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Line Lists for LiF and LiCl in the $X^1\Sigma^+$ Ground State

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Abstract

Vibration–rotation line lists for ${}^6\text{LiF}$, ${}^7\text{LiF}$, ${}^6\text{Li}^{35}\text{Cl}$, ${}^6\text{Li}^{37}\text{Cl}$, ${}^7\text{Li}^{35}\text{Cl}$, and ${}^7\text{Li}^{37}\text{Cl}$ in the $X^1\Sigma^+$ ground states have been prepared. The rovibrational energy levels have been calculated using potential energy surfaces determined by direct potential-fitting employing the rotational and rovibrational transition frequencies of all isotopologues, and required the inclusion of Born–Oppenheimer breakdown terms. Dipole moment functions calculated ab initio at the MRCI/aug-cc-pwCV5Z level have been used for line strength calculations. Partition functions for temperatures up to 5000 K have been calculated. LiF and LiCl are predicted to be present in the atmospheres of hot rocky exoplanets, brown dwarfs, and cool stars.

Key words: astronomical databases: miscellaneous – molecular data – opacity – techniques: spectroscopic

Supporting material: machine-readable tables

1. Introduction

Quantitative spectroscopic data are required to model the spectral energy distributions emitted by astronomical objects. The molecular opacities of a large variety of species are needed and are constantly being updated in support of these observations. Thermochemical equilibrium calculations (dependent on the assumed elemental composition) predict alkali metals and alkali halides to be present in the atmospheres of hot rocky super-Earths (Schaefer et al. 2012), low-mass dwarf stars, and brown dwarfs (Lodders 1999). Elemental lines of alkali metals and molecular bands of molecules containing such elements are predicted to be present in their atmospheric spectra.

Thermochemical equilibrium calculations by Lodders (1999) for low-mass dwarf stars and brown dwarfs have suggested LiCl to be the dominant Li-bearing gas over a significant portion of the calculated pressure–temperature (P – T) range. LiF was calculated to be the dominant Li-bearing gas over a smaller P – T range that is bounded by regions of higher and lower temperatures where LiCl is dominant.

Neutral Li resonance lines have typically been used to identify the substellar nature of objects by the “lithium test” (Martín et al. 1999). Core temperatures in stars are sufficiently high to burn lithium, resulting in rapid lithium depletion compared to substellar objects. Thus, Li I transitions have been used to discriminate between very low-mass (VLM) stars and young brown dwarfs, both having similar temperature and luminosity ranges.

As calculated by Lodders, the abundance of Li gas can be reduced by formation of Li-bearing molecules. In particular, the presence of LiOH, LiCl, and LiF can result in the misclassification of some brown dwarfs as VLM stars due to the reduction in neutral Li. The line wings of the alkali elements are also a significant source of opacity in substellar objects (Burrows & Volobuyev 2003). Thermochemical equilibrium calculations provide a temperature scale for M dwarfs and brown dwarfs that is based on the presence or absence of major element and alkali element gases in their atmospheres.

Weck et al. (2004a) calculated the radiative flux difference in the spectra of model atmospheres of brown dwarfs after the inclusion of LiCl. The radiative flux difference was found to be typically less than 20% and had the largest signature at $T_{\text{eff}} = 1200$ K and around the infrared fundamental band origin

at $15.8 \mu\text{m}$. The spectra, however, lack distinctive features and LiCl is hard to detect in spectra dominated by water absorption.

High-resolution rovibrational spectra of LiCl and LiF have been measured using tunable diode lasers (Maki 1983; Jones & Lindenmayer 1987) and Fourier transform infrared spectrometers (Thompson et al. 1987; Hedderich et al. 1991). High-resolution pure rotational spectra of LiCl and LiF are also available from older millimeter-wave and submillimeter-wave experiments (Pearson & Gordy 1969) and molecular-beam electric resonance (MBER) experiments.

