Contents

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The current file describes two ways to explore the current collection of results from the work on my thesis (partially performed together with our collaboration partners). The more comfortable way is to use the included evaluation program, while the alternative way is to directly look into the different types of text files. In this document I first explain how to use the evaluation program for this purpose, before I describe in the second section the content of the individual files and directories until I explain in the third section the used file formats.

Contents

1 How to use the included evaluation program to explore the current data collection

The most comfortable way to explore the current data collection is to use the included evaluation program 'MolSpektAnalysis' of which I included the source code as well as binaries for Linux and Windows. In the case none of the binaries runs on your system, you can try to compile the source code. The information about what is to consider in this case can be found at the end of the file 📂MolSpektAnalysis0_2_7📂Source📄README.txt. In the case you succeded in starting the program you can simply open the file for the molcule you are currently interested in (📄Sr2.mol, 📄LiRb.mol, 📄LiCa.mol, or 📄LiSr.mol) of which I added each a copy in the source and the binary folders of the program. In the opened molecule file you can see two tables, one for the observed electronic states and one for the observed electronic transitions between two of the electronic states. The table of electronic states contains combo boxes with the available term energy tables, Dunham coefficients, potentials and fit data sets and the table of the transitions the available line tables. The files currently selected in the combo boxes can be opened by either a double click on the according box or a right click on the same box and then the selection of the according entry in the opened context menu.

A term energy table contains a list of calculated energy levels from Dunham coefficients or a potential. The energies can be seen in a more compact view if one selects in the menu 'Show' the entry 'Show term view' while the term energy table is the active window. A term energy table I have added only for the ground state $X^1\Sigma_g^+$ of the molecule Sr_2, because this is the only electronic state of the investigated molecules where I know the full bound potential range sufficiently well to state that all the calculated energies are correct (in this case with a precision better than 0.005 cm^{-1}). For other electronic states you can use each of the given Dunham coefficient sets or potentials to calculate it on your own just by selecting the menu entry 'Calculate term energies' in the menus 'Dunham' or 'Potential' while the according window with Dunham coefficients or a potential is active. For potentials this can take many minutes (depending on the selected level range and the performance of you computer) in which the program does not react. Be aware that the term energies you calculate this way are precise only in the level range the used Dunham coefficients or potential is precise for. In which ranges the individual potentials and Dunham coefficients are precise you can read in the file listings in the following section.

If you open a potential file it gets visible as a table containing the coefficients the potential function gets calculated from or the spline points of a spline potential. The potential function can be drawn by selecting 'Plot potential' in the menu 'Potential'. This function you can use also to compare different potentials if you select the menu entry 'Add potential' in the menu 'Plot'. Wave functions can be drawn using the entry 'Show wave function' in the menu 'Show'. A table with Franck-Condon factors gets calculated on the fly if you select 'Show FCF view' in the menu 'Show'. For the Franck-Condon factors the same is valid as for the term energies, the factors are only precise in the range the used potentials are precise. The calculation of Franck-Condon factors can also cause a short freeze of the program for a few seconds.

A fit data set contains flourescence progressions and term energies collected

for fitting Dunham coefficients and potentials of a special electronic state. For an excited state it consists of term energies which are calculated from the observed fluorescence progressions or absorption or emnission lines and a ground state term energy table or as described in chapter 4.2 of my thesis from dense absorption spectra. Fit data sets for electronic ground states consist mainly out of flourescence progressions. In that of the Sr_2 ground state I added also cited term energies from photoassociation experiments. The fit data sets contain columns for the residuals of the last fit done with it, in the fit data files having in its name not only the electronic state but the name of a potential or Dunham coefficient set you can find the residuals of that fit. I sometimes used special fit data sets for special fits, because it had significant disadvantages to try to use all available levels for a particular fit. For example causes the large anharmonicity of a potential in and close to the asymptotic region the need of an extraordinary high number of coefficients if one wants to describe all existing levels of a potential with Dunham coefficients. To avoid this I often used a reduced data set for Dunham coefficient fits. Additional are derived energies for electronic ground states significantly different for a Dunham coefficient set and a potential, if both are fitted directly to the observed flourescence progressions. This causes the situation, that if both are published for the same electronic ground state, only one of it can be used to derive the correct transition frequencies to excited states. To avoid this situations I fitted additionally provided sets of Dunham coefficients not directly to the observations, but to level energies calcualted from the potential.

A new fit data set you can easily create by the menu entry 'File'→'New'→'Fit data set'. If you assign it to an electronic state of a molecule by selecting it in the according combo box in the table 'Known electronic states' of the molecule's window, you can easely fill it with content automatically generated from the available line tables by selecting the entry 'Update' in the menu 'Table'. There you can also select which line tables to use if more than one is available. To see how well a potential describes this set of fit data you can select the entry 'Show chiSq'. This fills also the deviation columns in the table of the fit data set.

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2.1   📁Analysis

This folder contains the most important final and intermediate results obtained during the work on my phd thesis.

2.1.1   📁Analysis📁Sr2

The molecule Sr_2 was the main object of investigation during the work on my thesis.

📄AnalyticalPotential_Sr2_XSiSigma.pot

This analytical potential for the ground state $X^1\Sigma_g^+$ of the molecule Sr_2 is precise for the full bound potential range. This means that all bound and quasi bound levels of all stable isotopes can be calculated from this potential with

a precision of 0.005 cm^{-1}. It describes all 67000 observations with a weighted standard deviation of $\sigma = 0.71$. All observations are included with their measurement uncertainty. This measurement uncertainty is for the largest part of my 67000 own observations in the quantum number range $0 \leq v'' \leq 60$ (≈ 51000) ≤ 0.005 cm^{-1}. Also included are ten highly precise photoassociation observations[1, 2, 3, 4] in the range $60 \leq v'' \leq 62$ with precisions varying from 7×10^{-6} to 7×10^{-9} cm^{-1}. This is the only electronic state for which we could derive precise experimental long range coefficients C_i. For the precise values averaged over many potential fits and its uncertainties see my thesis. The values included in the current file are fitted together with this potential and thus the correct ones to use as part of the potential, but for other purposes not as precise as the averaged values in the thesis.

DunhamCoefficients_Sr2_XSiSigma.dun

Dunham coefficients for the ground state X$^1\Sigma_g^+$ of the molecule Sr$_2$ which are fitted to term energies calculated from the potential in AnalyticalPotential_Sr2_XSiSigma.pot. The coefficients are valid for all levels below a straight line one could draw through the points $(v'' = 62, J'' = 4)$ and $(v'' = 0, J'' = 300)$ in figure 5.1 on page 89 of my thesis. The energies of the levels in the range one can calculate from the coefficients should be similar precise as if one calculates it directly from the potential. An exception to this are the levels close to the asymptote, there the potential reaches a much higher precision (relative to the asymptote) than the 0.005 cm^{-1} the Dunham coefficients can reproduce.

TermEnergies_Sr2_XSiSigma.term

Level energies calculated relative to the potential minimum for the electronic ground state X$^1\Sigma_g^+$ of the molecule Sr$_2$. The energies are calculated from the potential in AnalyticalPotential_Sr2_XSiSigma.pot with a precision of better than 0.005 cm^{-1} and are used to calculate the Dunham coefficients in DunhamCoefficients_Sr2_XSiSigma.dun.

