On the $X^1\Sigma^+$ rovibrational spectrum of lithium hydride

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ABSTRACT

The complete line list of rovibrational transitions of the $X^1\Sigma^+$ state of LiH is computed. The line list includes all possible dipole-allowed transition energies and oscillator strengths that cover the transition energy range $3.27\text{--}19476\text{ cm}^{-1}$. The line list was obtained using an accurate potential and dipole moment function constructed from available experimental and theoretical data. This paper discusses the agreement of the current calculations with previous theoretical and experimental results. We also provide the radiative cooling function in the high-density limit over a wide temperature range and compare them with previous results. A simulated collisionally-broadened LiH opacity relevant to cool dwarf stars is also presented.

Key words. molecular data – molecular processes

1. Introduction

Lithium hydride has been the subject of theoretical and experimental molecular physics investigations for many years (see for example [Partridge & Langhoff 1981](#)). As the simplest neutral heteronuclear diatomic molecule, LiH is a favorite benchmark for various quantum-chemical techniques ([Tung et al. 2011](#); [Holka et al. 2011](#)). In astrophysics, LiH may play a role at temperatures $T \leq 5000\text{ K}$ in the cooling of primordial clouds ([Stancil et al. 1996](#); [Bougleux & Galli 1997](#); [Galli & Palla 1998](#); [Bovino et al. 2011](#)) and is a means of monitoring the evolution of stars and interstellar clouds ([Dulick et al. 1998](#)). Furthermore, LiH, as well as other Li-bearing molecules (LiCl and LiOH), may be observable in cool ($T_{\text{eff}} \leq 2000\text{ K}$) dwarf atmospheres ([Lodders 1999](#); [Weck et al. 2004](#)). However, to date, searches for LiH at high redshift have proved unsuccessful ([Friedel et al. 2011](#)). Reviews of the lithium chemistry in the early Universe have been given by [Lepp et al. \(2002\)](#) and [Bovino et al. \(2011\)](#), while the status of laboratory infrared spectroscopy of LiH is outlined in [Dulick et al. \(1998\)](#). A complete and evaluated rovibrational line list for the ground electronic state, which is germane to its thermal evolution and needed for primordial spectral models, is needed¹.

In Sect. 2 we present the details of potential energy curve and dipole moment function for the electronic ground state of LiH. In Sect. 3, we briefly outline the relevant relations for computing transition energies, Einstein coefficients, oscillator strengths, and radiative cooling functions. Results of the current computation including the ground electronic-state rovibrational line list and cooling function are presented in Sect. 4 along with comparisons to previous work and astrophysical applications. Section 5 gives a summary of the current work. Atomic units are used throughout, unless otherwise noted.

2. Potential energy and dipole moment function

Within the well-known Born-Oppenheimer approximation, the motion of a diatomic molecule may be partitioned into its electronic and nuclear components. As such, the non-relativistic Hamiltonian of a molecule may be written as

$$\hat{H} = \hat{H}_e + \hat{T}_N \quad (1)$$

with the time-independent Schrödinger equation given by

$$\hat{H}\Psi(\mathbf{r}; \mathbf{R}) = E\Psi(\mathbf{r}; \mathbf{R}). \quad (2)$$

By separation of variables, the total wave function may be written as

$$\Psi(\mathbf{r}; \mathbf{R}) = \Psi_e(\mathbf{r}; \mathbf{R})\Psi_N(\mathbf{R}), \quad (3)$$

where $\mathbf{R}$ is the internuclear distance vector in body-fixed coordinates, and $\mathbf{r}$ the electron coordinate vector with respect to the center of mass of the nuclei. The motion of electrons (e) and nuclei (N) can be described by the electronic Schrödinger equation

$$\hat{H}_e\Psi_e(\mathbf{r}; \mathbf{R}) = E_e(\mathbf{R})\Psi_e(\mathbf{r}; \mathbf{R}) \quad (4)$$

and the nuclear Schrödinger equation

$$[\hat{T}_N + E_e(\mathbf{R})]\Psi_N(\mathbf{R}) = E_{v,J}\Psi_N(\mathbf{R}), \quad (5)$$

where $E_e(\mathbf{R})$ is the potential energy and $E_{v,J}$ the rovibrational energy or eigenvalue.

