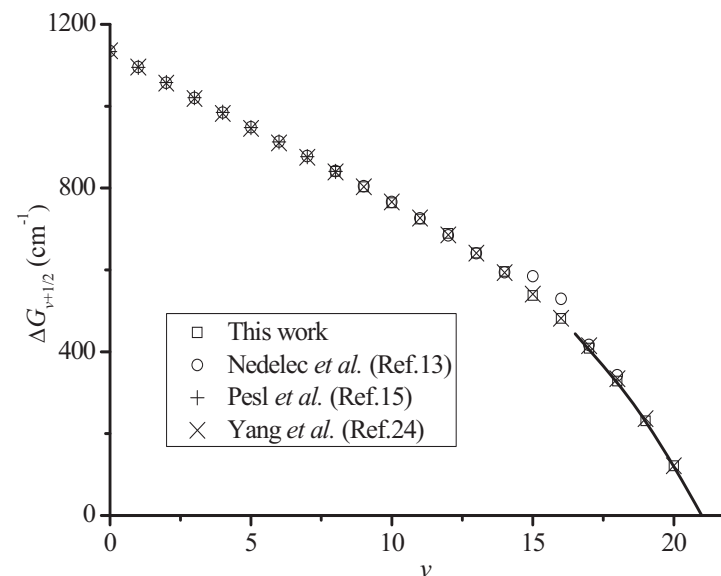
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*However*, their estimate of the dissociation energy was based on classical quadratic extrapolations of the vibrational spacings and vibrational energy that *neglected* the fact that Near-Dissociation theory shows that these plots should show *clear positive curvature at the intercept!*



Up to this point, all analyses of NaH and NaD data had been based on traditional Dunham analyses, one isotopologue at a time, and neglected the fact that since they were hydrides, *quantum mechanical deviations from semiclassical mass scaling and **B**orn-**O**ppenheimer breakdown (**BOB**) effects are expected to be relatively large !*

In contrast, the present paper reports a fully quantum mechanical *Direct Potential Fit (DPF) analysis* that takes full account of the different levels of precision of the various data set and accounts for all available data (on average) within their estimated uncertainties.

*But how is this done ?*

## *‘Direct Potential Fits’*

*{For 3-D Van der Waals molecules since 1974, and diatomics since  $\sim 1990$  }*

- Simulate level energies as eigenvalues of some parametrized analytic potential energy function  $V(r; \{p_j\})$
- Partial derivatives of observables w.r.t. parameters  $p_j$  required for fitting are generated readily using the Hellmann-Feynmann theorem:

$$\frac{\partial E(v, J)}{\partial p_j} = \left\langle \psi_{v,J} \left| \frac{\partial V(r; \{p_j\})}{\partial p_j} \right| \psi_{v,J} \right\rangle$$

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### *Advantages*

- final result is a global analytic potential energy function
- allows realistic predictions in ‘extrapolation’ region outside the data range, and of non-spectroscopic properties
- yields full quantum mechanical accuracy
- readily accounts for Born-Oppenheimer breakdown (BOB),  $\Lambda$ -doubling, and/or  $^2\Sigma$  splittings, in terms of radial functions



For the ground  $X^1\Sigma^+$  state of NaH, theory has given us good values of the leading long-range dispersion coefficients  $C_6$ ,  $C_8$  and  $C_{10}$ , so it is appropriate to use a potential function form that incorporates the theoretically predicted inverse-power long-range tail so we use:

The *Morse/Long-Range (MLR) Potential*.

If we define  $u_{\text{LR}}(r) = \frac{C_{m_1}}{r^{m_1}} + \frac{C_{m_2}}{r^{m_2}} + \dots$  we can write

$$V_{\text{MLR}}(r) = \mathfrak{D}_e \left\{ 1 - \frac{u_{\text{LR}}(r)}{u_{\text{LR}}(r_e)} e^{-\beta(r) y_p^{\text{eq}}(r)} \right\}^2$$

$$\xrightarrow{r \gg r_e} \mathfrak{D}_e - \left[ \frac{2\mathfrak{D}_e e^{-\beta_\infty}}{u_{\text{LR}}(r_e)} \right] u_{\text{LR}}(r) = \mathfrak{D}_e - \frac{C_{m_1}}{r^{m_1}} - \frac{C_{m_2}}{r^{m_2}} - \dots$$

in which  $\beta(r) = \beta_\infty y_p^{\text{ref}}(r) + [1 - y_p^{\text{ref}}(r)] \sum_{i=0}^{N_\beta} \beta_i y_q^{\text{ref}}(r)^i$

and  $\beta_\infty = \ln\{2\mathfrak{D}_e/u_{\text{LR}}(r_e)\}$ , where  $y_p^{\text{ref}}(r) \equiv \frac{r^q - r_{\text{ref}}^q}{r^q + r_{\text{ref}}^q}$

The physical parameters  $\mathfrak{D}_e$  and  $r_e$  and the exponent expansion parameters  $\{\beta_i\}$  are optimized using a standard automated least-squares technique.

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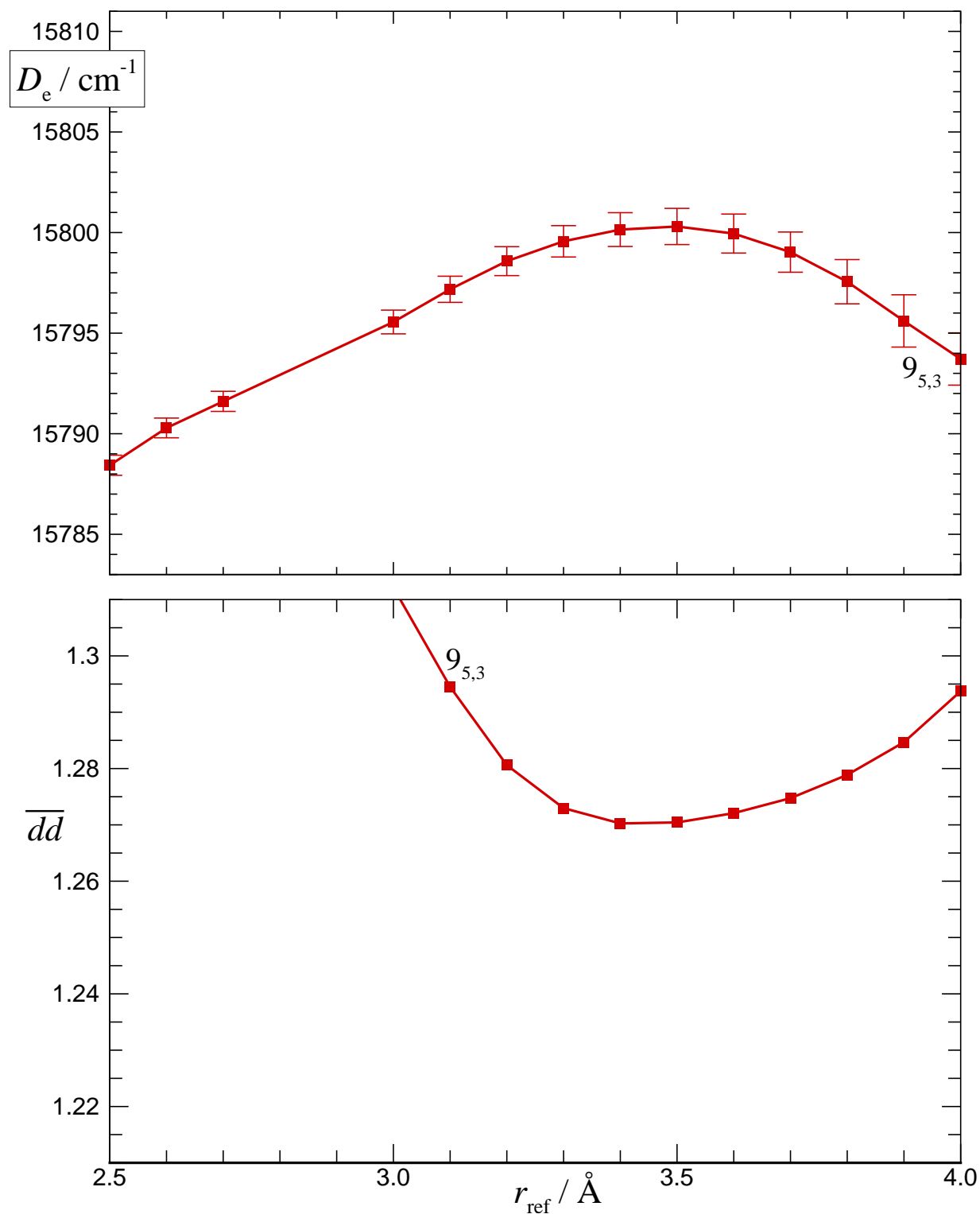
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With cases labelled by  
 $N_{p,q}$  where  $N \equiv N_\beta$ ,

The fitted dissociation  
 energy varies with the  
 choice of  $r_{\text{ref}}$

while we search for  
 a minimum of  $\overline{dd}$ .

