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Electronic structure with dipole moment and ionicity calculations of the low-lying electronic states of the ZnF molecule

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Abstract

Adiabatic potential energy curves of the 28 low-lying doublet and quartet electronic states in the representation $^{2s+1}\Lambda^{(\pm)}$ of the zinc monofluoride molecule are investigated using the complete active space self consistent field (CASSCF) with multi-reference configuration interaction MRCI method including single and double excitations with Davidson correction (+Q). The internuclear distance R_e , the harmonic frequency ω_e , the static and transition dipole moment μ , the rotational constant B_e and the electronic transition energy with respect to the ground state T_e are calculated for the bound states. The transition dipole moment between some doublet states is used to determine the Einstein spontaneous A_{21} and induced emission B_{21}^ω coefficients as well as the spontaneous radiative lifetime τ_{spont} , emission wavelength λ_{21} and oscillator strength f_{21} . The ground state ionicity q_{ionicity} and equilibrium dissociation energy $D_{e,e}$ are also computed. The comparison between the values of the present work and those available in the literature for several electronic states shows very good agreement. Twenty-three new electronic states have been studied in the present work for the first time.

1. Introduction

Though transition metal halides are not an easy target for structure determination, their study has received the attention of several theoretical and experimental researchers especially in the field of high temperature chemistry.¹ Under ordinary conditions most of them are crystals whose molecular forms can only be found in the gaseous phase. With full subshells, the zinc element of group IIB is a transition element of many unique characteristics due to the weak metallic bonding of the $4s^2$ electrons. The complexity of its diatomic halide systems makes theoretical spectroscopic investigations quite interesting; they can be used as guidance for further experimental work and may contribute in the advancement of high energy studies. Among the zinc monohalide species, ZnF and ZnCl have been the subject of many experimental and theoretical studies, but few included their excited states. Rochester and Olsson² analyzed an ultraviolet absorption spectrum of ZnF and reported the ground state vibrational frequency $\omega_e=628\text{ cm}^{-1}$ and its anharmonicity correction $\omega_e x_e=3.5\text{ cm}^{-1}$. For the same state, Moravec *et al.*³ determined $\omega_e=620\text{ cm}^{-1}$ from photoelectron spectrum of the ZnF⁻ anion and concluded that the $A^2\Pi$ state should lie at more than 21697 cm^{-1} . As a first gas-phase spectroscopic investigation, Flory *et al.*⁴ recorded the pure rotational spectrum of the ZnF radical using millimeter/submillimeter direct absorption techniques from which the spectroscopic constants of several isotopologues in the ground state are measured. They also estimated the ground state dissociation energy D_E and approximated the energy of the $A^2\Pi$ state. Theoretically, Bowmaker and Schwerdtfeger⁵ were first to carry out an *ab-initio* calculation using a modified version of Pople's SCF program GAUSSIAN 86. They reported the ground state equilibrium bond length, dissociation energy and force constant of the four diatomic zinc halides. Also for the ground state, the theoretical work of Liao *et al.*⁶ determined the constants R_e and ω_e of the ZnF free radical using the relativistic corrected local density methods. Boldyrev and Simons⁷ optimized those constants for the two lowest electronic states using analytical gradients and polarized split valence basis sets of 6-331++G(d,f) quality using different theoretical methods. Their calculations have shown that the ground state is strongly bound whereas the $^2\Pi$ state is a van der Waals complex. Few years later, Belanzoni *et al.*⁸ reported the bond distances for several molecules including ZnF molecule by using the density functional approach with the zero order regular approximation (ZORA) method. Based on the assumption that calcium is a pseudo-transition metal, Harrison *et al.*⁹ suggested that ZnF and CaF should have similar bonding properties. They studied the bonding characteristics of the zinc monofluoride system at the RCCSD(T) level and reported

$R_e=1.775 \text{ \AA}$ and $\omega_e=633 \text{ cm}^{-1}$ for its ground state. Hayashi *et al.*¹⁰ employed the multi-reference configuration interaction method with Davidson correction (MRCI+Q) to plot the adiabatic potential energy curves (PECs) and the dipole moment curves (DMCs) of several low-lying doublet and quartet electronic states. The spectroscopic constants R_e , ω_e , T_e and the absolute value of the dipole moment μ of 5 low-lying doublet states were reported. Lately, the two lowest excited $^2\Pi$ state of this molecule had been diabaticized in order to simulate the $^2\Pi \leftarrow X^2\Sigma^+$ vibronic spectrum using a wavepacket propagation technique and to study the predissociation of the $A^2\Pi$ state.¹¹ In this work, we employed the *ab-initio* method to plot the potential energy curves (PECs) and the static dipole moment curves (DMCs) of 28 low-lying doublet and quartet electronic states of ZnF molecule. The spectroscopic constants as the equilibrium internuclear distance R_e , the harmonic frequency ω_e , the vibrational constant B_e , the transition energy with respect to the ground state minimum T_e and the permanent dipole moment μ are calculated for the bound states. The ground state ionicity q_{ionicity} and dissociation energy D_E are also estimated using the obtained constants. The transition dipole moment between some doublet low-lying states is studied and employed to determine some emission coefficients as the Einstein spontaneous coefficient A_{21} , the spontaneous radiative lifetime τ_{spont} , the wavelength λ_{21} and the oscillator strength f_{21} .

2. Computational approach of the *ab-initio* calculations

Considering the complete active space self-consistent field (CASSCF) wave functions as reference, the calculations have been performed using the multi-reference configuration interaction (MRCI) method with Davidson correction (+Q), single and double excitations, as applied in the computational chemistry program MOLPRO¹² and taking the advantage of the graphical user interface GABEDIT.¹³ From the basis set library of the program, the neutral fluorine atom with two core electrons is treated using the ECP2SDF basis set where the 7 valence electrons are described by the associated $(4s4p)/[2s2p]$ basis sets. The neutral zinc atom with 30 electrons is treated via the energy-consistent ECP10MDF basis set as a system of 10 core electrons where the remaining 20 electrons are described by the energy optimized $(12s12p9d3f2g)/[6s6p4d3f2g]$ valence basis sets.¹⁴ Both effective core potentials consider quasi-relativistic level of theory. The quality of the selected basis sets is checked by comparing our CI calculations for the ground and several excited states of isolated zinc and fluorine atoms to the experimental data in NIST Atomic Spectra Database.¹⁵ The ionization potential of Zn and the electron affinity of F are calculated by comparing the ground state

atomic and ionic energies. The calculated values, 9.653 eV for Zn and 3.487 eV for F are in accordance with those obtained experimentally with the relative differences 2.75% and 2.54% respectively. Among the 39 electrons considered for the zinc mono-halide molecule (30 electrons for Zn and 9 for F), 12 electrons are treated within the core and the wavefunctions of 27 electrons are to be determined. The $3s$, $3p$ and $3d$ orbitals of Zn and the $2s$ orbital of F are kept doubly occupied and frozen in the subsequent calculations so that seven valence electrons are explicitly treated. The active space contains at least 6σ (Zn: $4s$, $4p_0$, $5s$; F: $2p_0$, $3s$, $4s$) and 2π (Zn: $4p_{\pm 1}$; F: $2p_{\pm 1}$) orbitals in the C_{2v} symmetry group distributed into irreducible representations a_1 , b_1 , b_2 , and a_2 in the following way $6a_1$, $2b_1$, $2b_2$, $0a_2$ noted by [6, 2, 2, 0]. In the range of the internuclear distance R around the equilibrium position of its ground state, the ZnF molecule is assumed to be mainly ionic. As function of R , the potential energy curves and static dipole moment curves of the doublet and quartet states in the representation of $^{2s+1}\Lambda^\pm$ have been calculated for 116 internuclear distances in the range $1.41\text{ \AA} \leq R \leq 4.8\text{ \AA}$.

3. Results and discussion

The calculations enabled the investigation of 14 low-lying doublet (five $^2\Sigma^+$, two $^2\Sigma^-$, two $^2\Delta$ and five $^2\Pi$) and 14 quartet electronic states (five $^4\Sigma^+$, two $^4\Sigma^-$, two $^4\Delta$ and five $^4\Pi$). Their PECs and DMCs are plotted as function of the internuclear distance R as shown in Figures (SM.1 - SM.6). Their numerical data is also provided as supplementary material [SM: B) Numerical data]. Among these states, 19 are found bound. The energy data around the equilibrium position is fitted into a polynomial in terms of the internuclear distance R in order to calculate the spectroscopic constants R_e , T_e , ω_e and B_e . These calculated constants together with the experimental and theoretical values available in literature are given in Table 1. The ground state, which is the most notably investigated electronic state of ZnF in literature, is determined to be $^2\Sigma^+$ state similar to the other zinc monohalides.¹⁶ Its calculated equilibrium bond length $R_e=1.802\text{ \AA}$ is in very good agreement with all the previously reported values, experimentally and theoretically, where the relative difference ranges between $(0.17\%) \leq \Delta R_e / R_e \leq (2.27\%)$.^{8,11} The spectroscopic constants $\omega_e=627.1\text{ cm}^{-1}$, $B_e=0.3501\text{ cm}^{-1}$ and $\alpha_e=2.690 \times 10^{-3}\text{ cm}^{-1}$ show reasonable agreement when compared to the most recent experimentally obtained values⁴ where the relative differences are 0.62%, 4.97% and 8.30% respectively. The calculated ground state vibrational frequency ω_e is 0.14% close to the value of $\omega_e=628\text{ cm}^{-1}$ obtained from UV absorption spectrum analysis.² The anharmonicity

correction $\omega_e x_e = 3.8 \text{ cm}^{-1}$ is also compared to the so far determined values, 3.5 cm^{-1} , 2 cm^{-1} , 4 cm^{-1} , 3.2 cm^{-1} and 2.8 cm^{-1} , available in literature.^{2-4,10,11}

The early experimental work of Rochester and Olsson have assigned a doublet splitting for the ${}^2\Pi \leftarrow {}^2\Sigma^+$ transition at 36975 cm^{-1} and 37399 cm^{-1} . Consistently, the photoelectron spectrum of the ZnF^- anion³ showed that no additional spectrum in the electronic structure of ZnF is obtained below 21697 cm^{-1} and that the first ${}^2\Pi$ state should lie higher. However while analyzing the second-order spin-orbit coupling for ZnF and considering the $A^2\Pi$ state as the main perturber to the ground state, the energy of the excited state is approximated to be 20400 cm^{-1} .⁴ The theoretical calculations of the lowest states of ZnF at the QCISD level⁷ reported that the lowest ${}^2\Pi$ state is a van der Waals complex whose minimum at $4.509 \text{ \AA}$ and $T_e = 22044 \text{ cm}^{-1}$ whereas RCCSD(T) calculations⁹ concluded that this state is an isolated one characterized by $T_e = 37344 \text{ cm}^{-1}$ at $1.757 \text{ \AA}$ and correlated with the second asymptote. Motivated by the wide range of the reported transition energy values T_e for the lowest ${}^2\Pi$ state of ZnF , a quasi-diabatic study at the MRCI level of theory has been carried out¹¹ at the region of 36300 cm^{-1} above the ground state in order to optimize a previous adiabatic study in which the electronic structure and the spectroscopic constants of few low-lying states were calculated within MRCI+Q method.¹⁰ The procedure lead to two ${}^2\Pi$ states; a repulsive one reaching the first dissociation limit and a bound one associated with the second limit. In this work, though the first ${}^2\Pi$ state that correlates with the first asymptote describes a very shallow PEC with minimum energy of $T_e = 19611 \text{ cm}^{-1}$ at $3.831 \text{ \AA}$ indicating a nearly dissociative nature; yet this state supports very few vibrational levels ($v=0,1,2$). However, the calculations predict that the transitions to this state are almost negligible (see the discussion of the transition dipole moment below). The shoulder of the first ${}^2\Pi$ state at the avoided crossing region with a higher ${}^2\Pi$ state at $1.83 \text{ \AA}$ yields a vertical excitation of 36247 cm^{-1} at the equilibrium geometry of the $X^2\Sigma^+$ state. A transition energy of $T_e = 37515 \text{ cm}^{-1}$ at $R_e = 1.884 \text{ \AA}$ of the $(2) {}^2\Pi$ state is in excellent agreement with the values existing in literature as the relative difference ranges between $(0.31\%) \leq \Delta T_e / T_e \leq (4.61\%)$.^{9,10}

In the absence of experimental data apart from the states discussed above, the spectroscopic constants of all other states, given in Table 1, are predictions that may guide future experiments concerning the low-lying excited states of ZnF molecule. The interaction of the $(2) {}^2\Sigma^+$ state with the ground state at the region near $2.523 \text{ \AA}$ results a well whose minimum corresponds to a transition energy of $T_e = 31091 \text{ cm}^{-1}$ and vibrational frequency $\omega_e = 326.2 \text{ cm}^{-1}$.

Such transition has received significant attention among the other zinc monohalides ever since the demonstration of the ZnI lasing.¹⁷ Our spectroscopic constants of the excited $^2\Sigma^+$ states are compared to those computed theoretically.^{10,11} Although diabatic approximation has yielded better vibrational frequency of the $(2)^2\Pi$ state, reasonable agreements are shown for the other constants. The PEC of each of the $(3)^2\Sigma^+$, $(4)^2\Sigma^+$ and $(5)^2\Sigma^+$ states interacts in turn with a lower and a higher $^2\Sigma^+$ state showing successive positions of avoided crossing as listed in Table 2. Such behavior leads to difficulty in accurate descriptions near the vicinity of these positions. Several crossing points take place between the PECs of the different doublet states as they exist at close energy levels. Table 2 shows these crossing points as well.

Relying on the good accordance obtained so far with literature for the doublet states of ZnF molecule, we were motivated to advance towards its quartet states. For the first time, the PECs of 8 quartet states are plotted as shown in Figure (SM.2). The spectroscopic constants of 7 bound quartet states are given in Table 1. The PECs of the $(1)^4\Sigma^+$, $(1)^4\Delta$ and $(1)^4\Sigma^-$ states are found in this work to be bound with shallow minima at 2.762 Å, 2.956 Å and 3.142 Å, respectively. These shallow electronic states, however, support few vibrational levels whose eigenvalues E_v , the rotational constants B_v , the centrifugal distortion constants D_v , the abscissas of the turning points $R_{\min}$ and $R_{\max}$ and some calculated wavelengths of possible vibronic transitions are given in Table (SM.3) in the supplementary material (SM: C).

With two ways to specify the dissociation energy, the zero point energy $D_{E,v=0}$ and the equilibrium dissociation energy $D_{E,e}$ can be estimated in terms of the molecular spectroscopic constants.¹⁸ Our value of $D_{E,e}=73.9$ kcal/mol has yielded $D_{E,v=0}=73.0$ kcal/mol. An excellent agreement is shown when the calculated equilibrium dissociation energy is compared to the values available in literature. The relative differences are 1.39%, 0.14%, 4.43% and 7.99% with respect to the values of 72 kcal/mol, 72.9 kcal/mol, 69.9 kcal/mol and 67.6 kcal/mol respectively.^{4,9,10,7} This agreement deteriorates upon comparison with the values of 50.2 kcal/mol and 46.8 kcal/mol reported from MP2 and CISDSD methods.⁵

Since the strength of the vibrational excitations depends on the variation of the dipole moment as function of geometry,¹⁹ the static dipole moment of the considered states is calculated and plotted as function of the internuclear distance R (Figures SM.3-6). With the zinc atom at the origin, the sign convention is defined such as the negative value corresponds to the $\text{Zn}^{\delta+}\text{F}^{\delta-}$

polarity. The curves will be mainly used here to indicate the bond nature, the polarity and interaction of the states. The DMC of the ground state presents negatively increased values with the largest magnitude $|\mu|=1.61$ a.u. near $R=2.31$ Å. The electric dipole moment curve shows a nearly linear trend close to the equilibrium position R_e for this ground state. One can understand the behavior of a bond from such curve by using the Paccinioni *et al.*²⁰ method: For two charges $+q$ and $-q$ separated by a distance R , the dipole moment is a straight line if the compound formed by the two charges is ionic, and curved if the compound has a dominating covalent character. This idea was quantified as the following: If $\mu = -q \times R$, then $\partial\mu/\partial R = -q$, the larger value of q , the more ionic charge (except in some case of polarization effects) and $\partial^2\mu/\partial R^2$ is closer to zero as the ionicity increases. In our case, $\partial\mu/\partial R = -1.48$ a.u./Å and $\partial^2\mu/\partial R^2=1.1$; the negative linear slope of value -1.48 confirms the presence of the ionic character of ZnF bond of the ground state, and the value 1.1 of the curvature indicates also a covalent nature of the same bond. This mixed nature has been confirmed experimentally by Flory *et al.*,⁴ who through the evaluation of hyperfine parameters has confirmed that ZnF is an ionic species, but with some covalent character. Another parameter that helps to quantify the nature of a molecular bond is the electric dipole moment charge, or the ionicity of a molecule defined as $q_{\text{ionicity}} = \mu/eR_e$.²¹ This quantity describes the fraction of ionic character of a molecular bond.^{22,23} We calculate the ionicity of the ZnF molecule by applying the formula given above for the ground state at its equilibrium distance R_e . The dipole moment μ and internuclear distance R_e are defined from the potential energy and dipole moment curves, Figures (SM.1, SM.3), at the equilibrium position. The comparison of the calculated value of the ionicity $q_{\text{ionicity}} = \frac{\mu}{eR_e} = 0.32$ for the ground state with other data

available in literature shows an overall good agreement (Table 3) which confirm the mixed nature (ionic/covalent) of the bond. At large internuclear distances where the molecule dissociates into its natural fragments, the dipole moment is expected to approach zero smoothly which is the case for the investigated states. However, the significant increase in the absolute dipole moment value of $(4)^2\Sigma^+$ state at distances between 3.4 Å and 6.4 Å points out a polarized state at this region where the fluorine atom strongly attract the bonding electrons. But upon extending the calculations to larger internuclear distances, the dipole moment possesses quasi-zero values at $R>8$ Å. The abrupt gradient change of the DMCs can be related to the occurrence of an avoided crossing between the PECs of two states of the same symmetry. At this region, the wavefunctions of these states will mix with each other to give

two adiabatic solutions such that the corresponding PECs do not cross. The DMCs mirror this region as a sharp change in their slopes indicating a reversed polarity of the atoms as for $(1)^2\Pi$ -(2) $^2\Pi$ at 1.83 Å and $(2)^2\Sigma^+$ -(3) $^2\Sigma^+$ at 1.68 Å. The behavior of the dipole moment of the $(5)^2\Sigma^+$ state between 1.86 Å and 1.77 Å is referred to its non-crossing interaction with a higher and a lower $^2\Sigma^+$ states successively. The validity of excited states calculations may be confirmed by noticing the agreement between regions of anti-crossing of two PECs and the crossing of their corresponding DMCs. Those positions are marked by dashed ovals on the DMCs.