FitData_Sr2_XSiSigma.fdat

The data set the potential in AnalyticalPotential_Sr2_XSiSigma.pot is fit to. It contains the fluorescence lines from the tables in Lines_CoupledSystem_1SiSigma_1TriPi_XSiSigma.lines, Lines_1SiPi_XSiSigma.lines and Lines_2SiSigma_XSiSigma.lines together with the level energies and energy differences from the photoassociation experiments[1, 2, 3, 4]. It contains all in all of about 67000 lines, which cover 4900 of the 5500 different levels of the most abundant isotopologue ^{88}Sr$_2$ and additionally 4600 and 3000 different levels of the next most frequent isotopologues ^{86}Sr^{88}Sr and ^{87}Sr^{88}Sr, respectively.

📄**AnalyticalPotential_Sr2_1SiSigma_Minimum.pot**

Analytical potential for the minimum of the electronic state $1^1\Sigma_u^+$ of the molecule Sr_2. It describes the 3145 level energies I have observed in the quantum number range with $0 \leq v' \leq 10$ and $J' \leq 220$ with a weighted standard deviation $\sigma = 0.89$. These levels are recognized with its measurement uncertainties of 0.01 cm^{-1} to 0.02 cm^{-1}, except 18 outliners wich are removed from the fit by setting an artificial uncertainty >9 cm^{-1}. The range of internuclear distances covered by the used data reaches from 3.60 Å to 4.54 Å. In the potential included long range coefficients C_i form only a continuous extension of the potential necessary for precisely solving the radial Schrödinger's equation but are furthermore absolutely without any meaning.

📄**AnalyticalPotential_Sr2_1SiSigma_Minimum.fdat**

The fit data set used for fitting the potential in 📄AnalyticalPotential_Sr2_1SiSigma_Minimum.pot. It contains the excerpt of the available level energies for the electronic state $1^1\Sigma_u^+$ which could be assigned to the quantum number range the potential describes. These level energies are derived either by adding the transition ernergies from the line table in 📄Lines_CoupledSystem_1SiSigma_1TriPi_XSiSigma.lines to the according ground state level energies from 📄TermEnergies_Sr2_XSiSigma.term or as described in chapter 4.2 of my thesis from the spectrum 📄29Sr_Av0_8_cut.spect in the folder 📂Spectra📂Sr2📂29Sr_Absorption.

📄**DunhamCoefficients_Sr2_1SiSigma.dun**

Dunham coefficients directly fitted to roughly the same level energies as the potential in 📄AnalyticalPotential_Sr2_1SiSigma_Minimum.pot. They describe the fit data set in 📄AnalyticalPotential_Sr2_1SiSigma_Minimum.fdat, which contains level energies in the range $0 \leq v' \leq 10$ and $J' \leq 220$, with a weighted standard deviation $\sigma = 0.98$.

📄**IPA_SplinePotential_Sr2_1SiSigma_1TriPi_1ad.pot**

This spline potential describes the energetically lower lying adiabatic state of the strongly coupled system $1^1\Sigma_u^+ - 1^3\Pi_{0u}$. Since the magnitude of the coupling is just that strong that the adiabatic picture describes the system a little better than the diabatic picture and these two electronic states are also perturbed by further electronic states, the average residuals of this fit are orders of magnitude larger than the ones of the potential in 📄AnalyticalPotential_Sr2_1SiSigma_Minimum.pot. While the residuals for the energetically higher lying vibrational states reach a few cm^{-1} for many rotational levels, the describtion of the absolute potential minimum is in its quality not very far away from the analytical potential. The overall standard deviation of this potential description is 0.66 cm^{-1}. Included long range coefficients C_i are only a continuous extension of the potential necessary for precisely solving

the radial Schrödinger's equation but are furthermore absolutely without any meaning.

🗎IPA_SplinePotential_Sr2_1SiSigma_1TriPi_2ad.pot

The standard deviation of the energetically higher lying adiabatic potential of the coupled system $1^1\Sigma_u^+$–$1^3\Pi_{0u}$ of the molecule Sr_2 is with 1.35 cm^{-1} even larger than that of the lower one, because it has no unperturbed part. Nevertheless, its description of the system is still orders of magnitude better than any *ab initio* potential I have seen so far. The potential describes only levels energetically below the asymptote $^1S_0$+$^3P_1$. Included long range coefficients C_i are only a continuous extension of the potential necessary for precisely solving the radial Schrödinger's equation but are furthermore absolutely without any meaning.

🗎IPA_SplinePotential_Sr2_1SiSigma_1TriPi_1ad.fdat

The fit data used for the fit of the potential in 🗎IPA_SplinePotential_Sr2_1SiSigma_1TriPi_1ad.pot consists of the known levels of the coupled system which could be assigned to the lower adiabatic state. As the fit data set in 🗎AnalyticalPotential_Sr2_1SiSigma_Minimum.fdat it consists of as well as level energies derived from fluorescence lines as of level energies derived from the spectrum 🗎29Sr_Av0_8_cut.spect. In the deviation columns it contains the detailed residuals of the fit.

🗎IPA_SplinePotential_Sr2_1SiSigma_1TriPi_2ad.fdat

The fit data set of the higher adiabatic state contains all the collected level energies of the coupled system, which fit rather to this higher adiabatic state than to the lower one.

🗎Lines_CoupledSystem_1SiSigma_1TriPi_XSiSigma.lines

This table of fluorescence lines contains the lines which I have observed for the coupled system $1^1\Sigma_u^+$–$1^3\Pi_{0u}$.

🗎IPA_SplinePotential_Sr2_1SiPi.pot

The spline potential for the electronic state $1^1\Pi_u$ describes all except 216 of the 4005 observed levels in the range from $v' = 0$ to $v' = 20$ with a weighted standard deviation of $\sigma = 1.22$ and thus almost whithin the measurement uncertainty of 0.01 cm^{-1} to 0.04 cm^{-1}. The 216 not as well described levels are affected by clearly visible local perturbations. The range of internuclear distances covered by the used data reaches from 3.52 Å to 4.97 Å. Included long range coefficients C_i are only a continuous extension of the potential necessary for precisely solving the radial Schrödinger's equation but are furthermore ab-

solutely without any meaning.

🗎IPA_SplinePotential_Sr2_1SiPi.fdat

The fit data set used to fit the potential in
🗎IPA_SplinePotential_Sr2_1SiPi.pot contains almost the same data as the
fit data set in 🗎FitData_Sr2_1SiPi.fdat. The difference between the two is,
that for the fit of the spline potential I subtracted the effect of the observed λ
doubling using the corresponding coefficients from the file
🗎DunhamCoefficients_Sr2_1SiPi.dun.

🗎DunhamCoefficients_Sr2_1SiPi.dun

The Dunham coefficients for the state $1^1\Pi_u$ describe the same set of observed
levels as the potential with a weighted standard deviation of $\sigma = 1.18$ and thus
similarily well.