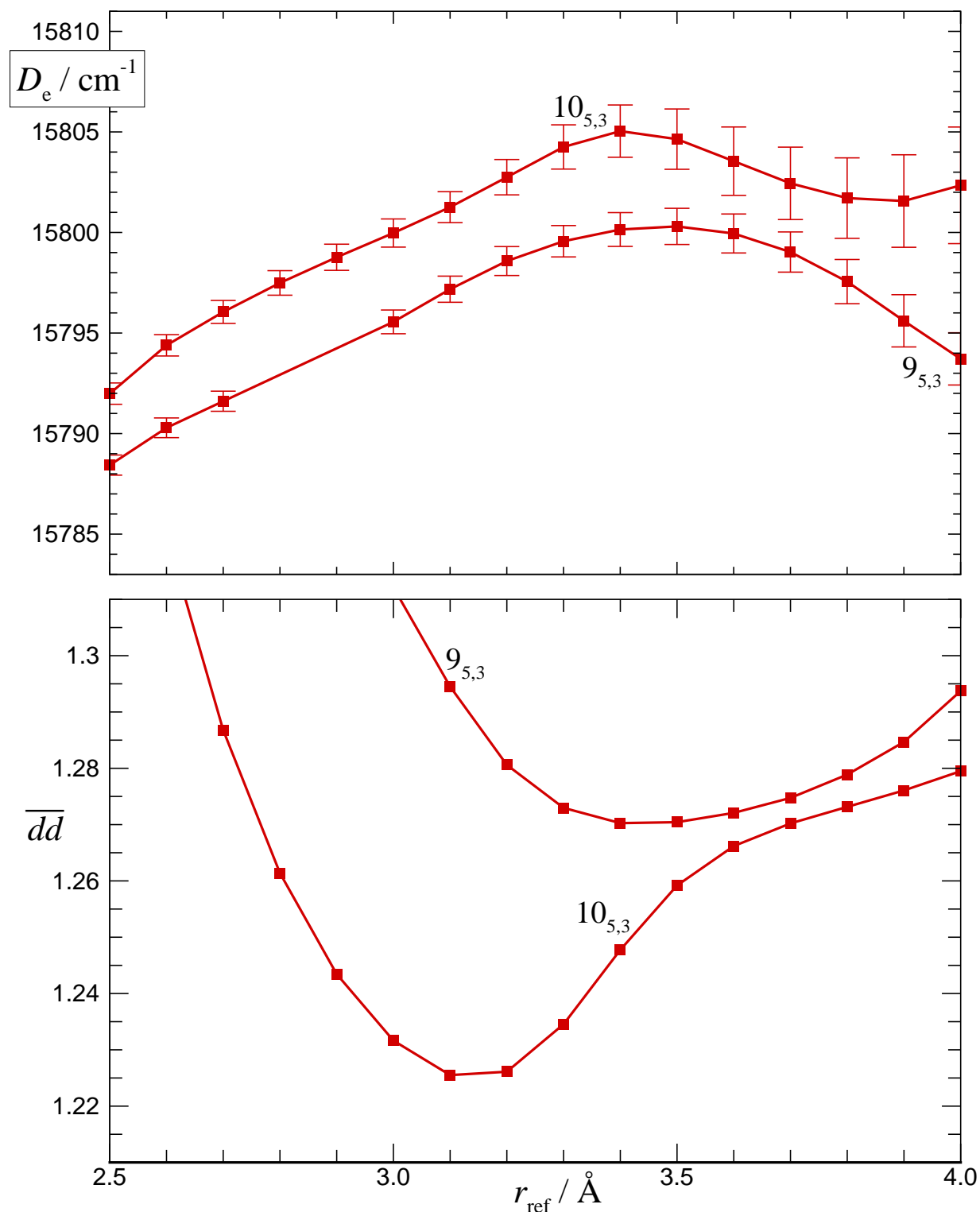


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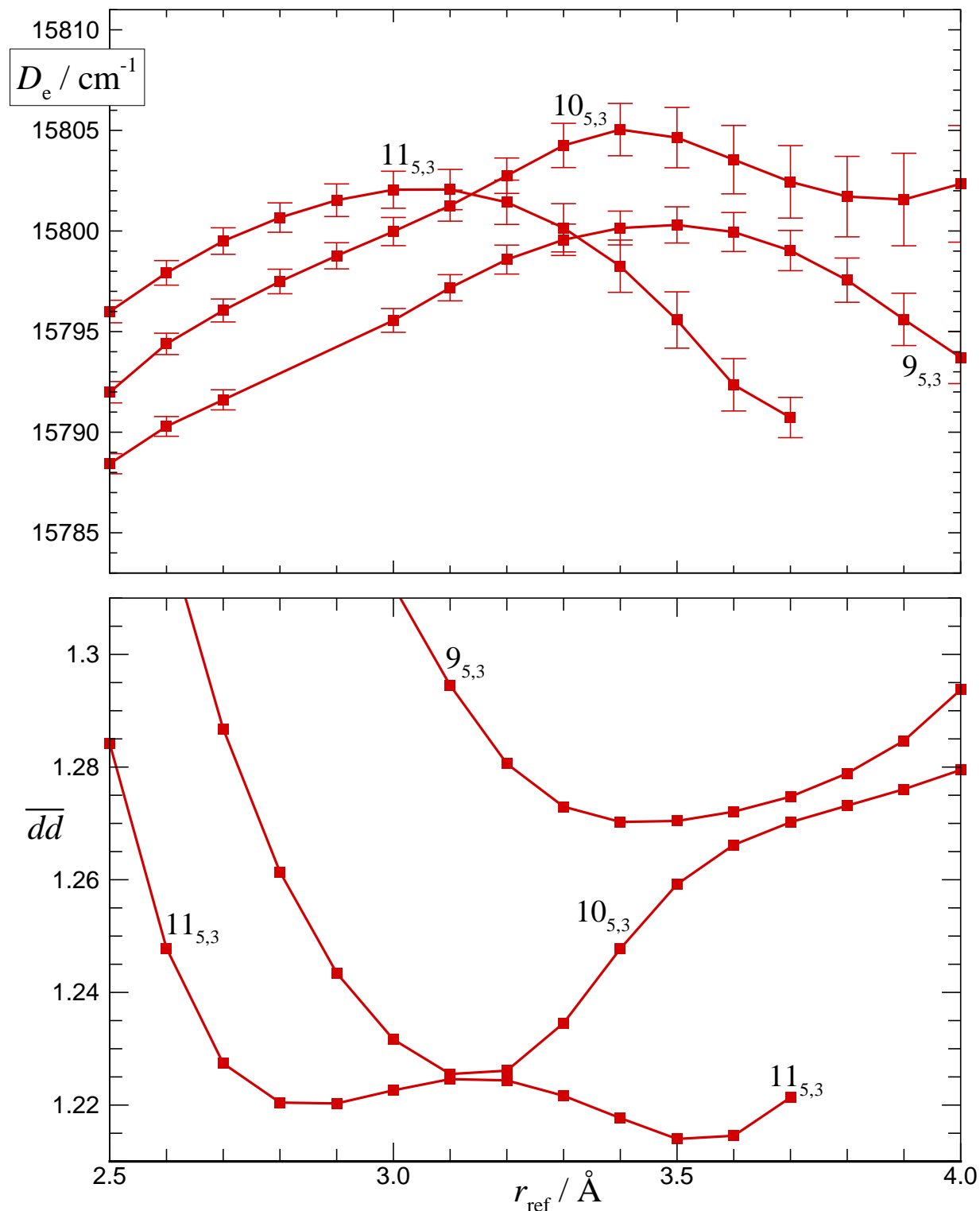


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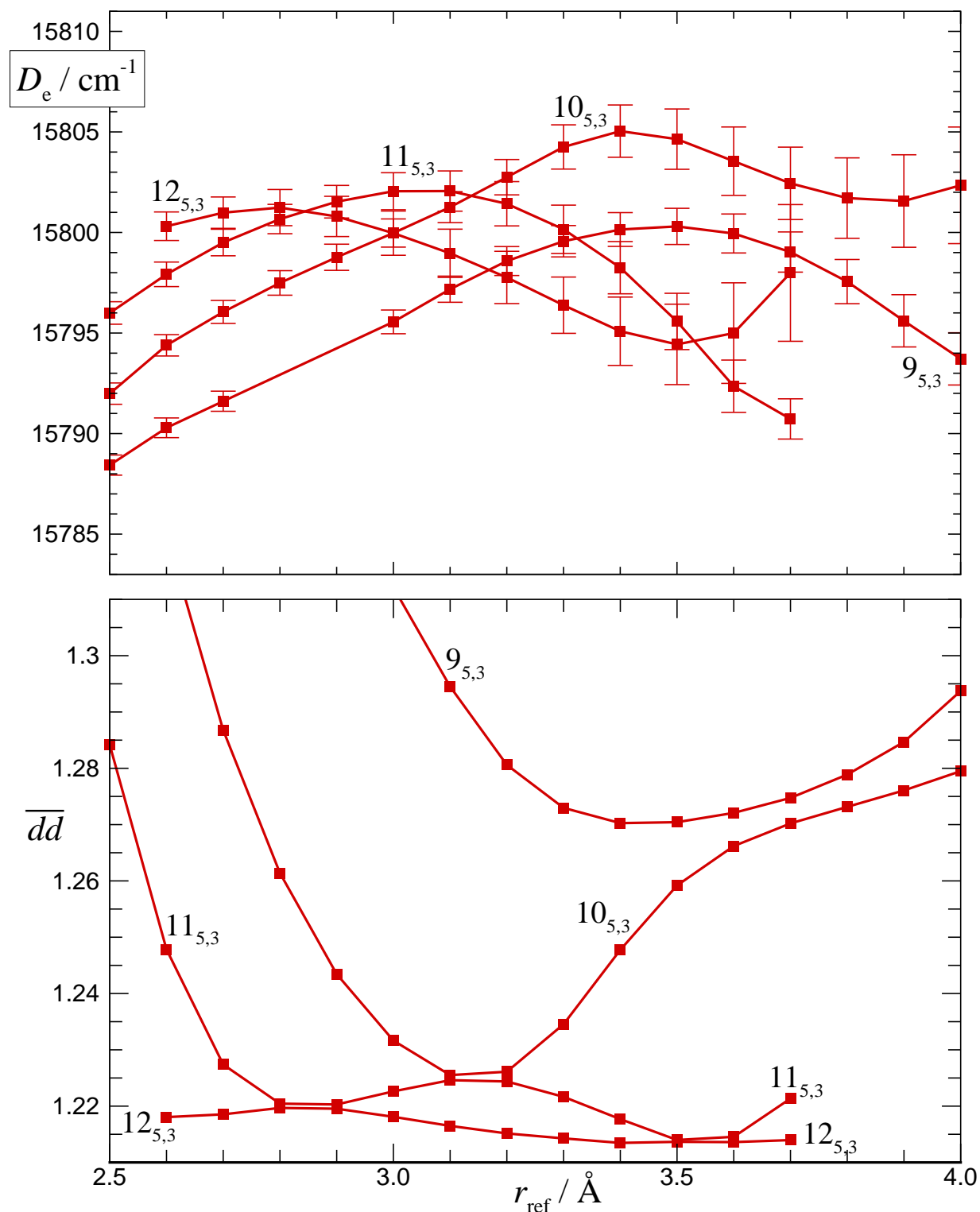


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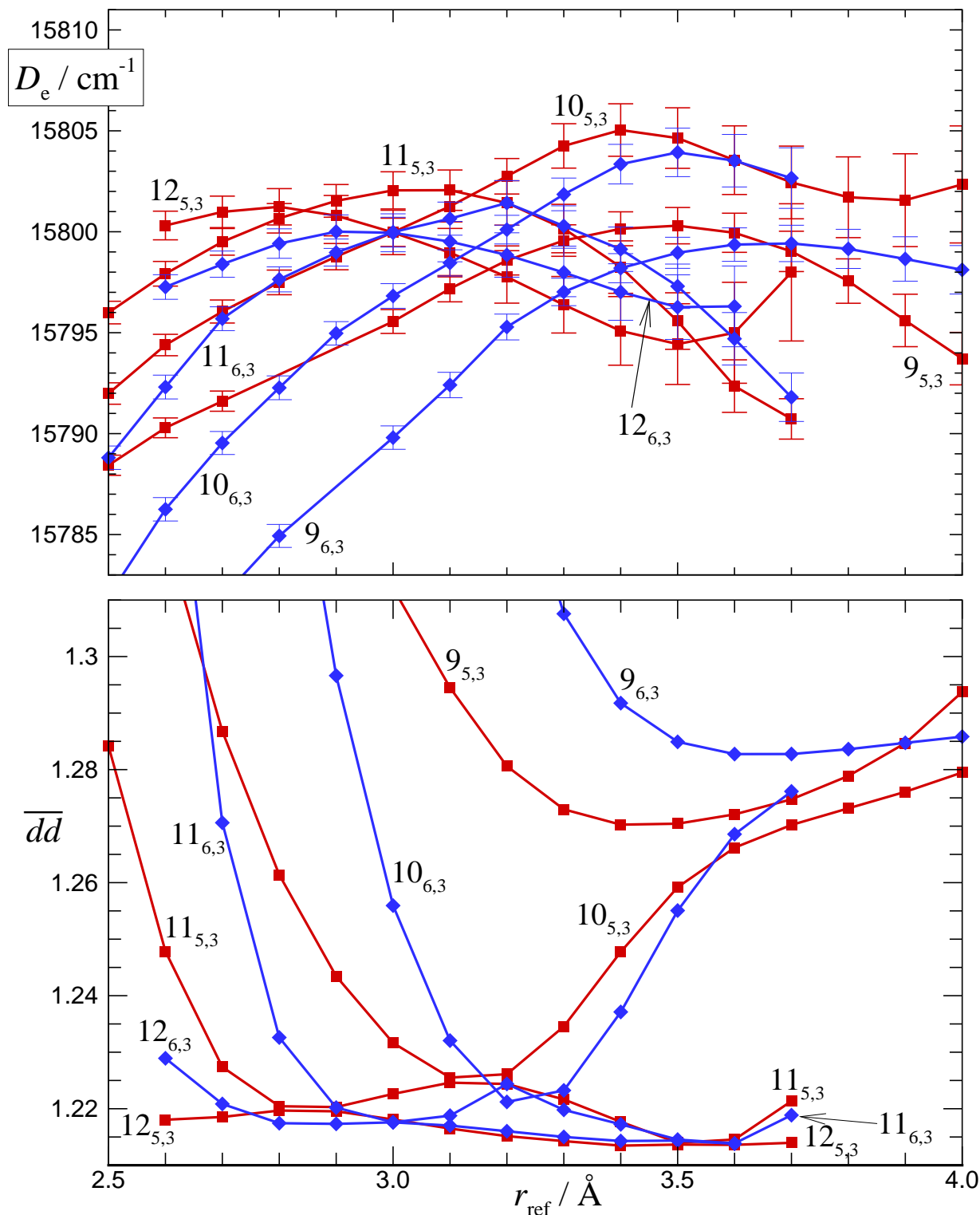
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The fitted dissociation energy varies with the choice of  $r_{\text{ref}}$  and  $N_\beta$  and of the power  $p$  in  $y_p^{\text{ref}}(r)$ .