Moreover, calculations of the PECs and DMCs show another importance for heteronuclear diatomic molecules as they allow noticing the non-zero permanent dipole moment at the equilibrium geometry (given in Table 1) which indicates the unequal distribution of electrons between the two nuclei. As a result, there can be a small excess of negative charge near one of the atoms and thus the molecule in this state is said to be a polar molecule. Polar molecules can be manipulated by external electric fields, allowing for the control of elementary chemical reactions at very low temperatures. There are several applications of such molecules in the physics of ultra-cold molecular gases. For example, the long-range electric dipole-dipole interaction between two polar molecules can significantly modify the many-body dynamics of trapped ultra-cold molecular Bose Einstein Condensates. For such application and others, it is known that the knowledge of the permanent or transition dipole moments is essential.²⁴ Therefore, the transition dipole moment curves (TDMs) between some doublet states are investigated and plotted in Figures (SM.7, SM.8). These curves are considered important as they can be very useful in designing the photoassociation experiments for a molecule²⁵ and helpful to predict transitions. Using the transition dipole moment value between two states μ_{21} at its equilibrium position of the upper state, we calculated the Einstein coefficient of spontaneous emission A_{21} from which the spontaneous radiative lifetime τ_{spont} , the Einstein coefficient of induced emission B_{21}^ω , the corresponding emission cross section σ_0 , the classical radiative decay rate of the single-electron oscillator at the emission frequency γ_{cl} and the emission oscillator strength f_{21} are determined by applying the following formulas:²⁶

$$\omega_{21} = 2 \pi \nu_{21}$$

$$A_{21} = \frac{2 \omega_{21}^3 \mu_{21}^2}{3 \epsilon_0 \hbar c^3}$$

$$\tau_{\text{spont}} = \frac{1}{A_{21}}$$

$$B_{21}^{\omega} = \frac{\pi^2 c^3 A_{21}}{\hbar \omega_{21}^3}$$

$$\sigma_0 = \frac{g_2 \lambda_{21}^2 A_{21}}{4 g_1}$$

$$\gamma_{cl} = \frac{e^2 \omega_{21}^2}{6 \pi \epsilon_0 m_e c^3}$$

$$f_{21} = \frac{-A_{21}}{3 \gamma_{cl}}$$

where ν_{21} is the transition frequency between the two states, h is Plank's constant, ϵ_0 is the vacuum permittivity, c is the velocity of light and g_1 and g_2 are the degeneracy factor of the lower and upper state, respectively, as indicated from the multiplicity and by neglecting the rotational and vibrational factors such that:²⁷

$$g_L = \begin{cases} (2S + 1) & \text{if } \Lambda = 0 \\ 2(2S + 1) & \text{if } \Lambda \neq 0 \end{cases}$$

The calculated constants are given in Table 4. It can be deduced that the intensity of some transitions is neglected as for the transitions from the $(1)^2\Delta$ and $(1)^2\Sigma^-$ states where $|f_{21}| < 10^{-4}$ is very small when compared to those of the experimentally verified transitions, i.e., $X^2\Sigma^+-(2)^2\Sigma^+$ and $X^2\Sigma^+-(2)^2\Pi$. It is also clear that most of these transitions take place in the ultraviolet region. As for the TDMCs, the sudden changes and jumps, that appear at different internuclear distances, can be explained either by the existence of avoided crossings between the potential energy curves at these particular distances ($(1)^2\Pi^+/(2)^2\Pi^+$, Figures (SM.1, SM.4)) or referred to a strong interaction of the covalent state with the ion-pair state (responsible for the electron transfer) and to the change of sign of the electronic wavefunctions around these internuclear distances. The curves as well as the corresponding numerical data of the TDMs between different electronic states in terms of the internuclear distance R are given as supplementary material in [SM: A), B)].

4. Conclusion

Using the *ab-initio* method as implemented in the MRCI+Q calculations, we have investigated the adiabatic potential energy curves and the dipole moment curves for 14 doublet and 14 quartet low-lying electronic states of ZnF molecule considering 7 valence electrons. The plots of these curves have been represented and the spectroscopic constants R_e , ω_e , T_e , and B_e are determined for 19 bound states. The ionicity q_{ionicity} and the equilibrium dissociation energy $D_{e,e}$ of the $X^2\Sigma^+$ state are also computed. The comparisons with the available low-lying theoretically plotted curves provide almost perfect agreement. The bond of the ground state is confirmed to be of mixed nature (ionic/covalent). The calculated spectroscopic constants are in very good accordance with other theoretical and experimental results. The calculated transition dipole moments were used to determine the Einstein spontaneous emission coefficients A_{21} from which other emission constants are calculated to shed light on few possible low-lying transitions.

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References

- ¹Carlson, K. D.; Claydon, C. R.. Adv. High Temp. Chem. **1967**, *1*, 43. [doi:10.1016/S0065-2741\(13\)70022-8](https://doi.org/10.1016/S0065-2741(13)70022-8)
- ²Rochester, G. D., Olsson, E. Z. Phys. **1939**, *114*, 495. [doi: 10.1007/BF01329529](https://doi.org/10.1007/BF01329529)
- ³Moravec, V. D.; Klopčič, S. A.; Chatterjee, B.; Jarrold, C. C. Chem. Phys. Lett. **2001**, *341*, 313. [doi:10.1016/S0009-2614\(01\)00465-1](https://doi.org/10.1016/S0009-2614(01)00465-1)
- ⁴Flory, M. A.; McLamarrah, S. K.; Ziurys, L. M. J. Chem. Phys. **2006**, *125*, 194304. [doi: 10.1063/1.2355495](https://doi.org/10.1063/1.2355495)
- ⁵Bowmaker, G. A.; Schwerdtfeger, P. J. Mol. Struct.: THEOCHEM. **1990**, *205*, 295. [doi: 10.1016/0166-1280\(90\)85129-B](https://doi.org/10.1016/0166-1280(90)85129-B)
- ⁶Liao, M.; Zhang, Q.; Schwarz, W. H. E. Inorg. Chem. **1995**, *34*, 5597. [doi: 10.1021/ic00126a033](https://doi.org/10.1021/ic00126a033)
- ⁷Boldyrev, A. I.; Simons, J. Mol. Phys. **1997**, *92*, 365-379. [doi:10.1080/002689797170103](https://doi.org/10.1080/002689797170103)
- ⁸Belanzoni, P.; Lenthe, E. van; Baerends, E. J. J. Chem. Phys. **2001**, *114*, 4421. [doi: 10.1063/1.1345509](https://doi.org/10.1063/1.1345509)
- ⁹Harrison, J. F.; Field, R. W.; Jarrold, C. C. ACS Sym. Ser. **2002**, *828*, 238. [doi: 10.1021/bk-2002-0828.ch011](https://doi.org/10.1021/bk-2002-0828.ch011)
- ¹⁰Hayashi, S.; Léonard, C.; Chambaud, G. J. Chem. Phys. **2008**, *129*, 044313. [doi: 10.1063/1.2960585](https://doi.org/10.1063/1.2960585)
- ¹¹Léonard, C.; Le Quéré, F. J. Chem. Phys. **2012**, *137*, 164318. [doi:10.1063/1.4762444](https://doi.org/10.1063/1.4762444)
- ¹²Werner, H. J.; Knowles, P. J.; Lindh, R.; Manby, F. R.; Schütz, M.; Celani, P.; Korona, T.; Rauhut, G.; Amos, R. D.; Bernhardsson, A.; Berning, A.; Cooper, D. L.; Deegan, M. J. O.; Dobbyn, A. J.; Eckert, F.; Hampel, C.; Hetzer, G.; Lloyd, A. W.; McNicholas, S. J.; Meyer, W.; Mura, M. E.; Nicklass, A.; Palmieri, P.; Pitzer, R.; Schumann, U.; Stoll, H.; Stone, A. J.; Tarroni, R.; Thorsteinsson, T. **2008**. Version 2012.1; <http://www.molpro.net/info/users>
- ¹³Allouche, A. R. Gabedit: J. Comp. Chem. **2011**, *32*, 174. [doi: 10.1002/jcc.21600](https://doi.org/10.1002/jcc.21600)
- ¹⁴Figgen, D.; Rauhut, G.; Dolg, M.; Stoll, H. Chem. Phys. **2005**, *311*, 227. [doi:10.1016/j.chemphys.2004.10.005](https://doi.org/10.1016/j.chemphys.2004.10.005)
- ¹⁵NIST Atomic Spectra Database. Levels Form. <http://www.nist.gov/pml/data/asd.cfm> (accessed April 15, 2016).
- ¹⁶Huber, K. P.; Herzberg, G. *Molecular Spectra and Molecular Structure: Constants of Diatomic Molecules*. Van Nostrand Reinhold Company; New York, **1979**; pp. 676-677. ISBN: 978-1-4757-0963-6 (Print) 978-1-4757-0961-2
- ¹⁷McCown, A. W.; Eden, J. G. Appl. Phys. Lett. **1981**, *39*, 371. [doi:10.1063/1.92741](https://doi.org/10.1063/1.92741)

- ¹⁸Herzberg, G. *Molecular Spectra and Molecular Structure: Spectra of Diatomic Molecules*. 2nd ed.; D. Van Nostrand Company (Canada), Inc.; Toronto, **1950**; pp 100. ISBN-13: 978-0894642685 / ISBN-10: 0894642685
- ¹⁹Tennyson, J. J. *Mol. Spectrosc.* **2014**, 298, 1. [doi:10.1016/j.jms.2014.01.012](https://doi.org/10.1016/j.jms.2014.01.012)
- ²⁰Gianfranco, P.; Illas, F. *Chem. phys.* **1995**, 199, 155. [doi: 10.1016/0301-0104\(95\)00202-Y](https://doi.org/10.1016/0301-0104(95)00202-Y)
- ²¹Stradella, O. G.; Eduardo, E. A.; Fernandez, F. M. *Inorganic. Chem.* **1951**, 24, 3631. [doi: 10.1021/ic00216a031](https://doi.org/10.1021/ic00216a031)
- ²²Rittner, E. S. J. *Chem. Phys.* **1951**, 19, 1030. [doi: 10.1063/1.1748448](https://doi.org/10.1063/1.1748448)
- ²³Noorizadeh, S.; Shakerzadeh, E. J. *Phys. Chem. A* **2008**, 112, 3486. [doi: 10.1021/jp709877h](https://doi.org/10.1021/jp709877h)
- ²⁴Kotochigova, S.; Julienne, P. S.; Tiesinga, E. *Phys. Rev. A* **2003**, 68, 022501. [doi: 10.1103/PhysRevA.68.022501](https://doi.org/10.1103/PhysRevA.68.022501)
- ²⁵de Lima, E. F.; Ho, T. S.; Rabitz, H. *Chem. Phys. Lett.* **2011**, 501, 267. [doi:10.1016/j.cplett.2010.12.018](https://doi.org/10.1016/j.cplett.2010.12.018)
- ²⁶Hilborn, R. C. *Am. J. Phys.* **1982**, 50, 982. Revised version, **2002**. [doi: 10.1119/1.12937](https://doi.org/10.1119/1.12937)
- ²⁷Loh, W. H. T. *Re-entry and Planetary Entry Physics and Technology. Part 1: Dynamics, Physics, Radiation, Heat Transfer and Ablation*. Springer-Verlag New York Inc. **1968**; pp. 235. ISBN 978-3-642-48927-3

Figure captions:

Figure (SM.1): Potential energy curves of the doublet electronic states of the ZnF molecule.

Figure (SM.2): Potential energy curves of the quartet electronic states of ZnF.

Figure (SM.3): Dipole moment curves of the $^2\Sigma^+$ electronic states of the ZnF molecule.

Figure (SM.4): Dipole moment curves of the $^2\Sigma^-$, $^2\Pi$ and $^2\Delta$ electronic states of the ZnF molecule.

Figure (SM.5): Dipole moment curves of the $^4\Sigma^+$ and $^4\Sigma^-$ electronic states of the ZnF molecule.

Figure (SM.6): Dipole moment curves of the $^4\Pi$ and $^4\Delta$ electronic states of the ZnF molecule.

Figure (SM.7): Transition dipole moment between the ground and $(2)^2\Sigma^+$, $(4)^2\Sigma^+$, $(1)^2\Pi$, and $(2)^2\Pi$ electronic states of the ZnF molecule.

Figures (SM.8-a) and (SM.8-b): Transition dipole moments between some doublet electronic states of the ZnF molecule.

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Table 1: Calculated spectroscopic constants for the bound doublet and quartet electronic states of the ZnF molecule.

State	R_e (Å)	T_e (cm ⁻¹)	ω_e (cm ⁻¹)	$B_e \times 10^2$ (cm ⁻¹)	μ (a.u.)	Asymptotic Energy (cm ⁻¹)
$X^2\Sigma^+$	1.802 ^(a) 1.768 ^(b) 1.784 ^(d1,d2) 1.787 ^(d3) 1.775 ^(e) 1.766 ^(g) 1.762 ^(h1) 1.799 ⁽ⁱ⁾ 1.796 ^(j) 1.780 ^(k)	0.00	627.1 ^(a) 631 ^(b) 620 ^(c) 600.7 ^(d1) 610 ^(d2) 599 ^(d3) 633 ^(e) 628 ^(f) 638.6 ^(g) 629.7 ^(h1) 593 ^(j) 609 ^(k)	35.01 ^(a) 36.84 ^(b)	1.09 ^(a) 1.23 ^(e) 0.94 ^(g) 1.28 ^(j) 0.98 ^(k)	0.0
$(1)^2\Pi$	3.831 ^(a) 4.509 ^(j)	19611 ^(a) 36247 ^{(a)*} 20400 ^{(b)†} >21697 ^(c) 37377 ^{(g)*} 22044 ^(j)	36.6 ^(a) 13 ^(j)	7.80 ^(a)	0.07 ^(a) 0.79 ^{(a)*} 1.00 ^{(g)*} 0.01 ^(j)	
$(2)^2\Sigma^+$	2.523 ^(a) 2.593 ^(g) 2.544 ^(h1)	31091 ^(a) 33078 ^(g) 31916 ^(h1)	326.2 ^(a) 327.7 ^(g) 311.9 ^(h1)	17.98 ^(a)	0.54 ^(a) 0.61 ^(g)	30711 ^(a) 32311 ^(l)
$(3)^2\Sigma^+$	1.816 ^(a) 1.760 ^(g)	51226 ^(a) 53992 ^(g)	712.8 ^(a) 705.1 ^(g)	34.74 ^(a)	1.32 ^(a) 1.30 ^(g)	
$(2)^2\Pi$	1.884 ^(a) 1.757 ^(e) 1.861 ^(g) 1.965 ^(h1) 1.876 ^(h2)	37515 ^(a) 37344 ^(e) 37399 ^(f) 39328 ^(g) 38490 ^(h1) 37376 ^(h2)	950.6 ^(a) 659 ^(e) 601.5 ^(f) 935.3 ^(g) 962.9 ^(h1) 614.8 ^(h2)	32.25 ^(a)	1.35 ^(a) 1.50 ^(e) 1.07 ^(g) 1.10 ^(h1) 1.82 ^(h2)	
$(1)^2\Delta$	3.176 ^(a)	49794 ^(a)	56.2 ^(a)	11.33 ^(a)	0.15 ^(a)	
$(1)^2\Sigma^-$	3.289 ^(a)	49916 ^(a)	48.9 ^(a)	10.60 ^(a)	0.13 ^(a)	
$(1)^4\Sigma^-$	2.761 ^(a)	49474 ^(a)	85.0 ^(a)	15.00 ^(a)	0.25 ^(a)	
$(1)^4\Delta$	2.956 ^(a)	49826 ^(a)	55.3 ^(a)	13.10 ^(a)	0.19 ^(a)	
$(1)^4\Sigma^-$	3.146 ^(a)	50023 ^(a)	50.7 ^(a)	11.59 ^(a)	0.15 ^(a)	
$(4)^2\Sigma^+$	3.794 ^(a)	55637 ^(a)	141.0 ^(a)	7.96 ^(a)	3.08 ^(a)	44918 ^(l)
$(5)^2\Sigma^+$	1.925 ^(a)	63672 ^(a)	789.0 ^(a)	30.91 ^(a)	0.88 ^(a)	45053 ^(a)
$(4)^2\Pi$	2.325 ^(a)	63585 ^(a)	264.6 ^(a)	21.19 ^(a)	0.36 ^(a)	46745 ^(l)
$(2)^2\Delta$	2.808 ^(a)	63592 ^(a)	62.7 ^(a)	14.52 ^(a)	0.29 ^(a)	
$(2)^2\Sigma^-$	2.919 ^(a)	63791 ^(a)	55.8 ^(a)	13.43 ^(a)	0.24 ^(a)	
$(3)^4\Sigma^+$	3.371 ^(a)	74973 ^(a)	51.8 ^(a)	10.12 ^(a)	0.28 ^(a)	54955 ^(a)
$(3)^4\Pi$	2.690 ^(a)	73185 ^(a)	114.2 ^(a)	15.84 ^(a)	0.34 ^(a)	53672 ^(l)
$(4)^4\Pi$	2.503 ^(a)	84131 ^(a)	156.1 ^(a)	18.28 ^(a)	0.32 ^(a)	64929 ^(a) 65432 ^(l)
$(5)^4\Pi$	2.276 ^(a)	91835 ^(a)	210.9 ^(a)	22.11 ^(a)	0.33 ^(a)	74758 ^(a) 73964 ^(l)

- (a) This work {^{Theo}: MRCI+Q}
- (b) Flory *et al.*⁴ {^{Exp}: Direct absorption techniques}, † By calculation.
- (c) Moravec *et al.*³ {^{Exp}: Photoelectron spectra}
- (d) Bowmaker and Schwerdtfeger⁵ {^{Theo}: d¹MP2, d²CISD, d³CISDSC}
- (e) Harrison *et al.*⁹ {^{Theo}: RCCSD(T)}
- (f) Rochester and Olsson² {^{Exp}: UV absorption spectrum}
- (g) Hayashi *et al.*¹⁰ {^{Theo}: MRCI+Q}
- (h) Léonard and Le Quéré¹¹ {^{Theo}: h¹ adiabatic MRCI, h² diabatic MRCI}
- (i) Belanzoni *et al.*⁸ {^{Theo}: DFT-ZORA}
- (j) Boldyrev and Simons⁷ {^{Theo}: QCISD}
- (k) Liao *et al.*⁶ {^{Theo}: LDF}
- (l) NIST Atomic Spectra Database¹⁵
- * absolute energy/dipole moment calculated at the minimum of the ground state X²Σ⁺.