The dipole moment function can be defined as

$$D(\mathbf{R}) = \int \Psi_e^*(\mathbf{r}; \mathbf{R}) \left(\sum_i e\mathbf{r}_i \right) \Psi_e(\mathbf{r}; \mathbf{R}) d\mathbf{r}, \quad (6)$$

where $\Psi_e(\mathbf{r}; \mathbf{R})$ is the electronic eigenfunction. In this work we consider $X^1\Sigma^+ \leftarrow X^1\Sigma^+$ rovibrational transitions so that only the z -component of the $\mathbf{r}$ operator contributes.

¹ A previous, though unevaluated, line list is available on the ExoMol database: <http://www.exomol.com>

Fig. 1. Potential energy (solid line) and the dipole moment function (dashed line) of the $X^1\Sigma^+$ state for LiH.

For a diatomic molecule, the potential energy is only a function of nuclear distance and can be written as $E_e(R)$. We applied an empirical potential (Coxon & Dickinson 2004), which was generated by directly fitting the spectroscopic LiH line positions, for $2 < R < 20 a_0$. The long-range potential is given by $V^{LR}(R) = -\frac{C_6}{R^6} - \frac{C_8}{R^8} - \frac{C_{10}}{R^{10}}$ for $R > 20 a_0$, where $C_6 = 66.536$, $C_8 = 3279.99$ and $C_{10} = 223016.6$ (Yan et al. 1996). For $R < 2 a_0$, the potential has been extrapolated with the short-range form $V^{SR}(R) = A \exp(-BR) + C$.

In a similar way, the dipole moment function of the X state calculated by Partridge & Langhoff (1981) has been used over the range $R = 1.75$ to $17.5 a_0$. For $R > 17.5 a_0$, the long-range form of Bottcher & Dalgarno (1974), $D^{LR}(R) = d_7/R^7$, was adopted. For $R < 1.75 a_0$, the short-range form $D^{SR}(R) = AR^2 + BR$ was fit to the ab initio data. The potential and dipole moment function are displayed in Fig. 1.

3. Rovibrational eigenvalues, transition probabilities, and related quantities

The radial nuclear Schrödinger equation of a diatomic molecule may be written as

$$\left[-\frac{1}{2\mu} \frac{d^2}{dR^2} + E_e(R) + \frac{J(J+1)}{2\mu R^2} - E_{vJ} \right] \chi_{vJ}(R) = 0, \quad (7)$$

which can be solved numerically by the Numerov-Cooley method (Johnson 1977), for example. Here μ is the reduced mass of ^7LiH , v is vibrational quantum number, J the rotational quantum number, and $\chi_{vJ}(R)$ is the corresponding rovibrational eigenfunction. The Einstein A coefficient, or transition probability, in the dipole approximation, can be calculated given $\chi_{vJ}(R)$ and $D(R)$, and is defined as (Weissbluth 1978)

$$A_{v'J',v''J''} = \frac{4}{3} \frac{c\alpha^4}{a_0} \Delta E_{v'J',v''J''}^3 \frac{S_{J'J''}}{2J''+1}, \quad (8)$$

where $\alpha = e^2/\hbar c$, is the fine-structure constant, a_0 is the Bohr radius, and $\Delta E_{v'J',v''J''}$ the transition energy. Here $S_{J'J''}$ is the line strength and defined as

$$S_{J'J''} = |\langle \chi_{v'J'} | D(R) | \chi_{v''J''} \rangle|^2 \varphi_{J'J''}. \quad (9)$$

Table 1. Vibrational binding energies $G_{v'}$ of the $X^1\Sigma^+$ state of ^7LiH in units of cm^{-1} .