Empirical potentials determined from spectroscopic data have been published for LiF and LiCl. Dunham potentials have been determined by Ogilvie (1992) for LiF and LiCl from Dunham coefficients. A potential referred to as a modified Lennard-Jones function was determined for LiCl by Melville & Coxon (2001) using 2620 transitions, obtaining a weighted standard deviation of 0.904. A description of the potential is provided by Hajigeorgiou & Le Roy (2000). The fits included rotational and vibrational transitions from all the naturally occurring isotopologues and required that adiabatic and non-adiabatic Born–Oppenheimer breakdown terms be included in the Hamiltonian.

Experimental dipole moments are available mainly from the MBER method. Stark transitions up to $v = 5$ (Mariella et al. 1973) and rotational transitions up to $v = 3$ (Wharton et al. 1963) have been measured for ${}^7\text{LiF}$ and ${}^6\text{LiF}$. Hyperfine transitions up to $v = 3$ were measured for ${}^6\text{LiCl}$ (Marple & Trischka 1956). The equilibrium dipole moments of ${}^7\text{LiF}$, ${}^6\text{LiF}$, and ${}^6\text{Li}^{35}\text{Cl}$ (Lide et al. 1964) are 6.2854(12), 6.28446 D, and 7.075 D, respectively. The dipole moment functions of LiF and LiCl have been obtained using a Herman–Wallis analysis (Ito et al. 1999). A discrepancy was found with these results compared to analyses of MBER work and it is likely due to the assumptions used for the Herman–Wallis analysis.

An ab initio potential energy surface (PES) of LiCl in the $X^1\Sigma^+$ state calculated over a large range of internuclear separations has been presented by Weck et al. (2004b). These calculations were performed at the multi-reference single- and double-excitation configuration interaction (MRSDCI) level of theory. The dipole moment function and transition moments have also been calculated at the same level of theory. The theoretical PES was found to be in good agreement with the

Table 1
Fitting Parameters of the Empirical EMO Potential for LiF and LiCl

	LiF	LiCl
β_0	1.142235140(95) ^a	0.956113250(93)
β_1	-0.5233536(20)	-0.3766661(19)
β_2	0.0405430(46)	0.006567(12)
β_3	0.017960(68)	0.034660(87)
β_4	-0.06547(17)	-0.09110(47)
β_5	...	0.0600(18)
u_1^{Li}	-4.470(92)	-3.66(11)
u_2^{Li}	8.00(22)	7.30(25)
u_1^{Cl}	...	0.860(62)
t_1^{Li}	0.0000600(50)	...
$r_e/\text{\AA}$	1.563864240(62)	2.020671500(97)
$r_{\text{ref}}/\text{\AA}$	[1.56] ^b	[2.02]
$D_e \times 10^{-4}/\text{cm}^{-1}$	[4.84] ^c	[3.92] ^c
$\sigma_{\text{r.m.s.}}$	0.424225	0.692743

Notes.

^a Parameters were determined using sequential rounding and a refitting procedure (Le Roy 1998).

^b Values in squared brackets have been fixed during fitting.

^c Calculated as $D_0+G(0)$ (Luo 2007).

experimental PES by Ogilvie (1992). Previous theoretical investigations were mainly focused on the PESs in the vicinity of the avoided crossing between the two lowest $^1\Sigma^+$ states (Kahn et al. 1974; Werner & Meyer 1981). Weck et al. also provided vibrationally averaged dipole moments and vibrational matrix elements using vibrational wavefunctions obtained by solving the radial nuclear Schrödinger equation (SE). The vibrationally averaged dipole moments were found to systematically overestimate the experimentally determined value by 0.2 D ($\sim 3\%$). Kurosaki & Yokoyama (2012) have calculated PESs of 13 spin-orbit (SO) Ω states as well as dipole moment functions and transition moments at the MRSDCI level of theory. Core-electron correlation was included in the MRSDCI calculation and was found to be necessary to reliably predict spectroscopic constants. The goal of this work was to assess the role of spin-orbit coupling in the low-lying electronic states of LiCl, not to carry out a highly accurate ground-state calculation; in fact, the agreement with experiments for dipole moments and vibrational frequencies is not as good as that obtained by Weck et al. (2004b). Ab initio studies of the PESs of the low $^1\Sigma^+$ states of LiF and a dipole moment function calculated at the full configuration interaction level of theory have been published by Bauschlicher & Langhoff (1988). Recently, Nkambule et al. (2015) also calculated LiF PESs for the two lowest singlet states in order to study the Li^+ and F^- neutralization reaction.