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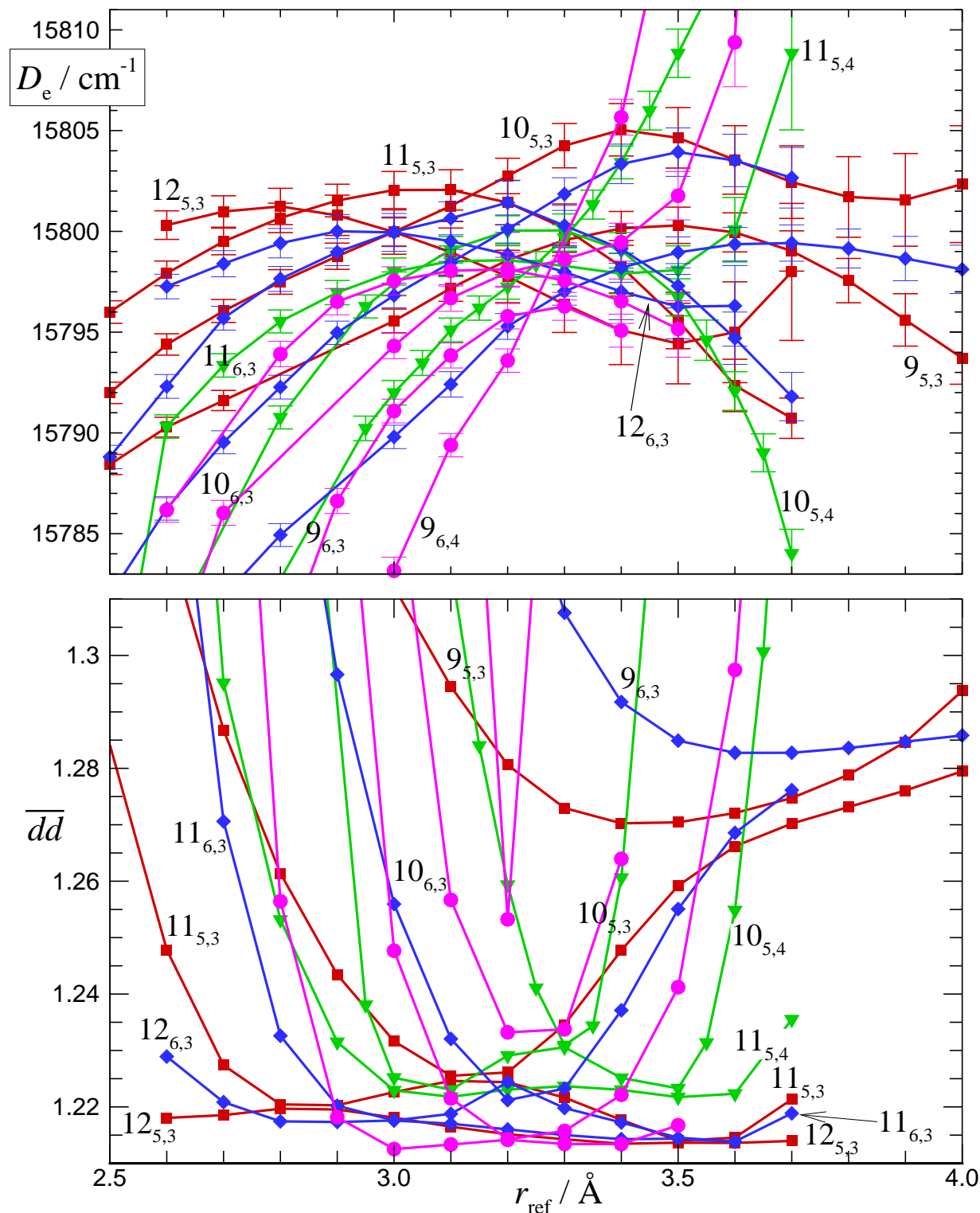
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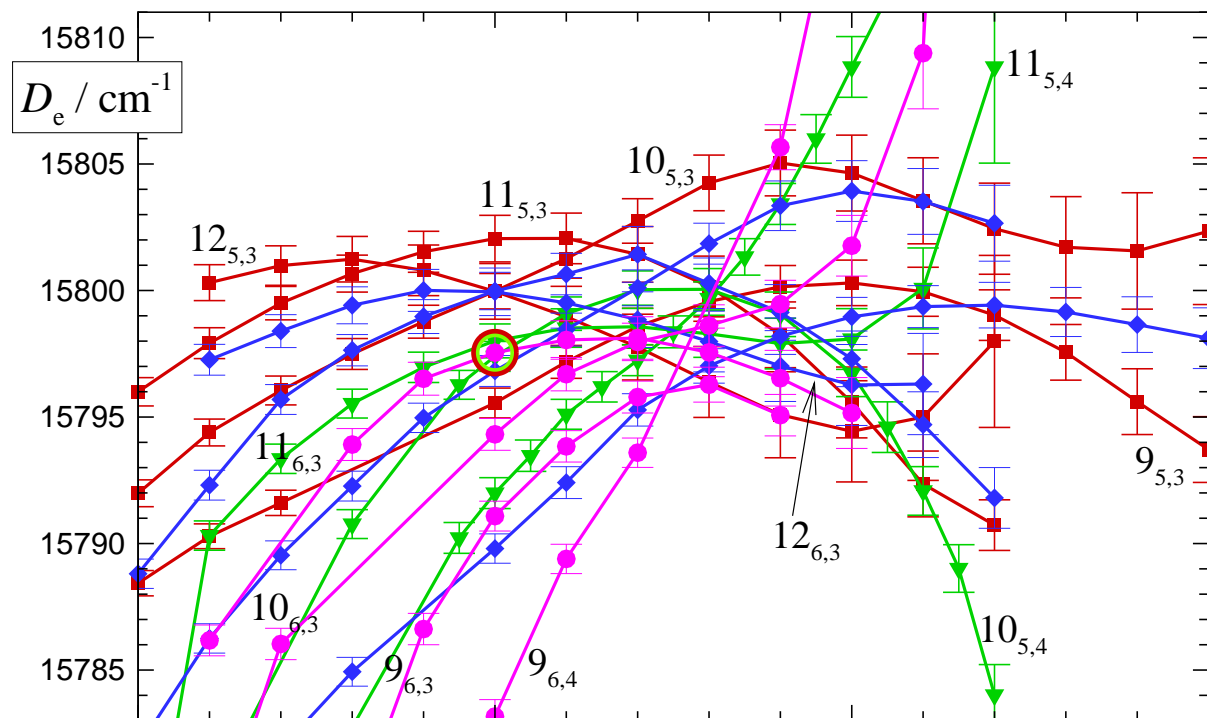
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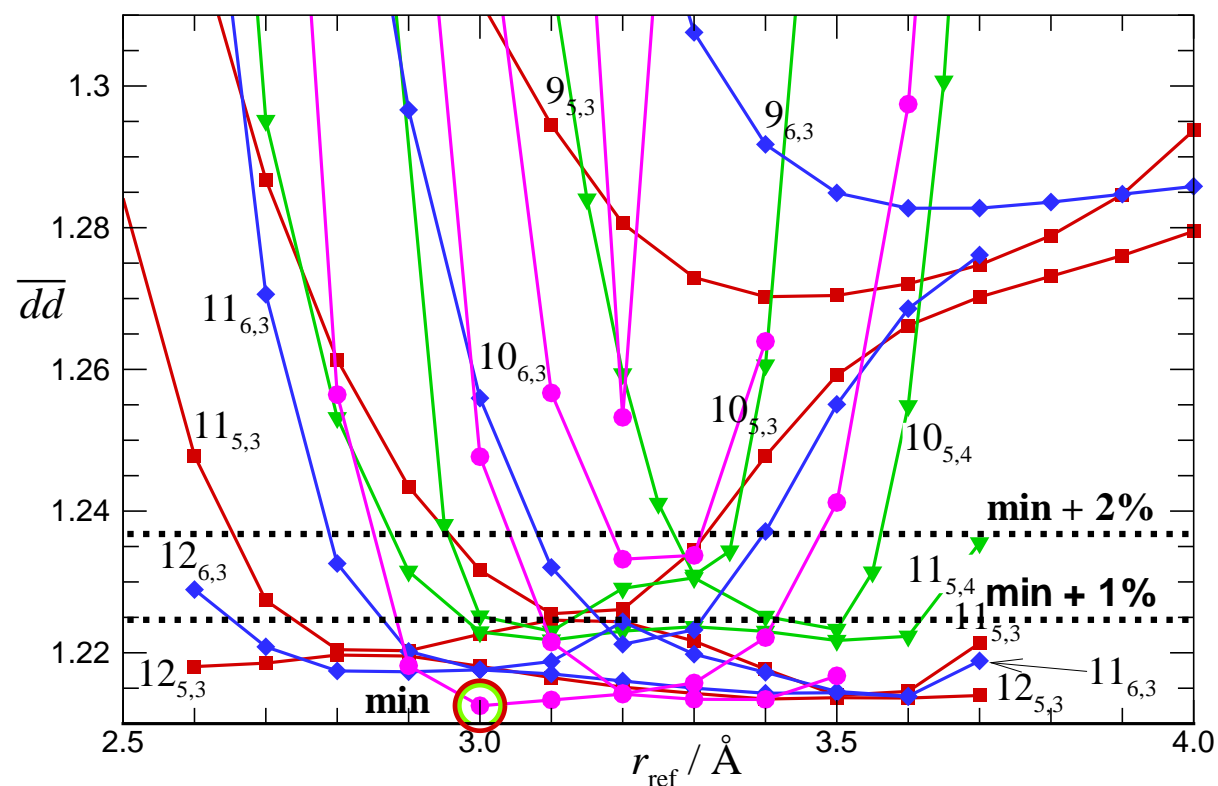




Now ... what about  
finding the best model, and  
the best estimate of  $\mathfrak{D}_e$   
*and of its uncertainty?*



the **best model** has  
 $\overline{dd}$  at its minimum  
for a minimum of  $N_\beta$ , but  
the uncertainty in its  $\mathfrak{D}_e$   
value is small relative to the  
variation between models.