v	$J_{\max}^a$	Present	Experiment ^b	Holka ^c
0	61	19 588.05	19 589.820	19 593.55
1	59	18 228.34	18 230.110	18 232.97
2	57	16 913.49	16 915.220	16 917.44
3	55	15 642.58	15 644.330	15 646.02
4	54	14 414.77	14 416.560	14 417.86
5	52	13 229.32	13 231.120	13 232.2
6	50	12 085.58	12 087.350	12 088.36
7	48	10 983.01	10 984.750	10 985.82
8	46	9921.24	9922.970	9924.17
9	44	8900.06	8901.800	8903.2
10	42	7919.47	7921.280	7922.91
11	40	6979.78	6981.660	6983.55
12	38	6081.62	6083.570	6085.76
13	36	5226.11	5228.090	5230.59
14	33	4414.92	4416.900	4419.72
15	31	3650.52	3652.460	3655.55
16	28	2936.31	2938.340	2941.52
17	25	2277.00	2278.970	2282.34
18	23	1678.99	1681.080	1684.42
19	20	1151.01	1153.170	1156.35
20	16	704.78	706.560	709.36
21	12	354.95	355.570	357.48
22	8	115.39	117.860	117.34

Notes. ^(a) $J_{\max}$ is the maximum rotational level determined in the present calculation.

References. ^(b) Chan et al. (1986). ^(c) Holka et al. (2011).

Here $\varphi_{J'J''}$ is a Hönl-London factor (Herzberg 1989) given by

$$\varphi_{J'J''} = \begin{cases} J'', & \text{P-branch} \\ J'' + 1, & \text{R-branch.} \end{cases} \quad (10)$$

The oscillator strength may then be defined (Weissbluth 1978) as

$$f_{v'J',v''J''} = \frac{2}{3} \Delta E_{v'J',v''J''} \frac{S_{J'J''}}{2J''+1}. \quad (11)$$

In a variety of applications, it is useful to obtain the radiative cooling function in the high-density or local thermodynamic equilibrium (LTE) limit (see for example Coppola et al. 2011). In LTE, the radiative cooling function only depends on the rovibrational energies, degeneracies, and transition probabilities. It is only a function of the gas kinetic temperature T and is given (in ergs/s) by

$$\Lambda_{\text{LTE}}(T) = \frac{(2J'+1) \sum_{v'',J'' \leftarrow v',J'} \Delta E_{v'J',v''J''} e^{-\Delta E_{v'J',v''J''}/kT} A_{v'J',v''J''}}{(2J''+1) \sum_{v'',J''} e^{-\Delta E_{v'',J'',00}/kT}}. \quad (12)$$

The sum is over all possible rovibrational deexcitation transitions within the electronic ground state and the denominator is the rovibrational partition function $Q(T)$.

4. Results and discussion

The radial Schrödinger Eq. (7) was solved with a step size $1.0 \times 10^{-3} a_0$, over a range of internuclear distances from $R = 1.0$ to $60.0 a_0$. The reduced mass of ^7LiH was 0.881238162 u (Stwalley & Zemke 1993).

The vibrational energies $G_{v'}$ and corresponding vibrational energy spacings $\Delta G_{v'+1/2}$ of the $X^1\Sigma^+$ state obtained in the

Table 2. Vibrational level spacings $\Delta G_{v'+1/2}$ of the $X^1\Sigma^+$ state of ^7LiH where $\Delta G_{v'+1/2} = G_{v'+1} - G_{v'}$ is in units of cm^{-1} .

v	Present	Experiment ^a	Holka ^b
0	1359.71	1359.71	1360.58
1	1314.85	1314.89	1315.53
2	1270.91	1270.89	1271.42
3	1227.81	1227.77	1228.16
4	1185.45	1185.44	1185.66
5	1143.75	1143.77	1143.84
6	1102.57	1102.60	1102.54
7	1061.77	1061.78	1061.65
8	1021.18	1021.17	1020.97
9	980.58	980.52	980.29
10	939.69	939.62	939.36
11	898.16	898.09	897.79
12	855.52	855.48	855.17
13	811.18	811.19	810.87
14	764.40	764.44	764.17
15	714.21	714.12	714.03
16	659.31	659.37	659.18
17	598.01	597.89	597.92
18	527.98	527.91	528.07
19	446.23	446.61	446.99
20	349.83	350.99	351.88
21	239.56	237.71	240.14

References. ^(a) Chan et al. (1986). ^(b) Holka et al. (2011).