A line list for the ground electronic state of $^7\text{Li}^{35}\text{Cl}$ has been presented by Weck et al. (2004a). A hybrid potential consisting of a shifted potential by Ogilvie (1992) at internuclear distances $3.25a_0 \leq R \leq 4.80a_0$ was combined with an ab initio potential. For internuclear distances of $R > 4.80a_0$, a van der Waals dispersion expansion was used.

We present the line lists of both LiCl and LiF in the ground electronic states. To the best of our knowledge, the first line list of LiF is provided herein. The dependence of the vibrational matrix elements on the rotational state due to the Herman-Wallis effect (Herman & Wallis 1963) has been accounted for in the calculation of the line strengths.

2. Computational Methods

Ab initio calculations have been performed using the MOLPRO 2012 package (Werner et al. 2012). The dipole moments have been calculated as expectation values at the internally contracted MRSDCI level of theory employing the aug-cc-pwCV5Z basis set. All electrons were included in the correlation treatment. Weck et al. (2004b) used a similar method for LiCl, but with a Slater-type basis set and without core correlation. The wavefunctions used for the MRCI calculations have been obtained from state-averaged CASSCF calculations of the two lowest $^1\Sigma^+$ states, having equal weights. The active space included all orbitals obtained from the atomic valence orbitals ($3-6a_1$, $1-2b_1$, and $1-2b_2$ for LiF and $5-8a_1$, $2-3b_1$, and $2-3b_2$ for LiCl in the C_{2v} point group symmetry used).

3. Results

3.1. PES Fitting

Direct potential-fitting employing the program dPotFit by Le Roy (2017a) has been used to determine the empirical expanded Morse oscillator (EMO) potential for LiF and LiCl by least squares fitting of spectroscopic transitions:

$$V_{\text{EMO}}(r) = D_e[1 - e^{-\beta(r)(r-r_e)}]^2, \quad (1)$$

where

$$\beta(r) = \beta_{\text{EMO}}(y_q^{\text{ref}}(r)) = \sum_{i=0}^{N_\beta} \beta_i y_q^{\text{ref}}(r)^i, \quad (2)$$

$$y_q^{\text{ref}}(r) = \frac{r^q - r_{\text{ref}}^q}{r^q + r_{\text{ref}}^q}. \quad (3)$$

For LiF, 1032 rovibrational transitions up to $v = 8$ and $J = 67$, and 33 rotational transitions up to $J = 6$ have been used. For LiCl, 2520 rovibrational transitions up to $v = 8$ and $J = 80$ and 67 rotational transitions up to $J = 11$ have been used. The EMO potential is expected to give a good reproduction of the potential surface, even beyond the region that is typically well

determined by the experimental data as previously demonstrated by direct potential-fitting of the alkali halides NaCl and KCl (Barton et al. 2014). The q parameter in Equation (3) was set to 2 (p and q , occurring in the Born–Oppenheimer breakdown correction terms, were set to 2 (Le Roy 2017b)). To fit the potentials using the available data for all naturally abundant isotopologues (^6LiF and ^7LiF for LiF and $^6\text{Li}^{35}\text{Cl}$, $^6\text{Li}^{37}\text{Cl}$, $^7\text{Li}^{35}\text{Cl}$, and $^7\text{Li}^{37}\text{Cl}$ for LiCl), an effective radial SE derived by Watson, accounting for the atomic-mass-dependent BOB, had to be used. The approach employed by dPotFit to account for the BOB correction functions is described in detail by Le Roy & Huang (2002) and results in the determination of the fitted parameters u_n^X and t_n^X (Table 1). ^7LiF and $^7\text{Li}^{35}\text{Cl}$ were set as the reference isotopologues in the BOB correction functions. The fitted parameters are provided in Table 1.