Table 2: Positions of the crossings R_C and avoided crossings R_{AC} between electronic states of ZnF molecule.

(n_1) state 1/ (n_2) state 2	R_C (Å)	R_{AC} (Å)	ΔE (cm ⁻¹)
$(2)^2\Sigma^+/(2)^2\Pi$	1.59		
	1.98		
$(3)^2\Sigma^+/(1)^2\Delta$	2.16		
$(3)^2\Sigma^+/(1)^2\Sigma^-$	2.19		
$(4)^2\Sigma^+/(1)^2\Delta$	1.86		
$(4)^2\Sigma^+/(1)^2\Sigma^-$	1.89		
$(4)^2\Sigma^+/(3)^2\Pi$	2.43		
$(5)^2\Sigma^+/(3)^2\Pi$	2.06		
$(5)^2\Sigma^+/(4)^2\Pi$	2.08		
	2.67		
$(5)^2\Sigma^+/(1)^2\Delta$	1.71		
$(5)^2\Sigma^+/(1)^2\Sigma^-$	1.73		
$(5)^2\Sigma^+/(2)^2\Delta$	2.13		
$(5)^2\Sigma^+/(2)^2\Sigma^-$	2.19		
$(4)^4\Sigma^+/(5)^4\Pi$	1.98		
$(2)^2\Sigma^+/(3)^2\Sigma^+$		1.68	2499
$(3)^2\Sigma^+/(4)^2\Sigma^+$		1.47	681
		2.10	4284
$(4)^2\Sigma^+/(5)^2\Sigma^+$		1.86	5103
$(1)^2\Pi/(2)^2\Pi$		1.83	2398
$(4)^4\Pi/(5)^4\Pi$		1.56	235

Table 3: Calculation of ionicity for the ground $X^2\Sigma^+$ state of ZnF molecule.

μ (a.u)	R_e (Å)	μ/eR_e
1.092	1.802	3.211
1.23 ^(a)	1.787	3.643
0.98 ^(b)	1.780	2.914
1.28 ^(c)	1.796	3.772

First entry is for the present work
(a)Bowmaker and Schwerdtfeger⁵ {^{Theo}: CISDSC}
(b)Liao *et al.*⁶ {^{Theo}: LDF}
(c)Boldyrev and Simons⁷ {^{Theo}: QCISD}

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Table 4: The transition dipole moment values of the upper state at its equilibrium position $|\mu|$, the emission angular frequency ω_{21} , the Einstein coefficients of spontaneous and induced emissions (A_{21} and B_{21}^ω), the spontaneous radiative lifetime τ_{spont} , the emission cross section σ_0 , the classical radiative decay rate of the single-electron oscillator γ_{cl} and the emission oscillator strength f_{21} of some transitions among the doublet states of ZnF.

Transition	$ \mu_{21} $ (a.u.)	$ \mu_{21} \times 10^{30}$ (C.m)	$\omega_{21} \times 10^{-15}$ (rad.s ⁻¹)	$A_{21} \times 10^{-7}$ (s ⁻¹)	τ_{spont} (ns)	$B_{21}^\omega \times 10^{-20}$ (m ³ .rad.J ⁻¹ .s ⁻²)	$\sigma_0 \times 10^6$ (m ² .rad.s ⁻¹)	λ_{21} (nm)	$\gamma_{cl} \times 10^{-7}$ (s ⁻¹)	$ f_{21} $
X ² Σ ⁺ - (1) ² Π	0.018	0.15	3.694	< 10 ⁻³	> 10 ⁵	< 10 ⁻³	0.001	510.0	8.55	< 10 ⁻⁴
X ² Σ ⁺ - (2) ² Σ ⁺	1.223	10.37	5.856	9.11	10.98	11.43	2.355	321.7	21.49	0.141
(1) ² Π-(1) ² Δ	0.001	0.01	5.685	< 10 ⁻³	> 10 ⁵	< 10 ⁻³	< 10 ⁻³	331.3	20.25	< 10 ⁻⁴
(2) ² Π - (1) ² Δ	0.003	0.03	2.313	< 10 ⁻³	> 10 ⁵	< 10 ⁻³	< 10 ⁻³	814.5	3.35	< 10 ⁻⁴
(1) ² Π-(1) ² Σ ⁻	0.001	0.01	5.708	< 10 ⁻³	> 10 ⁵	< 10 ⁻³	< 10 ⁻³	330.0	20.42	< 10 ⁻⁴
(2) ² Π - (1) ² Σ ⁻	0.021	0.18	2.336	< 10 ⁻³	> 10 ⁵	< 10 ⁻³	< 10 ⁻³	806.4	3.42	< 10 ⁻⁴
(1) ² Π - (2) ² Π	1.044	8.85	3.372	1.27	78.92	8.33	0.988	558.6	7.13	0.059
X ² Σ ⁺ - (2) ² Π	1.067	9.05	7.066	12.18	8.21	8.70	4.327	266.6	31.29	0.130
X ² Σ ⁺ - (3) ² Σ ⁺	0.767	6.50	9.648	16.02	6.24	4.50	1.526	195.2	58.34	0.092
X ² Σ ⁺ - (4) ² Σ ⁺	0.415	3.52	10.479	6.01	16.64	1.32	0.485	179.7	68.82	0.029
(2) ² Σ ⁺ - (3) ² Σ ⁺	0.146	1.24	3.792	0.04	2837.06	0.16	0.022	496.7	9.01	0.001

Supplementary Material:

A. Curves:

Figure (SM.1): Potential energy curves of the doublet electronic states of the ZnF molecule.

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Figure (SM.7): Transition dipole moment between the ground and $(2)^2\Sigma^+$, $(4)^2\Sigma^+$, $(1)^2\Pi$, and $(2)^2\Pi$ electronic states of the ZnF molecule.

Figure (SM.8): Transition dipole moments between some doublet electronic states of the ZnF molecule.

B. Numerical data of energy and dipole moments:

Table (SM.1): Numerical data corresponding to the potential energy E (cm^{-1}) and dipole moment μ (a.u.) of zinc monofluoride ZnF molecule as function of the internuclear distance R ($\text{\AA}$).

$X^2\Sigma^+$			$(2)^2\Sigma^+$			$(3)^2\Sigma^+$		
R ($\text{\AA}$)	E (cm^{-1})	μ (a.u.)	R ($\text{\AA}$)	E (cm^{-1})	μ (a.u.)	R ($\text{\AA}$)	E (cm^{-1})	μ (a.u.)
1.41	30559.4	-0.410	1.41	78936.4	-1.812	1.41	88577.2	-0.759
1.44	24399.0	-0.473	1.44	73146.0	-1.811	1.44	82655.5	-0.506
1.47	19245.3	-0.533	1.47	68329.6	-1.805	1.47	77560.0	-0.064
1.50	14930.3	-0.590	1.50	64324.1	-1.794	1.50	73071.4	0.430
1.53	11412.4	-0.646	1.53	61072.1	-1.777	1.53	69017.9	0.842
1.56	8538.4	-0.701	1.56	58425.9	-1.748	1.56	65324.7	1.045
1.59	6214.0	-0.754	1.59	56288.1	-1.697	1.59	61991.8	1.100
1.62	4360.9	-0.805	1.62	54569.0	-1.595	1.62	59017.7	1.045
1.65	2912.5	-0.855	1.65	53148.2	-1.346	1.65	56425.2	0.815
1.68	1811.6	-0.905	1.68	51821.4	-0.739	1.68	54320.4	0.215
1.71	1009.2	-0.953	1.71	50324.1	0.077	1.71	52883.8	-0.599
1.74	463.0	-1.000	1.74	48653.8	0.546	1.74	52061.7	-1.069
1.77	137.1	-1.047	1.77	46990.9	0.733	1.77	51616.3	-1.255
1.80	0.0	-1.092	1.80	45421.9	0.801	1.80	51402.3	-1.320
1.83	24.8	-1.137	1.83	43970.3	0.819	1.83	51347.3	-1.331
1.86	187.9	-1.180	1.86	42636.2	0.813	1.86	51407.1	-1.312
1.89	468.9	-1.223	1.89	41413.1	0.794	1.89	51548.9	-1.271
1.92	849.8	-1.264	1.92	40292.3	0.768	1.92	51744.9	-1.212
1.95	1315.1	-1.305	1.95	39265.7	0.736	1.95	52009.8	-1.135
1.98	1850.9	-1.344	1.98	38325.8	0.700	1.97	52229.2	-1.063
2.01	2444.9	-1.381	2.01	37464.9	0.661	1.99	52426.8	-0.995
2.04	3086.6	-1.417	2.04	36676.7	0.619	2.01	52580.4	-0.936
2.07	3766.3	-1.451	2.07	35955.6	0.576	2.03	52690.1	-0.859
2.10	4475.6	-1.483	2.10	35296.4	0.530	2.05	52799.9	-0.759
2.13	5207.3	-1.512	2.13	34695.9	0.481	2.07	52942.5	-0.642
2.16	5954.2	-1.538	2.16	34149.1	0.429	2.09	52997.4	-0.519
2.19	6710.6	-1.561	2.19	33653.1	0.375	2.11	52975.4	-0.442
2.22	7470.9	-1.580	2.22	33205.4	0.319	2.13	52880.2	-0.334
2.25	8230.3	-1.594	2.25	32803.7	0.258	2.16	52868.9	-0.203
2.28	8984.3	-1.604	2.28	32446.3	0.194	2.19	52818.3	-0.092
2.31	9728.7	-1.609	2.31	32132.0	0.125	2.22	52737.9	-0.002
2.34	10459.6	-1.607	2.34	31859.5	0.052	2.25	52636.3	0.068
2.37	11173.3	-1.599	2.37	31628.3	-0.028	2.28	52521.0	0.122
2.40	11866.3	-1.583	2.40	31438.2	-0.113	2.31	52397.6	0.162
2.43	12535.2	-1.559	2.43	31288.4	-0.205	2.34	52270.5	0.192
2.46	13176.9	-1.527	2.46	31179.1	-0.304	2.37	52142.5	0.213
2.49	13788.6	-1.487	2.49	31110.8	-0.410	2.40	52015.7	0.227
2.52	14368.4	-1.438	2.52	31083.6	-0.524	2.43	51891.4	0.236
2.55	14914.6	-1.380	2.55	31097.8	-0.644	2.46	51770.3	0.241

2.58	15425.0	-1.315	2.58	31153.4	-0.771	2.49	51652.9	0.243
2.61	15898.2	-1.242	2.61	31250.2	-0.903	2.52	51540.1	0.242
2.64	16333.3	-1.165	2.64	31387.4	-1.039	2.55	51433.1	0.239
2.67	16729.8	-1.083	2.67	31564.0	-1.177	2.58	51332.2	0.235
2.70	17088.6	-0.999	2.70	31778.3	-1.315	2.61	51237.4	0.229
2.73	17410.5	-0.915	2.73	32028.2	-1.452	2.64	51148.2	0.223
2.76	17697.4	-0.833	2.76	32310.9	-1.585	2.67	51064.5	0.216
2.79	17951.5	-0.754	2.79	32623.4	-1.713	2.70	50986.1	0.209
2.82	18175.4	-0.679	2.82	32962.3	-1.836	2.73	50912.7	0.202
2.85	18371.6	-0.609	2.85	33324.5	-1.951	2.76	50844.0	0.194
2.88	18543.0	-0.544	2.88	33706.3	-2.059	2.79	50779.7	0.186
2.91	18692.3	-0.485	2.91	34104.5	-2.159	2.82	50719.8	0.178
2.94	18822.0	-0.431	2.94	34515.9	-2.251	2.85	50663.9	0.170
2.97	18934.6	-0.383	2.97	34937.8	-2.335	2.88	50611.9	0.162
3.00	19032.2	-0.340	3.00	35367.3	-2.413	2.91	50563.4	0.154
3.03	19116.9	-0.302	3.03	35802.2	-2.482	2.94	50518.5	0.147
3.06	19190.4	-0.268	3.06	36240.5	-2.546	2.97	50476.8	0.139
3.09	19254.1	-0.238	3.09	36680.2	-2.602	3.00	50438.1	0.132
3.12	19309.6	-0.212	3.12	37119.8	-2.653	3.03	50402.4	0.125
3.15	19357.9	-0.189	3.15	37557.9	-2.697	3.06	50369.5	0.119
3.18	19400.0	-0.168	3.18	37993.4	-2.736	3.09	50339.1	0.112
3.21	19436.9	-0.150	3.21	38425.2	-2.770	3.12	50311.2	0.106
3.24	19469.2	-0.134	3.24	38852.3	-2.799	3.15	50285.6	0.100
3.27	19497.5	-0.120	3.27	39274.3	-2.822	3.18	50262.2	0.094
3.30	19522.6	-0.107	3.30	39690.3	-2.841	3.21	50240.9	0.089
3.33	19544.7	-0.096	3.33	40099.9	-2.855	3.24	50221.4	0.083
3.36	19564.3	-0.086	3.36	40502.5	-2.864	3.27	50203.7	0.078
3.39	19581.8	-0.078	3.39	40897.8	-2.868	3.30	50187.7	0.074
3.42	19597.4	-0.070	3.42	41285.4	-2.868	3.33	50173.3	0.069
3.45	19611.4	-0.063	3.45	41665.1	-2.863	3.36	50160.4	0.065
3.48	19624.1	-0.058	3.48	42036.5	-2.854	3.39	50148.8	0.061
3.51	19635.5	-0.052	3.51	42399.6	-2.840	3.42	50138.5	0.057
3.54	19645.8	-0.048	3.54	42754.1	-2.821	3.45	50129.3	0.053
3.57	19655.3	-0.043	3.57	43099.8	-2.797	3.48	50121.3	0.050
3.60	19663.9	-0.040	3.60	43436.5	-2.769	3.51	50114.2	0.046
3.63	19671.8	-0.036	3.63	43764.2	-2.737	3.54	50108.1	0.043
3.66	19679.1	-0.033	3.66	44082.7	-2.699	3.57	50102.8	0.040
3.69	19685.9	-0.031	3.69	44391.8	-2.657	3.60	50098.4	0.038
3.72	19692.2	-0.028	3.72	44691.5	-2.611	3.63	50094.7	0.035
3.75	19698.1	-0.026	3.75	44981.7	-2.560	3.66	50091.7	0.032
3.78	19703.6	-0.024	3.78	45262.2	-2.505	3.69	50089.2	0.030
3.81	19708.9	-0.023	3.81	45533.1	-2.446	3.72	50087.4	0.028
3.84	19713.7	-0.021	3.84	45794.3	-2.383	3.75	50086.1	0.026
3.87	19718.4	-0.020	3.87	46045.6	-2.316	3.78	50085.2	0.024