present study are listed in Tables 1 and 2, along with the theoretical values of Holka et al. (2011) and the measurements of Chan et al. (1986). The largest discrepancy for $G_{v'}$ between our calculations and the experiment is 2.47 cm^{-1} , which occurs for $v = 22$, while the largest difference for $\Delta G_{v'+1/2}$ is smaller at 1.85 cm^{-1} for $v = 22$. Some select transition energies are listed in Table 3 along with the corresponding experimental results of Dulick et al. (1998) and the calculations of Coppola et al. (2011). It can be seen that the current results are in excellent agreement with experiments, the largest discrepancy being 0.027 cm^{-1} .

Transition probabilities for some band-averaged transitions in the $X^1\Sigma^+$ state are compared in Table 4 with the previous calculation of Partridge & Langhoff (1981). The maximum difference is less than 6.79%. As a further illustration, the J -dependent dipole moment matrix elements for $v = 1$ to $v = 0$ are shown in Fig. 2, which are similar to those given in Gianturco et al. (1996). It can be seen that the transition probabilities for the P-branch are much higher than those for the R-branch. The line oscillator strengths as a function of wavelength are shown in Fig. 3 for the $X^1\Sigma^+ \leftarrow X^1\Sigma^+$ transition. The most intense line of the R-branch is at $22.968 \mu\text{m}$ (band 0-0, R(60)). For the P-branch, the strongest is at $16.822 \mu\text{m}$ (band 8-7, P(31)). The complete line list is available on the UGA Molecular Opacity Project website (<http://www.physast.uga.edu/ugamop/>) and in the format of the Leiden Atomic and Molecular Database (LAMDA, Schöier et al. 2005).

Utilizing the theoretical rovibrational energies and transition probabilities, the LTE radiative cooling function was calculated as a function of temperature as shown in Fig. 4. It is compared with the previous results of Dalgarno (1994, priv. comm.) and Coppola et al. (2011), along with the low-density limit cooling function ($n_{\text{H}} \leq 100 \text{ cm}^{-3}$) due to H collisions (Galli & Palla 1998) (see the Appendix for a further discussion). All three LTE cooling functions are seen to be in excellent agreement over the considered temperature range.

Table 3. Rovibrational transition energies for in the $X^1\Sigma^+$ state of ^7LiH .

Band	Line	Transition energy (cm^{-1})			
		Present	Experiment ^a	ΔE_{cp}^b	ΔE^c
1–0	P(28)	858.1193	858.0924	0.31	2.7E-02
	P(23)	953.1177	953.0989	0.38	1.9E-02
	P(18)	1048.2419	1048.231	0.46	1.1E-02
	P(13)	1141.6388	1141.6337	0.54	5.1E-03
	P(8)	1231.0873	1231.0857	0.63	1.6E-03
	P(3)	1314.0901	1314.0902	0.72	−1.0E-04
	R(2)	1401.5064	1401.5062	0.82	2.0E-04
	R(7)	1461.2703	1461.2695	0.88	8.0E-04
	R(12)	1506.8725	1506.8724	0.93	1.0E-04
	R(17)	1536.7646	1536.7673	0.95	−2.7E-03
	R(22)	1550.0615	1550.0721	0.94	−1.1E-02
2–1	P(27)	844.9443	844.9214	0.33	2.3E-02
	P(22)	937.6974	937.6828	0.38	1.5E-02
	P(17)	1030.1894	1030.1815	0.45	7.9E-03
	P(12)	1120.5469	1120.5438	0.53	3.1E-03
	P(7)	1206.5402	1206.5394	0.62	8.0E-04
	P(2)	1285.6869	1285.6872	0.71	−3.0E-04
	R(3)	1368.0210	1368.0208	0.80	2.0E-04
	R(8)	1423.2838	1423.2834	0.86	4.0E-04
	R(13)	1464.2863	1464.2873	0.90	−1.0E-03
	R(17)	1485.8610	1485.8639	0.92	−2.9E-03
3–2	P(23)	885.7266	885.7132	0.39	1.3E-02
	P(18)	976.0542	976.0472	0.44	7.0E-03
	P(12)	1081.9646	1081.9626	0.53	2.0E-03
	P(7)	1165.6453	1165.645	0.61	3.0E-04
	P(2)	1242.5862	1242.5865	0.69	−3.0E-04
	R(3)	1322.4840	1322.4835	0.78	5.0E-04
	R(8)	1375.9434	1375.9434	0.85	0.0E+00
	R(13)	1415.3862	1415.3881	0.89	−1.9E-03
	R(18)	1439.4378	1439.4452	0.92	−7.4E-03
	R(18)	1439.4378	1439.4452	0.92	−7.4E-03
4–3	P(21)	888.1921	888.1827	0.42	9.4E-03
	P(16)	975.7737	975.7707	0.48	3.0E-03
	P(11)	1060.7999	1060.7993	0.55	6.0E-04
	P(6)	1141.0946	1141.0945	0.63	1.0E-04
	R(1)	1253.6893	1253.6882	0.75	1.1E-03
	R(6)	1310.3681	1310.3676	0.82	5.0E-04
	R(11)	1353.9579	1353.9574	0.88	5.0E-04
5–4	P(15)	957.1386	957.1371	0.51	1.5E-03
	P(10)	1039.1932	1039.1925	0.57	7.0E-04
	P(4)	1130.6447	1130.6442	0.66	5.0E-04
	R(4)	1244.8800	1244.8819	0.79	−1.9E-03
	R(5)	1255.3743	1255.3722	0.81	2.1E-03
	R(8)	1283.7835	1283.7859	0.85	−2.4E-03