3.2. Line Strengths

The program LEVEL by Le Roy (2017b) has been employed to calculate the vibrational wavefunctions of LiF and LiCl by solving the radial SE with the potentials provided in Section 3.1. Using LEVEL, the Einstein A coefficients, in s^{-1} units, have been calculated as

$$A_{J' \rightarrow J''} = \frac{16\pi^2\nu^3 S_{J''}^{\Delta J}}{3\epsilon_0 hc^3 (J' + 1)} |\langle \psi_{v',J'} | M(r) | \psi_{v'',J''} \rangle|^2, \quad (4)$$

where ν is the transition frequency, $S_{J''}^{\Delta J}$ is the Hönl–London factor, and $M(r)$ is the dipole moment function (Bernath 2016). The dipole moment matrix elements are J -dependent for the Herman–Wallis effect (Herman & Wallis 1963). $M(r)$ was calculated ab initio as described in Section 2 and is provided in Table 2. The ab initio dipole moments at the calculated equilibrium structures at 1.5583 and 2.0149 Å were 6.324 D and 7.236 D for LiF and LiCl, respectively. The ab initio equilibrium structures are found to be shorter by 0.0056 and 0.0058 Å from the values determined by the direct potential-fitting for LiF and LiCl and the ab initio equilibrium dipole moments are larger by 0.040 D and 0.161 D from the values obtained from the MBER data for LiF and LiCl, respectively.

The oscillator strengths ($f_{J' \leftarrow J''}$) have been calculated from $A_{J' \rightarrow J''}$ by Bernath (2016) as

$$f_{J' \leftarrow J''} = 1.4991938 \frac{1}{\tilde{\nu}^2} \frac{(2J' + 1)}{(2J'' + 1)} A_{J' \rightarrow J''}, \quad (5)$$

where $\tilde{\nu}$ is the transition wavenumber in units of cm^{-1} . Calculated transition frequencies, Einstein A coefficients, dipole moment matrix elements, and the oscillator strengths for transitions with upper vibrational levels up to $v = 11$ and rotational levels up to $J = 200$ for all isotopologues of LiF and LiCl are provided in Table 3. Transitions up to $\Delta v = 2$ and $\Delta v = 8$ have been provided for LiF and LiCl, respectively, because the calculations for larger Δv values are not reliable. As noted by Medvedev et al. (2016) and others, transition dipole moments should decrease in a regular pattern as Δv increases, but various numerical problems can prevent this. For LiF and LiCl, the calculated transition moments no longer decrease as expected for $\Delta v > 2$ and $\Delta v > 8$,

Table 2
Dipole Moment Functions of the $X^1\Sigma^+$ States of LiF and LiCl in Debye

$r/\text{Å}$	LiF	LiCl
1.0	3.856	3.701
1.5	6.049	5.185
2.0	8.259	7.149
2.5	10.556	9.333
3.0	12.888	11.582
3.5	15.177	13.642
4.0	17.361	15.295
4.5	...	16.125
5.0	...	14.331

(This table is available in its entirety in machine-readable form.)

respectively, so they are not provided in Table 3. Refinement of the ab initio pointwise dipole moment function grids and calculations with quadruple precision have been used in attempts to prevent this flattening of the intensities, but without much success.

3.3. Partition Function

The partition functions for LiF and LiCl isotopologues have been calculated with vibrational levels up to the dissociation limit with all rotational levels (including quasibound levels) as follows:

$$Q = \sum_{v=0}^{v_{\max}} \left(\sum_{J=0}^{J_{\max}} (2J + 1) e^{-\frac{E_{v,J}}{kT}} \right). \quad (6)$$

The partition function has been calculated in the temperature range 1–5000 K in steps of 1 K. A polynomial regression has been performed on the following expression:

$$\log_{10} Q = \sum_{n=0}^{n_{\max}} a_n \log_{10} T^n. \quad (7)$$

The calculated partition functions and the determined a_n coefficients are provided in Tables 4 and 5, respectively.