Thus ... we need a scheme for averaging to get a best estimate of  $\mathfrak{D}_e$  and of its overall uncertainty, while taking account of model-dependence. We use the scheme introduced in *J. Chem. Phys.* **101**, 10217 (1994).

If a fit to a particular model, model  $k$ , with an overall dimensionless standard deviation of  $\overline{dd}_k$  yields the value  $P_k$  and uncertainty  $u(P_k)$  for parameter  $P$ , then the weight given to this  $P_k$  value is

$$w_k^P = \frac{1}{[u(P_k) \overline{dd}_k]^2}$$

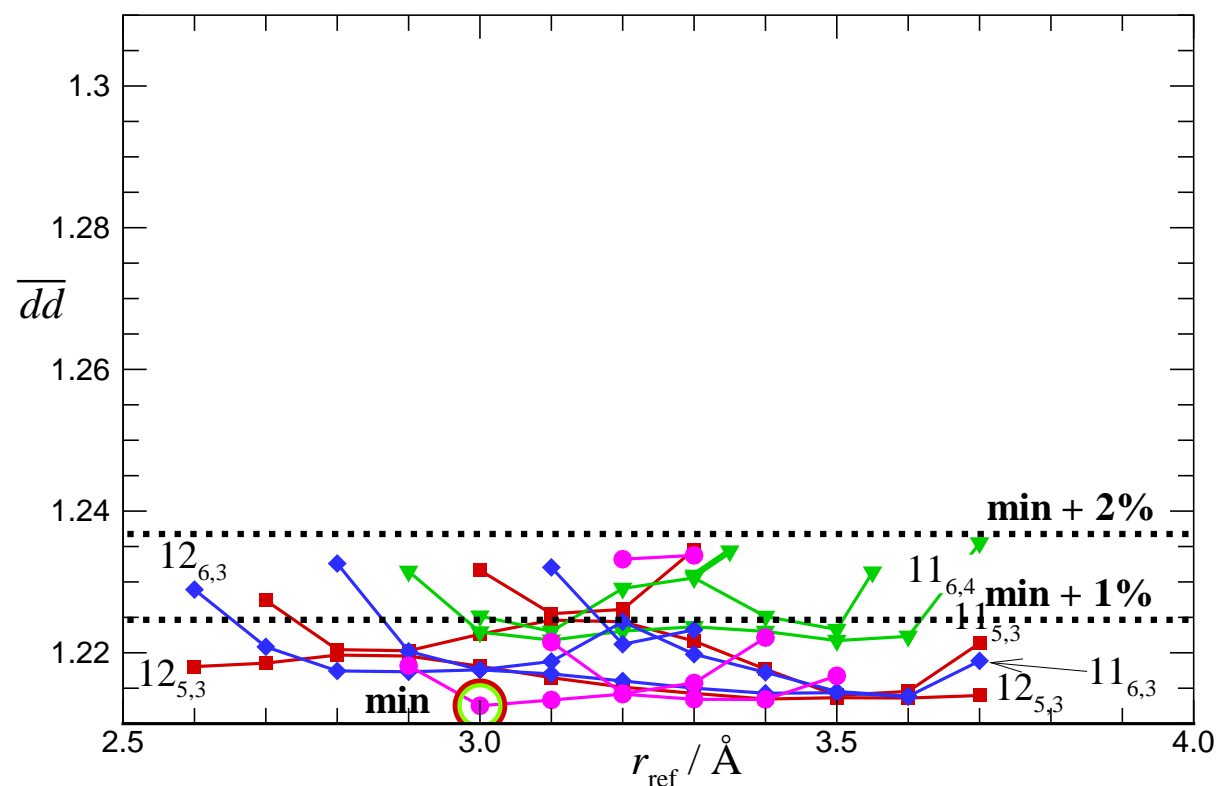
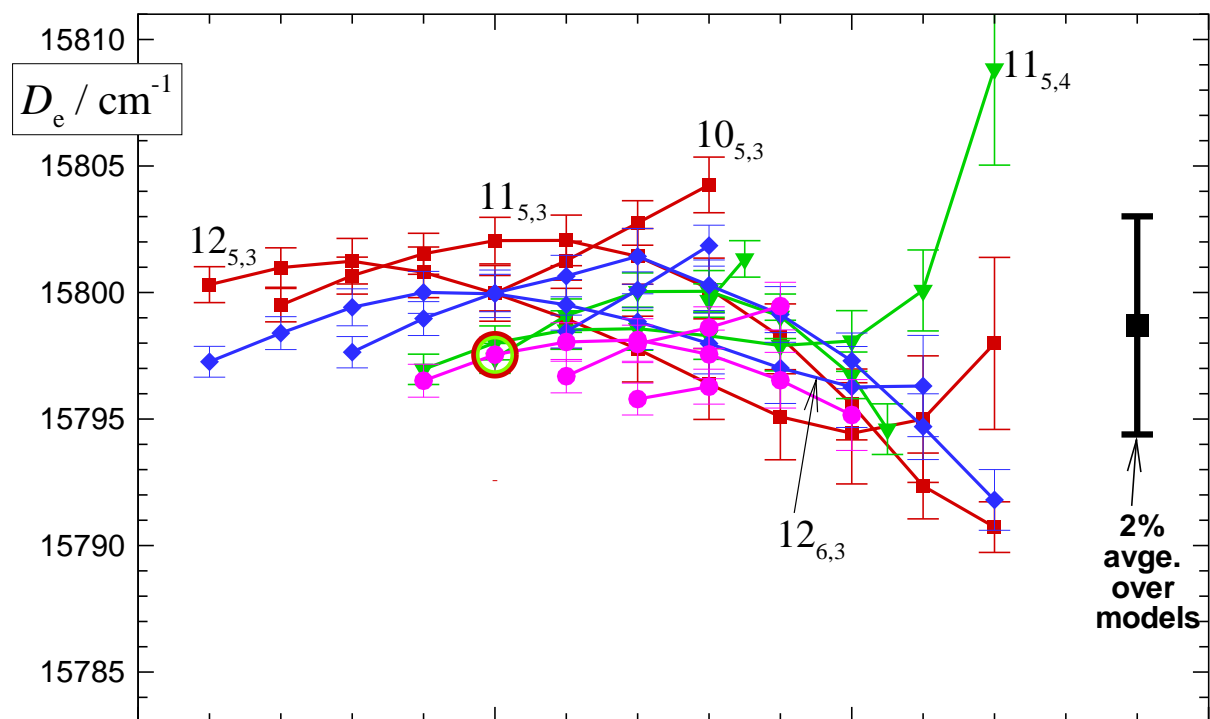
The recommended value of this parameter would then be based on an average over the values from all models whose  $\overline{dd}_k$  values lay within, say, 1% or 2% of the  $\overline{dd}_k$  minimum

$$\overline{P} = \frac{\sum_k (w_k^P P_k)}{\sum_k w_k^P}$$

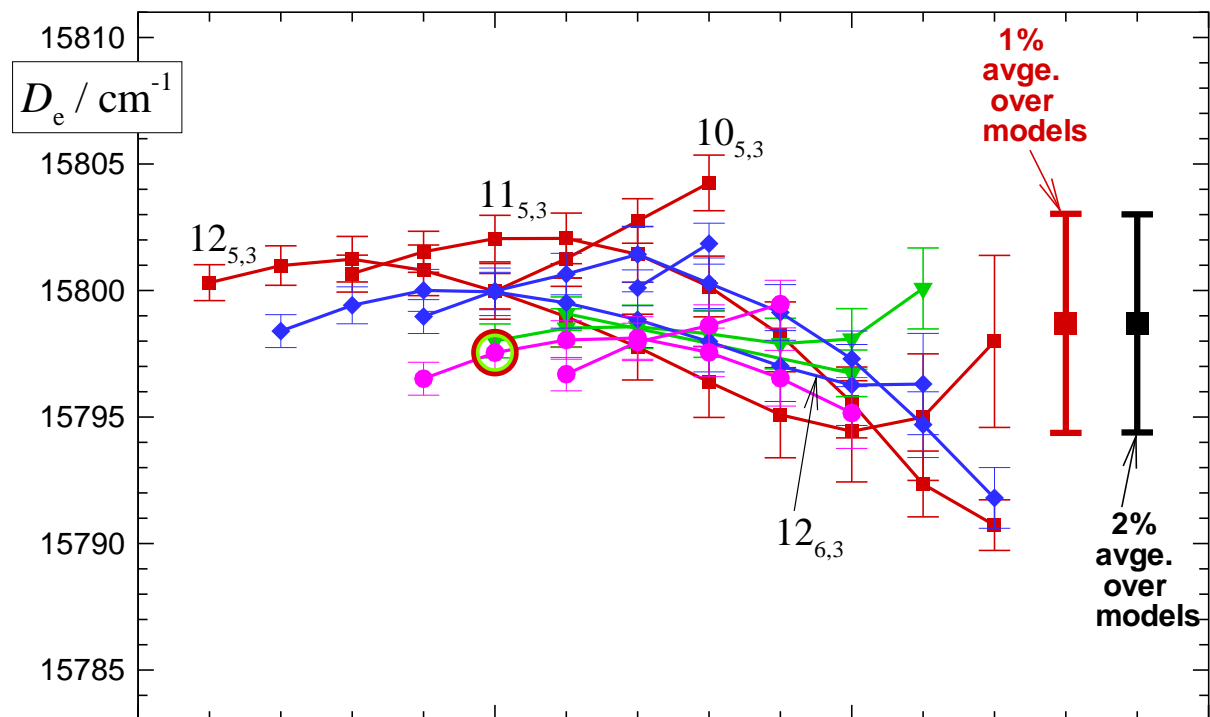
and the associated uncertainty in this estimate is

$$u(\overline{P}) = \left\{ \left[ \frac{\sum_k w_k^P (P_k - \overline{P})^2}{\sum_k w_k^P} \right] + \left[ \frac{\sum_k w_k^P u(P_k)}{\sum_k w_k^P} \right]^2 \right\}^{1/2}$$