Notes. ^(a) Dulick et al. (1998). ^(b) Comparison between Coppola et al. (2011) and Dulick et al. (1998), $\Delta E_{\text{cp}} = E_{\text{cp}} - E_{\text{expt}}$. ^(c) $\Delta E = E_{\text{th}} - E_{\text{expt}}$.

To simulate the opacity of LiH in a cool dwarf atmosphere, we computed the absorption cross section using Eq. (6) of Dulick et al. (2003) for a temperature of 1800 K, as an example. The line absorption cross section, which is a function of the transition probability, line frequency, partition function, and temperature, is multiplied by a Lorentzian line profile (Bernath 1995) with width corresponding to collisional broadening. Assuming a canonical collisional broadening cross section of 10^{-16} cm^2 with a line width proportional to the pressure, Figure 5 displays the opacity for 100 atm. There is a series of strong individual pure rotational lines for $\lambda > 20 \mu\text{m}$, while the fundamental vibrational band occurs near $8 \mu\text{m}$. Comparison is made to the LiCl opacity (Weck et al. 2004) for the same temperature and pressure. The LiCl fundamental vibrational band falls in the gap between the pure LiH rotational lines and the LiH 0-1 band, but is typically

Table 4. A-values for transitions in the $X^1\Sigma^+$ state of ${}^7\text{LiH}$.

$v' - v''$	$A_{v'v''}(\text{s}^{-1})$			$\Delta(\%)^d$
	Present ^a	Coppola ^b	Partridge ^c	
1–0	45.4	46.6	43.1	5.32
2–0	2.0	2.1	1.9	4.66
2–1	82.8	85.3	78.5	5.43
3–1	6.4	6.6	6.3	2.15
3–2	112.5	115.9	106.7	5.47
4–2	13.4	13.6	13.3	0.72
4–3	134.5	138.7	127.3	5.63
5–3	23.1	23.5	22.7	1.87
5–4	148.7	153.7	140.3	6.01
6–4	35.9	36.3	34.5	3.96
6–5	155.6	161.3	145.7	6.79
7–5	51.8	52.3	49.3	4.99

Notes. ^(a) Using the P(1) transition. ^(b) Coppola et al. (2011). ^(c) Table V in Partridge & Langhoff (1981). ^(d) Percent difference between current results and Partridge & Langhoff (1981).