4. Conclusions

The line lists for LiF and for LiCl in their $X^1\Sigma^+$ states have been calculated using ab initio dipole moment functions. EMO empirical potentials have been determined for both molecules by direct potential-fitting using rovibrational and rotational transitions. The observed minus calculated residuals for LiCl transitions are improved by about 3 orders of magnitude from the transitions calculated by Weck et al. (2004a). This difference is likely due to the use of the potential by Ogilvie (1992), which was not obtained by direct potential-fitting. The vibrationally averaged dipole moments and the ab initio calculated r_e and μ_e are in better agreement with experiments than the values calculated previously by Weck et al. (2004b) for LiCl. The line lists can be used in model atmosphere calculations for spectroscopic measurements of astronomical objects that contain LiF and LiCl.

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Appendix A

Line Lists

Table 3
Line Lists of ${}^6\text{LiF}$, ${}^7\text{LiF}$, ${}^6\text{Li}^{35}\text{Cl}$, ${}^7\text{Li}^{35}\text{Cl}$, ${}^6\text{Li}^{37}\text{Cl}$, and ${}^7\text{Li}^{37}\text{Cl}$ in the $X^1\Sigma^+$ State

Isotopologue	Branch	J''	v'	v''	$E_{v'',J''}/\text{cm}^{-1}$	$\tilde{\nu}/\text{cm}^{-1}$	$A_{J''\rightarrow J''}/\text{s}^{-1}$	$f_{J''\rightarrow J''}$
${}^6\text{LiF}$	R	2	1	1	1435.273	8.837	3.891×10^{-3}	1.046×10^{-4}
${}^6\text{LiF}$	R	48	1	0	3919.919	1028.822	6.429×10^0	9.293×10^{-6}
${}^6\text{LiF}$	R	3	2	2	2372.137	11.594	9.389×10^{-3}	1.346×10^{-4}
${}^6\text{LiF}$	R	49	2	1	4948.740	1009.994	1.159×10^1	1.738×10^{-5}
${}^6\text{LiF}$	P	50	3	1	5088.857	1587.667	4.289×10^{-1}	2.500×10^{-7}
${}^6\text{LiF}$	R	50	3	1	5088.857	1861.396	4.044×10^{-1}	1.784×10^{-7}
${}^6\text{LiF}$	R	50	3	2	5958.734	991.519	1.588×10^1	2.469×10^{-5}
${}^7\text{LiF}$	R	2	1	1	1355.875	7.890	2.763×10^{-3}	9.316×10^{-5}
${}^7\text{LiF}$	R	48	1	0	3529.675	971.499	5.304×10^0	8.599×10^{-6}
${}^7\text{LiF}$	R	3	2	2	2241.957	10.361	6.675×10^{-3}	1.198×10^{-4}
${}^7\text{LiF}$	R	49	2	1	4501.174	954.836	9.593×10^0	1.609×10^{-5}
${}^7\text{LiF}$	P	50	3	1	4626.965	1521.284	3.080×10^{-1}	1.956×10^{-7}
${}^7\text{LiF}$	R	50	3	1	4626.965	1767.512	2.859×10^{-1}	1.399×10^{-7}
${}^7\text{LiF}$	R	50	3	2	5456.010	938.467	1.320×10^1	2.292×10^{-5}
