Selected Bibliography on Ground and Excited
State Potential Curves of H_2 , LiH and Li_2 . *

William C. Stwalley[†],
Department of Chemistry
University of Iowa
Iowa City, Iowa 52242

and

Warren T. Zemke,
Department of Chemistry
Wartburg College
Waverley, Iowa 50677

July 26, 1974

* Acknowledgment is made to the United States Atomic Energy Commission [Contract AT(11-1)-2326] for support of this work.

[†] Alfred P. Sloan Foundation Fellow.

MASTER

DISTRIBUTION OF THIS DOCUMENT UNLIMITED

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

General Bibliographies

- A. W. G. Richards, T. E. H. Walker, and R. K. Hinkley, A Bibliography of ab initio Molecular Wave Functions (Oxford University Press, London 1971).
- B. B. Rosen (Ed.), Selected Constants: Spectroscopic Data Relative to Diatomic Molecules (Pergamon, New York 1970).
- C. T. E. Sharp, "Potential Energy Curves for Molecular Hydrogen and Its Ions", Atomic Data 2, 119 (1971).
- D. W. Kolos, "The Adiabatic Approximation and Its Accuracy", Advan. Quantum Chem. 5, 99 (1970).
- E. A. Dalgarno, "New Methods for Calculating Long-Range Intermolecular Forces", Advan. Chem. Phys. 12, 143 (1967).

References included in these bibliographies are not included below.

SUMMARY OF INFORMATION ON POTENTIALS

Molecule	State	Sym.	Potential					Long-Range				
			<i>ab initio</i>									
			Fix. N	AD	NA	RKR	OTHER	C ₃ or C ₄	C ₆	C ₈	C ₁₀	D ₀
I. H ₂	1. X	1 Σ_g^+	X	X	X	X		na	X	X	X	X
	2. B	1 Σ_u^+	X	X	e	(X)	X	X	X	X	X	X
	3. C	1 Π_u	X	X		X		X	X	X	X	X
	4. B'	1 Σ_u^+	(X)			(X)		na	X	X	X	X
	5. D	1 Π_u	X			X						X
H ₂ ⁺	6. X	2 Σ_g^+	X	X	X			X	X	X	X	X
II. LiH	1. X	1 Σ^+	X	e		X		na	X	X	X	X
	2. Z	1 Σ^+	X	e		X		na	X	X		X
	3. B	1 Π	X	e		X	X	na	X	X		X
	4. X	2 Σ^+	X						X	X		
III. Li ₂	1. X	1 Σ_g^+	X			X		na	X	X		X
	2. A	1 Σ_u^+	X			X		X	X	X		X
	3. B	1 Π_u	X			X		X				X
	4. X	2 Σ_g^+	X					X	X			