🗎FitData_Sr2_1SiPi.fdat

The fit data set used for the fit of the Dunham coefficients and the spline
potential consists as the fit data set for the coupled system $1^1\Sigma_u^+ - 1^3\Pi_{0u}$ of
level energies derived from fluorescence lines and a white light absorption spec-
trum. For the higher excited electronic states as this one I specially recorded
the spectrum in the folder 📂Spectra📂Sr2📂30Sr_Absorption. The used level
energies I have derived from 🗎30Sr_Av2_11_norm_cut.spect.

🗎Lines_1SiPi_XSiSigma.lines

The fluorescence lines I have observed for the electronic transition $1^1\Pi_u \longrightarrow X^1\Sigma_g^+$.

🗎IPA_SplinePotential_Sr2_2SiSigma.pot

The spline potential for the electronic state $2^1\Sigma_u^+$ describes all observed vi-
brational levels of this state up to $v' = 38$ with a weighted standard deviation
$\sigma = 1.02$. The speciality of this potential fit is, that because of the high density
of local perturbations in the vibrational levels with $v' \geq 26$ all levels in this
range were not included with their measurement uncertainty of 0.01 cm^{-1} to
0.04 cm^{-1}, but artificially increased uncertainty values of 0.1 cm^{-1} to 1 cm^{-1}, to
decrease the weigth of these strongly perturbed levels. Additionally, I removed
with its weight from the fit further 1062 levels which are significantly affected
by local perturbations in the lower vibrational levels with $v' \leq 25$ by setting
artificially uncertainties > 9 cm^{-1}. The range of internuclear distances covered
by the used data reaches from 3.62 Å to 5.92 Å. Included long range coefficients
C_i are only a continuous extension of the potential necessary for precisely solv-
ing the radial Schrödinger's equation but are furthermore absolutely without

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any meaning.

📄DunhamCoefficients_Sr2_2SiSigma.dun

In contrast to the potential the Dunham coefficients for the state $2^1\Sigma_u^+$ only describe the vibrational levels with $0 \leq v' \leq 12$. They describe the 4712 levels in this range which have mearement uncertainties of 0.01 cm^{-1} to 0.04 cm^{-1} with a weighted standard deviation of $\sigma = 0.77$, in which 229 levels affected by local perturbations were removed by an artifical uncertainty value > 9 cm^{-1}.

📄FitData_Sr2_2SiSigma.fdat

The fit data set used for the fits to levels of the electronic state $2^2\Sigma_u^+$ consists as the one for the state $1^1\Pi_u$ of level energies derived from fluorescence lines and from the absorption spectrum in 📄30Sr_Av2_11_norm_cut.spect.

📄Lines_2SiSigma_XSiSigma.lines

The fluorescence lines I have observed for the transition $1^1\Sigma_u^+ \longrightarrow \mathrm{X}^1\Sigma_g^+$ of the molecule Sr$_2$.

2.1.2   📁Analysis📁LiRb

The molecule LiRb I have investigated together with our coloboration partners.

📄IPA_SplinePotential_LiRb_XSiSigma.pot

Spline potential for the electronic ground state $\mathrm{X}^1\Sigma^+$ of the molecule LiRb I have taken from our article[5]. This potential describes about 3400 lines in the quantum number range of $0 \leq v' \leq 45$ and measurement uncertainties between 0.005 cm^{-1} and 0.02 cm^{-1} with a weighted standard deviation of $\sigma = 0.60$. The data covers an energy range up to of about 40 cm^{-1} below the asymptote[5]. The included long range coefficients C_6 and C_8 are citations from [6].

📄DunhamCoefficients_LiRb_XSiSigma.dun

This Dunham coefficients I have fitted to levels calculated from the spline potential in 📄IPA_SplinePotential_LiRb_XSiSigma.pot which are below a straigth line one could draw through the points $(v'' = 9, J'' = 100)$ and $(v'' = 40, J'' = 22)$. The coefficients should describe the levels in this range similar well as the potential itself.

📄AnalyticalPotential_LiRb_XSiSigma.pot

Analytical potential for the electronic ground state $X^1\Sigma^+$ of the molecule LiRb I have taken from our article. This potential describes the same data set as the spline potential in 📄IPA_SplinePotential_LiRb_XSiSigma.pot with a similar precision. The advantage of the current potential is that it is fitted together with the potential of the asymptotically coupling state $a^3\Sigma^+$ in 📄AnalyticalPotential_LiRb_aTriSigma.pot including the usage of Feshbach resonance data from [7, 8, 9] and that it recognized a correction to the Born-Oppenheimer approximation regarding the mass difference between ^{7}Li and ^{6}Li. The disadvantage of the current potential with respect of the current data collection is, that it did not get used for the estimation of the excited states energies the Dunham coefficient sets and potentials for the excited electronic states are fitted to. Because of this, only the spline potential in 📄IPA_SplinePotential_LiRb_XSiSigma.pot or the Dunham coefficients in 📄DunhamCoefficients_LiRb_XSiSigma.dun can be used together with the Dunham coefficients and potentials for the excited states to derive transition frequencies without the loss of precsion.

📄IPA_SplinePotential_LiRb_XSiSigma.pot

Analytical potential for the electronic state $a^3\Sigma^+$ of the molecule LiRb which I have taken from our article[5] and which got fitted together with the potential of the state $X^1\Sigma^+$ in 📄AnalyticalPotential_LiRb_XSiSigma.pot. Since we observed only 18 levels for two neighboring vibrational states the *ab initio* potential from [10] was taken and only slightly adjusted to describe the few observations and to obtain the current potential.

📄DunhamCoefficients_LiRb_BSiPi_f.dun

These Dunham coefficients for the f levels of the state $B^1\Pi$ of the state LiRb describe 1446 levels in the quantum number range $0 \leq v' \leq 22$ having a mesurement precision of 0.01 cm^{-1} with a weighted standard deviation of $\sigma = 0.82$. To reach the full precision in the calculation of transition frequencies to the ground state $X^1\Sigma^+$ these Dunham coefficients must be used together with the spline potential in 📄IPA_SplinePotential_LiRb_XSiSigma.pot or the Dunham coefficients in 📄DunhamCoefficients_LiRb_XSiSigma.dun.

📄AnalyticalPotential_LiRb_BSiPi.pot

I have taken this potential from our article [11]. If used together with the potential of the state $C^1\Sigma^+$ in 📄AnalyticalPotential_LiRb_CSiSigma.pot and the coupling function you can find in table 6.39 of my thesis or table III in[11] it describes 1441 levels of the isotopologues ^{7}Li^{85}Rb and ^{7}Li^{87}Rb of which 1195 levels of our own mesurements are included with an uncertainty of 0.01 cm^{-1} and additional 246 levels from [12] which are included with an uncertainty of 0.03 cm^{-1} with a weighted standard deviation $\sigma = 1.20$. To reach

the full precision in the calculation of transition frequencies to the ground state $X^1\Sigma^+$ these coupled potentials must be used together with the spline potential in 🗎IPA_SplinePotential_LiRb_XSiSigma.pot or the Dunham coefficients in 🗎DunhamCoefficients_LiRb_XSiSigma.dun. The energy range of the potential curves covered by the measured levels energies reaches up to an energy of 18500 cm^{-1} above the minimum of the ground state potential or 160 cm^{-1} below the asymptote of the state $B^1\Pi$. Included long range coefficients C_i are only a continuous extension of the potential necessary for precisely solving the radial Schrödinger's equation but are furthermore absolutely without any meaning.