3.90	19722.6	-0.019		3.90	46287.1	-2.247		3.81	50084.9	0.022
3.93	19726.8	-0.017		3.93	46518.9	-2.174		3.84	50084.9	0.020
3.96	19730.8	-0.016		3.96	46740.8	-2.099		3.87	50085.4	0.019
3.99	19734.6	-0.016		3.99	46952.9	-2.021		3.90	50086.2	0.017
4.02	19738.3	-0.015		4.02	47155.4	-1.942		3.93	50087.4	0.016
4.05	19741.8	-0.014		4.05	47348.4	-1.862		3.96	50088.8	0.014
4.08	19745.2	-0.013		4.08	47531.8	-1.781		3.99	50090.4	0.013
4.11	19748.4	-0.013		4.11	47706.0	-1.700		4.02	50092.4	0.012
4.14	19751.6	-0.012		4.14	47871.1	-1.619		4.05	50094.6	0.011
4.17	19754.6	-0.012		4.17	48027.3	-1.539		4.08	50096.8	0.010
4.20	19757.6	-0.011		4.20	48174.9	-1.459		4.11	50099.5	0.009
4.23	19760.4	-0.011		4.23	48314.2	-1.381		4.14	50102.2	0.008
4.26	19763.2	-0.010		4.26	48445.4	-1.305		4.17	50105.0	0.007
4.29	19765.8	-0.010		4.29	48568.7	-1.231		4.20	50108.2	0.006
4.32	19768.5	-0.010		4.32	48684.6	-1.159		4.23	50111.3	0.005
4.35	19771.2	-0.009		4.35	48793.4	-1.090		4.26	50114.6	0.005
4.38	19773.7	-0.009		4.38	48895.3	-1.024		4.29	50117.8	0.004
4.41	19776.1	-0.009		4.41	48990.8	-0.960		4.32	50121.3	0.003
4.44	19778.3	-0.009		4.44	49080.2	-0.900		4.35	50124.8	0.003
4.47	19780.6	-0.008		4.47	49163.7	-0.842		4.38	50128.4	0.002
4.50	19782.9	-0.008		4.50	49241.7	-0.787		4.41	50132.0	0.002
4.53	19785.1	-0.008		4.53	49314.5	-0.735		4.44	50135.7	0.001
4.56	19787.2	-0.008		4.56	49382.6	-0.686		4.47	50139.3	0.001
4.59	19789.2	-0.008		4.59	49446.1	-0.640		4.50	50142.9	0.001
4.62	19791.3	-0.007		4.62	49505.1	-0.597		4.53	50146.6	0.000
4.65	19793.1	-0.007		4.65	49560.4	-0.556		4.56	50150.3	0.000
4.68	19795.0	-0.007		4.68	49611.8	-0.518		4.59	50154.0	0.000
4.71	19797.0	-0.007		4.71	49659.8	-0.482		4.62	50157.6	0.000
4.74	19798.8	-0.007		4.74	49704.6	-0.448		4.65	50161.3	0.000
4.77	19800.7	-0.007		4.77	49746.6	-0.417		4.68	50164.9	0.000
4.80	19802.7	-0.007		4.80	49785.4	-0.388		4.71	50168.4	0.000
								4.74	50172.0	0.000
								4.77	50175.9	0.000
								4.80	50179.3	0.000

(4) ² Σ ⁺			(5) ² Σ ⁺			(1) ² Π		
R (Å)	E (cm ⁻¹)	μ (a.u.)	R (Å)	E (cm ⁻¹)	μ (a.u.)	R (Å)	E (cm ⁻¹)	μ (a.u.)
1.41	89817.3	0.633	1.41	96424.7	-0.464	1.41	66130.5	-1.276
1.44	83590.0	0.359	1.45	89957.7	-0.560	1.44	60151.6	-1.314
1.47	78240.8	-0.105	1.47	86490.0	-0.632	1.47	55149.8	-1.348
1.50	73794.1	-0.619	1.49	83373.4	-0.707	1.50	50945.3	-1.379
1.53	70211.8	-1.052	1.51	80739.7	-0.814	1.53	47534.1	-1.406
1.56	67390.0	-1.280	1.54	77930.5	-0.900	1.56	44751.3	-1.429
1.59	65181.8	-1.375	1.58	73826.3	-0.995	1.59	42504.0	-1.448

1.62	63468.0	-1.400	1.61	71719.3	-1.100	1.62	40716.1	-1.462
1.65	62158.9	-1.386	1.65	69502.4	-1.207	1.65	39324.6	-1.468
1.69	60997.9	-1.330	1.68	68436.1	-1.291	1.68	38273.9	-1.463
1.76	59888.8	-1.100	1.71	67669.9	-1.359	1.71	37509.5	-1.436
1.83	59291.5	-0.641	1.74	67163.1	-1.344	1.74	36971.2	-1.366
1.86	59117.2	-0.372	1.77	66851.1	-1.140	1.77	36589.1	-1.196
1.89	58888.2	-0.110	1.80	65950.3	-0.012	1.80	36251.5	-0.789
1.92	58596.3	0.092	1.83	64939.6	-0.113	1.83	35707.5	-0.083
1.95	58269.2	0.204	1.86	64220.1	-0.369	1.86	34857.8	0.493
1.98	57947.8	0.234	1.89	63807.9	-0.640	1.89	33840.9	0.747
2.01	57667.5	0.198	1.92	63681.4	-0.859	1.92	32811.5	0.840
2.04	57452.5	0.116	1.95	63784.6	-0.994	1.95	31832.3	0.870
2.07	57315.6	0.006	1.98	64047.7	-1.045	1.98	30919.3	0.873
2.10	57259.4	-0.117	2.01	64401.8	-1.021	2.01	30076.5	0.863
2.13	57279.9	-0.235	2.04	64780.1	-0.917	2.04	29300.3	0.846
2.16	57362.0	-0.336	2.07	65102.7	-0.721	2.07	28585.7	0.826
2.19	57490.9	-0.418	2.10	65283.4	-0.434	2.10	27927.8	0.804
2.22	57650.7	-0.478	2.13	65271.6	-0.120	2.13	27321.2	0.780
2.25	57826.8	-0.518	2.16	65149.4	0.131	2.16	26761.0	0.756
2.28	58006.9	-0.540	2.19	65005.0	0.262	2.19	26242.6	0.731
2.31	58181.3	-0.549	2.26	64650.3	0.358	2.22	25762.1	0.707
2.34	58342.9	-0.546	2.31	64573.4	0.372	2.25	25316.0	0.682
2.37	58486.8	-0.537	2.34	64512.3	0.355	2.28	24901.0	0.658
2.40	58610.0	-0.522	2.37	64468.3	0.334	2.31	24514.3	0.635
2.43	58711.2	-0.506	2.40	64436.9	0.312	2.34	24153.4	0.611
2.46	58790.2	-0.489	2.43	64415.6	0.291	2.37	23816.0	0.588
2.49	58847.2	-0.474	2.46	64402.5	0.269	2.40	23499.9	0.566
2.52	58883.1	-0.462	2.49	64396.1	0.250	2.43	23203.5	0.545
2.55	58899.0	-0.453	2.52	64392.9	0.231	2.46	22925.1	0.524
2.58	58896.1	-0.448	2.55	64388.0	0.215	2.49	22663.1	0.503
2.61	58876.2	-0.447	2.58	64379.9	0.200	2.52	22416.6	0.484
2.64	58840.6	-0.450	2.61	64369.1	0.186	2.55	22184.6	0.464
2.67	58791.2	-0.458	2.64	64352.9	0.173	2.58	21966.0	0.446
2.70	58729.3	-0.470	2.67	64337.0	0.161	2.61	21759.7	0.428
2.73	58656.5	-0.486	2.70	64319.7	0.150	2.64	21564.8	0.411
2.76	58574.0	-0.507	2.73	64300.7	0.139	2.67	21380.6	0.394
2.79	58483.6	-0.531	2.76	64281.2	0.129	2.70	21206.2	0.378
2.82	58385.5	-0.559	2.79	64260.8	0.119	2.73	21040.9	0.362
2.85	58281.3	-0.591	2.82	64240.1	0.110	2.76	20884.4	0.348
2.88	58172.2	-0.625	2.85	64219.5	0.101	2.79	20735.6	0.333
2.91	58058.9	-0.663	2.88	64199.9	0.092	2.82	20594.3	0.319
2.94	57942.4	-0.704	2.91	64180.4	0.084	2.85	20459.8	0.306
2.97	57823.6	-0.748	2.94	64161.9	0.076	2.88	20354.8	0.293
3.00	57703.3	-0.795	2.97	64144.4	0.068	2.91	20282.8	0.281

3.03	57582.1	-0.844	3.00	64128.0	0.061	2.94	20216.4	0.269
3.06	57460.8	-0.896	3.03	64112.8	0.054	2.97	20155.2	0.258
3.09	57339.9	-0.951	3.06	64099.0	0.047	3.00	20099.0	0.247
3.12	57220.2	-1.009	3.09	64086.6	0.041	3.03	20047.3	0.237
3.15	57101.9	-1.069	3.12	64075.3	0.035	3.06	19999.9	0.227
3.18	56985.9	-1.132	3.15	64065.4	0.029	3.09	19956.4	0.217
3.21	56872.3	-1.197	3.18	64056.9	0.024	3.12	19916.7	0.208
3.24	56761.5	-1.265	3.21	64049.6	0.019	3.15	19880.5	0.199
3.27	56654.2	-1.336	3.24	64043.3	0.014	3.18	19847.4	0.191
3.30	56550.6	-1.409	3.27	64038.1	0.010	3.21	19817.4	0.182
3.33	56451.1	-1.486	3.30	64034.2	0.005	3.24	19790.2	0.175
3.36	56355.9	-1.565	3.33	64031.2	0.002	3.27	19765.6	0.167
3.39	56265.4	-1.648	3.36	64029.4	-0.002	3.30	19743.4	0.160
3.42	56179.8	-1.733	3.39	64028.3	-0.006	3.33	19723.4	0.153
3.45	56099.4	-1.822	3.42	64027.8	-0.009	3.36	19705.5	0.147
3.48	56024.6	-1.915	3.45	64028.1	-0.012	3.39	19689.5	0.140
3.51	55955.5	-2.010	3.48	64029.1	-0.015	3.42	19675.3	0.134
3.54	55892.3	-2.110	3.51	64030.7	-0.018	3.45	19662.7	0.129
3.57	55835.4	-2.212	3.54	64032.8	-0.020	3.48	19651.6	0.123
3.60	55784.9	-2.319	3.57	64035.4	-0.023	3.51	19642.0	0.118
3.63	55741.1	-2.429	3.60	64038.8	-0.025	3.54	19633.6	0.113
3.66	55704.1	-2.543	3.63	64042.3	-0.027	3.57	19626.4	0.108
3.69	55674.1	-2.660	3.66	64046.3	-0.029	3.60	19620.2	0.103
3.72	55651.4	-2.782	3.69	64050.6	-0.031	3.63	19615.3	0.099
3.75	55636.2	-2.907	3.72	64055.2	-0.033	3.66	19610.9	0.094
3.78	55628.5	-3.035	3.75	64060.0	-0.035	3.69	19607.5	0.090
3.81	55628.9	-3.167	3.78	64065.1	-0.037	3.72	19604.9	0.087
3.84	55636.6	-3.301	3.81	64070.4	-0.038	3.75	19603.2	0.083
3.87	55652.8	-3.439	3.84	64075.8	-0.040	3.78	19601.8	0.079
3.90	55676.5	-3.579	3.87	64081.5	-0.041	3.81	19601.2	0.076
3.93	55709.2	-3.722	3.90	64087.4	-0.043	3.83	19601.0	0.073
3.96	55749.5	-3.866	3.93	64093.5	-0.044	3.87	19601.4	0.070
3.99	55797.4	-4.012	3.96	64099.5	-0.045	3.90	19602.4	0.067
4.02	55854.0	-4.158	3.99	64105.5	-0.047	3.93	19603.7	0.064
4.05	55919.2	-4.306	4.02	64111.9	-0.048	3.96	19605.4	0.061
4.08	55991.2	-4.453	4.05	64118.3	-0.049	3.99	19607.5	0.058
4.11	56071.5	-4.600	4.08	64124.6	-0.051	4.02	19609.8	0.056
4.14	56159.4	-4.747	4.11	64131.1	-0.052	4.05	19612.6	0.053
4.17	56254.6	-4.891	4.14	64137.6	-0.053	4.08	19615.3	0.051
4.20	56356.8	-5.035	4.17	64144.2	-0.054	4.11	19618.4	0.049
4.23	56465.4	-5.175	4.20	64151.2	-0.055	4.14	19621.7	0.047
4.26	56581.3	-5.314	4.23	64157.9	-0.057	4.17	19625.2	0.045
4.29	56702.2	-5.449	4.26	64163.9	-0.057	4.20	19629.1	0.043
4.32	56829.3	-5.582	4.29	64170.9	-0.059	4.23	19632.8	0.041

4.35	56961.5	-5.710	4.32	64177.6	-0.060	4.26	19636.7	0.039
4.38	57098.7	-5.836	4.35	64184.2	-0.061	4.29	19640.7	0.037
4.41	57240.3	-5.957	4.38	64191.2	-0.062	4.32	19644.8	0.036
4.44	57385.9	-6.075	4.41	64197.7	-0.063	4.35	19649.0	0.034
4.47	57535.0	-6.189	4.44	64204.3	-0.065	4.38	19653.2	0.033
4.50	57687.5	-6.298	4.47	64210.7	-0.066	4.41	19657.4	0.031
4.53	57842.7	-6.404	4.50	64217.0	-0.067	4.44	19661.7	0.030
4.56	57999.9	-6.505	4.53	64223.3	-0.068	4.47	19666.0	0.029
4.59	58159.5	-6.603	4.56	64229.5	-0.069	4.50	19670.3	0.027
4.62	58320.6	-6.696	4.59	64236.5	-0.070	4.53	19674.5	0.026
4.65	58483.0	-6.785	4.62	64242.4	-0.072	4.56	19678.8	0.025
4.68	58646.5	-6.870	4.65	64248.7	-0.073	4.59	19682.9	0.024
4.71	58811.0	-6.951	4.68	64254.8	-0.075	4.62	19687.1	0.023
4.74	58976.0	-7.028	4.71	64260.6	-0.076	4.65	19691.2	0.022
4.77	59143.8	-7.101	4.74	64266.4	-0.077	4.68	19695.3	0.021
4.80	59308.5	-7.170	4.77	64272.2	-0.078	4.71	19699.2	0.020
			4.80	64278.2	-0.080	4.74	19703.2	0.019
						4.77	19707.1	0.018
						4.80	19710.9	0.018

(2) ² Π			(3) ² Π			(4) ² Π		
R (Å)	E (cm ⁻¹)	μ (a.u.)	R (Å)	E (cm ⁻¹)	μ (a.u.)	R (Å)	E (cm ⁻¹)	μ (a.u.)
1.41	87887.7	1.268	1.43	108735.4	0.962	1.41	119740.9	-0.478
1.44	81036.6	1.327	1.44	107244.3	0.963	1.44	112654.1	-0.412
1.47	74797.4	1.336	1.46	103026.6	0.953	1.47	106423.8	-0.344
1.50	69229.2	1.326	1.50	96673.6	0.938	1.50	100951.4	-0.270
1.53	64302.4	1.306	1.53	92874.0	0.911	1.53	96180.5	-0.208
1.56	59948.0	1.280	1.56	89211.2	0.886	1.56	92026.7	-0.145
1.59	56096.6	1.250	1.59	85982.0	0.848	1.59	88378.0	-0.075
1.62	52687.4	1.215	1.62	83219.8	0.802	1.62	85202.5	-0.001
1.65	49664.5	1.174	1.65	80695.8	0.753	1.65	82298.0	0.065
1.68	46982.1	1.123	1.68	78437.2	0.700	1.68	79971.6	0.134
1.71	44603.0	1.052	1.71	76532.8	0.643	1.70	78193.8	0.190
1.74	42503.5	0.941	1.74	74432.7	0.562	1.74	75801.6	0.260
1.77	40680.6	0.731	1.77	73193.5	0.466	1.77	73870.2	0.334
1.80	39169.8	0.287	1.80	71819.1	0.389	1.80	72333.9	0.409
1.83	38105.1	-0.454	1.83	70525.2	0.354	1.83	70973.1	0.437
1.86	37623.1	-1.062	1.86	69336.0	0.343	1.86	69722.1	0.435
1.89	37578.9	-1.345	1.89	68163.8	0.355	1.89	68515.0	0.413
1.92	37772.3	-1.464	1.92	67174.9	0.391	1.92	67483.5	0.373
1.95	38104.0	-1.515	1.93	66228.7	0.406	1.95	66770.0	0.334
1.98	38524.4	-1.535	1.94	65927.4	0.420	1.96	66626.5	0.324
2.01	39007.8	-1.538	1.95	65633.2	0.434	1.97	66476.4	0.313
2.04	39535.3	-1.530	1.96	65345.8	0.448	1.98	66323.6	0.300