I. 1. $X^1\Sigma_g^+ H_2$

- (a) A. L. Ford, "Nonadiabatic Effects in the Ground State of the Hydrogen Molecule", to be published.
- (b) A. L. Ford, E. M. Greenawalt, and J. C. Browne, "The Computation of Nuclear Motion and Mass Polarization Energy Corrections for Several States of the Hydrogen Molecule", to be published.
- (c) W. Kołos and L. Wolniewicz, "Improved Potential Energy Curve and Vibrational Energies for the Electronic Ground State of the Hydrogen Molecule", to be published.
- (d) L. I. Kleinman and M. Wolfsberg, "Corrections to the Born-Oppenheimer Approximation and Electronic Effects on Isotopic Exchange Equilibria", J. Chem. Phys., 60, 4740 (1974).
- (e) L. I. Kleinman and M. Wolfsberg, "Shifts in Vibrational Constants from Corrections to the Born-Oppenheimer Approximation: Effects on Isotopic Exchange Equilibria", J. Chem. Phys., 60, 4749 (1974).
- (f) W. Kołos and L. Wolniewicz, "Variational Calculation of the Long-Range Interaction between Two Ground-State Hydrogen Atoms", Chem. Phys. Lett., 24, 457 (1974).
- (g) T. Orlikowski and L. Wolniewicz, "Nonadiabatic Corrections to the Vibrational Energies of the Hydrogen Molecule", Chem. Phys. Lett., to be published (1974).
- (h) P. R. Bunker, "Forbidden Transitions in Homopolar Isotopically Unsymmetric Diatomic Molecules and the Dipole Moment of HD", J. Mol. Spec., 46, 119 (1973).
- (i) L. I. Kleinman and M. Wolfsberg, "Corrections to the Born-Oppenheimer Approximation and Electronic Effects on Isotopic Exchange Equilibria", J. Chem. Phys., 59, 2043 (1973).
- (j) J. D. Poll and G. Karl, "Electric Dipole Transitions in HD", Can. J. Phys., 51, 594 (1973).
- (k) L. Wolniewicz and T. Kowalski, "Rotational-Vibrational Dipole Transitions in HD", Chem. Phys. Lett., 18, 55 (1973).
- (l) T. R. Singh, J. F. Bukta, and W. J. Meath, "Long Range Interaction Energies Using Gaussian Basis Sets and a One-Center Method", Intl. J. Quant. Chem., 6, 201 (1972).
- (m) F. M. Wu and C. L. Beckel, "Theoretical Determination of H_2 Ground-State Spectroscopic Properties", Intl. J. Quant. Chem., 7, 135 (1973).
- (n) P. R. Bunker, "On The Breakdown of the Born-Oppenheimer Approximation for a Diatomic Molecule", J. Mol. Spec., 42, 478 (1972).
- (o) W. J. Deal, "The Long-Range Interaction between Two Hydrogen Atoms", Int. J. Quant. Chem., VI, 593 (1972).
- (p) H. L. Buijs and H. P. Gush, "Static Field Induced Spectrum of Hydrogen", Can. J. Phys., 49, 2366 (1971).
- (q) G. Chalasinski, W. Kołos, B. Petelenz, and L. Piela, "Gaussian Orbitals in Calculations of the Second-Order Corrections to the Interaction Energy of Two Hydrogen Atoms", Chem. Phys. Lett., 12, 233 (1971).
- (r) R. J. LeRoy, "Eigenvalues and Certain Expectation Values for all Bound and Quasibound Levels of Ground-State ($X^1\Sigma_g^+$) H_2 , HD, and D_2 ", J. Chem. Phys., 54, 5433 (1971).
- (s) R. J. LeRoy and R. B. Bernstein, "Shape Resonances and Rotationally Predissociating Levels: The Atomic Collision Time-Delay Functions and Quasibound Level Properties of $H_2(X^1\Sigma_g^+)$ ", J. Chem. Phys., 54, 5114 (1971).
- (t) M. A. Marchetti and S. R. LaPaglia, "Electronic Transition Moment of the Lyman Bands of $H_2(B^1\Sigma_u^+ - X^1\Sigma_g^+)$ as a Function of Internuclear Separation", J. Chem. Phys., 55, 8655 (1971).