🗎AnalyticalPotential_LiRb_CSiSigma.pot

The analytical potential for the state $C^1\Sigma^+$ of the molecule LiRb which is needed to derive precise level energies for the e levels of the state $B^1\Pi$ in a coupled channel calculation I have taken from our article [11]. Since no direct observations of the state $C^1\Sigma^+$ were available during the time the deperturbation analysis was carried out the current potential will have a significantly lower precision that that of the state $B^1\Pi$. Included long range coefficients C_i are only a continuous extension of the potential necessary for precisely solving the radial Schrödinger's equation but are furthermore absolutely without any meaning.

🗎IPA_SplinePotential_LiRb_DSiPi.pot

This spline potential for the state $D^1\Pi$ of the molecule LiRb describes a data set of 1051 level energies observed with an uncertainty of 0.01 cm^{-1} with a weighted standard deviation of $\sigma = 0.92$ where 45 levels affected by local perturbations were removed with its weight from the fit by using an artifical uncertainty > 9 cm^{-1}. The quantum number range covered by the data set is $0 \leq v' \leq 10$ plus three additional levels with $v' = 11$, $v' = 13$ and $v' = 15$. The internuclear distance range covered by the more dense part of the data is 3.48 Å to 5.39 Å, by the highest observed level with $v' = 15$, $J' = 34$ 3.38 Å to 6.13 Å (of about 300 cm^{-1} below the asymptote of this state). To reach the full precision in the calculation of transition frequencies to the ground state $X^1\Sigma+$ this potential must be used together with the spline potential in 🗎IPA_SplinePotential_LiRb_XSiSigma.pot or the Dunham coefficients in 🗎DunhamCoefficients_LiRb_XSiSigma.dun. Included long range coefficients C_i are only a continuous extension of the potential necessary for precisely solving the radial Schrödinger's equation but are furthermore absolutely without any meaning.

🗎IPA_SplinePotential_LiRb_DSiPi.fdat

The level energies I have fitted the potential in 🗎IPA_SplinePotential_LiRb_DSiPi.pot to. Contains the residuals of this fit. The energies are derived by adding the observed transition energies from 🗎Lines_LiRb_DSiPi_XSiSigma.lines to ground state level energies calculated

from the spline potential in 🖹IPA_SplinePotential_LiRb_XSiSigma.pot.

🖹DunhamCoefficients_LiRb_DSiPi.dun

The Dunham coefficients for the state $D^1\Pi$ of the molecule LiRb describes the data set with 1051 levels observed with an uncertainty of 0.01 cm^{-1} with a weighted standard deviation of $\sigma = 0.91$ with 46 likely perturbed levels removed with its weight from the fit. To reach the full precision in the calculation of transition frequencies to the ground state $X^1\Sigma^+$ these Dunham coefficients must be used together with the spline potential in 🖹IPA_SplinePotential_LiRb_XSiSigma.pot or the Dunham coefficients in 🖹DunhamCoefficients_LiRb_XSiSigma.dun.

🖹DunhamCoefficients_LiRb_DSiPi.fdat

This collection of level energies I have used for the fit of the Dunham coefficients in 🖹DunhamCoefficients_LiRb_DSiPi.dun contains exactly the same level energies as the file 🖹IPA_SplinePotential_LiRb_DSiPi.fdat, but additionally to this the information which levels where removed with its weight from the fit, together with the residuals of the Dunham fit.

🖹Lines_LiRb_BSiPi_XSiSigma.lines

My collection of fluorescence lines we have observed for the electronic transition $B^1\Pi \longrightarrow X^1\Sigma^+$ of the molecule LiRb.

🖹Lines_LiRb_DSiPi_XSiSigma.lines

My collection of fluorescence lines we have observed for the electronic transition $D^1\Pi \longrightarrow X^1\Sigma^+$ of the molecule LiRb.

2.1.3   📁Analysis📁LiCa

🖹IPA_SplinePotential_LiCa_XDoublSigma.pot

I have taken this spline potential for the electronic state $X^2\Sigma^+$ of the molecule LiCa from our article [13]. It describes a data set of more than 2000 lines of the isotopologue $^7\text{Li}^{40}\text{Ca}$ in the quantum number range with $0 \leq v' \leq 19$ having a measurement uncertainty on average of about 0.01 cm^{-1} with a weighted standard deviation of $\sigma = 0.68$. The included long range coefficient C_6 is calculated by the use of formulas from [14] and [15] from the coefficients C_6 and dipole polarizabilities of Li and Ca from [16]. The also included coefficient C_8 is fitted to the fluorescence line data, but since this data only reaches an internuclear distance of 10.27 Å about 80 cm^{-1} below the asymptote and the LeRoy radius for LiCa is 11.4 Å, it is considered to be not very precise for other uses.

The file does not include any information of the observed fine structure splitting, but the eigenvalues $E_{v,N}$ calculated from the potential can be corrected by $E_{v,N,F_1} = E_{v,N} + a_v N$ and $E_{v,N,F_2} = E_{v,N} - a_v(N+1)$ with $a_v = a_0 + bv$, $a_0 = 1.71 \times 10^{-3}$ cm^{-1} and $b = -1.08 \times 10^{-4}$ cm^{-1}.

📄AnalyticalPotential_LiCa_2DoublSigma.pot

The analytical potential for the state $2^2\Sigma^+$ of the molecule ^{7}Li^{40}Ca I have already used for our article [17]. It describes 251 levels in the range $0 \leq v' \leq 2$ with a weighted standard deviation $\sigma = 0.95$. Because of the small quantum number range of observed levels it is precise only in the region directly around the potential minimum. It also does not include coefficients for the observed fine structure splitting, but these coefficients you can find inside the table of Dunham coefficients 📄DunhamCoefficients_LiCa_2DoublSigma.dun.

📄DunhamCoefficients_LiCa_2DoublSigma.dun

These Dunham coefficients for the state $2^2\Sigma^+$ of the molecule ^{7}Li^{40}Ca, I have already used for our article [17], describe the 251 observed levels in the range $0 \leq v' \leq 2$ with a weighted standard deviation of $\sigma = 0.92$.

📄FitData_LiCa_2DoublSigma.fdat

My collection of level energies of the state $2^2\Sigma^+$ of the molecule LiCa which I have derived by adding the frequencies of the observed lines to the ground state level energies calculated from the spline potential in 📄IPA_SplinePotential_LiCa_XDoublSigma.pot.

📄Lines_LiCa_2DoublSigma_XDoublSigma.lines

My collection of thermal emission and fluorescence lines we have observed for the electronic transition $2^2\Sigma^+ \longrightarrow X^2\Sigma^+$.

📄Lines_LiCa_4DoublSigma_XDoublSigma.lines

My collection of fluorescence lines we have observed for the electronic transition $4^2\Sigma^+ \longrightarrow X^2\Sigma^+$.