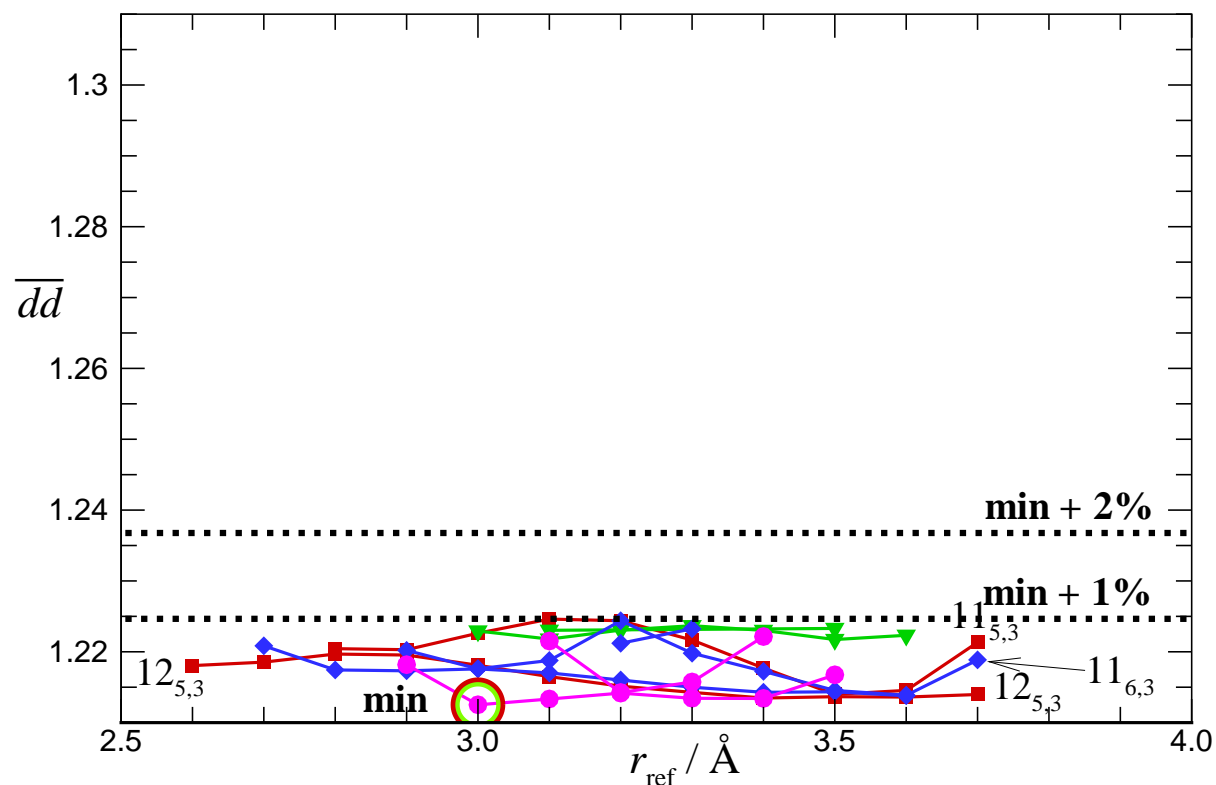
Now let us apply this  
“averaging-over-models”  
method to our fitted  $\mathcal{D}_e$   
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2% of the minimum,  
or 1% of the minimum!



*The close similarity of  
these two averages  
gives us confidence in  
their predictions!*



## Experimental estimates of the NaH well depth energy

source	$\mathfrak{D}_e / \text{cm}^{-1}$	method
<b>present work (2013)</b>	<b>15 799 <math>\pm</math> 4</b>	<b>direct fit to an MLR potential function</b>
Huang <i>et al.</i> (2010)	15 815 $\pm$ 5	polynomial extrapolation from $v'' = 21$
Stwalley <i>et al.</i> (1991)	15 900 $\pm$ 100	<i>ab initio</i> tail + binding energy of $v'' = 19$
Nedelec and Grioud (1983)	15 785 $\pm$ 20	Polynomial Birge-Sponer extrapolation from $v = 19$
Grioud and Nedelec (1980)	16 300 $\pm$ 500	Polynomial Birge-Sponer extrapolation from $v = 16$
Pankhurst (1949)	17 410 $\pm$ ??	Morse extrapolation from $v'' = 8$
Hori (1931)	18 100 $\pm$ ??	polynomial extrapolation from $v'' = 20$

Now that we have an optimum model for the  $X^1\Sigma^+$  state, ...

**what about the  $A^1\Sigma^+$  state?**

This state dissociates to  $\text{Na}(3p)+\text{H}(1s)$ , and there are no reported theoretical dispersion coefficients for the long-range interaction of these atoms, so we *cannot* model this state with an MLR function. Instead, let us use the

*Extended Morse Oscillator (EMO) Potential.*

$$V_{\text{EMO}}(r) = \mathfrak{D}_e \left\{ 1 - e^{-\beta(r) (r-r_e)} \right\}^2$$

in which  $\beta(r) = \sum_{i=0}^{N_\beta} \beta_i y_q^{\text{ref}}(r)^i$  where  $y_q^{\text{ref}}(r) = \frac{r^q - r_{\text{ref}}^q}{r^q + r_{\text{ref}}^q}$

Once again, the physical parameters  $\mathfrak{D}_e$  and  $r_e$  and the exponent expansion parameters  $\{\beta_i\}$  may be optimized using our standard automated least-squares technique.

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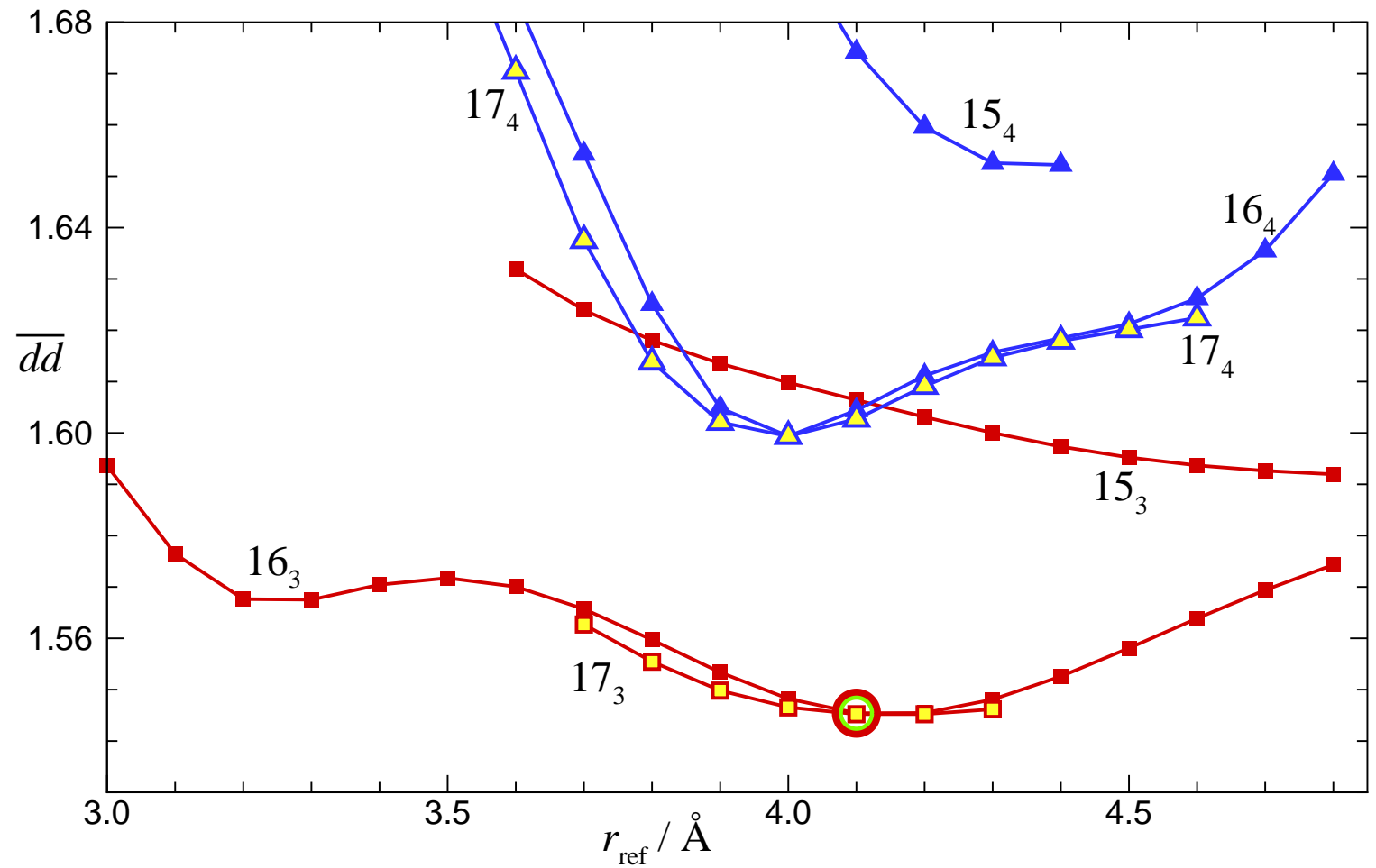
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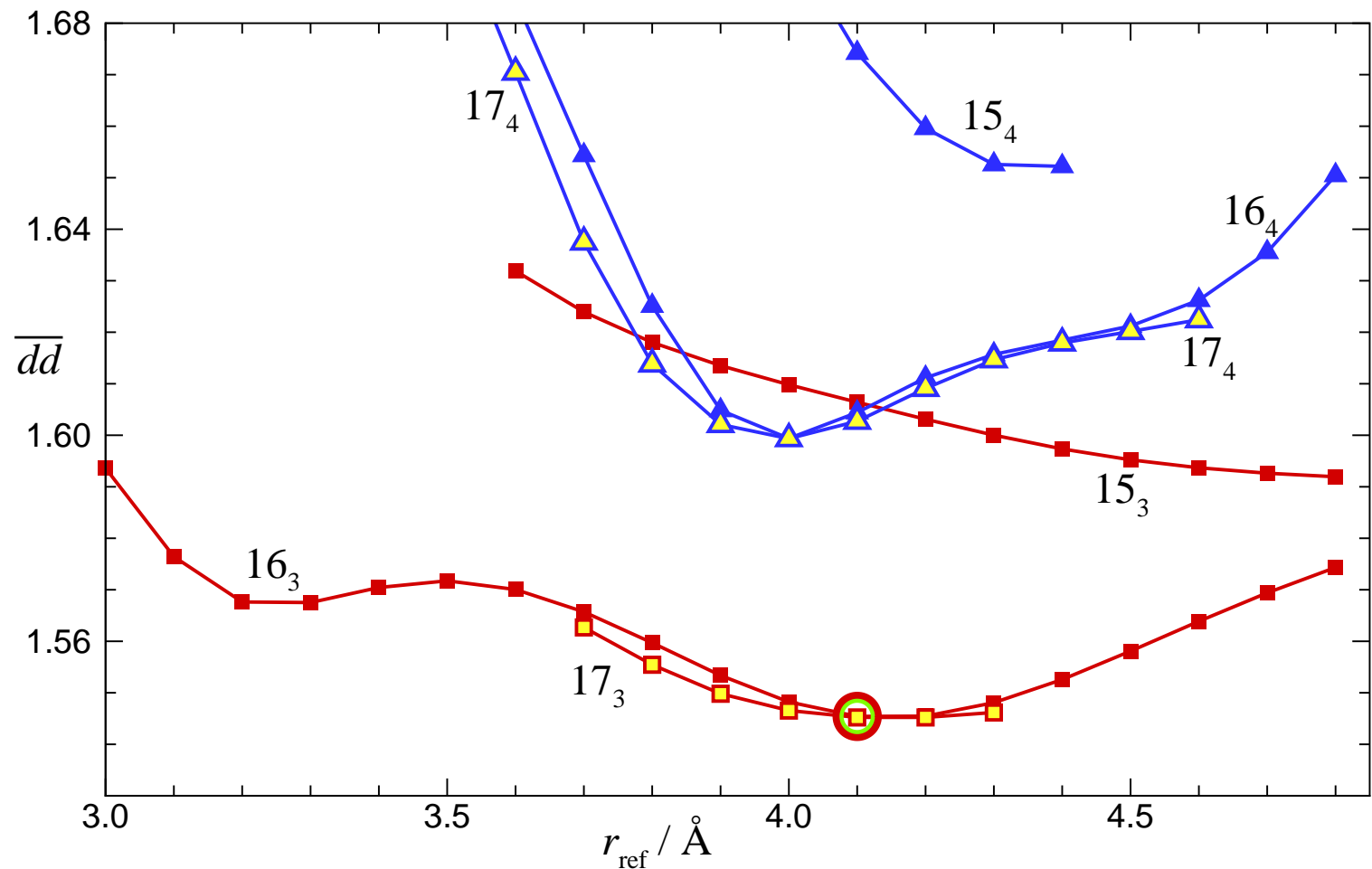
while the expansion centre  $r_{\text{ref}}$  and the power  $q$  defining the expansion variable, and the exponent polynomial order  $N_\beta$  must be determined by manual (trial-and-error) fits.