- (u) K. Pecul, "The Energy of the Interaction between Two Atoms Calculated by using the Variational Method", *Acta Phys. Polonica*, A39 9 (1971).
 - (v) A. C. Allison and A. Dalgarno, "Band Oscillator Strengths and Transition Probabilities for the Lyman and Werner Systems of H_2 , HD, and D_2 ", *Atomic Data*, 1, 289 (1970).
 - (w) P. R. Bunker, "The Effect of the Breakdown of the Born-Oppenheimer Approximation on the Determination of B_e and ω_e for a Diatomic Molecule", *J. Mol. Spec.*, 35, 306 (1970).
 - (x) P. R. Bunker, "The Electronic Isotope Shift in Diatomic Molecules and the Partial Breakdown of the Born-Oppenheimer Approximation", *J. Mol. Spec.*, 28, 422 (1968).
2. $B \ ^1\Sigma_u^+ H_2$
- (a) I. D. Dabrowski and G. Herzberg, "The Absorption Spectrum of D_2 from 1100 to 840 $\text{\AA}$ ", *Can. J. Phys.*, 52, to be published (1974).
 - (b) A. L. Ford, E. M. Greenawalt, and J. C. Browne, "The Computation of Nuclear Motion and Mass Polarization Energy Corrections for Several States of the Hydrogen Molecule", to be published.
 - (c) R. Grice and D. R. Herschbach, "Long-Range Configuration Interactions of Ionic and Covalent States", *Mol. Phys.*, 27, 159 (1974).
 - (d) W. Kołos, "Long- and Intermediate-Range Interaction between Hydrogen Atoms in the $B \ ^1\Sigma_u^+$ State", to be published.
 - (e) T. L. Stephens and A. Dalgarno, "Long Range Interactions of Excited Hydrogen Atoms", *Mol. Phys.*, to be published (1974).
 - (f) W. C. Stwalley and W. T. Zemke, "The Potential Energy Curves for the $B \ ^1\Sigma_u^+$ and $C \ ^1\Pi_u$ States of H_2 : A Comparison of Spectroscopic and ab initio Results", presented at the 29th Symposium on Molecular Structure and Spectroscopy (Columbus, Ohio, June 1974).
 - (g) P. S. Julienne, "Nonadiabatic Effects in the B, C, B' and D States of H_2 ", *J. Mol. Spec.*, 48, 508 (1973).
 - (h) R. W. Dreyfus and R. T. Hodgson, "Molecular-hydrogen Laser: 1098-1613 $\text{\AA}$ ", *Phys. Rev. A*, 9, 2635 (1974) (and references therein).
 - (i) A. C. Allison and W. C. Stwalley, "Comment on Continuity at the Dissociation Threshold in Molecular Absorption", *J. Chem. Phys.*, 58, 1187 (1973).
 - (j) H. Bredohl and G. Herzberg, "The Lyman and Werner Bands of Deuterium", *Can. J. Phys.*, 51, 867 (1973).
 - (k) J. F. Bukta and W. J. Meath, "Long Range Interaction Energies between Ground and First Excited State Hydrogen Atoms using a One Centre Method", *Mol. Phys.*, 25, 412 (1972).
 - (l) A. F. Shestakov, S. I. Vetchinkin, and S. V. Khristenko, "Dispersion Interaction of Hydrogen Atoms in Excited States", *Opt. Spektrosk.*, 35, 608 (1973).
 - (m) W. C. Stwalley, "Potential Energy Curve of the $B \ ^1\Sigma_u^+$ State of H_2 ", *J. Chem. Phys.*, 58, 536 (1972).
 - (n) D. L. Huestis and W. A. Goddard, II, "The Valence Bond Aufbau Principle for Molecular Excited States", *Chem. Phys. Lett.*, 16, 157 (1972).
 - (o) D. L. Huestis, Ph.D. Thesis, California Institute of Technology, 1972.
 - (p) A. C. Allison and A. Dalgarno, "Continuity at the Dissociation Threshold in Molecular Absorption", *J. Chem. Phys.*, 55, 4342 (1971).
 - (q) H. M. Crosswhite (Ed.), "The Hydrogen Molecule Wavelength Tables of Gerhard Heinrich Dieke", (Wiley, New York 1972).
 - (r) T. L. Stephens and A. Dalgarno, "Spontaneous Radiative Dissociation in Molecular Hydrogen", *J. Quant. Spectrosc. Radiant. Transfer*, 12, 569 (1972).