Fig. 2. Dipole moment matrix elements for the P-branch and R-branch rovibrational transitions for ${}^7\text{LiH}$ for the $v = 0$ to $v = 1$ transition.

one to two orders of magnitude smaller. According to the cool dwarf atmosphere models of Lodders (1999), the abundances of LiH and LiCl, as well as LiOH, are comparable at 1800 K, but for higher temperatures, LiH becomes the dominant Li-bearing molecule. Weck et al. (2004) suggest that it would be difficult to detect LiCl in cool dwarfs due to strong absorption features from other more abundant molecules (e.g., water) in the same wavelength range. LiH, with its somewhat higher opacity, might be a better candidate for detecting lithium molecules.

5. Conclusions

The rovibrational energy levels of ${}^7\text{LiH}$ were computed with an empirical potential generated from a direct fit of available spectroscopic line positions. The computed vibrational energies and transition energies are found to be in very good agreement with experiments. Oscillator strengths and transition probabilities were also computed and used to construct a complete rovibrational line list. The transition energies were evaluated against available experimental data and found to be reliable to better than 0.03 cm^{-1} . The line list was used to compute an LTE radiative cooling function for LiH and to explore its infrared opacity. Among all dominant Li-bearing molecules, LiH is a better candidate for detecting lithium in cool dwarf atmospheres.

Fig. 3. Oscillator strengths for the $X^1\Sigma^+ \leftarrow X^1\Sigma^+$ transition of ${}^7\text{LiH}$ versus wavelength. R-branch (red) and P-branch (black). **Fig. 4.** Radiative cooling functions of LiH in the LTE (upper three lines) and the low-density limit ($n_{\text{H}} \leq 100 \text{ cm}^{-3}$, lower solid red and black lines) considering only H collisions. **Fig. 5.** Opacity of the LiH (red) rovibrational transitions in the infrared compared to the LiCl (blue) opacity for a temperature of 1800 K and a pressure of 100 atms.

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Appendix: Collisional excitation of LiH

While in this work, we present an LTE radiative cooling function (i.e., valid within the high-density limit), [Bougleux & Galli \(1997\)](#) have approximated a density-dependent non-LTE (NLTE) cooling function (see also [Galli & Palla 1998](#)). In this approach, the NLTE cooling function is parameterized in terms of the LTE radiative cooling function and a collisional cooling function in the zero-density limit. For applications to the early Universe, they considered only collisions due to atomic hydrogen. Unfortunately, rotational or vibrational excitation rate coefficients of LiH due to H are not available, requiring [Bougleux & Galli \(1997\)](#) to adopt the LiH-He calculations of [Jendrek & Alexander \(1980\)](#), but adjusted to emulate LiH-H collisions via mass-scaling of the collisional rate coefficients. The mass-scaling approach is typically adopted when rate coefficients due to He impact are used to approximate para-H₂ impact. Recent work on other molecules suggests this approach is questionable at best (e.g., [Cernicharo et al. 2011](#)) even though the PESs for He- and H₂-complexes are expected to be similar, being characterized by weakly bound van der Waals minima. Collision complexes involving H, on the other hand, typically involve very deep wells leading to very fast exothermic reactive channels. As a consequence, mass-scaling to deduce H-impact excitation rate coefficients from He- or H₂-impact data is likely to be a poor approximation.

For general astrophysical applications, collisions due to the most abundant species, H, H₂, He, e⁻, and H⁺, should be included in an NLTE cooling function, though H₂ dominates in most interstellar environments. LiH-He collisional excitation calculations have been more recently given by [Taylor & Hinde \(1999, 2005\)](#) and [Bodo et al. \(2001a\)](#), and discussed in a review of lithium chemistry by [Bodo et al. \(2003\)](#). The reactive process

and the H-exchange process

have been considered in a number of recent studies ([Prudente et al. 2009](#); [Bovino et al. 2009](#)), but to date, inelastic collisional excitation of LiH due to H has not been investigated because it is a very computationally demanding problem that would

require simultaneous treatment with reactions (13) and (14). We are unaware of any inelastic data due to H₂, e⁻, or H⁺ impacts, though an excited state PES for the LiH₂⁺ complex is available ([Bodo et al. 2001b](#)), which could be used later. It is therefore, not currently possible to construct an accurate, comprehensive NLTE cooling function for LiH. Figure 4 gives an indication of the expected range of the NLTE cooling function.

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