2.1.4   📁Analysis📁LiSr

📄DunhamCoefficients_LiSr_XDoublSigma.dun

The Dunham coefficients for the electronic ground state $X^2\Sigma^+$ of the molecule ^{7}Li^{88}Sr describe a data set of 435 lines of this isotopologue in the quantum

number range $0 \leq v' \leq 1$ with a weighted standard deviation of $\sigma = 0.50$. The uncertainties of the lines are individually estimated depending on how much they overlap with other lines. The most frequent uncertainties within this data set are 0.005 cm^{-1} (195 lines), 0.02 cm^{-1} (129 lines) and 0.05 cm^{-1} (101 lines). Note the fact, that the available quantum number range is too small to obtain a good estimation for ω_e. The coefficient which is in its value normally very close to ω_e is in the current coefficient set rather close to $G_{1/2}$ (though not exactly $G_{1/2}$).

🗎FitData_LiSr_XDoublSigma.fdat

My collection of line frequencies useful for the fit of the Dunham coefficients for the ground state X$^2\Sigma^+$ of the molecule LiSr. Since I did a separate fit for the ground state I needed differences of frequencies of lines with the same excited states level. Because of this this fit data set does not contain the full list of observed lines from 🗎Lines_LiSr_2DoublSigma_XDoublSigma.lines but only the lines which form groups of at least two lines having the same excited states level.

🗎DunhamCoefficients_LiSr_2DoublSigma.dun

The Dunham coefficients for the state $2^2\Sigma^+$ of the molecule LiSr describe a set of 196 levels of the isotopologue ^{7}Li^{88}Sr in the quantum number range $0 \leq v' \leq 1$ with measurement uncertainties of 0.01 cm^{-1} and 53 outliners removed with its weight from the fit because of clearly visible local perturbations with a weighted standard deviation $\sigma = 1.89$. Note that this data set is more than ever not sufficient to give a good estimation for ω_e and that the observed local perturbations significantly reduce the reached precision in the determination of rotational constants.

🗎FitData_LiSr_2DoublSigma.fdat

My collection of level energies for the electronic state $2^2\Sigma^+$ of the molecule ^{7}Li^{88}Sr. This energies are derived by adding the observed line frequencies to ground state level energies calculated from the set of Dunham coefficients in 🗎DunhamCoefficients_LiSr_XDoublSigma.dun.

🗎Lines_LiSr_2DoublSigma_XDoublSigma.lines

My collection of thermal emission and laser induced fluorescence lines we have observed for the electronisc transition $2^2\Sigma^+ \longrightarrow$X$^2\Sigma^+$ of the molecule ^{7}Li^{88}Sr.

2.2   📁MolSpektAnalysis0_2_7

The evaluation program I developed during the work on my diploma and phd thesises and used to generate the largest part of my results I present in my thesis. It can also be very useful to explore the current data collection.

2.2.1   📁MolSpektAnalysis0_2_7📁Linux_Binary

The Linux executable 📄MolSpektAnalysis I have tested with OpenSuse Leap 42.1, 📄*.atom files containing needed atomic informations as its chemical appreviation, the mass numbers, natural abundancies and core spins of its natural available isotopes, and 📄*.mol files containing links to the other files with collected input data and results relevant for the molecule.

2.2.2   📁MolSpektAnalysis0_2_7📁Windows_Binary

The Windows executable 📄MolSpektAnalysis.exe, the 📄*.dll files needed for the execution of the program, 📄*.atom files containing needed atomic informations as its chemical appreviation, the mass numbers, natural abundancies and core spins of its natural available isotopes, and 📄*.mol files containing links to the other files with collected input data and results relevant for the molecule.

2.2.3   📁MolSpektAnalysis0_2_7📁Source

The source code you can use to build your own binary if you want to modify something or if both of the included executables should not be suited for your system, a 📄README.txt file containing information you should recognize if you want to modify or build the source code, 📄*.atom files containing needed atomic informations as its chemical appreviation, the mass numbers, natural abundancies and core spins of its natural available isotopes, and 📄*.mol files containing links to the other files with collected input data and results relevant for the molecule.

3   The used file formats

Common in most file formats used in my evaluation program which I also use for this data collection are the first two rows: The first row starts with "Source: " and the following space can be freely filled with text. It is ment for information describing the orign of the data included in the file, for example for the journal reference if the important part of the content i.e. the numbers are citations from a publication. The second row starts with "Name: " and must contain an identifier string for the file which should be unique at least for the type of file (📄*.mol, 📄*.atom, 📄*.pot...). If two files with same name and type are loaded at the same time, the evaluation program automatically modifies the name of the second loaded file by adding a "0" to the end if the last character is not the end of a number, if the last character are a number it gets increased by one.

3.1   The molecule file (📄*.mol)

The molecule file holds first of all tables with links to the files relevant for the current analysis regarding the molecule its named after. The first two rows of

the file start with "Atom 1: " and "Atom 2: " followed each by the relative paths of the atom files (📄*.atom) which can be both times the same if the molecule is a homonuclear one as Sr_2. The third row starts with "Reference isotopologue: " followed by an abreviation close to the chemical correct one for the name of the reference isotopologue, i.e. "88Sr2" for $^{88}Sr_2$, or "7Li85Rb" for $^{7}Li^{85}Rb$. The fourth row starts with "name of molecule: " followed by a similar abreviation, i.e. "Sr2".

Next follow the tables, after an empty row and separated by empty rows. Separator for the table columns is each time the string " | ". The first row of each table is a describing head line followed next by a row with column heads and then by the rows with the content. The head lines for the first four tables are "List of term energy tables:", "List of Dunham coefficient sets:", "List of potentials:" and "List of fit datasets:". The column heads are each time the same: "State: | name: | file name: | source:". The "State:" column contains the name identifier for the electronic state the file in the current row is assigned to, the "name:" column the name identifier of the file, the "file name:" column the path of the file relative to the path of the current 📄*.mol file and the "source:" column the source string from the file. The fields of these tables get filled automatically, if the user assigns a file to the electronic state of the molecule and also updated automatically, if a value gets changed while both files are opened or the referenced file gets opened while the molecule file is already opened.

The next two tables have the head lines "List of line tables:" and "List of FCF tables:", of which the second table is always empty, because the feature of writeable FCF tables is not completely implemented. These two tables have both the column heads "Upper state: | lower state: | name: | file name: | source:" with identifiers for two different electronic states, the energetically higher ("upper") and the energetically lower state. Both, flourescence lines and Franck-Condon factors are not specific for a single electronic state but a transition between two electronic states. Despite from this everything mentioned for the four tables above is valid for these two tables, too.

More special are the lowest two tables, the "Table of states:" and "Table of transitions:". The first, the table of states, has the following column heads: "Name: | lambda: | S: | +/- - symmetry: | g/u - symmetry: | Omega: | term energies: | dunham coeff.: | potential: | fit data:". Here contains the first column again the name identifier of the electronic state, the second column the quantum number λ of the electronic state, which can take positive whole-number values or 0, the third column its electronic spin quantum number S, taking depending on the molecule whole-number or half-integral values noted as floating point number. The fourth column can contain a "+" for positive symmetry and a "-" for negative symmetry, the fifth column a "g" for even symmetry and a "u" for odd symmetry and the quantum number Ω in the sixth column again positive integer values or 0. The seventh, eighth, nineth and tenth column contain the relative path to the default term energy table, Dunham coefficient set, potential or fit data set. These default objects are used by the part of the program functions, which does not ask the user which one to take.