- (s) S. Z. Moody and C. L. Beckel, "Theoretical Determination of Vibration-Rotation Properties for the $B^1\Sigma_u^+$ State of H_2 ", *Intl. J. Quant. Chem.*, IIIS, 469 (1970).
 - (t) W. C. Stwalley, "The Dissociation Energy of the Hydrogen Molecule using Long-Range Forces", *Chem. Phys. Lett.*, 6, 241 (1970).
 - (u) J. Geiger and H. Schmoranz, "Electronic and Vibrational Transition Probabilities of Isotopic Hydrogen Molecules H_2 , HD, and D_2 Based on Electron Energy Loss Spectra", *J. Mol. Spec.*, 32, 39 (1969).
 - (v) L. Wolniewicz, "Theoretical Investigation of the Transition Probabilities in the Hydrogen Molecule", *J. Chem. Phys.*, 51, 5002 (1969).
 - (w) W. Kołos, "Long-Range Interaction between 1s and 2s or 2p Hydrogen Atoms", *Intl. J. Quant. Chem.*, 1, 169 (1967).
 - (x) See also I.1.(b), (t), (v), (x)
3. $C^1\Pi_u H_2$
- (a) A. L. Ford, "Lambda-Doubling in the $C^1\Pi_u$ State of H_2 ", to be published.
 - (b) H. Schmoranz and J. Geiger, "Light Emission of Electron Impact Excited Hydrogen Molecules and the Dependence of Electronic Transition Moment on Internuclear Distance", *J. Chem. Phys.*, 59, 6153 (1973).
 - (c) E. J. Stone and E. C. Zipf, "Excitation of the Werner Bands of H_2 by Electron Impact", *J. Chem. Phys.*, 56, 4646 (1972).
 - (d) See also I.1. (b), (v).
 - (e) See also I.2. (a), (e), (f), (g), (h), (j), (k), (l), (n), (o), (p), (q), (r), (u), (v), (w).
4. $B'^1\Sigma_u^+ H_2$
- (a) W. J. Deal and R. H. Young, "Long-Range Dispersion Interactions Involving Excited Atoms; the $H(1s)$ - $H(2s)$ Interaction", *Int. J. Quant. Chem.*, 7, 877 (1973).
 - (b) O. Goscinski and O. Tapia, "Predissociation by Rotational and Long-Range Interactions", *Mol. Phys.*, 24, 641 (1972).
 - (c) W. R. Thorson, "Absorption Edge Doubling in the HD Dissociation Continuum", *J. Mol. Spectry.*, 37, 199 (1971).
 - (d) See also I.1. (b).
 - (e) See also I.2. (a), (e), (g), (k), (l), (n), (o), (q), (w).
5. $D^1\Pi_u H_2$
- (a) See I.1. (b); 2. (e), (g), (l), (q).
6. $X^2\Sigma_g^+ H_2^+$
- (a) D. M. Bishop, "Properties of the Adiabatic Energy Curves for the Ground States of H_2 , HD, and D_2 ", to be published.
 - (b) S. Takezawa and Y. Tanaka, "Absorption Spectrum of HD in the Vacuum UV-Region. Rydberg States and Ionization Energy", to be published.
 - (c) D. M. Bishop and R. W. Wetmore, "Adiabatic Vibrational Energy Spacings for HD", *J. Mol. Spec.*, 46, 502 (1973).
 - (d) D. M. Bishop and R. W. Wetmore, "Vibrational Spacings for H_2^+ , D_2^+ , and H_2 ", *Mol. Phys.*, 26, 145 (1973).
 - (e) P. R. Bunker, "Nonadiabatic Effects on the Vibrational Intervals of H_2^+ ", *J. Mol. Spec.*, 46, 504 (1973).
 - (f) M. M. Madsen and J. M. Peek, "Eigenparameters for the Lowest Twenty Electronic States of the Hydrogen Molecule Ion", *Atomic Data*, 2, 171 (1971).