2.07	40092.5	-1.513		1.97	65065.1	0.462		1.99	66170.7	0.286
2.10	40668.8	-1.489		1.98	64790.7	0.475		2.00	66019.7	0.271
2.13	41254.9	-1.458		1.99	64473.0	0.488		2.01	65871.8	0.255
2.16	41842.0	-1.421		2.00	63724.5	0.501		2.02	65727.8	0.233
2.19	42423.6	-1.379		2.01	63010.1	0.515		2.07	65084.2	0.153
2.22	42993.4	-1.332		2.04	62334.1	0.543		2.08	64972.3	0.135
2.25	43547.4	-1.280		2.07	61694.5	0.576		2.09	64866.0	0.116
2.28	44081.0	-1.225		2.10	61140.0	0.604		2.10	64765.4	0.098
2.31	44591.1	-1.166		2.13	60720.4	0.628		2.11	64671.2	0.080
2.34	45074.9	-1.105		2.16	60370.0	0.649		2.12	64581.8	0.062
2.37	45531.0	-1.042		2.19	60030.1	0.666		2.13	64497.8	0.044
2.40	45957.8	-0.978		2.22	59730.1	0.679		2.18	64062.6	-0.073
2.43	46354.8	-0.914		2.25	59430.0	0.689		2.20	63898.7	-0.134
2.46	46721.8	-0.851		2.28	59189.9	0.695		2.23	63768.0	-0.193
2.49	47059.3	-0.789		2.31	58900.3	0.699		2.25	63673.6	-0.250
2.52	47368.9	-0.729		2.34	58580.7	0.700		2.28	63612.5	-0.304
2.55	47653.1	-0.671		2.37	58320.4	0.699		2.31	63582.1	-0.352
2.58	47913.0	-0.617		2.40	58040.2	0.696		2.34	63579.4	-0.394
2.61	48150.0	-0.565		2.43	57758.0	0.691		2.37	63601.1	-0.430
2.64	48365.5	-0.516		2.46	57402.4	0.684		2.40	63643.6	-0.457
2.67	48560.6	-0.471		2.49	57062.0	0.676		2.43	63702.5	-0.476
2.70	48737.0	-0.429		2.52	56735.9	0.667		2.46	63774.5	-0.487
2.73	48896.2	-0.391		2.55	56423.7	0.657		2.49	63855.8	-0.489
2.76	49040.1	-0.355		2.58	56124.8	0.645		2.52	63942.7	-0.483
2.79	49169.3	-0.323		2.61	55838.8	0.633		2.55	64032.3	-0.470
2.82	49285.6	-0.293		2.64	55565.3	0.621		2.58	64121.0	-0.452
2.85	49390.2	-0.266		2.67	55303.7	0.608		2.61	64207.1	-0.429
2.88	49484.3	-0.242		2.70	55053.7	0.594		2.64	64289.2	-0.403
2.91	49569.2	-0.219		2.73	54814.7	0.580		2.67	64365.9	-0.375
2.94	49645.4	-0.199		2.76	54586.5	0.566		2.70	64436.7	-0.347
2.97	49714.4	-0.181		2.79	54368.7	0.552		2.73	64501.2	-0.318
3.00	49776.4	-0.164		2.82	54161.2	0.537		2.76	64560.5	-0.289
3.03	49832.9	-0.150		2.85	53963.0	0.523		2.79	64612.1	-0.261
3.06	49884.8	-0.136		2.88	53773.9	0.509		2.82	64657.6	-0.235
3.09	49933.0	-0.124		2.91	53593.9	0.494		2.85	64697.6	-0.211
3.12	49977.8	-0.113		2.94	53422.0	0.480		2.88	64732.3	-0.188
3.15	50019.0	-0.103		2.97	108735.4	0.465		2.91	64763.1	-0.168
3.18	50056.6	-0.093		3.00	107244.3	0.451		2.94	64788.9	-0.149
3.21	50090.9	-0.085		3.03	53258.0	0.437		2.97	64811.1	-0.132
3.24	50122.0	-0.078		3.06	53101.9	0.423		3.00	64829.7	-0.116
3.27	50150.4	-0.071		3.09	52952.3	0.410		3.03	64845.4	-0.103
3.30	50176.2	-0.065		3.12	52809.6	0.396		3.06	64858.6	-0.090
3.33	50199.6	-0.059		3.15	52673.8	0.383		3.09	64869.5	-0.079
3.36	50221.0	-0.054		3.18	52544.5	0.370		3.12	64878.5	-0.069

3.39	50240.6	-0.049	3.21	52421.7	0.357	3.15	64885.8	-0.061
3.42	50258.4	-0.045	3.24	52305.1	0.345	3.18	64891.7	-0.053
3.45	50274.7	-0.041	3.27	52194.4	0.333	3.21	64896.5	-0.046
3.48	50289.5	-0.037	3.30	52089.5	0.321	3.24	64900.1	-0.040
3.51	50303.1	-0.034	3.33	51989.9	0.309	3.27	64902.9	-0.035
3.54	50315.5	-0.031	3.36	51895.5	0.298	3.30	64905.0	-0.030
3.57	50327.0	-0.028	3.39	51806.0	0.286	3.33	64905.8	-0.026
3.60	50337.4	-0.025	3.42	51721.2	0.276	3.36	64906.8	-0.022
3.63	50347.0	-0.022	3.45	51640.8	0.265	3.39	64907.4	-0.019
3.66	50355.8	-0.020	3.48	51564.7	0.255	3.42	64907.6	-0.016
3.69	50363.9	-0.017	3.51	51492.6	0.245	3.45	64907.6	-0.014
3.72	50371.4	-0.015	3.54	51424.4	0.235	3.48	64907.4	-0.011
3.75	50378.4	-0.013	3.57	51359.8	0.225	3.51	64906.9	-0.009
3.78	50384.9	-0.010	3.60	51298.7	0.216	3.54	64906.4	-0.008
3.81	50397.6	-0.008	3.63	51240.8	0.207	3.57	64905.8	-0.006
3.84	50403.5	-0.006	3.66	51186.0	0.198	3.60	64905.0	-0.005
3.87	50409.1	-0.003	3.69	51134.2	0.190	3.63	64904.2	-0.003
3.90	50414.6	0.000	3.72	51085.1	0.181	3.66	64903.5	-0.002
3.93	50420.1	0.003	3.75	51038.7	0.173	3.69	64902.6	-0.001
3.96	50425.5	0.006	3.78	50994.5	0.165	3.72	64901.8	0.000
3.99	50434.3	0.010	3.81	50954.0	0.156	3.75	64901.0	0.001
4.02	50440.3	0.014	3.84	50914.4	0.148	3.78	64900.3	0.002
4.05	50446.6	0.019	3.87	50876.7	0.140	3.81	64905.8	0.003
4.08	50453.2	0.024	3.90	50842.0	0.132	3.84	64904.7	0.003
4.11	50460.0	0.029	3.93	50807.8	0.124	3.87	64903.8	0.004
4.14	50466.8	0.035	3.96	50774.8	0.115	3.90	64903.5	0.005
4.17	50473.2	0.040	3.99	50743.9	0.106	3.93	64911.1	0.006
4.20	50478.7	0.045	4.02	50712.9	0.097	3.96	64910.5	0.007
4.23	50483.0	0.049	4.05	50682.8	0.088	3.99	64914.6	0.008
4.26	50485.8	0.052	4.08	50653.2	0.079	4.02	64913.9	0.009
4.29	50486.6	0.055	4.11	50624.4	0.069	4.05	64913.5	0.010
4.32	50472.3	0.056	4.14	50596.6	0.059	4.08	64913.2	0.011
4.35	50460.4	0.057	4.17	50570.1	0.050	4.11	64913.2	0.012
4.38	50450.6	0.057	4.20	50545.6	0.041	4.14	64913.6	0.014
4.41	50442.5	0.056	4.23	50523.1	0.033	4.17	64914.3	0.015
4.44	50435.9	0.055	4.26	50503.5	0.026	4.20	64915.2	0.017
4.47	50430.5	0.054	4.32	50486.7	0.015	4.23	64916.9	0.019
4.50	50426.0	0.053	4.35	50485.2	0.011	4.26	64919.0	0.021
4.53	50422.3	0.051	4.38	50482.7	0.008	4.32	64925.4	0.026
4.56	50419.3	0.049	4.41	50479.4	0.006	4.35	64929.4	0.029
4.59	50416.7	0.048	4.44	50475.6	0.004	4.38	64934.5	0.033
4.62	50414.6	0.046	4.47	50471.4	0.002	4.41	64941.2	0.038
4.65	50412.8	0.044	4.50	50467.1	0.001	4.44	64948.0	0.043
4.68	50411.3	0.042	4.53	50462.7	0.000	4.47	64956.4	0.048

4.71	50410.1	0.041		4.56	50458.3	-0.001		4.50	64965.7	0.054
4.74	50409.0	0.039		4.59	50453.9	-0.001		4.53	64967.0	0.060
4.77	50408.2	0.037		4.62	50449.7	-0.002		4.56	64937.8	0.066
4.80	50407.5	0.035		4.65	50445.7	-0.002		4.59	64909.1	0.071
				4.68	50441.8	-0.002		4.62	64881.7	0.077
				4.71	50438.1	-0.003		4.65	64856.1	0.081
				4.74	50434.7	-0.003		4.68	64832.7	0.085
				4.77	50431.5	-0.003		4.71	64811.3	0.087
				4.80	50428.4	-0.003		4.74	64794.0	0.090
								4.77	64777.9	0.091
								4.80	64763.9	0.092

(5) ² Π			(1) ² Δ			(2) ² Δ		
R (Å)	E (cm ⁻¹)	μ (a.u.)	R (Å)	E (cm ⁻¹)	μ (a.u.)	R (Å)	E (cm ⁻¹)	μ (a.u.)
1.41	124149.6	0.275	1.41	109361.7	1.103	1.41	119268.0	1.125
1.44	117123.0	0.319	1.44	102154.7	1.100	1.44	112217.9	1.128
1.47	110979.8	0.347	1.47	95853.7	1.093	1.47	106057.2	1.126
1.50	105594.0	0.372	1.50	90325.5	1.086	1.50	100626.8	1.123
1.53	100929.2	0.389	1.53	85509.1	1.073	1.53	95935.0	1.114
1.56	96858.0	0.402	1.56	81291.6	1.058	1.56	91837.9	1.102
1.59	93301.6	0.416	1.59	77593.1	1.041	1.59	88253.6	1.089
1.62	90191.7	0.428	1.62	74346.3	1.024	1.62	85114.9	1.074
1.64	87762.9	0.437	1.65	71493.0	1.005	1.65	82363.8	1.057
1.66	86490.0	0.443	1.68	68982.9	0.986	1.68	79952.3	1.040
1.68	85085.2	0.449	1.71	66772.7	0.966	1.71	77836.6	1.022
1.71	82995.1	0.456	1.74	64824.9	0.946	1.74	75981.2	1.003
1.74	81061.2	0.466	1.77	63107.0	0.925	1.77	74352.0	0.984
1.77	79373.8	0.473	1.80	61591.0	0.903	1.80	72922.5	0.964
1.80	78143.2	0.479	1.83	60252.4	0.882	1.83	71668.6	0.943
1.83	76723.8	0.486	1.86	59069.9	0.860	1.86	70569.4	0.922
1.86	75814.8	0.492	1.89	58024.7	0.837	1.89	69606.5	0.901
1.89	74807.5	0.499	1.92	57100.7	0.815	1.92	68763.9	0.879
1.92	74015.0	0.504	1.95	56283.3	0.792	1.95	68027.3	0.856
1.95	73292.4	0.510	1.98	55559.9	0.769	1.98	67384.4	0.834
1.98	72751.5	0.517	2.01	54919.4	0.746	2.01	66823.9	0.811
2.01	72042.8	0.522	2.04	54351.9	0.723	2.04	66336.4	0.788
2.04	71530.6	0.526	2.07	53848.7	0.701	2.07	65913.0	0.765
2.05	71380.7	0.528	2.10	53402.1	0.678	2.10	65545.5	0.742
2.06	71236.0	0.530	2.13	53005.5	0.655	2.13	65230.7	0.718
2.07	71096.5	0.532	2.16	52652.7	0.633	2.16	64957.4	0.695
2.08	70962.1	0.533	2.19	52338.9	0.611	2.19	64723.3	0.673
2.09	70832.6	0.535	2.22	52059.0	0.589	2.22	64523.1	0.650
2.10	70707.8	0.536	2.25	51809.1	0.567	2.25	64351.8	0.627
2.11	70588.2	0.538	2.28	51585.6	0.546	2.28	64205.3	0.605

2.12	70472.3	0.539	2.31	51385.7	0.525	2.31	64082.8	0.583
2.13	70360.8	0.540	2.34	51206.5	0.505	2.34	63980.0	0.561
2.14	70253.5	0.541	2.37	51045.7	0.485	2.37	63894.5	0.540
2.16	69870.8	0.543	2.40	50901.2	0.466	2.40	63824.5	0.519
2.19	69668.9	0.544	2.43	50771.0	0.447	2.43	63768.7	0.499
2.22	69438.7	0.545	2.46	50653.2	0.429	2.46	63725.4	0.479
2.25	69220.9	0.546	2.49	50546.4	0.411	2.49	63694.9	0.460
2.28	69019.6	0.546	2.52	50449.9	0.394	2.52	63673.0	0.441
2.31	68834.4	0.548	2.55	50363.4	0.378	2.55	63654.1	0.423
2.34	68665.0	0.548	2.58	50286.5	0.362	2.58	63637.6	0.405
2.37	68508.2	0.548	2.61	50218.2	0.346	2.61	63623.1	0.388
2.40	68364.5	0.547	2.64	50157.6	0.331	2.64	63611.5	0.372
2.43	68231.5	0.546	2.67	50103.7	0.317	2.67	63601.6	0.356
2.46	68109.1	0.543	2.70	50055.8	0.303	2.70	63593.5	0.340
2.49	67994.7	0.541	2.73	50013.5	0.290	2.73	63588.0	0.325
2.52	67888.7	0.538	2.76	49976.2	0.277	2.76	63584.5	0.311
2.55	67789.4	0.534	2.79	49943.4	0.265	2.79	63582.7	0.297
2.58	67696.4	0.531	2.82	49915.0	0.253	2.82	63582.4	0.284
2.61	67610.5	0.527	2.85	49890.1	0.242	2.85	63583.8	0.271
2.64	67527.1	0.523	2.88	49868.5	0.231	2.88	63586.5	0.259
2.67	67447.8	0.518	2.91	49850.0	0.221	2.91	63590.4	0.247
2.70	67372.2	0.514	2.94	49834.4	0.211	2.94	63595.5	0.236
2.73	67299.9	0.509	2.97	49821.2	0.202	2.97	63601.5	0.225
2.76	67231.0	0.505	3.00	49810.5	0.193	3.00	63608.6	0.215
2.79	67164.3	0.500	3.03	49801.9	0.184	3.03	63616.4	0.205
2.82	67099.9	0.495	3.06	49795.3	0.176	3.06	63625.0	0.196
2.85	67037.6	0.490	3.09	49790.4	0.168	3.09	63634.3	0.187
2.88	66977.5	0.485	3.12	49787.2	0.160	3.12	63644.2	0.178
2.91	66919.1	0.480	3.15	49785.4	0.153	3.15	63654.6	0.170
2.94	66862.1	0.475	3.18	49785.0	0.146	3.18	63665.6	0.162
2.97	66809.0	0.468	3.21	49785.8	0.140	3.21	63677.1	0.155
3.00	66754.9	0.463	3.24	49787.7	0.134	3.24	63688.8	0.148
3.03	66702.2	0.457	3.27	49790.5	0.128	3.27	63700.8	0.141
3.06	66649.2	0.452	3.30	49794.3	0.122	3.30	63713.1	0.135
3.09	66599.8	0.445	3.33	49798.8	0.117	3.33	63725.6	0.128
3.12	66548.0	0.440	3.36	49804.0	0.112	3.36	63738.2	0.123
3.15	66498.9	0.433	3.39	49809.8	0.107	3.39	63750.9	0.117
3.18	66451.0	0.427	3.42	49816.1	0.102	3.42	63763.7	0.112
3.21	66404.1	0.421	3.45	49822.9	0.098	3.45	63776.5	0.107
3.24	66357.9	0.414	3.48	49830.1	0.094	3.48	63789.3	0.102
3.27	66312.7	0.407	3.51	49837.6	0.090	3.51	63802.1	0.097
3.30	66268.2	0.401	3.54	49845.4	0.086	3.54	63814.9	0.093
3.33	66224.5	0.394	3.57	49853.4	0.082	3.57	63827.5	0.089
3.36	66181.6	0.387	3.60	49861.7	0.079	3.60	63840.1	0.085