Once again, we perform fits for a variety of  $N_q$  models, plot  $\overline{dd}$  vs.  $r_{\text{ref}}$  and search for a minimum.





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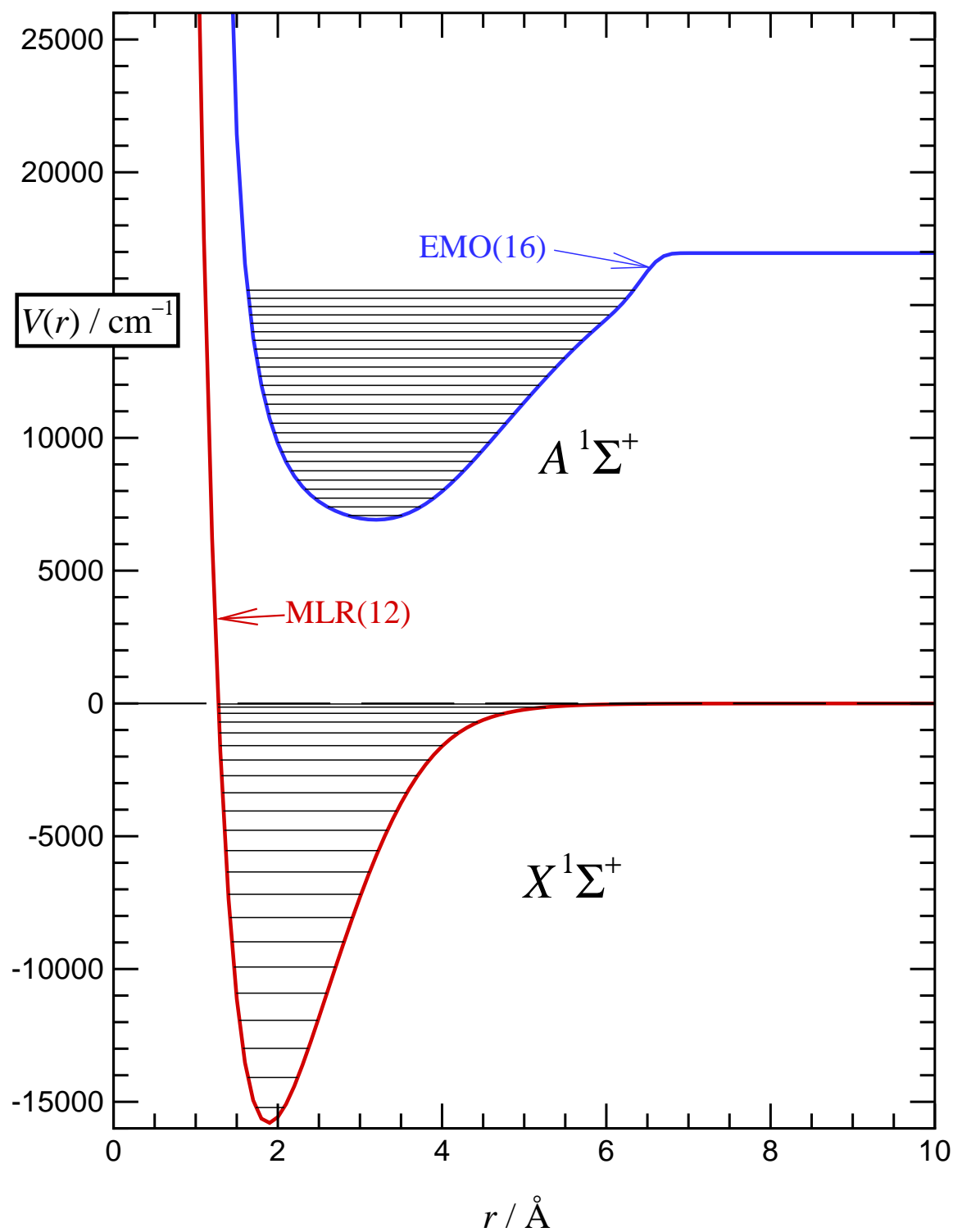
Our optimum model is the one for which:  $N_\beta = 16$  ,  $q = 3$  , and  $r_{\text{ref}} = 4.1 \text{ \AA}$ .

Now we can perform a global fit to all of the data, varying all parameters simultaneously, and then perform “*sequential rounding and refitting*” to obtain an optimally compact set of parameter values.

*But what are these  
potential functions like ?*

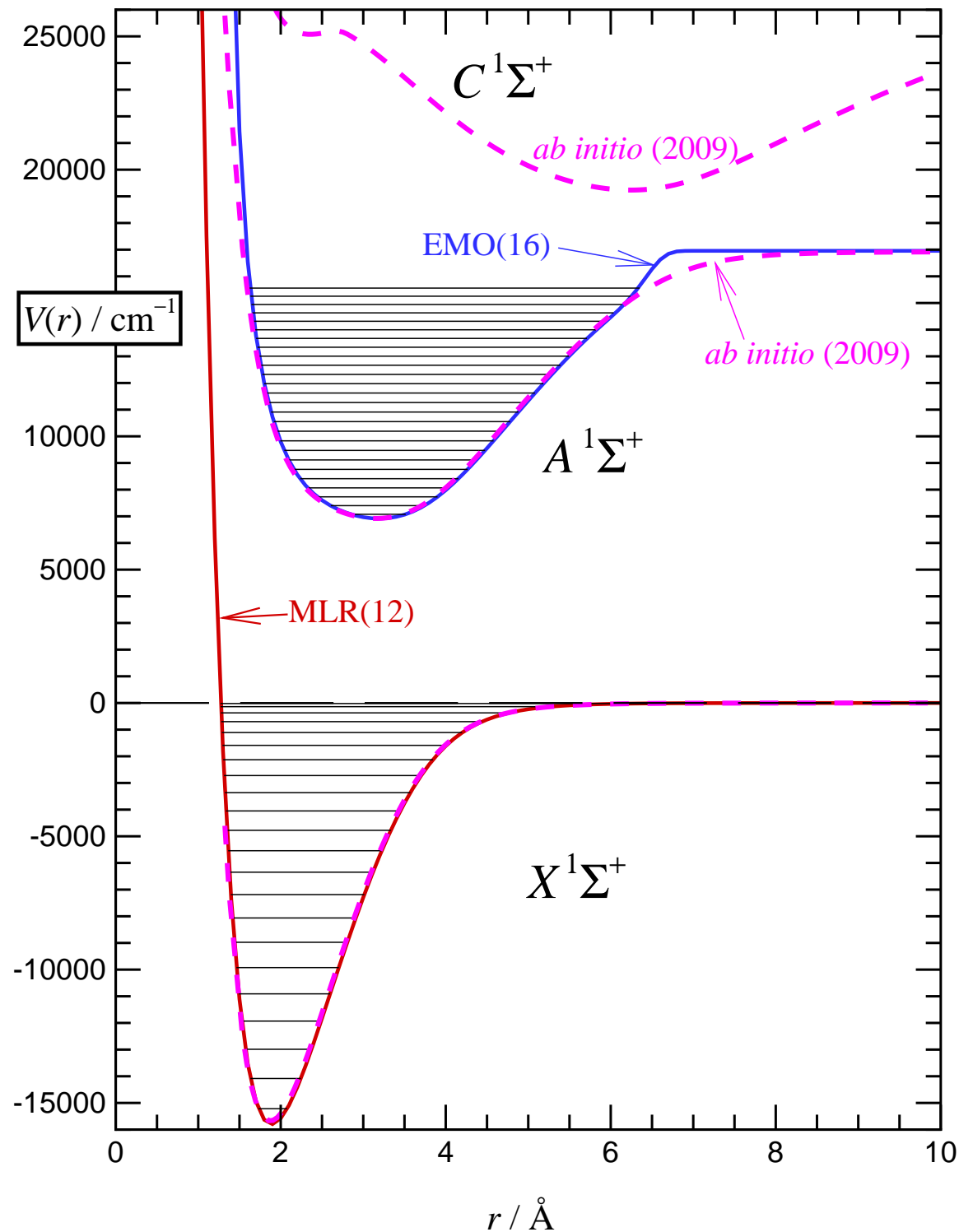
	$X\ ^1\Sigma_g^+$	$A\ ^1\Sigma_u^+$
model	<b>MLR(12)</b>	<b>EMO(18)</b>
$\mathfrak{D}_e$	15797.9 (4.9)	9353.167 (4)
$r_e$	1.8870239 (15)	3.107856 (5)
$C_6$	$[3.57502 \times 10^5]$	—
$C_8$	$[5.41796 \times 10^6]$	—
$C_{10}$	$[1.12920 \times 10^8]$	—
$\{p, q\} =$	$\{6, 4\}$	$\{q\} = \{3\}$
$r_{\text{ref}}$	[3.00]	[4.1]
$\beta_0$	0.07318223	0.50113700
$\beta_1$	−4.1817932	0.3566980
$\beta_2$	−5.794976	−0.039330
$\beta_3$	−6.28633	−0.15659
$\beta_4$	−6.31251	0.30030
$\beta_5$	−5.8552	1.5283
$\beta_6$	−4.6227	8.3540
$\beta_7$	−3.177	−18.233
$\beta_8$	−4.406	−104.69
$\beta_9$	−9.290	103.57
$\beta_{10}$	−11.94	666.1
$\beta_{11}$	−7.76	−12.4
$\beta_{12}$	−2.00	−2037.
$\beta_{13}$	—	−1443.
$\beta_{14}$	—	2070.
$\beta_{15}$	—	3070.
$\beta_{16}$	—	1100.