- (g) G. Herzberg and C. Jungen, "Rydberg Series and Ionization Potential of the H_2 Molecule", *J. Mol. Spec.*, 41, 425 (1972).
- (h) D. M. Bishop, "Cubic and Quartic Force Constants for H_2^+ ", *J. Chem. Phys.*, 54, 2761 (1971).
- (i) L. Asbrink, "The Photoelectron Spectrum of H_2 ", *Chem. Phys. Lett.*, 7, 549 (1970).
- (j) C. L. Beckel and B. D. Hansen III, "Theoretical Study of H_2^+ Ground Electronic State Spectroscopic Properties", *J. Chem. Phys.*, 53, 3681 (1970).
- (k) D. M. Bishop, "Ab initio Calculations of Harmonic Force Constants. III. An Exact Calculation of the H_2^+ Force Constant", *J. Chem. Phys.*, 53, 1541 (1970).
- (l) L. J. Schaad and W. V. Hicks, "Equilibrium Bond Length in H_2^+ ", *J. Chem. Phys.*, 53, 851 (1970).
- (m) W. Kołos, "Some Accurate Results for Three-Particle Systems", *Acta Physica Academiae Scientiarum Hungaricae*, 27, 241 (1969).
- (n) S. K. Luke, G. Hunter, R. P. McEachran, and M. Cohen, "Relativistic Theory of H_2^+ ", *J. Chem. Phys.*, 50, 1644 (1969).

II.1. X $1\Sigma^+$ LiH

- (a) R. Velasco and F. Rivero, "Espectro de Absorción de la Molécula 6LiH ", to be published.
- (b) H. J. T. Preston and M. Yoshimine, unpublished calculations.
- (c) W. C. Stwalley and T. R. Proctor, "Long-Range Interaction of Alkali Metals and Rare Gases in S States", presented at the 7th Midwest Theoretical Chemistry Conference (Lexington, KY, May 1974), and related unpublished work.
- (d) W. C. Stwalley, K. R. Way, K. C. Li and W. T. Zemke, "The Potential Energy Curves for the X $1\Sigma^+$, A $1\Sigma^+$ and B 1Π States of LiH", Presented at the 29th Symposium on Molecular Structure and Spectroscopy (Columbus, Ohio, June 1974).
- (e) J. E. Kouba and W. J. Meath, "Lithium Dipole Properties and van der Waals Constants using a Pseudo Spectral One-Centre Method", *Mol. Phys.*, 26, 1397 (1973).
- (f) K. K. Docken and J. Hinze, "LiH Potential Curves and Wavefunctions for X $1\Sigma^+$, A $1\Sigma^+$, B 1Π , $3\Sigma^+$, and 3Π ", *J. Chem. Phys.*, 57, 4928 (1972).
- (g) K. K. Docken and J. Hinze, "LiH Properties, Rotation-Vibrational Analysis, and Transition Moments for X $1\Sigma^+$, A $1\Sigma^+$, B 1Π , $3\Sigma^+$ and 3Π ", *J. Chem. Phys.*, 57, 4936 (1972).
- (h) I. Fernandez-Florez and R. Velasco, *Optica Pura y Aplicada*, 2, 123 (1969).
- (i) E. F. Pearson and W. Gordy, "Millimeter-Wave Spectra and Molecular Constants of 6LiD and 7LiD ", *Phys. Rev.*, 177, 59 (1969).
- (j) R. M. Predny, Ph.D. Thesis, 1969, University of Florida.
- (k) E. Rothstein, Ph.D. Thesis, 1968, University of California at Berkeley.
- (l) G. M. Stacey and A. Dalgarno, "Dipole Spectrum of Lithium", *J. Chem. Phys.*, 48, 2515 (1968).
- (m) See also I.1. (d), (e), (i), (x).

2. A $1\Sigma^+$ LiH

- (a) See also I.1. (x).
- (b) See also II.1. (a), (c), (d), (f), (g), (h), (j).

3. B $^1\Pi$ LiH

- (a) R. Velasco, "New Experimental Results on the B-X Band System of Lithium Hydride", to be published.
- (b) W. C. Stwalley, and K. R. Way, "Dissociation Energies of ^7LiD ", J. Chem. Phys., 60, 3611 (1974).
- (c) K. R. Way and W. C. Stwalley, "Accurate Dissociation Energies from Rotational Predissociation and Long-Range Forces: B $^1\Pi$ ", J. Chem. Phys., 59, 5298 (1973).
- (d) See also I.1. (x).
- (e) See also II.1. (c), (d), (f), (g), (j).