3.39	66139.4	0.380		3.63	49870.0	0.075		3.63	63852.5	0.081
3.42	66098.0	0.373		3.66	49878.5	0.072		3.66	63864.8	0.078
3.45	66057.4	0.366		3.69	49887.1	0.069		3.69	63877.0	0.074
3.48	66017.4	0.359		3.72	49895.8	0.066		3.72	63889.0	0.071
3.51	65978.4	0.352		3.75	49904.6	0.064		3.75	63901.0	0.068
3.54	65939.7	0.345		3.78	49913.4	0.061		3.78	63912.7	0.065
3.57	65901.6	0.338		3.81	49922.1	0.059		3.81	63924.3	0.062
3.60	65868.4	0.331		3.84	49930.9	0.056		3.84	63935.6	0.059
3.63	65838.5	0.325		3.87	49939.7	0.054		3.87	63947.1	0.057
3.66	65799.7	0.318		3.90	49948.4	0.052		3.90	63958.1	0.054
3.69	65764.1	0.311		3.93	49957.0	0.050		3.93	63968.9	0.052
3.72	65730.0	0.304		3.96	49965.6	0.048		3.96	63979.6	0.050
3.75	65696.8	0.297		3.99	49974.1	0.046		3.99	63990.3	0.048
3.78	65661.3	0.290		4.02	49982.6	0.044		4.02	64000.6	0.046
3.81	65629.0	0.283		4.05	49990.9	0.042		4.05	64010.7	0.044
3.84	65596.6	0.276		4.08	49999.2	0.040		4.08	64020.6	0.042
3.87	65565.0	0.269		4.11	50007.4	0.039		4.11	64030.4	0.040
3.90	65534.1	0.262		4.14	50015.5	0.037		4.14	64039.9	0.039
3.93	65504.0	0.255		4.17	50023.5	0.036		4.17	64049.3	0.037
3.96	65474.3	0.248		4.20	50031.4	0.034		4.20	64058.3	0.035
3.99	65445.7	0.241		4.23	50039.2	0.033		4.23	64067.3	0.034
4.02	65417.2	0.233		4.26	50046.9	0.032		4.26	64076.1	0.033
4.05	65386.5	0.225		4.29	50054.5	0.030		4.29	64085.8	0.031
4.08	65362.0	0.219		4.32	50061.9	0.029		4.32	64094.3	0.030
4.11	65335.2	0.212		4.35	50069.3	0.028		4.35	64103.3	0.029
4.14	65309.0	0.204		4.38	50076.5	0.027		4.38	64111.4	0.028
4.17	65283.1	0.197		4.41	50083.5	0.026		4.41	64119.3	0.026
4.20	65259.3	0.190		4.44	50090.4	0.025		4.44	64127.0	0.025
4.23	65232.9	0.182		4.47	50097.1	0.024		4.47	64134.2	0.024
4.26	65207.8	0.174		4.50	50103.7	0.023		4.50	64141.6	0.023
4.29	65181.4	0.165		4.53	50110.2	0.022		4.53	64148.7	0.022
4.32	65156.2	0.156		4.56	50116.5	0.021		4.56	64155.7	0.021
4.35	65132.6	0.148		4.59	50122.8	0.020		4.59	64163.3	0.021
4.38	65107.4	0.140		4.62	50129.1	0.020		4.62	64169.9	0.020
4.41	65078.2	0.129		4.65	50135.0	0.019		4.65	64176.3	0.019
4.44	65053.4	0.120		4.68	50140.7	0.018		4.68	64182.5	0.018
4.47	65025.2	0.110		4.71	50146.2	0.017		4.71	64188.6	0.017
4.50	64996.3	0.099		4.74	50151.6	0.017		4.74	64194.5	0.017
4.53	64975.7	0.089		4.77	50156.8	0.016		4.77	64201.2	0.016
4.56	64986.0	0.078		4.80	50161.9	0.015		4.80	64206.7	0.015
4.59	64996.2	0.068								
4.62	65005.6	0.059								
4.65	65013.9	0.050								
4.68	65020.8	0.042								

4.71	65026.1	0.035							
4.74	65029.7	0.030							
4.77	65032.1	0.025							
4.80	65033.1	0.021							

(1) ² Σ ⁻			(2) ² Σ ⁻			(1) ⁴ Σ ⁺		
R (Å)	E (cm ⁻¹)	μ (a.u.)	R (Å)	E (cm ⁻¹)	μ (a.u.)	R (Å)	E (cm ⁻¹)	μ (a.u.)
1.41	110050.6	1.117	1.41	119956.7	1.136	1.41	105651.1	1.044
1.44	102832.2	1.114	1.44	112875.5	1.138	1.44	98542.4	1.032
1.47	96519.1	1.107	1.47	106685.8	1.136	1.47	92340.2	1.018
1.50	90977.6	1.099	1.50	101223.0	1.133	1.50	86926.4	1.003
1.53	86148.4	1.086	1.53	96508.5	1.123	1.53	82198.0	0.987
1.56	81917.9	1.071	1.56	92391.2	1.111	1.56	78065.8	0.970
1.59	78206.4	1.054	1.59	88788.4	1.097	1.59	74452.1	0.953
1.62	74946.4	1.037	1.62	85632.9	1.082	1.62	71289.9	0.934
1.65	72079.9	1.018	1.65	82866.9	1.066	1.65	68521.0	0.916
1.68	69556.6	0.998	1.68	80440.9	1.048	1.68	66095.2	0.897
1.71	67333.3	0.978	1.71	78311.9	1.030	1.71	63969.3	0.878
1.74	65372.6	0.957	1.74	76444.4	1.011	1.74	62105.6	0.859
1.77	63641.8	0.936	1.77	74803.7	0.991	1.77	60471.6	0.839
1.80	62113.0	0.914	1.80	73363.3	0.971	1.80	59039.1	0.819
1.83	60761.8	0.892	1.83	72099.3	0.950	1.83	57783.5	0.799
1.86	59566.8	0.870	1.86	70990.4	0.929	1.86	56683.5	0.779
1.89	58509.3	0.847	1.89	70018.3	0.907	1.89	55720.1	0.759
1.92	57573.0	0.825	1.92	69166.9	0.885	1.92	54877.0	0.738
1.95	56743.7	0.802	1.95	68421.9	0.863	1.95	54139.6	0.718
1.98	56008.5	0.779	1.98	67770.8	0.840	1.98	53495.4	0.697
2.01	55356.3	0.756	2.01	67202.5	0.817	2.01	52933.0	0.677
2.04	54777.3	0.733	2.04	66707.3	0.794	2.04	52442.7	0.656
2.07	54262.8	0.709	2.07	66276.4	0.771	2.07	52015.4	0.636
2.10	53805.1	0.687	2.10	65901.7	0.747	2.10	51643.7	0.616
2.13	53397.5	0.664	2.13	65577.7	0.724	2.13	51320.6	0.596
2.16	53034.0	0.641	2.16	65297.5	0.701	2.16	51040.2	0.576
2.19	52709.6	0.619	2.19	65056.5	0.678	2.19	50797.0	0.556
2.22	52419.2	0.597	2.22	64851.9	0.655	2.22	50586.6	0.536
2.25	52159.1	0.575	2.25	64674.0	0.632	2.25	50404.8	0.517
2.28	51925.8	0.554	2.28	64519.8	0.610	2.28	50248.0	0.498
2.31	51715.8	0.533	2.31	64391.5	0.588	2.31	50113.0	0.480
2.34	51527.1	0.512	2.34	64282.2	0.566	2.34	49997.2	0.462
2.37	51356.8	0.492	2.37	64190.2	0.545	2.37	49898.3	0.444
2.40	51203.0	0.473	2.40	64113.9	0.524	2.40	49814.0	0.427
2.43	51063.7	0.454	2.43	64051.8	0.503	2.43	49742.5	0.410
2.46	50937.1	0.435	2.46	64002.1	0.483	2.46	49682.4	0.394
2.49	50821.6	0.417	2.49	63965.4	0.464	2.49	49632.1	0.378

2.52	50716.6	0.400		2.52	63936.6	0.445		2.52	49590.5	0.363
2.55	50621.8	0.383		2.55	63912.3	0.426		2.55	49556.4	0.348
2.58	50536.8	0.367		2.58	63889.8	0.409		2.58	49529.1	0.333
2.61	50460.6	0.352		2.61	63869.3	0.391		2.61	49507.5	0.320
2.64	50392.3	0.336		2.64	63851.6	0.375		2.64	49491.1	0.306
2.67	50331.0	0.322		2.67	63835.9	0.359		2.67	49479.1	0.293
2.70	50275.8	0.308		2.70	63822.1	0.343		2.70	49471.1	0.281
2.73	50226.4	0.295		2.73	63811.0	0.328		2.73	49466.6	0.269
2.76	50182.2	0.282		2.76	63801.9	0.314		2.76	49465.0	0.257
2.79	50142.7	0.269		2.79	63794.7	0.300		2.79	49466.1	0.246
2.82	50107.7	0.257		2.82	63789.1	0.286		2.82	49469.6	0.235
2.85	50076.5	0.246		2.85	63785.3	0.274		2.85	49475.0	0.225
2.88	50048.8	0.235		2.88	63782.9	0.261		2.88	49485.4	0.215
2.91	50024.3	0.225		2.91	63781.8	0.250		2.91	49496.6	0.206
2.94	50002.9	0.215		2.94	63782.0	0.238		2.94	49508.3	0.197
2.97	49984.2	0.205		2.97	63783.4	0.227		2.97	49519.6	0.188
3.00	49968.0	0.196		3.00	63785.8	0.217		3.00	49531.9	0.180
3.03	49954.1	0.187		3.03	63789.1	0.207		3.03	49545.2	0.172
3.06	49942.4	0.179		3.06	63793.4	0.198		3.06	49559.3	0.164
3.09	49932.6	0.171		3.09	63798.4	0.189		3.09	49574.0	0.157
3.12	49924.5	0.163		3.12	63804.1	0.180		3.12	49589.3	0.150
3.15	49918.1	0.156		3.15	63810.5	0.172		3.15	49605.0	0.144
3.18	49913.2	0.149		3.18	63817.5	0.164		3.18	49621.1	0.137
3.21	49909.7	0.142		3.21	63825.2	0.156		3.21	49637.6	0.131
3.24	49907.4	0.136		3.24	63833.2	0.149		3.24	49654.3	0.126
3.27	49906.2	0.130		3.27	63841.6	0.142		3.27	49671.2	0.120
3.30	49906.0	0.124		3.30	63850.3	0.136		3.30	49688.3	0.115
3.33	49906.8	0.119		3.33	63859.4	0.130		3.33	49705.4	0.110
3.36	49908.3	0.114		3.36	63868.6	0.124		3.36	49722.5	0.105
3.39	49910.6	0.109		3.39	63878.1	0.118		3.39	49739.6	0.101
3.42	49913.5	0.104		3.42	63887.7	0.113		3.42	49756.7	0.096
3.45	49917.0	0.100		3.45	63897.4	0.108		3.45	49773.6	0.092
3.48	49921.0	0.095		3.48	63907.2	0.103		3.48	49790.4	0.088
3.51	49925.4	0.091		3.51	63917.1	0.098		3.51	49807.0	0.085
3.54	49930.3	0.087		3.54	63927.0	0.094		3.54	49823.4	0.081
3.57	49935.4	0.084		3.57	63936.9	0.090		3.57	49839.9	0.078
3.60	49940.9	0.080		3.60	63946.8	0.086		3.60	49855.9	0.074
3.63	49946.6	0.077		3.63	63956.6	0.082		3.63	49871.6	0.071
3.66	49952.6	0.074		3.66	63966.4	0.078		3.66	49887.1	0.068
3.69	49958.7	0.071		3.69	63976.1	0.075		3.69	49902.3	0.065
3.72	49965.0	0.068		3.72	63985.7	0.072		3.72	49917.3	0.063
3.75	49971.5	0.065		3.75	63995.3	0.069		3.75	49932.0	0.060
3.78	49978.0	0.062		3.78	64004.7	0.066		3.78	49946.4	0.058
3.81	49984.6	0.060		3.81	64014.1	0.063		3.81	49960.5	0.055

3.84	49991.2	0.057		3.84	64023.3	0.060		3.84	49974.4	0.053
3.87	49998.1	0.055		3.87	64032.5	0.058		3.87	49988.0	0.051
3.90	50004.9	0.053		3.90	64041.5	0.055		3.90	50001.3	0.049
3.93	50011.7	0.051		3.93	64050.3	0.053		3.93	50014.3	0.047
3.96	50018.4	0.048		3.96	64059.0	0.051		3.96	50027.9	0.045
3.99	50025.3	0.047		3.99	64067.9	0.048		3.99	50040.4	0.043
4.02	50032.0	0.045		4.02	64076.4	0.046		4.00	50044.5	0.042
4.05	50038.8	0.043		4.05	64084.7	0.044		4.03	50056.6	0.041
4.08	50045.5	0.041		4.08	64092.9	0.043		4.06	50068.6	0.039
4.11	50052.2	0.040		4.11	64100.9	0.041		4.09	50080.2	0.037
4.14	50058.9	0.038		4.14	64108.8	0.039		4.12	50091.6	0.036
4.17	50065.5	0.036		4.17	64116.6	0.037		4.15	50102.8	0.034
4.20	50072.0	0.035		4.20	64124.0	0.036		4.18	50113.7	0.033
4.23	50078.5	0.034		4.23	64131.5	0.034		4.21	50124.4	0.032
4.26	50085.0	0.032		4.26	64138.9	0.033		4.24	50134.8	0.030
4.29	50091.4	0.031		4.29	64146.6	0.032		4.27	50145.0	0.029
4.32	50097.6	0.030		4.32	64153.8	0.030		4.30	50155.0	0.028
4.35	50103.9	0.029		4.35	64161.1	0.029		4.33	50164.8	0.027
4.38	50109.9	0.027		4.38	64167.9	0.028		4.36	50174.3	0.026
4.41	50116.0	0.026		4.41	64174.5	0.027		4.39	50183.6	0.025
4.44	50121.8	0.025		4.44	64181.0	0.026		4.42	50192.6	0.024
4.47	50127.6	0.024		4.47	64187.0	0.025		4.45	50201.5	0.023
4.50	50133.3	0.023		4.50	64193.1	0.024		4.48	50210.1	0.022
4.53	50138.8	0.022		4.53	64199.1	0.023				
4.56	50144.3	0.022		4.56	64204.9	0.022				
4.59	50149.7	0.021		4.59	64211.5	0.021				
4.62	50155.2	0.020		4.62	64217.0	0.020				
4.65	50160.3	0.019		4.65	64222.4	0.019				
4.68	50165.3	0.018		4.68	64227.6	0.018				
4.71	50170.1	0.018		4.71	64232.7	0.018				
4.74	50174.8	0.017		4.74	64237.5	0.017				
4.77	50179.3	0.016		4.77	64243.4	0.016				
4.80	50183.8	0.016		4.80	64247.9	0.016				

(2) ⁴ Σ ⁺			(3) ⁴ Σ ⁺			(4) ⁴ Σ ⁺		
R (Å)	E (cm ⁻¹)	μ (a.u.)	R (Å)	E (cm ⁻¹)	μ (a.u.)	R (Å)	E (cm ⁻¹)	μ (a.u.)
1.41	120935.2	-0.497	1.41	131014.7	1.659	1.41	146500.6	2.302
1.44	114881.3	-0.431	1.44	125028.8	1.640	1.44	140186.9	2.242
1.47	109563.7	-0.369	1.47	119770.9	1.619	1.47	134542.6	2.170
1.50	104881.8	-0.308	1.50	115146.4	1.593	1.50	129493.8	2.089
1.53	100748.4	-0.248	1.53	111072.4	1.565	1.53	124968.4	1.997
1.56	97087.4	-0.188	1.56	107476.4	1.533	1.56	120951.9	1.880
1.59	93833.0	-0.128	1.59	104294.6	1.498	1.59	117316.0	1.748
1.62	90927.8	-0.067	1.62	101469.7	1.460	1.62	114051.7	1.592

1.65	88322.4	-0.006	1.68	96685.9	1.373	1.65	111117.4	1.413
1.68	85974.1	0.055	1.71	94639.8	1.325	1.68	108482.6	1.214
1.71	83846.4	0.117	1.74	92808.3	1.272	1.71	106130.8	0.981
1.74	81907.8	0.178	1.77	91052.8	1.215	1.74	104130.1	0.600
1.77	80131.6	0.238	1.80	89637.8	1.161	1.77	101835.9	1.843
1.80	78495.1	0.296	1.83	88308.9	1.101	1.80	100186.3	1.396
1.83	76979.4	0.353	1.86	87140.2	1.042	1.83	98684.4	1.155
1.86	75568.3	0.406	1.89	86075.1	0.981	1.86	97334.2	1.004
1.89	74248.6	0.456	1.92	85100.8	0.919	1.89	96127.3	0.891
1.92	73009.3	0.502	1.95	84199.5	0.856	1.92	95051.3	0.795
1.95	71841.4	0.543	1.98	83376.6	0.795	1.95	94093.2	0.710
1.98	70737.6	0.580	2.01	82619.2	0.737	1.98	93240.6	0.632
2.01	69691.8	0.611	2.04	81923.4	0.681	2.01	92482.0	0.560
2.04	68699.3	0.638	2.07	81286.0	0.628	2.04	91807.0	0.492
2.07	67756.0	0.660	2.10	80702.6	0.579	2.07	91206.5	0.432
2.10	66858.5	0.678	2.13	80169.4	0.534	2.10	90671.3	0.371
2.13	66004.1	0.691	2.19	79236.9	0.455	2.13	90194.4	0.315
2.16	65190.3	0.700	2.22	78830.8	0.421	2.16	89769.1	0.261
2.19	64415.2	0.706	2.25	78460.3	0.391	2.19	89390.4	0.216
2.22	63676.8	0.708	2.28	78122.3	0.364	2.22	89051.6	0.169
2.25	62973.7	0.707	2.31	77814.3	0.340	2.25	88748.9	0.125
2.28	62304.1	0.704	2.34	77533.5	0.319	2.28	88478.5	0.085
2.31	61666.8	0.698	2.37	77277.7	0.301	2.31	88236.8	0.049
2.34	61060.5	0.691	2.40	77044.7	0.285	2.34	88020.6	0.016
2.37	60484.0	0.682	2.43	76832.6	0.271	2.37	87827.1	-0.013
2.40	59935.9	0.671	2.46	76639.6	0.259	2.40	87653.9	-0.039
2.43	59415.1	0.660	2.49	76464.0	0.249	2.43	87498.9	-0.062
2.46	58920.7	0.647	2.52	76304.4	0.240	2.46	87359.5	-0.084
2.49	58451.2	0.633	2.55	76159.5	0.233	2.49	87234.9	-0.101
2.52	58005.7	0.619	2.58	76027.9	0.227	2.52	87123.0	-0.115
2.55	57583.1	0.605	2.61	75908.5	0.223	2.55	87022.4	-0.127
2.58	57182.5	0.590	2.64	75800.5	0.219	2.58	86931.7	-0.136
2.61	56802.8	0.574	2.67	75702.7	0.217	2.61	86849.8	-0.143
2.64	56443.1	0.559	2.70	75614.3	0.215	2.64	86775.7	-0.148
2.67	56102.3	0.543	2.73	75534.6	0.214	2.67	86708.2	-0.151
2.70	55779.7	0.527	2.76	75462.8	0.214	2.70	86646.6	-0.153
2.73	55474.3	0.512	2.79	75398.2	0.214	2.73	86590.0	-0.153
2.76	55185.3	0.496	2.82	75340.3	0.215	2.76	86537.6	-0.152
2.79	54911.9	0.480	2.85	75288.4	0.216	2.79	86488.8	-0.150
2.82	54653.3	0.465	2.88	75230.5	0.221	2.82	86443.0	-0.147
2.85	54408.7	0.450	2.91	75189.8	0.223	2.85	86399.7	-0.143
2.88	54189.1	0.437	2.94	75153.7	0.226	2.88	86358.8	-0.141
2.91	53970.1	0.422	2.97	75121.8	0.228	2.91	86319.5	-0.138
2.94	53763.2	0.407	3.00	75093.9	0.231	2.94	86281.6	-0.134