The table of transitions has the column heads "State 1: | State 2: | table of lines: | FCF: | Strength:". The first two columns contain here again the name identifiers for the two electronic states involved in the transition, the third column the relative path to the default line table, the fourth column

would contain the one for the default FCF table and the fifth column contains a by the user manually estimateable relative transition strength.

3.2   The atom file (📄*.atom)

The atom file contains the atomic information needed by the evaluation program. Many information in this file is already textbook knowledge, but the important masses of the isotopes are still measured from time to time with more precision. Because of this, the "Source" row here is named "Source of masses:" and contains the journal reference for the isotopic masses. The rows after the "Name:" row are for the symbol and the atomic number of the atom and are named accordingly "Chemical symbol:" and "Atomic number:". After a free row follows the "Table of isotopes:" with the column heads "Number of nuclides | mass [u] | relative abundance | nuclear spin" and table content as the column heads suggest. In contrast to the electronic spin in the table of states of the molecule file the nuclear spin here is coded in integer values, half numbered spins are written with fraction line, e.g. "9/2" for the nuclear spin of ^{87}Sr.

3.3   The term energy file (📄*.term)

The term energy file contains level energies calculated from Dunham coefficients or a potential energy curve needed especially for the assignment of fluorescence, absorption and emmission lines. The source row of this file is named "Source of data:" and after the "Name:" row the large table filling this file directly starts with the column heads "Iso 1: | Iso 2: | component: | v: | J: | term energy:". The two "Iso" columns simply contain the mass numbers of the isotopes, e.g. "84" for ^{84}Sr. The component column contains an integer number in which can be encoded if it is an e or f level or if it is an F_1 or F_2 level. For an electronic state with $\lambda = 0$ and $S > 0$, the value of the component column would be "0" for F_1, "1" for F_2 and so on. If it is an electronic state with $\lambda > 0$ and λ doubling information would be available, the values for the F components would be multiplied by two and a value be added which is 0 for e levels and 1 for f levels. The content of the remaining columns is simply what the label in the column head tells, except that the column J can also contain the value of N, if the latter quantum number should be more appropriate for denoting the rotational energy levels of the current electronic state.

3.4   The Dunham coefficients file (📄*.dun)

The file contains after the "Source:" and "Name:" rows four rows with information about the usability of the current Dunham coefficients. The third row starting with "Max v:" gives a maximum v for the range of level energies which can be safely derived from the coefficient set, the fourth row starting with "Max J:" a maximum J for this range. The fifth row starting with "Error:" contains an uncertainty estimate for the level energies calculated from the coefficients. The sixth row looks typically "Border line points: vp1 = 0, Jp1 = 0, vp2 = 0, Jp2 = 0" and can give a further limit for the range of derivable level energies. It defines two points (v, J) which, if unequal to each other, define a straight line in a picture as the one in figure 5.1 on page 89 of my thesis giving an additional maximum confinement for the range of levels to be calculated.

After a free row starts the "Table of coefficients:" with the column heads "k: | l: | type: | coefficient: | error:". The meaning of the individual coefficients depends here not only on the values of the integers "k" and "l", but even more on their "type". The "error" values are uncertainty estimates derived from the covariance matrix of the linear system of equations which was set up for the fit.

A "type" named "coeff" means, that the coefficient in the row is a standard Dunham cofficient. All these Dunham coefficients together can be used to calculate the level energies by using the well known formula:

$$E_{IvJ} = \sum_{k,l} Y_{kl} \left(\sqrt{\frac{\mu_0}{\mu_I}} \right)^{k+2l} \left(v + \frac{1}{2} \right)^k \cdot \left[J(J+1) - \Omega^2 \right]^l ,\qquad (1)$$

where Y_{kl} is the value from the "coefficient" column and μ_I the reduced mass $\mu = \frac{m_1 \cdot m_2}{m_1 + m_2}$ with m_1 and m_2 the masses of the isotopes of atom 1 and atom 2, respectively, and μ_0 the reduced mass of the "Reference isotopologue" from the molecule file. A difference of my Dunham coefficients to the classical Dunham coefficients is, that the coefficient with $k = l = 0$ is for simplicity the difference between a virtual level with $J = 0$ and $v = -\frac{1}{2}$ (for electronic states with $\Omega = 0$) and the potential minimum of the electronic ground state, so simply the energy offset of the whole coefficient set needed to obtain the correct level energies fitting to the other Dunham coefficients and potentials of this collection.

If in the "type" column the string "adCorr" is used, it means that the current coefficients is an adiabatic correction, a correction to the normal mass scaling done by the factor $\left(\sqrt{\frac{\mu_0}{\mu_I}} \right)^{k+2l}$. In the current implementation it is implemented as a correction to Y_{kl} in equation (1):

$$Y_{Ikl} = Y_{kl} + v_{kl} \left(1 - \frac{\mu_{ref}}{\mu_I} \right) ,\qquad (2)$$

where Y_{Ikl} is a replacement for Y_{kl} in equation (1) and v_{lk} the value from the "coefficient" column.

If in the "type" column the string "ldcorr" is used, it means that the current cofficient is a λ doubling correction which in the current implemention is a energy correction, which is applied as a correction to Y_{kl} in equation (1) for e levels only:

$$Y_{e,kl} = Y_{f,kl} + g_{kl} ,\qquad (3)$$

where g_{kl} is the value from the "coefficient" column and $Y_{f,kl}$ identical to the uncorrected Y_{kl}. It is to note, that it is with the current implementation physically not reasonable to use λ doubling coefficients with $l = 0$, since the λ doubling is caused by a rotational perturbation which has an effect proportional to $J(J+1)$.

The fourth string which can be used in the "type" column is "SpinRot". The use of this string means that the current coefficient describes an energy splitting between fine structure levels F_1 and F_2 of a state of type $^2\Sigma$ caused by a spin-rotation perturbation. It is applied as

$$E_{v,N,F_1} = E_{v,N} + a_{v,N} N$$
$$E_{v,N,F_2} = E_{v,N} - a_{v,N}(N+1) ,\qquad (4)$$

with

$$a_{v,N} = \sqrt{\frac{\mu_0}{\mu_I}} \sum_{k,l} a_{kl} \left(\sqrt{\frac{\mu_0}{\mu_I}} \right)^{k+2(l-1)} \left(v + \frac{1}{2} \right)^k \cdot [N(N+1)]^{l-1} \tag{5}$$

for $l > 0$. "SpinRot" coefficients with $l = 0$ must not be used and would not lead to physically meaningful results. The coefficient a_{kl} is the value from the "coefficient" column and $E_{v,N}$ gets calculated by a variant of equation (1), where J got replaced by N.