4. X $^2\Sigma^+$ LiH $^+$

- (a) M. E. Schwartz and J. D. Switalski, "Valence Electron Studies with Gaussian-Based Model Potentials and Gaussian Basis Functions. II. Discussion of the One-Valence-Electron Molecular Theory and Applications to Li_2^+ , Na_2^+ , and LiH^+ ", J. Chem. Phys., 57, 4132 (1972).

III. 1. X $^1\Sigma_g^+$ Li $_2$

- (a) D. Hsu and M. M. Hessel, "A Complete Analysis on the Absorption Spectra of the Excited States of Li_2^+ ", presented at the 29th Symposium on Molecular Structure and Spectroscopy (Columbus, Ohio, June, 1974).
- (b) T. Caves, "van der Waals Interactions between Excited Li Atoms", J. Chem. Phys., 59, 6177 (1973).
- (c) G. Emmen, Ph.D. Thesis, 1972, Universitat Gottingen.
- (d) W. Kutzelnigg, V. Staemmler, and M. Gelus, "Potential Curve of the Lowest Triplet State of Li_2 ", Chem. Phys. Lett., 13, 496 (1972).
- (e) A. C. Roach, "Theoretical Ground State and Excited State Potential Energy Curves for Alkali Diatomic Molecules", J. Mol. Spec., 42, 27 (1972).
- (f) J. N. Bardsley, "Pseudopotential Calculations of Alkali Interactions", Chem. Phys. Lett., 7, 517 (1970).
- (g) W. Kutzelnigg and M. Gelus, "Potential Curve of the Li_2 Ground State for Large Internuclear Distances. A Contribution to the Understanding of Interatomic Forces", Chem. Phys. Lett., 7, 296 (1970).
- (h) R. Velasco, C. Ottinger, and R. N. Zare, "Dissociation Energy of Li_2 from Laser-Excited Fluorescence", J. Chem. Phys., 51, 5522 (1969).
- (i) See also I.1. (f).
- (j) See also II.1. (e), (l).

2. A $^1\Sigma_u^+$ Li $_2$

- (a) I. Fernandez-Florez and R. Velasco, "Contribución al Estudio de la Molécula LiH : Distribución de Intensidades en el Sistema A-X", Optica pura y Aplicada, 11, 123 (1969).
- (b) R. Velasco and F. Rivero, "El Sistema de Bandas A-X en el Espectro de la Molécula $^6\text{Li}_2$ ", Optica pura y Aplicada, 5, 76 (1972).
- (c) See also III.1. (a), (e).

3. $B^1\Pi_u Li_2$

- (a) L. R. Kahn, T. H. Dunning and N. W. Winter, "The Theoretical Determination of the $Li_2 B^1\Pi_u$ Potential Energy Curve", to be published.
- (b) R. Velasco and G. Ennen and C. Ottinger, "A Splitting in Vibrationally Excited $Li_2(B^1\Pi_u)$ ", to be published.
- (c) R. Velasco and V. Morales, "El Sistema de Bandas B-X en la Molecular 6Li_2 ", Optica pura y Aplicada, 6, 52 (1973).

4. $X^2\Sigma_g^+ Li_2^+$

- (a) G. A. Henderson, W. T. Zemke, and A. C. Wahl, "Hartree-Fock Potential Energy Curves, Spectroscopic Constants, and 1-Electron Properties for the Lowest $^2\Sigma_g^+$ and $^2\Pi_g$ States of Li_2^+ ", J. Chem. Phys., 58, 2654 (1973).
- (b) W. L. McMillan, "Theory of One-Electron Molecules. I. Li_2^+ ", Phys. Rev. A, 4, 69 (1971).
- (c) A. Dalgarno, C. Bottcher, and G. A. Victor, "Pseudo-Potential Calculation of Atomic Interactions", Chem. Phys. Lett., 7, 265 (1970).
- (d) W. S. Struve, "Semi-Empirical Pseudopotential Calculations of Alkali Dimer-Ion Dissociation Energies", Chem. Phys. Lett., 7, 382 (1970).
- (e) See also II.4. (a).
- (f) See also III.1. (f).