2.97	53567.7	0.393	3.03	75069.5	0.235	2.97	86244.4	-0.130
3.00	53383.0	0.379	3.06	75048.3	0.238	3.00	86208.1	-0.124
3.03	53208.6	0.365	3.09	75030.1	0.242	3.03	86172.2	-0.119
3.06	53043.9	0.352	3.12	75014.7	0.246	3.06	86136.5	-0.114
3.09	52888.4	0.339	3.15	75001.7	0.250	3.09	86101.0	-0.108
3.12	52741.7	0.326	3.18	74991.0	0.254	3.12	86065.4	-0.101
3.15	52603.2	0.313	3.21	74982.3	0.258	3.15	86027.3	-0.095
3.18	52472.6	0.301	3.27	74970.4	0.266	3.21	85950.8	-0.088
3.21	52349.4	0.289	3.30	74966.8	0.270	3.24	85914.2	-0.086
3.24	52233.1	0.278	3.33	74964.6	0.274	3.27	85877.4	-0.084
3.27	52123.5	0.267	3.36	74963.6	0.278	3.30	85840.4	-0.082
3.30	52020.2	0.256	3.39	74963.6	0.282	3.33	85803.0	-0.081
3.33	51922.9	0.245	3.42	74964.7	0.286	3.36	85765.6	-0.080
3.36	51831.1	0.235	3.45	74966.7	0.290	3.39	85728.0	-0.080
3.39	51744.7	0.225	3.48	74969.4	0.294	3.42	85690.4	-0.080
3.42	51663.2	0.215	3.51	74972.9	0.297	3.45	85652.9	-0.081
3.45	51586.5	0.206	3.54	74976.9	0.301	3.48	85615.1	-0.083
3.48	51514.3	0.197	3.57	74981.5	0.304	3.51	85577.3	-0.084
3.51	51446.2	0.188	3.60	74986.5	0.307	3.54	85539.6	-0.086
3.54	51382.2	0.180	3.63	74991.9	0.310	3.57	85502.1	-0.088
3.57	51322.0	0.172	3.66	74997.7	0.313	3.60	85464.7	-0.090
3.60	51265.3	0.164	3.69	75003.7	0.316	3.63	85427.5	-0.092
3.63	51211.9	0.157	3.72	75009.9	0.319	3.69	85199.5	-0.097
3.66	51161.8	0.149	3.75	75016.4	0.321	3.72	85184.4	-0.100
3.69	51114.6	0.142	3.78	75023.0	0.323	3.75	85189.9	-0.103
3.72	51070.4	0.135	3.81	75029.6	0.325	3.78	85162.0	-0.106
3.75	51028.8	0.129	3.84	75036.2	0.327	3.81	85135.8	-0.109
3.78	50989.6	0.123	3.87	75042.9	0.329	3.84	85106.9	-0.112
3.81	50952.9	0.117	3.90	75049.6	0.330	3.87	85076.5	-0.114
3.84	50918.3	0.111	3.93	75056.2	0.331	3.90	85048.8	-0.117
3.87	50885.9	0.105	3.96	75062.7	0.332	3.93	85020.2	-0.119
3.90	50855.5	0.100	3.99	75069.2	0.333	3.96	84991.1	-0.121
3.93	50827.0	0.095	4.02	75075.5	0.334	3.99	84963.8	-0.122
3.96	50801.0	0.090	4.05	75081.6	0.334	4.02	84935.3	-0.124
3.99	50775.9	0.086	4.08	75087.6	0.334	4.05	84909.4	-0.125
4.00	50768.0	0.084	4.11	75093.5	0.334	4.08	84881.7	-0.126
4.03	50745.0	0.080	4.14	75099.1	0.334	4.11	84855.8	-0.127
4.06	50723.5	0.076	4.17	75104.5	0.334	4.14	84830.4	-0.127
4.09	50703.4	0.072	4.20	75109.6	0.333	4.17	84805.1	-0.127
4.12	50684.6	0.068	4.23	75114.5	0.333	4.20	84780.9	-0.127
4.15	50667.1	0.064	4.26	75119.2	0.332	4.23	84757.6	-0.127
4.18	50650.7	0.061	4.29	75123.6	0.331	4.26	84734.8	-0.127
4.21	50635.4	0.058	4.32	75127.7	0.329	4.29	84712.7	-0.126
4.24	50621.1	0.054	4.35	75131.5	0.328	4.32	84691.2	-0.125

4.27	50607.9	0.051		4.38	75135.0	0.326		4.35	84670.5	-0.124
4.30	50595.5	0.049		4.41	75138.2	0.324		4.38	84650.4	-0.123
4.33	50584.0	0.046		4.44	75141.0	0.323		4.41	84631.5	-0.121
4.36	50573.3	0.043		4.48	75143.6	0.321		4.44	84613.0	-0.120
4.39	50563.3	0.041						4.48	84595.0	-0.118
4.42	50554.1	0.038								
4.45	50545.6	0.036								
4.48	50537.6	0.034								

(5) ⁴ Σ ⁺			(1) ⁴ Π			(2) ⁴ Π		
R (Å)	E (cm ⁻¹)	μ (a.u.)	R (Å)	E (cm ⁻¹)	μ (a.u.)	R (Å)	E (cm ⁻¹)	μ (a.u.)
1.41	152401.4	-0.920	1.41	108606.2	1.080	1.41	119107.6	-0.455
1.44	145376.8	-0.851	1.44	102527.0	1.078	1.44	112002.3	-0.401
1.47	139284.3	-0.786	1.47	97168.0	1.070	1.47	105802.4	-0.350
1.50	133998.1	-0.721	1.50	92437.0	1.059	1.50	100386.4	-0.300
1.53	129408.7	-0.658	1.53	88253.8	1.043	1.53	95649.0	-0.251
1.56	125420.0	-0.597	1.56	84548.7	1.025	1.56	91498.5	-0.202
1.59	121954.4	-0.535	1.59	81260.9	1.005	1.59	87855.5	-0.153
1.62	118943.1	-0.473	1.62	78337.6	0.982	1.62	84651.4	-0.104
1.65	116326.9	-0.411	1.65	75732.9	0.958	1.65	81826.9	-0.054
1.68	114050.8	-0.350	1.68	73407.2	0.932	1.68	79330.8	-0.004
1.71	112066.0	-0.288	1.71	71326.1	0.906	1.71	77118.9	0.046
1.74	110331.5	-0.228	1.74	69460.0	0.878	1.74	75153.1	0.096
1.77	108814.2	-0.169	1.77	67783.1	0.850	1.77	73400.8	0.146
1.80	107485.2	-0.111	1.80	66273.2	0.822	1.80	71833.2	0.195
1.83	106319.2	-0.055	1.83	64910.9	0.794	1.83	70425.9	0.243
1.86	105295.4	-0.001	1.86	63679.7	0.765	1.86	69158.1	0.290
1.89	104395.1	0.050	1.89	62564.8	0.737	1.89	68011.3	0.334
1.92	103602.3	0.100	1.92	61553.6	0.708	1.92	66969.9	0.377
1.95	102901.7	0.146	1.95	60635.0	0.680	1.95	66020.1	0.417
1.98	102282.2	0.190	1.98	59799.2	0.653	1.98	65150.3	0.454
2.01	101732.8	0.231	2.01	59037.7	0.625	2.01	64350.3	0.488
2.04	101244.3	0.270	2.04	58342.8	0.598	2.04	63611.4	0.518
2.07	100808.8	0.304	2.07	57707.9	0.572	2.07	62926.1	0.546
2.10	100418.7	0.336	2.10	57127.1	0.546	2.10	62288.0	0.570
2.13	100068.3	0.365	2.13	56595.2	0.521	2.13	61691.8	0.591
2.16	99751.7	0.391	2.16	56107.5	0.497	2.16	61132.6	0.608
2.19	99464.5	0.413	2.19	55659.9	0.473	2.19	60606.6	0.622
2.22	99202.3	0.433	2.22	55248.8	0.450	2.22	60110.4	0.633
2.25	98961.9	0.449	2.25	54870.7	0.428	2.25	59641.2	0.641
2.28	98740.5	0.463	2.28	54522.9	0.407	2.28	59196.5	0.646
2.31	98535.4	0.475	2.31	54202.6	0.386	2.31	58774.4	0.649
2.34	98344.8	0.484	2.34	53907.6	0.366	2.34	58373.0	0.650
2.37	98166.9	0.490	2.37	53635.6	0.347	2.37	57990.9	0.649

2.40	98000.1	0.495		2.40	53384.9	0.328		2.40	57626.7	0.646
2.43	97843.3	0.498		2.43	53153.6	0.311		2.43	57279.4	0.641
2.46	97695.3	0.499		2.46	52940.2	0.294		2.46	56947.9	0.635
2.49	97555.2	0.499		2.49	52743.3	0.278		2.49	56631.4	0.627
2.52	97422.3	0.497		2.52	52561.6	0.262		2.52	56329.0	0.618
2.55	97295.9	0.494		2.55	52393.8	0.248		2.55	56040.2	0.609
2.58	97175.4	0.490		2.58	52239.0	0.234		2.58	55764.2	0.598
2.61	97060.5	0.485		2.61	52096.2	0.220		2.61	55500.5	0.587
2.64	96950.5	0.479		2.64	51964.4	0.208		2.64	55248.4	0.576
2.67	96845.3	0.472		2.67	51842.7	0.196		2.67	55007.6	0.563
2.70	96744.4	0.464		2.70	51730.5	0.184		2.70	54777.5	0.551
2.73	96647.7	0.456		2.73	51627.0	0.173		2.73	54557.7	0.538
2.76	96554.9	0.448		2.76	51531.6	0.163		2.76	54347.8	0.525
2.79	96465.7	0.439		2.79	51443.6	0.153		2.79	54147.2	0.512
2.82	96380.1	0.430		2.82	51362.7	0.144		2.82	53955.8	0.498
2.85	96297.9	0.420		2.85	51288.0	0.136		2.85	53773.2	0.484
2.88	96214.9	0.409		2.88	51227.0	0.131		2.88	53597.7	0.470
2.91	96139.0	0.399		2.91	51163.8	0.123		2.91	53431.4	0.457
2.94	96066.2	0.389		2.94	51105.8	0.116		2.94	53272.6	0.443
2.97	95996.0	0.379		2.97	51052.5	0.109		2.97	53121.2	0.430
3.00	95928.8	0.369		3.00	51003.8	0.102		3.00	52976.9	0.417
3.03	95864.4	0.359		3.03	50959.1	0.096		3.03	52839.3	0.404
3.06	95802.6	0.349		3.06	50918.2	0.090		3.06	52708.2	0.391
3.09	95743.3	0.339		3.09	50880.7	0.085		3.09	52583.5	0.378
3.12	95686.5	0.329		3.12	50846.5	0.080		3.12	52464.8	0.365
3.15	95631.5	0.319		3.15	50815.2	0.075		3.15	52352.1	0.353
3.18	95581.0	0.309		3.18	50786.9	0.071		3.18	52245.2	0.341
3.21	95531.6	0.299		3.21	50760.7	0.066		3.21	52143.4	0.329
3.24	95484.4	0.290		3.24	50736.7	0.062		3.24	52046.8	0.317
3.27	95439.3	0.280		3.27	50714.7	0.059		3.27	51955.1	0.306
3.30	95396.2	0.271		3.30	50694.6	0.055		3.30	51868.1	0.295
3.33	95355.2	0.262		3.33	50676.2	0.052		3.33	51785.7	0.284
3.36	95315.9	0.254		3.36	50659.5	0.049		3.36	51707.6	0.273
3.39	95278.4	0.245		3.39	50644.1	0.046		3.39	51633.6	0.263
3.42	95242.7	0.237		3.42	50630.1	0.044		3.42	51563.6	0.253
3.45	95208.7	0.229		3.45	50617.4	0.042		3.45	51497.2	0.243
3.48	95176.4	0.221		3.48	50605.7	0.039		3.48	51434.5	0.234
3.51	95145.6	0.213		3.51	50595.1	0.037		3.51	51375.1	0.224
3.54	95116.4	0.205		3.54	50585.3	0.036		3.54	51319.0	0.215
3.57	95088.5	0.198		3.57	50576.4	0.034		3.57	51265.9	0.206
3.60	95062.1	0.191		3.60	50568.3	0.032		3.60	51215.8	0.198
3.63	95037.0	0.184		3.63	50560.9	0.031		3.63	51168.4	0.189
3.66	95012.7	0.177		3.66	50554.1	0.030		3.66	51123.7	0.181
3.69	94990.0	0.170		3.69	50547.9	0.029		3.69	51081.6	0.173

3.72	94968.5	0.164	3.72	50542.2	0.028	3.72	51041.8	0.166
3.75	94949.2	0.158	3.75	50537.0	0.027	3.75	51004.3	0.158
3.78	94929.9	0.152	3.78	50533.4	0.026	3.78	50969.2	0.151
3.81	94911.6	0.146	3.81	50529.0	0.025	3.81	50936.0	0.144
3.84	94894.3	0.140	3.84	50524.9	0.025	3.84	50904.7	0.137
3.87	94878.0	0.135	3.87	50521.3	0.024	3.87	50875.3	0.130
3.90	94862.6	0.130	3.90	50517.9	0.024	3.90	50847.7	0.124
3.93	94848.1	0.124	3.93	50514.7	0.024	3.93	50821.8	0.117
3.96	94834.4	0.119	3.96	50512.4	0.024	3.96	50798.1	0.111
3.99	94821.6	0.115	3.99	50509.7	0.024	3.99	50775.3	0.105
4.02	94809.6	0.110	4.00	50508.4	0.024	4.00	50767.3	0.103
4.05	94798.3	0.105	4.03	50506.4	0.024	4.03	50747.2	0.097
4.08	94787.8	0.101	4.06	50504.1	0.024	4.06	50727.8	0.092
4.11	94777.9	0.097	4.09	50501.9	0.024	4.09	50709.6	0.086
4.14	94768.7	0.093	4.12	50499.9	0.025	4.12	50692.7	0.081
4.17	94760.1	0.089	4.15	50498.0	0.025	4.15	50677.0	0.075
4.20	94752.2	0.086	4.18	50496.2	0.026	4.18	50662.4	0.070
4.23	94744.8	0.082	4.21	50494.5	0.026	4.21	50648.8	0.065
4.26	94738.0	0.079	4.24	50492.8	0.027	4.24	50636.2	0.060
4.29	94731.8	0.075	4.27	50491.2	0.028	4.27	50624.6	0.055
4.32	94726.0	0.072	4.30	50489.8	0.028	4.30	50613.9	0.051
4.35	94720.6	0.069	4.33	50488.3	0.029	4.33	50604.0	0.046
4.38	94715.6	0.066	4.36	50486.9	0.029	4.36	50595.0	0.042
4.41	94711.0	0.064	4.39	50485.5	0.030	4.39	50586.6	0.038
4.44	94706.8	0.061	4.42	50484.1	0.030	4.42	50579.0	0.035
4.48	94702.9	0.058	4.45	50482.8	0.031	4.45	50572.0	0.031
			4.48	50481.5	0.031	4.48	50565.7	0.028

(3) ⁴ Π			(4) ⁴ Π			(5) ⁴ Π		
R (Å)	E (cm ⁻¹)	μ (a.u.)	R (Å)	E (cm ⁻¹)	μ (a.u.)	R (Å)	E (cm ⁻¹)	μ (a.u.)
1.41	129873.5	1.683	1.41	142350.1	0.414	1.41	144373.2	2.352
1.44	122817.9	1.660	1.44	135352.2	0.424	1.44	137028.9	2.270
1.47	116664.1	1.637	1.47	129275.0	0.431	1.47	130518.6	2.187
1.50	111294.0	1.613	1.50	123997.9	0.437	1.50	124753.9	2.104
1.53	106604.7	1.588	1.53	119415.0	0.448	1.53	119649.8	2.017
1.56	102506.5	1.561	1.56	115122.4	1.931	1.56	115441.0	0.459
1.59	98921.5	1.533	1.59	111112.9	1.862	1.59	111988.1	0.445
1.62	95782.3	1.504	1.62	107554.6	1.749	1.62	108992.9	0.444
1.65	93030.4	1.473	1.65	104400.0	1.637	1.65	106396.0	0.443
1.68	90615.3	1.440	1.68	102200.0	1.543	1.68	104146.0	0.442
1.71	88493.3	1.406	1.71	100200.0	1.464	1.71	102199.1	0.440
1.74	86626.7	1.370	1.73	98700.0	1.403	1.74	100517.1	0.438
1.77	84982.8	1.332	1.77	96519.2	1.312	1.77	99066.9	0.435
1.80	83533.5	1.292	1.80	94873.2	1.237	1.80	97819.6	0.431