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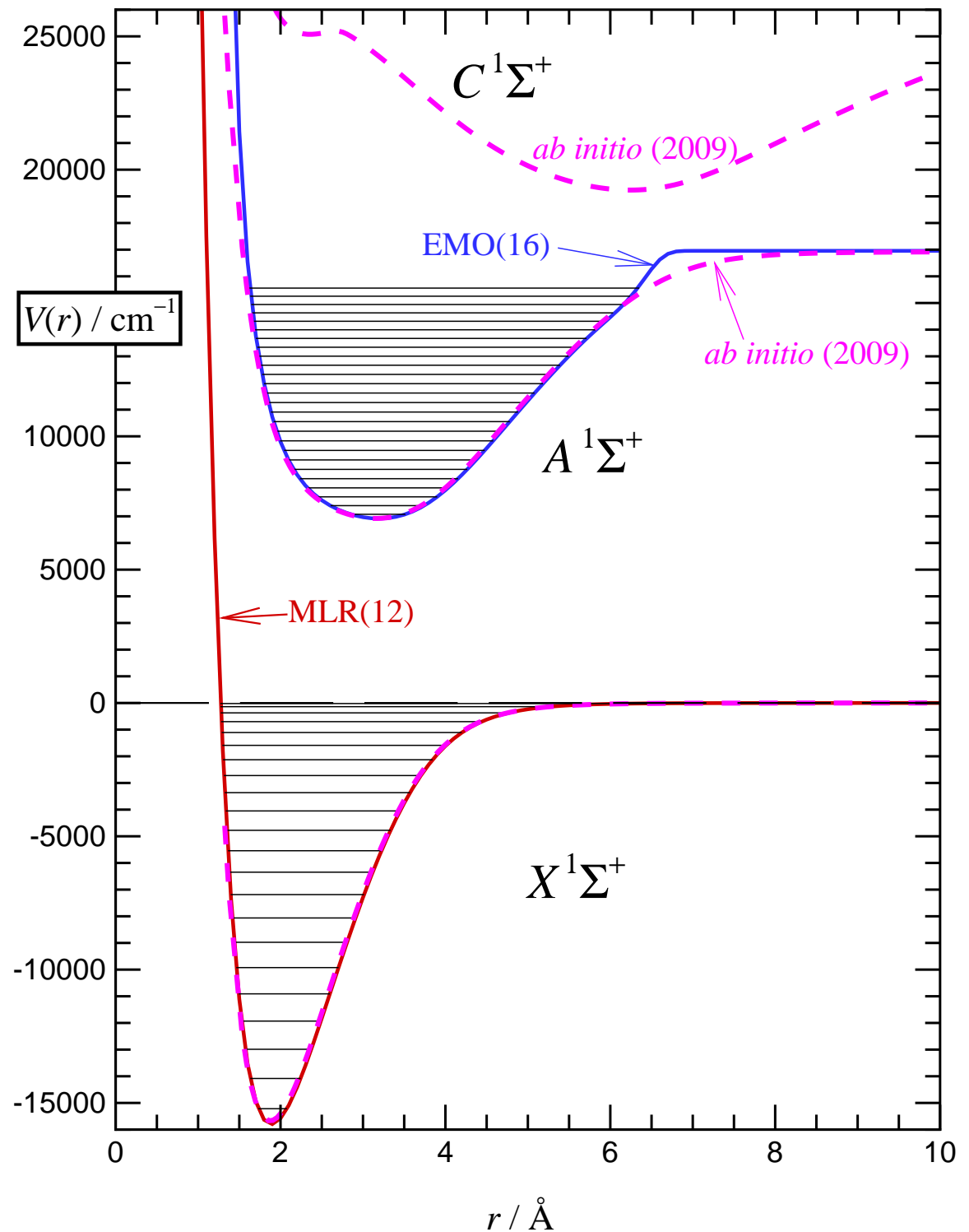
The *ab initio* calculations by Aymar, Deiglmayr and Dulieu [Can. J. Phys. **87**, 543 (2009)] show that this is due to an avoided crossing with the  $C^1\Sigma^+$ -state potential.



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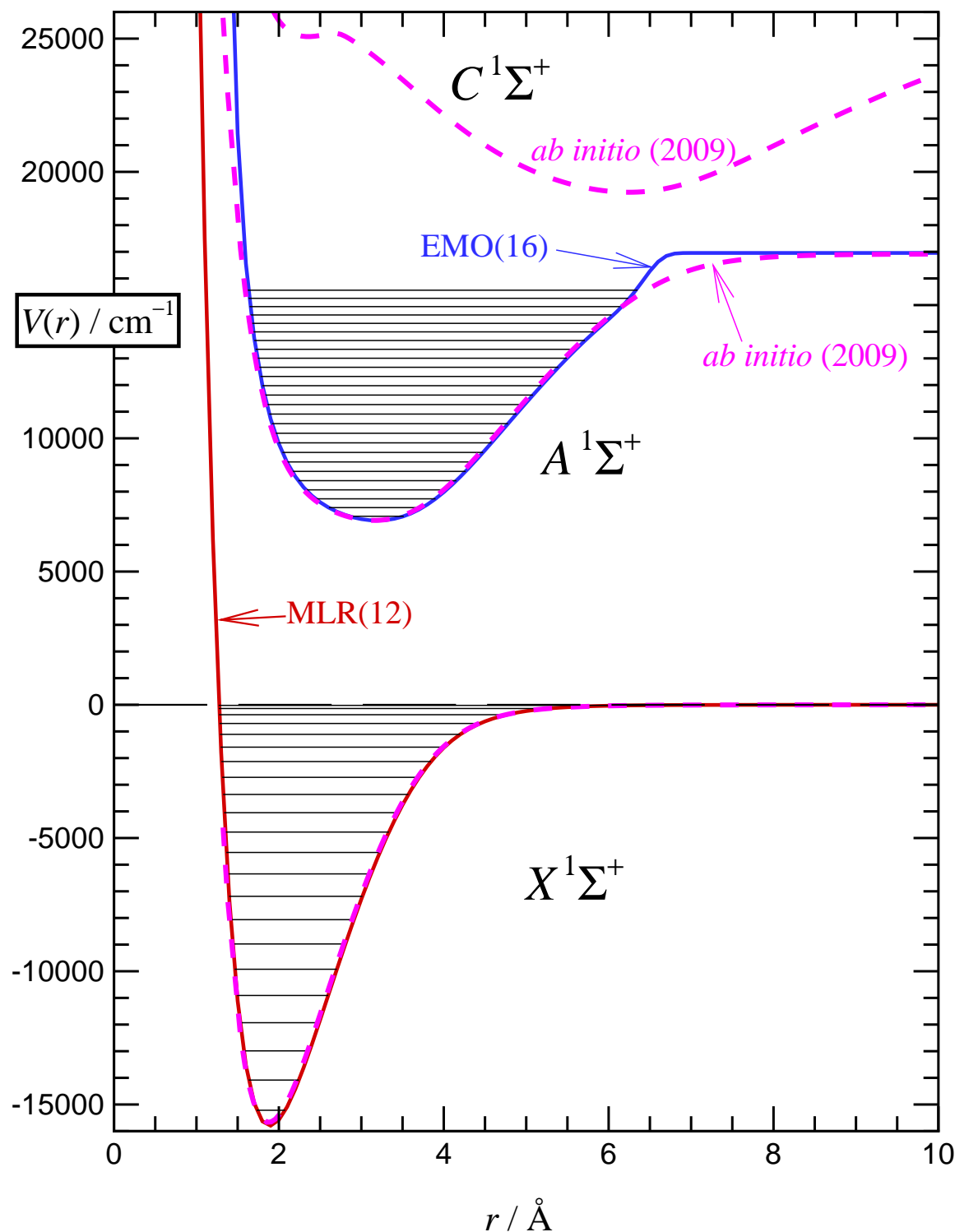
**This confirms that our exponential-cutoff EMO potential needs an improved form at large  $r$ .**



## Conclusions

Our DPF analysis gives:

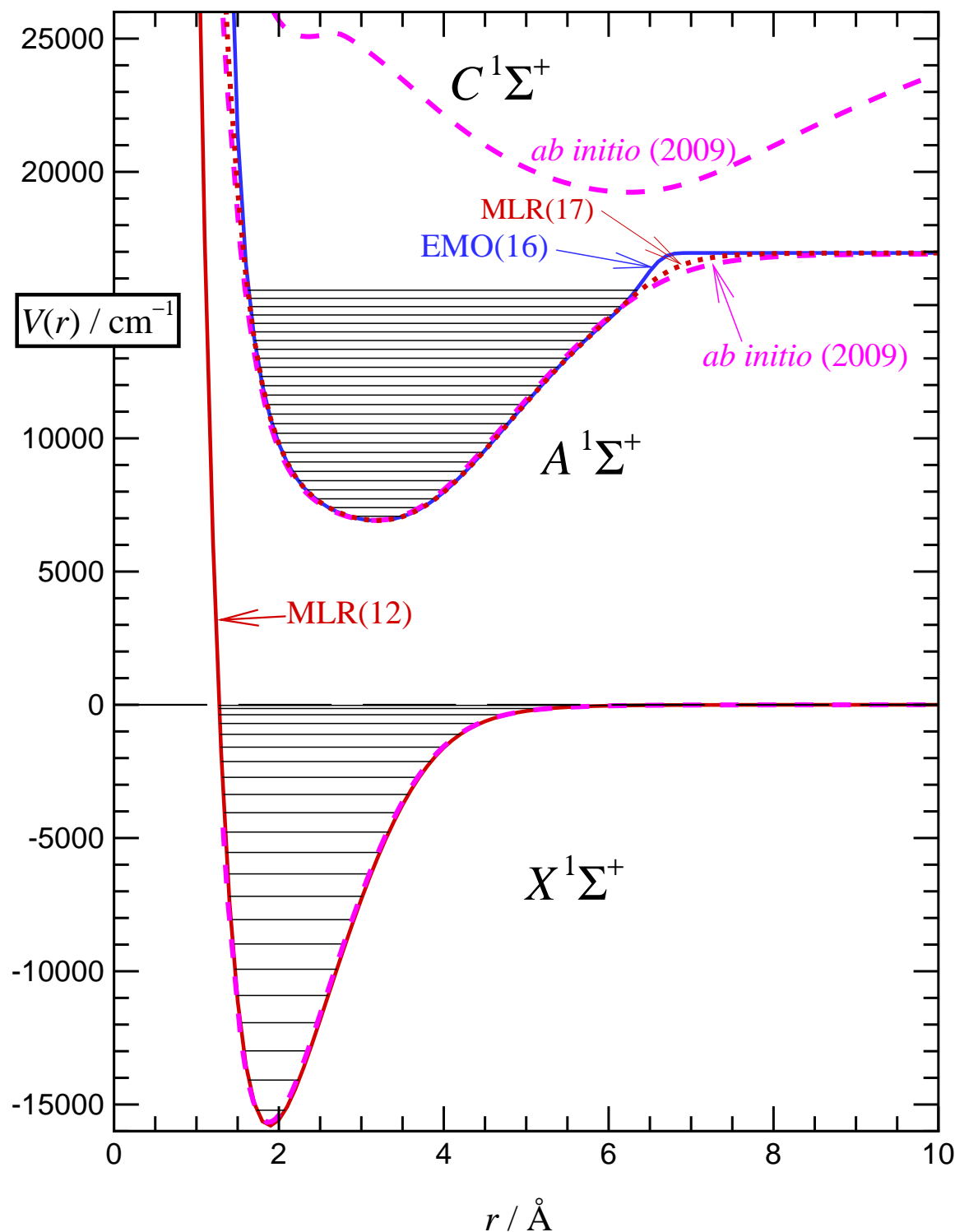
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- an EMO potential for the  $A^1\Sigma^+$  state whose abrupt cutoff at the asymptote correctly reflects the avoided-crossing physics there.
- *A DPF using an MLR form does capture that turnover properly!*



*Diatomic DPF analyses may be performed ‘routinely’ using*

## **program DPotFit (*‘Diatomic Potential Fits’*)**

{ available with manual from <http://leroy.uwaterloo.ca/programs/> }

*which performs DPF fits to spectroscopic data and can:*

- simultaneously treat any combination of microwave, infrared, electronic, fluorescence series, tunneling level widths, & photo-association data
  - \* for one or multiple isotopologues
  - \* for one or multiple electronic states
- take account of atomic-mass dependent Born-Oppenheimer breakdown
- take account of  $\Lambda$ -doubling of singlet states or  $^2\Sigma$  splittings
- use “*sequential rounding and re-fitting*” to automatically yield fitted parameters with a minimum number of significant digits and no loss of precision in representing data
- use Watson’s “*robust*” data weighting technique to damp the effect of “outlier” observations which give anomalously large discrepancies with the model, and might unreasonably mislead a fit.
- allow four types of potential forms: EMO, MLR, DELR, or polynomials.