${}^6\text{Li}^{35}\text{Cl}$	R	2	1	1	1022.674	4.739	7.762×10^{-4}	7.253×10^{-5}
${}^6\text{Li}^{35}\text{Cl}$	R	48	1	0	2198.305	728.833	3.478×10^0	1.002×10^{-5}
${}^6\text{Li}^{35}\text{Cl}$	R	3	2	2	1693.291	6.242	1.883×10^{-3}	9.316×10^{-5}
${}^6\text{Li}^{35}\text{Cl}$	R	49	2	1	2927.138	718.707	6.667×10^0	1.974×10^{-5}
${}^6\text{Li}^{35}\text{Cl}$	P	50	3	1	3003.956	1199.271	2.559×10^{-1}	2.614×10^{-7}
${}^6\text{Li}^{35}\text{Cl}$	R	50	3	1	3003.956	1350.587	2.980×10^{-1}	2.498×10^{-7}
${}^6\text{Li}^{35}\text{Cl}$	R	50	3	2	3645.845	708.698	9.583×10^0	2.917×10^{-5}
${}^7\text{Li}^{35}\text{Cl}$	R	2	1	1	958.793	4.167	5.265×10^{-4}	6.364×10^{-5}
${}^7\text{Li}^{35}\text{Cl}$	R	48	1	0	1954.136	682.022	2.738×10^0	9.008×10^{-6}
${}^7\text{Li}^{35}\text{Cl}$	R	3	2	2	1588.177	5.493	1.279×10^{-3}	8.168×10^{-5}
${}^7\text{Li}^{35}\text{Cl}$	R	49	2	1	2636.158	673.202	5.267×10^0	1.778×10^{-5}
${}^7\text{Li}^{35}\text{Cl}$	P	50	3	1	2703.936	1136.174	1.891×10^{-1}	2.153×10^{-7}
${}^7\text{Li}^{35}\text{Cl}$	R	50	3	1	2703.936	1269.903	2.180×10^{-1}	2.067×10^{-7}
${}^7\text{Li}^{35}\text{Cl}$	R	50	3	2	3309.361	664.478	7.596×10^0	2.630×10^{-5}
${}^6\text{Li}^{37}\text{Cl}$	R	2	1	1	1018.637	4.702	7.579×10^{-4}	7.195×10^{-5}
${}^6\text{Li}^{37}\text{Cl}$	R	48	1	0	2182.467	725.877	3.427×10^0	9.953×10^{-6}
${}^6\text{Li}^{37}\text{Cl}$	R	3	2	2	1686.652	6.194	1.839×10^{-3}	9.242×10^{-5}
${}^6\text{Li}^{37}\text{Cl}$	R	49	2	1	2908.344	1009.99	6.572×10^0	1.962×10^{-5}
${}^6\text{Li}^{37}\text{Cl}$	P	50	3	1	2984.576	1195.339	2.512×10^{-1}	2.584×10^{-7}
${}^6\text{Li}^{37}\text{Cl}$	R	50	3	1	2984.576	1345.515	2.923×10^{-1}	2.469×10^{-7}
${}^6\text{Li}^{37}\text{Cl}$	R	50	3	2	3624.180	705.911	9.448×10^0	2.899×10^{-5}
${}^7\text{Li}^{37}\text{Cl}$	R	2	1	1	954.482	4.130	5.124×10^{-4}	6.306×10^{-5}
${}^7\text{Li}^{37}\text{Cl}$	R	48	1	0	1938.152	678.861	2.693×10^0	8.941×10^{-6}
${}^7\text{Li}^{37}\text{Cl}$	R	3	2	2	1581.079	5.444	1.244×10^{-3}	8.093×10^{-5}
${}^7\text{Li}^{37}\text{Cl}$	R	49	2	1	2617.013	670.126	5.181×10^0	1.764×10^{-5}
${}^7\text{Li}^{37}\text{Cl}$	P	50	3	1	2684.199	1131.849	1.852×10^{-1}	2.124×10^{-7}
${}^7\text{Li}^{37}\text{Cl}$	R	50	3	1	2684.199	1264.425	2.133×10^{-1}	2.039×10^{-7}
${}^7\text{Li}^{37}\text{Cl}$	R	50	3	2	3287.139	661.485	7.473×10^0	2.611×10^{-5}

(This table is available in its entirety in machine-readable form.)