3.5   The potential file (📄*.pot)

Of the potential file I have created several different variants for different types of potential representations. Common to all variants is that the text file consists after the obligatory two rows for source and name of one table. In the following I will explain the two variants which I have used most often and which are also used for the current data collection. The first is for the analytical potential energy curve. It has the third row with the column heads: "Column titles: coefficient | value | error | sig. digits". Of the four columns are the first two important and the remaining two often empty. The first contains the name of the potential coefficient or constant in ascii representation and the second its value. The potential energy curve ($V(R)$) is defined by three different functions ($V_c(R)$, $V_i(R)$ and $V_o(R)$) valid in different internuclear distance ranges. The $V_c(R)$ is valid in the range $R_i \leq R \leq R_a$ and is defined as follows:

$$V_c(R) = T_m + \sum_{n=1}^{N} a_n \xi(R)^n \tag{6}$$

with

$$\xi(R) = \frac{R - R_m}{R + bR_m}. \tag{7}$$

The $V_i(R)$ is valid in the range $R \leq R_i$ and is defined as

$$V_i(R) = A + \frac{B}{R^s} \tag{8}$$

and the $V_c(R)$ is valid in the range $R_a \leq R$ and defined as

$$V_a(R) = U_\infty \pm E_{exch}(R) - \sum_{n}^{n} \frac{C_n}{R^n} \tag{9}$$

with

$$E_{exch}(R) = A_{exch} R^\alpha e^{-\gamma R}. \tag{10}$$

The following table shows which ascii representation belongs to which coefficient or constant:

coefficient	ascii
a_*	a* [cm^-1]
b	b
R_m	Rm [A]
T_m	Tm [cm^-1]
R_i	Ri [A]
s	n
A	A [cm^-1]
B	B [cm^-1 A^s]
R_o	Ra [A]
C_*	C* [cm^-1 A^*]
U_∞	U infinity [cm^-1]
A_{exch}	A_ex [cm^-1 A^γ]
γ	gamma
α	beta [A^-1]

The "*" is here a replacement for an integer > 0, "s" and "γ" in the right column must be exchanged by the respective values of these constants. The names of some of the coefficients and constants where changed some time ago, "n" got "s" and "β" got "α", but their ascii representations in the potential file were kept unchanged. "A_{exch}", "γ" and "α" are missing in most potential files which means that the exchange interaction was not found to be important for the affected potential descriptions.

The second potential representation I want to describe here is the IPA spline potential. The file format I use for these potentials has the third row "Column titles: R [A] | E [cm^-1] | d^2E/dR^2". Each row of the table contains one spline point, the first column the internuclear distance, the second column the energy and the third column the for the reconstruction of the splines also important second derivative of the energy. These points can be used to reconstruct the potential function V_s (applying [18]) by:

$$V_s(R) = A_j(R)V_j + B_j(R)V_{j+1} + C_j(R)V_j'' + D_j(R)V_{j+1}'' \tag{11}$$

with

$$A_j(R) = \frac{R_{j+1} - R}{R_{j+1} - R_j} \tag{12}$$

$$B_j(R) = \frac{R - R_j}{R_{j+1} - R_j} = 1 - A_j(R) \tag{13}$$

$$C_j(R) = \frac{1}{6}(A_j(R)^3 - A_j(R))(R_{j+1} - R_j)^2 \tag{14}$$

$$D_j(R) = \frac{1}{6}(B_j(R)^3 - B_j(R))(R_{j+1} - R_j)^2 \tag{15}$$

and R_j the internuclear distance of the jth spline point, V_j its energy and V_j'' its second derivative of the energy. Of this IPA spline potential exist again two different variants. In my own interpretation I use the functions $V_i(R)$ and $V_o(R)$ from the analytical potential description for the extrapolation to smaller and larger internuclear distances, respectively, and calculate the second derivatives of the energy in the way that the first derivative of the potential energy function

at the first spline point matches the first derivative of the energy of the function $V_i(R)$ at this internuclear distance and the first derivative at the last spline point matches that of the function $V_o(R)$ at that point.

The second variant developed earlier by a collaboration partner uses natural splines where the second derivatives of the spline function are set to 0 at the first and the last spline point. The function $V_i(R)$ is not used here and the transition point to the long range function $V_o(R)$ starts at the point R_o which is at a significantly smaller internuclear distance than the last spline point.

The ascii representations for the coefficients of the functions $V_i(R)$ and $V_o(R)$, which are located directly subsequent to the table of spline points, are in the file format of the spline potentials a little different compared to the file format of the analytical potentials, as the following table containing the ascii representations in the spline potential files shows:

coefficient	ascii
s	iExp
A	iA
B	iO
R_o	R_o
C_*	C_*
U_∞	U_inf

The constant "s" is missing in some potential files using $V_i(R)$, in these cases the default value of $s = 6.0$ is used.

Some of the potential files in the current collection contain an adiabatic correction, a correction to the Born-Oppenheimer approximation. The adiabatic correction used here ($V_{ad}(R)$) which has to be added to the potential energy function $V(R)$ of the affected isotopologue, is defined as follows:

$$V_{ad}(R) = \left(1 - \frac{M_{ref}}{M}\right)\left(\frac{2R_m}{R + R_m}\right)^n \sum_i v_i \xi^i . \tag{16}$$

The v_* (v_i) have in the file the ascii representations "AdCorr*" with "*" integers starting from 0. The masses M and M_{ref} are, depending on the parameter called in the files "Type AdCorr", either isotopic masses of one of the atoms of the molecule, or reduced masses of the isotopologues of the molecule. The values of "Type AdCorr" of 1 or 2 mean, that the isotopic masses of atom 1 or atom 2 has to be used, respectively, while the value of 3 stands for the reduced masses of the molecule. The constant n is named in the files "Pow AdCorr". The function ξ is the function $\xi(R)$ from V_c of the analytical potential. In the two rows after "Pow AdCorr" are constants "RIso1AdCorr" and "RIso2AdCorr" which give the isotopic masses for atom 1 and atom 2, respectively, which have to be used to determine M_{ref}. In the file of a spline potential two further rows are following containing the constants "AdCorr b" and "AdCorr Rm" which are the constants R_m and b, respectively, to use for the calculation of $V_{ad}(R)$ with $\xi(R)$. For analytical potentials the constants R_m and b from $V_c(R)$ are used.

3.6   The fit data file (📄*.fdat)

The fit data file holds line frequencies and/or level energies collected for fitting potentials or Dunham coefficients together with the residuals of the fit it was

last used for. After the source row and the name row it has a row starting with
"Max v:" and then a row starting with "Max J:" which hold the maximum
vibrational and rotational levels to use for the next fit, respectively. The fifth
row contains with "Column titles: Iso v J v' J' Source Prog File Energy uncert.
obs-calc DevR" already the column heads of the table filling most of the fit data
file. In contrast to the most other file formats in this data collection, the fit
data file uses tabulators as column delimiters.