# *In the beginning there was Hori . . .*

Zeitschrift für Physik **62**, 352-367 (1930):

## **Das Absorptionsspektrum des Natriumhydrids.**

Von **Takeo Hori** in Port-Arthur.

Mit 2 Abbildungen. (Eingegangen am 20. März 1930.)

Ein neues Absorptionsspektrum in der Gegend von 3680 bis 4450 Å wurde aufgefunden. Es ähnelt dem neulich von Nakamura mitgeteilten Lithiumhydrid-Viellinienspektrum und gehört zu einem Übergangstypus  ${}^1\Sigma \rightarrow {}^1\Sigma$ . Der angeregte  ${}^1\Sigma$ -Zustand ist dadurch charakterisiert, daß sich seine Kernschwingungsniveaus nicht durch die von der gewöhnlichen Theorie verlangte Formel darstellen lassen. Eine Anomalie ähnlicher Art tritt auch in der Abhängigkeit der Rotationsenergien im Anregungszustand von der Schwingungsquantenzahl zutage.

Zeitschrift für Physik  
**71**, 478-537 (1931):

who observed  $P/R$

transitions for

for  $v''(X) = 0 - 3$

and  $v'(A) = 0 - 20$

with  $J = 0 - 35$ .

*However*, his data

uncertainties were

only  $\pm 0.3 \text{ cm}^{-1}$ .

## **Das Emissionsspektrum des Natriumhydrids.**

Von **Takeo Hori** in Port Arthur.

Mit 2 Abbildungen. (Eingegangen am 8. Juni 1931.)

Das in der Gegend von 3680 bis 4450 Å auftretende Absorptionsspektrum des Natriumhydrids<sup>1)</sup> wurde durch das Emissionsspektrum ergänzt, welches sich von 3540 bis 5050 Å erstreckt und viel komplizierter als das Absorptionsspektrum ist. Als Folge der Analyse, die nur mit Hilfe der des Absorptionsspektrums durchführbar ist, erweist sich, daß das ganze Spektrum einem System  ${}^1\Sigma \rightarrow {}^1\Sigma$  angehört. Das Trägheitsmoment des Normalzustandes ergibt sich gleich  $5,65 \cdot 10^{-40} \text{ g cm}^2$ , das des angeregten Zustandes  $14,66 \cdot 10^{-40} \text{ g cm}^2$ . Die aus den Nulllinien berechnete Kernschwingungsformel lautet:

$$\nu = 23696,1 + 335,24 \nu' + 4,416 \nu'^2 - 0,3147 \nu'^3 + 0,00756 \nu'^4 - 0,000089 \nu'^5 - (1170,8 \nu'' - 18,9 \nu''^2),$$

wobei das positive Vorzeichen des dritten Gliedes eine merkwürdige Anomalie in dem Verlauf der Schwingungsintervalle  $\Delta \nu'$  aufweist. Die Dissoziationsenergien der normalen und angeregten Zustände betragen 2,24 und 1,47 Volt. Der Zerfall des normalen Moleküls erfolgt in ein Na- und ein H-Atom im Grundzustand, der des angeregten in ein angeregtes  $2^2P$ -Na-Atom und ein normales H-Atom. Für die Anregung des NaH-Bandenspektrums eignet sich ein Natriumbogen in Wasserstoffatmosphäre von 20 cm Druck (Betriebsspannung 450 Volt, Strom 2,5 bis 3 Amp.).

*... and then there was Olsson ...*

Zeitschrift für Physik **93**, 206-219 (1935):

## **Das Absorptionsspektrum des NaD.**

Von **E. Olsson** in Stockholm.

(Eingegangen am 22. November 1934.)

Das Bandenspektrum des NaD ist ausgemessen und analysiert worden. Die wahren Quantenzahlen in NaD und NaH werden mittels des Isotopieeffektes festgestellt. Eine von Hulthén und Holst an AlH/AlD beobachtete und gedeutete Einwirkung der Teilnahme der Elektronen an der Kernschwingung und Kernrotation findet sich auch in NaH/NaD vor. Der Isotopieeffekt im erregten Zustande ist ganz normal, was für das Verständnis des sonst auffallend unregelmäßigen Verlaufes wichtig erscheint.

who observed  $P/R$  series of NaH for  $v''(X) = 0, 1$  and  $v'(A) = 4 - 13$  with  $J$  up to 23 at slightly higher precision of  $\sim 0.2 \text{ cm}^{-1}$ , as well as

NaD data for  $v''(X) = 0, 1$  and  $v'(A) = 4 - 17$  with  $J$  up to 23.

His results showed that Hori's  $v'(A)$  numbering for NaH had to be increased by 3

... then after the war there was Pankhurst (1949) ...

Proceedings of the Physical Society **A 62**, 191-199, (1949):

## **The Emission Spectrum of Sodium Hydride**

By R. C. PANKHURST

Imperial College, London \*

*Communicated by R. W. B. Pearse ; MS. received 27th July 1948*

**ABSTRACT.** Observations on the spectrum of sodium hydride have been extended to longer wavelengths (from 4600 Å. to 6450 Å.) and photographed under high dispersion. Analysis of the data thus obtained gives values of the vibrational and rotational constants for several new vibrational levels, among which the lowest levels of the excited state are of especial interest.

The intensity distribution has been calculated from the wave functions appropriate to potential energy curves based on the constants derived from the analysis of the band system. The theoretical estimates are found to be in fair agreement with the experimental results.

whose NaH measurements for  $v''(X) = 0 - 8$  and  $v'(A) = 1 - 20$  with  $J$  up to 31 had improved precision of ca.  $\pm 0.1 \text{ cm}^{-1}$ .

He reported his fitted band origins, as well as tables of combination differences (which we treat as pure rotational data) for the  $X$  and  $A$  states.

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He reported his fitted band origins, as well as combination differences (which we treat as pure rotational data) for the  $X$  and  $A$  states.

**However, he never presented the actual data**, which were then lost.

... *Finally, the 'modern era' began in 1980 with ...*

JOURNAL OF MOLECULAR SPECTROSCOPY **79**, 314–322 (1980)

## New Spectroscopic Analyses and Potential Energy Curves for the $X^1\Sigma^+$ and $A^1\Sigma^+$ States of NaH<sup>1</sup>

F. B. ORTH<sup>2</sup> AND W. C. STWALLEY

*Departments of Chemistry and Physics, University of Iowa, Iowa City, Iowa 52242*

AND

S. C. YANG AND Y. K. HSIEH

*Department of Chemistry, National Taiwan University, Taipei, Taiwan, Republic of China*

The emission spectrum of NaH has been photographed in the  $\sim 6000\text{--}7300\text{-}\text{\AA}$  region. Additional bands of the  $A^1\Sigma^+ \text{--} X^1\Sigma^+$  electronic transition have been analyzed and in particular the observed vibrational structure of the excited  $A$  state has been extended down to  $v' = 0$ . New spectroscopic constants have been obtained, the  $v' = 0$  data leading to especially large changes in the constants of the anomalous  $A^1\Sigma^+$  state. New Rydberg–Klein–Rees (RKR) potential energy curves have been calculated up to  $v'' = 8$  of the  $X^1\Sigma^+$  state and up to  $v' = 20$  in the  $A^1\Sigma^+$  state.

While still of relatively low precision ( $\pm 0.3 \text{ cm}^{-1}$ ) they finally extended measurements for the  $A^1\Sigma^+$  state down to  $v' = 0$ .



*... This was followed by a number of high resolution microwave and infrared studies ...*

J. Chem. Phys. 75(10), 15 Nov. 1981

0021-9606/81/224753-05\$01.00

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4753

## **The millimeter wave spectra of NaH and NaD**

K. V. L. N. Sastry,<sup>a)</sup> Eric Herbst, and Frank C. De Lucia

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(Received 3 June 1981; accepted 16 July 1981)

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JOURNAL OF MOLECULAR SPECTROSCOPY **122**, 150–156 (1987)

## **Far-Infrared Spectrum of Sodium Hydride<sup>1</sup>**

K. R. LEOPOLD,<sup>2</sup> L. R. ZINK, K. M. EVENSON, AND D. A. JENNINGS

*National Bureau of Standards, Boulder, Colorado 80303*

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13 May 1988

## **THE GROUND-STATE INFRARED SPECTRUM OF SODIUM HYDRIDE**

Ulrich MAGG and Harold JONES

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Received 3 March 1988

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J. Chem. Phys. **90** (12), 15 June 1989

6887

## **Infrared spectrum of sodium hydride**

Arthur G. Maki and Wm. Bruce Olson

*Molecular Spectroscopy Division, National Institute of Standards and Technology, Gaithersburg, Maryland 20899*

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*... which were followed by more electronic work ...*

J. Phys. B: At. Mol. Opt. Phys. **26** (1993) L129–L134. Printed in the UK

**Near-dissociation photoabsorption spectra of LiH, NaH  
and KH**

M Rafiq§, N Ali†, K Ahmad†, I A Khan†, M A Baig‡ and Zafar Iqbal‡

† Department of Physics, Karachi University, Karachi-32, Pakistan

‡ Atomic and Molecular Physics Laboratory, Department of Physics, Quaid-I-Azam  
University, Islamabad, Pakistan

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Z. Phys. D 38, 35–40 (1996)

**New Dunham coefficients of the  $A^1\Sigma^+$ -State of NaH and NaD**

S. Lochbrunner<sup>1</sup>, M. Motzkus<sup>1</sup>, G. Pichler\*, K. L. Kompa<sup>1</sup>, P. Hering<sup>1, 2</sup>

<sup>1</sup> Max-Planck-Institut für Quantenoptik, D-85748 Garching, Germany

<sup>2</sup> Institut für Lasermedizin, Universität Düsseldorf, D-40225 Düsseldorf, Germany

---

*However, no one had attempted to collect and  
synthesize all of these data prior to ...*

*... which were followed by more electronic work ...*

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**Pesl, Lutz & Bergman: Euro. Phys. J. D 10, 247 (2000)**

**Improved molecular constants  
for the  $X^1\Sigma^+$  and  $A^1\Sigma^+$  states of NaH**

F.P. Pesl, S. Lutz, and K. Bergmann<sup>a</sup>

Fachbereich Physik, Universität Kaiserslautern, 67663 Kaiserslautern, Germany

They reported new electronic data for  $v(A) = 6 - 9$  and  $v(X) = 2 - 8$ .

*More important* – they collected all accessible older data and provided a global Dunham analysis and RKR potentials for  $v(X) = 0 - 9$  and  $v(A) = 0 - 25$ .