Appendix B

Partition Functions

Table 4
Partition Functions for LiF and LiCl Isotopologues in the $X^1\Sigma^+$ State

Temperature/K	^6LiF	^7LiF	$^6\text{Li}^{35}\text{Cl}$	$^6\text{Li}^{37}\text{Cl}$	$^7\text{Li}^{35}\text{Cl}$	$^7\text{Li}^{37}\text{Cl}$
100	46.817	52.443	87.353	88.047	99.381	100.281
1000	636.447	733.365	1431.103	1445.912	1693.778	1713.927
2000	1981.341	2313.141	4801.169	4854.464	5750.349	5823.470
3000	4179.595	4905.242	10459.375	10578.467	12583.535	12747.427
4000	7352.349	8653.075	18780.320	18996.965	22647.416	22946.027
5000	11659.720	13746.367	30297.167	30649.460	36588.359	37074.397

(This table is available in its entirety in machine-readable form.)

Table 5
Polynomial Coefficients Determined from Regression of Equation (7)

	^6LiF	^7LiF	$^6\text{Li}^{35}\text{Cl}$	$^6\text{Li}^{37}\text{Cl}$	$^7\text{Li}^{35}\text{Cl}$	$^7\text{Li}^{37}\text{Cl}$
a_0	6.8206×10^{-3}	6.90834×10^{-3}	$1.70478170 \times 10^{-3}$	$1.71280669 \times 10^{-3}$	$-9.20021938 \times 10^{-4}$	$-9.29760672 \times 10^{-4}$
a_1	$-1.1043657 \times 10^{-1}$	$-1.1090837 \times 10^{-1}$	$-4.20647598 \times 10^{-2}$	$-4.22347486 \times 10^{-2}$	$2.68161062 \times 10^{-2}$	$2.70764455 \times 10^{-2}$
a_2	7.2913102×10^{-1}	7.2535382×10^{-1}	$4.56549683 \times 10^{-1}$	$4.58082306 \times 10^{-1}$	$-3.50877969 \times 10^{-1}$	$-3.53984516 \times 10^{-1}$
a_3	-2.52739313×10^0	-2.48763218×10^0	-2.86436422×10^0	-2.87196228×10^0	2.72091505×10^0	2.74274425×10^0
a_4	4.96718579×10^0	4.82925764×10^0	1.14856700×10^1	1.15077702×10^1	-1.39057880×10^1	-1.40061576×10^1
a_5	-5.61040922×10^0	-5.37260927×10^0	-3.07411541×10^1	-3.07769655×10^1	4.92817535×10^1	4.95992208×10^1
a_6	3.60769185×10^0	3.38254701×10^0	5.57128762×10^1	5.57330978×10^1	-1.24105141×10^2	-1.24812375×10^2
a_7	-3.841394×10^{-1}	$-2.5824791 \times 10^{-1}$	-6.79345281×10^1	-6.79001413×10^1	2.23870445×10^2	2.24988110×10^2
a_8	2.090878×10^{-2}	3.034117×10^{-2}	5.42595574×10^1	5.41782728×10^1	-2.87855061×10^2	-2.89100759×10^2
a_9	-2.69358717×10^1	-2.69358717×10^1	2.59092174×10^2	2.60052583×10^2
a_{10}	7.65298031×10^0	7.61694319×10^0	-1.57558206×10^2	-1.58051520×10^2
a_{11}	$-2.10802154 \times 10^{-1}$	$-2.00741107 \times 10^{-1}$	6.06530153×10^1	6.08111736×10^1
a_{12}	$1.16002042 \times 10^{-1}$	$1.17661007 \times 10^{-1}$	-1.28632005×10^1	-1.28926168×10^1
a_{13}	1.85471989×10^0	1.85941586×10^0
a_{14}	$1.48905023 \times 10^{-1}$	$1.51363997 \times 10^{-1}$

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