The first column called "Iso" contains the number internally used in the eval-
uation program to identify an isotopologue. The following tables gives the trans-
lations of the identifying number to a human readable value for the molecules
data is contained in the current collection:

Sr$_2$:

number	translation
0	^{84}Sr$_2$
1	^{84}Sr^{86}Sr
2	^{84}Sr^{87}Sr
3	^{84}Sr^{88}Sr
4	^{86}Sr$_2$
5	^{86}Sr^{87}Sr
6	^{86}Sr^{88}Sr
7	^{87}Sr$_2$
8	^{87}Sr^{88}Sr
9	^{88}Sr$_2$

LiRb:

number	translation
0	^{7}Li^{85}Rb
1	^{7}Li^{87}Rb
2	^{6}Li^{85}Rb
3	^{6}Li^{87}Rb

LiCa:

number	translation
0	^{7}Li^{40}Ca
1	^{7}Li^{42}Ca
2	^{7}Li^{43}Ca
3	^{7}Li^{44}Ca
4	^{7}Li^{46}Ca
5	^{7}Li^{48}Ca
6	^{6}Li^{40}Ca
7	^{6}Li^{42}Ca
8	^{6}Li^{43}Ca
9	^{6}Li^{44}Ca
10	^{6}Li^{46}Ca
11	^{6}Li^{48}Ca

	number	translation
	0	$^{6}\text{Li}^{84}\text{Sr}$
	1	$^{6}\text{Li}^{86}\text{Sr}$
	2	$^{6}\text{Li}^{87}\text{Sr}$
LiSr:	3	$^{6}\text{Li}^{88}\text{Sr}$
	4	$^{7}\text{Li}^{84}\text{Sr}$
	5	$^{7}\text{Li}^{86}\text{Sr}$
	6	$^{7}\text{Li}^{87}\text{Sr}$
	7	$^{7}\text{Li}^{88}\text{Sr}$

Note that the default numbering starts with the light isotopes of each atom as it is visible for Sr_2 and LiSr. For LiRb and LiCa I changed the order, because a colaboration partner started the analysis using a different numbering and I did not want to produce confusion by keeping my own.

The second column has at his head the string "v" and the third "J". They contain the vibrational and rotational quantum numbers of the electronic state the energy level or fluorescence line is assigned to, respectively. The fourth and the fifth column have the headings "v" and "J", respectively. These columns contain the quantum numbers indicated by their names only if the current row contains a fluorescence line of a decay to our electronic state the fit data set is assigned to. If the electronic states involved in the transition have a spin quantum number $S > 0$ the numbers shown in the fourth column can be $v' + 1000$ if the involved levels are F_1 levels, $v' + 2000$ if they are F_2 levels, and so on. The content of this column can also be not a number. In the case the row contains not a fluorescence line, but an energy level which is derived from accumulated information of several lines which have the same excited states level common, so our electronic state the current fit data file is assigned to is an excited electronic state, this quantum number v' is already the quantum number given as v in the second column. In this case simply the string "TE" is given in the fourth column. This column can also contain the string "nA", indicating that the quantum number of the line in the current row is currently not assigned to an excited states level. Even if in the current row is an energy level, the value of J' in the fifth column is needed to identify, if it is an e or an f level. Because of this, it contains for energy levels indicated by "TE" in the fourth column the value $J + 1$ or J with J the value from the third column, wether it is an e or f level, respectively.

The sixth column has the head "Source" and contains the name of the line table if the line in the row is derived from a line table or the name of the absorption spectrum if it is an energy level directly derived from the absorption spectrum. If the line or the level is a citation it can also contain the names of the authors of the publication our the full journal reference. The seventh column having the head "Prog" contains the progression number from the line table if in the current row is a line from a line table or is empty otherwise. The eighth column "File" contains the path to the spectrum file the line or level energy is derived from or the second part of a journal reference. The nineth column "Energy" contains the level energy of the energy level in cm^{-1} or the line frequency of the line if it is a line, also in cm^{-1}. The tenth column "uncert." contains the uncertainty of the level energy or line frequency [cm^{-1}]. The eleventh column "obs-calc" contains the *obs-calc* value [cm^{-1}] from the last fit the current fit data file was used for, where *obs* is the value from the nineth

column and calc the value derived for the level/line at the end of the fit. The dimensionless value "DevR" in the twelvth and last column is calculated by dividing the *obs-calc* value from the eleventh column by the uncertainty value from the tenth column.

If the fit data file contains close to its end a row with the text "SourceOffsets:", it means that the following row(s) contain a small table with defined offsets for special source files. The first column of this table contains the name of the source as it is also used in the sixth column of the main table for the affected rows, and the second column the offset which gets subtracted from the level energies or line frequencies before they get used for a fit. Such offsets occur, because in most of the recorded spectra the absolute frequencies are significantly less precisely measured[1] as the frequencies within a spectrum relative to each other. The appearing offset of a spectrum can be determined from the average deviations the energies/frequencies from this source have compared to the ones derived from other sources if the number of level energies or line frequencies from this spectrum is high enough to be statistically relevant or if the spectrum contains with good signal to noise ratio lines which are already precisely known from the literature, e.g. atomic lines.

3.7   The line table file (📄*.lines)

The line table file contains usually the lines assigned to the electronic transition the line table is assigned to. After the source and the name row it contains the row with the column heads for the table filling the remaining file: " PN vo Jo vu Ju FC Eout err Iso File SNR deviation comment". This file has also a special column delimiter, here spaces are used and most columns have a fixed size. The first column with the head "PN" and a with of five characters contains the progression number used to identify lines belonging to the same progression and to distinguish between lines from different progressions. The next five columns have all a width of four characters. The first four of this five having the heads "vo", "Jo", "vu" and "Ju" contain the quantum numbers v', J', v'' and J'', respectively. A value of -1 in one of these columns means unassigned. The sixth column having the head "FC" contains a number indicating the finestructure component of the involved ground state level, -1 if the electronic ground state has no fine structure splitting. The number used for a certain fine structure component differs from molecule to molecule. For LiCa a value of 2 means F_1 and a value of 3 means F_2, while all other values mean that the affected line did not get assigned to a certain fine structure component, for LiSr means a value of 0 F_1 and 1 F_2 while only -1 would mean unassigned. The molecules LiRb and Sr_2 have no fine structure splitting in the electronic ground state.

The seventh column with the width of 15 characters and the head "Eout" contains the line frequency in cm^{-1}, the eight column with the head "err" and a width of ten characters its uncertainty, in cm^{-1}, too. The nineth column with the head "Iso" and a width of five characters contains an identifier number for the isotopologue, if the line can be unhesitatingly used for fitting it is simply the number used in the fit data file increased by one and then multiplied by ten.

The tenth column "File" with a variable with contains the path to the spectrum the line is originating from or only its name. The eleventh column "SNR"

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[1]In the spectra recorded for the current work its a factor of ten, according to the specification of the used instrument.

is filled with automatically estimated signal to noise ratios of the lines. The twelveth colum "deviation" contains distance or deviation values originating from the fully or partially automated assignment routines. The precise meaning depends on the used routine which is not indicated in the current file. Because of this the exact meaning is partially unknown and thus the content of this column should be considered as irrelevant since anyway not important. The thirtheenth and last column has again a variable width, the head "comment" and contains mostly automatically generated additional information about the line. A comment "overlap" means, that the according line overlaps with other lines and the frequency cannot be estimated as precise as for other lines because of that. The comment "laser" means that the line matches the laser excitation. These laser lines can often also not be measured very precise, because of the scattered laser light intruding the spectrometer from various angles. A comment "satellite" means, that the line is a collisional induced satellite of a laser induced fluorescence (LIF) line.

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