1.83	82254.4	1.250	1.83	93453.6	1.159	1.83	96750.1	0.427
1.86	81124.4	1.207	1.86	92098.0	1.096	1.86	95836.7	0.423
1.89	80125.4	1.162	1.89	90901.9	1.035	1.89	95060.1	0.418
1.92	79241.7	1.115	1.92	89885.8	0.976	1.92	94403.5	0.413
1.95	78459.6	1.068	1.95	89016.3	0.926	1.95	93851.8	0.408
1.98	77767.5	1.020	1.98	88179.1	0.878	1.98	93391.9	0.402
2.01	77155.0	0.972	2.01	87499.8	0.829	2.01	93012.1	0.395
2.04	76613.4	0.924	2.04	86913.2	0.778	2.04	92702.0	0.389
2.07	76134.8	0.877	2.07	86409.2	0.730	2.07	92452.5	0.381
2.10	75712.6	0.831	2.10	85979.7	0.688	2.10	92255.5	0.374
2.13	75340.6	0.787	2.13	85648.4	0.635	2.13	92103.8	0.366
2.16	75013.6	0.745	2.16	85291.7	0.596	2.16	91991.0	0.358
2.19	74726.9	0.704	2.19	85053.1	0.557	2.19	91911.5	0.350
2.22	74476.2	0.666	2.22	84824.2	0.530	2.22	91860.3	0.342
2.25	74257.7	0.630	2.25	84647.7	0.504	2.25	91833.1	0.333
2.28	74067.9	0.597	2.28	84495.1	0.483	2.28	91826.2	0.324
2.31	73904.0	0.566	2.31	84388.2	0.452	2.31	91836.2	0.316
2.34	73763.1	0.537	2.34	84295.6	0.426	2.34	91860.3	0.307
2.37	73642.7	0.511	2.37	84237.4	0.396	2.37	91895.9	0.298
2.40	73540.6	0.486	2.40	84185.0	0.381	2.40	91941.0	0.289
2.43	73454.8	0.464	2.43	84151.1	0.362	2.43	91993.7	0.280
2.46	73383.5	0.444	2.46	84131.3	0.343	2.46	92052.3	0.271
2.49	73325.2	0.425	2.49	84123.1	0.325	2.49	92115.5	0.262
2.52	73278.3	0.408	2.52	84124.7	0.308	2.52	92182.1	0.253
2.55	73241.6	0.393	2.55	84134.4	0.292	2.55	92251.0	0.244
2.58	73214.0	0.379	2.58	84150.9	0.278	2.58	92321.5	0.235
2.61	73194.3	0.367	2.61	84172.9	0.264	2.61	92392.8	0.227
2.64	73181.7	0.356	2.64	84199.3	0.250	2.64	92464.4	0.219
2.67	73175.3	0.346	2.67	84231.5	0.235	2.67	92535.6	0.210
2.70	73174.5	0.337	2.69	84250.6	0.230	2.70	92606.7	0.202
2.73	73178.4	0.329	2.72	84283.5	0.216	2.73	92676.4	0.195
2.76	73186.6	0.322	2.76	84331.2	0.199	2.76	92744.9	0.187
2.79	73198.6	0.316	2.79	84366.9	0.188	2.79	92811.9	0.180
2.82	73213.9	0.311	2.82	84402.7	0.177	2.82	92877.4	0.173
2.85	73231.9	0.306	2.85	84438.0	0.166	2.85	92941.0	0.166
2.88	73254.3	0.302	2.88	84477.9	0.156	2.88	93005.8	0.159
2.91	73276.9	0.298	2.91	84511.1	0.147	2.91	93065.5	0.152
2.94	73301.5	0.295	2.94	84542.9	0.138	2.94	93123.4	0.146
2.97	73327.6	0.293	2.97	84573.1	0.130	2.97	93179.3	0.140
3.00	73355.2	0.291	3.00	84601.8	0.121	3.00	93233.4	0.134
3.03	73383.9	0.290	3.03	84627.0	0.115	3.03	93285.6	0.128
3.06	73413.6	0.289	3.06	84653.2	0.107	3.06	93336.2	0.123
3.09	73444.1	0.288	3.09	84672.9	0.099	3.09	93384.7	0.118
3.12	73475.4	0.288	3.12	84699.8	0.091	3.12	93431.5	0.113

3.15	73507.1	0.288	3.15	84713.5	0.086	3.15	93476.7	0.108
3.18	73539.6	0.289	3.18	84727.5	0.078	3.18	93520.1	0.104
3.21	73572.0	0.289	3.21	84742.6	0.072	3.21	93561.9	0.099
3.24	73604.7	0.290	3.24	84754.0	0.064	3.24	93602.2	0.095
3.27	73637.4	0.291	3.27	84763.5	0.057	3.27	93641.1	0.091
3.30	73670.2	0.292	3.30	84771.0	0.049	3.30	93678.4	0.088
3.33	73702.9	0.293	3.33	84777.1	0.042	3.33	93714.2	0.084
3.36	73735.4	0.295	3.36	84780.0	0.035	3.36	93748.8	0.080
3.39	73767.8	0.296	3.39	84782.0	0.030	3.39	93782.0	0.077
3.42	73799.9	0.298	3.42	84783.1	0.028	3.42	93813.8	0.074
3.45	73831.7	0.300	3.45	84785.9	0.027	3.45	93844.5	0.071
3.48	73863.2	0.301	3.48	84809.9	0.026	3.48	93873.9	0.068
3.51	73895.1	0.304	3.51	84783.6	0.027	3.51	93902.2	0.065
3.54	73925.8	0.305	3.54	84778.4	0.029	3.54	93929.4	0.063
3.57	73956.0	0.307	3.57	84771.8	0.031	3.57	93955.6	0.060
3.60	73985.8	0.309	3.60	84764.9	0.029	3.60	93980.7	0.058
3.63	74015.2	0.311	3.63	84757.0	0.028	3.63	94004.8	0.056
3.66	74044.0	0.313	3.66	84748.3	0.026	3.66	94028.0	0.053
3.69	74072.3	0.314	3.69	84738.9	0.026	3.69	94050.4	0.051
3.72	74100.0	0.316	3.72	84728.8	0.025	3.72	94071.9	0.049
3.75	74127.2	0.317	3.75	84718.2	0.026	3.75	94092.6	0.047
3.78	74153.9	0.319	3.78	84707.1	0.026	3.78	94112.5	0.046
3.81	74180.0	0.320	3.81	84695.5	0.028	3.81	94131.7	0.044
3.84	74205.6	0.321	3.84	84683.6	0.029	3.84	94150.2	0.042
3.87	74230.7	0.322	3.87	84671.3	0.030	3.87	94168.1	0.041
3.90	74255.2	0.324	3.90	84658.8	0.031	3.90	94185.3	0.039
3.93	74279.1	0.324	3.93	84646.1	0.031	3.93	94201.9	0.038
3.96	74302.5	0.325	3.96	84633.1	0.030	3.96	94218.0	0.036
3.99	74325.4	0.326	3.99	84620.0	0.028	3.99	94233.5	0.035
4.00	74332.4	0.326	4.02	84606.9	0.026	4.02	94248.5	0.034
4.03	74355.0	0.327	4.05	84593.8	0.023	4.05	94263.0	0.032
4.06	74376.6	0.327	4.08	84580.6	0.019	4.08	94277.0	0.031
4.09	74397.7	0.327	4.11	84568.4	0.015	4.11	94290.6	0.030
4.12	74418.2	0.327	4.14	84555.5	0.010	4.14	94303.7	0.029
4.15	74438.1	0.327	4.17	84542.9	0.006	4.17	94316.4	0.028
4.18	74457.5	0.327	4.20	84530.6	0.005	4.20	94328.7	0.027
4.21	74476.4	0.326	4.23	84518.7	0.005	4.23	94340.7	0.026
4.24	74494.6	0.326	4.26	84507.1	0.004	4.26	94352.2	0.025
4.27	74512.6	0.325	4.29	84496.1	0.003	4.29	94363.4	0.024
4.30	74529.6	0.325	4.32	84485.6	0.002	4.32	94374.3	0.023
4.33	74546.4	0.324	4.35	84475.7	0.002	4.35	94384.8	0.022
4.36	74562.5	0.323	4.38	84466.6	0.001	4.38	94395.0	0.021
4.39	74578.1	0.322	4.41	84458.4	0.001	4.41	94404.8	0.020
4.42	74593.1	0.320	4.44	84451.3	0.000	4.44	94414.4	0.020

4.45	74607.5	0.319		4.47	84445.5	0.000		4.48	94423.6	0.019
4.48	74621.4	0.317								

(1) ⁴ Δ			(2) ⁴ Δ			(1) ⁴ Σ ⁻		
R (Å)	E (cm ⁻¹)	μ (a.u.)	R (Å)	E (cm ⁻¹)	μ (a.u.)	R (Å)	E (cm ⁻¹)	μ (a.u.)
1.41	107486.6	1.078	1.41	154184.1	-0.897	1.41	108952.3	1.108
1.44	100335.8	1.066	1.44	147115.7	-0.828	1.44	101767.6	1.096
1.47	94091.0	1.052	1.47	140978.7	-0.762	1.47	95487.9	1.082
1.50	88634.2	1.037	1.50	135647.4	-0.698	1.50	89995.5	1.067
1.53	83862.7	1.020	1.53	131013.0	-0.635	1.53	85188.0	1.050
1.56	79687.2	1.003	1.56	126981.3	-0.572	1.56	80976.1	1.032
1.59	76030.3	0.984	1.59	123470.7	-0.510	1.59	77282.8	1.013
1.62	72824.9	0.965	1.62	120411.0	-0.449	1.62	74041.0	0.994
1.65	70013.0	0.946	1.65	117741.4	-0.388	1.65	71192.7	0.974
1.68	67544.6	0.926	1.68	115409.7	-0.327	1.68	68688.0	0.954
1.71	65376.2	0.906	1.71	113370.8	-0.266	1.71	66483.5	0.933
1.74	63470.5	0.886	1.74	111585.8	-0.207	1.74	64541.9	0.912
1.77	61795.0	0.865	1.77	110021.0	-0.148	1.77	62830.9	0.891
1.80	60321.5	0.845	1.80	108647.6	-0.091	1.80	61322.3	0.870
1.83	59025.4	0.824	1.83	107440.3	-0.035	1.83	59991.8	0.848
1.86	57885.4	0.802	1.86	106377.4	0.020	1.86	58818.1	0.826
1.89	56882.8	0.781	1.89	105439.9	0.072	1.89	57782.4	0.805
1.92	56001.1	0.760	1.92	104611.1	0.121	1.92	56868.4	0.783
1.95	55225.9	0.739	1.95	103876.7	0.168	1.95	56061.9	0.761
1.98	54544.6	0.717	1.98	103224.2	0.213	1.98	55350.1	0.738
2.01	53946.0	0.696	2.01	102642.5	0.254	2.01	54721.7	0.716
2.04	53420.2	0.674	2.04	102122.1	0.292	2.04	54167.0	0.694
2.07	52958.5	0.653	2.07	101654.8	0.326	2.07	53677.2	0.672
2.10	52553.1	0.632	2.10	101233.5	0.358	2.10	53244.5	0.651
2.13	52197.3	0.611	2.13	100851.9	0.386	2.13	52862.3	0.629
2.16	51885.0	0.590	2.16	100504.8	0.411	2.16	52524.4	0.608
2.19	51610.9	0.570	2.19	100187.6	0.433	2.19	52225.5	0.586
2.22	51370.5	0.550	2.22	99896.5	0.452	2.22	51961.1	0.566
2.25	51159.6	0.530	2.25	99627.9	0.468	2.25	51727.0	0.545
2.28	50974.6	0.510	2.28	99379.2	0.481	2.28	51519.6	0.525
2.31	50812.4	0.491	2.31	99147.9	0.492	2.31	51335.9	0.505
2.34	50670.3	0.472	2.34	98931.9	0.500	2.34	51173.0	0.486
2.37	50545.8	0.454	2.37	98729.5	0.506	2.37	51028.4	0.467
2.40	50436.9	0.436	2.40	98539.0	0.510	2.40	50900.3	0.449
2.43	50341.8	0.419	2.43	98359.3	0.513	2.43	50786.5	0.431
2.46	50258.7	0.402	2.46	98189.2	0.513	2.46	50685.6	0.414
2.49	50186.4	0.386	2.49	98027.9	0.512	2.49	50596.1	0.397
2.52	50123.5	0.370	2.52	97874.5	0.510	2.52	50516.7	0.381
2.55	50069.1	0.355	2.55	97728.4	0.506	2.55	50446.4	0.365

2.58	50022.0	0.340		2.58	97589.0	0.502		2.58	50384.2	0.350
2.61	49981.5	0.325		2.61	97455.9	0.496		2.61	50329.1	0.335
2.64	49946.9	0.312		2.64	97328.7	0.489		2.64	50280.5	0.321
2.67	49917.4	0.298		2.67	97206.9	0.482		2.67	50237.7	0.307
2.70	49892.6	0.285		2.70	97090.2	0.474		2.70	50200.1	0.294
2.73	49871.9	0.273		2.73	96978.2	0.466		2.73	50167.1	0.282
2.76	49854.9	0.261		2.76	96870.9	0.457		2.76	50138.3	0.270
2.79	49841.2	0.250		2.79	96767.9	0.448		2.79	50113.3	0.258
2.82	49830.3	0.239		2.82	96669.1	0.438		2.82	50091.7	0.247
2.86	49822.2	0.228		2.85	96574.2	0.428		2.85	50073.2	0.236
2.88	49820.0	0.218		2.88	96479.0	0.416		2.87	50063.7	0.225
2.90	49818.5	0.208		2.91	96391.6	0.406		2.91	50050.5	0.215
2.94	49816.7	0.199		2.94	96307.8	0.396		2.94	50043.0	0.204
2.97	49816.5	0.190		2.97	96227.4	0.385		2.97	50034.0	0.195
3.00	49817.8	0.182		3.00	96150.2	0.375		3.00	50026.8	0.187
3.03	49820.4	0.174		3.03	96076.3	0.365		3.03	50021.4	0.178
3.06	49824.3	0.166		3.06	96005.4	0.354		3.06	50017.5	0.170
3.09	49829.3	0.159		3.09	95937.5	0.344		3.09	50015.3	0.163
3.12	49835.3	0.152		3.12	95872.5	0.334		3.12	50014.1	0.156
3.15	49842.1	0.145		3.15	95809.6	0.324		3.15	50013.9	0.149
3.18	49849.5	0.138		3.18	95742.8	0.313		3.18	50014.2	0.142
3.21	49857.8	0.132		3.21	95685.3	0.304		3.21	50016.2	0.136
3.24	49866.7	0.126		3.24	95630.1	0.294		3.24	50019.2	0.130
3.27	49876.0	0.121		3.27	95577.6	0.284		3.27	50022.9	0.124
3.30	49885.8	0.116		3.30	95527.4	0.275		3.30	50027.2	0.119
3.33	49896.0	0.111		3.33	95479.4	0.266		3.33	50032.2	0.114
3.36	49906.5	0.106		3.36	95433.6	0.257		3.36	50037.7	0.109
3.39	49917.3	0.101		3.39	95389.9	0.248		3.39	50043.7	0.104
3.42	49928.2	0.097		3.42	95348.1	0.240		3.42	50050.1	0.099
3.45	49939.3	0.093		3.45	95308.3	0.231		3.45	50056.8	0.095
3.48	49950.4	0.089		3.48	95270.3	0.223		3.48	50063.8	0.091
3.51	49961.7	0.085		3.51	95234.0	0.215		3.51	50071.0	0.087
3.54	49972.9	0.081		3.54	95199.7	0.207		3.54	50078.4	0.083
3.57	49984.4	0.078		3.57	95166.8	0.200		3.57	50086.0	0.080
3.60	49995.6	0.075		3.60	95135.5	0.192		3.60	50093.7	0.077
3.63	50006.8	0.071		3.63	95105.7	0.185		3.63	50101.5	0.073
3.66	50017.9	0.068		3.66	95077.4	0.178		3.66	50109.4	0.070
3.69	50029.0	0.066		3.69	95050.5	0.172		3.69	50117.3	0.067
3.72	50039.9	0.063		3.72	95025.0	0.165		3.72	50125.2	0.065
3.75	50050.7	0.060		3.75	95000.7	0.159		3.75	50133.2	0.062
3.78	50061.3	0.058		3.78	94977.8	0.153		3.78	50141.1	0.059
3.81	50071.9	0.055		3.81	94956.0	0.147		3.81	50149.0	0.057
3.84	50082.3	0.053		3.84	94935.4	0.141		3.84	50156.9	0.055
3.87	50092.6	0.051		3.87	94914.7	0.135		3.87	50164.8	0.052

3.90	50102.7	0.049	3.90	94896.3	0.130	3.90	50172.6	0.050
3.93	50112.6	0.047	3.93	94878.9	0.125	3.93	50180.4	0.048
3.96	50123.1	0.045	3.96	94862.6	0.120	3.96	50188.0	0.046
3.99	50132.8	0.043	3.99	94848.4	0.115	4.00	50199.5	0.044
4.00	50136.5	0.043	4.02	94833.9	0.110	4.03	50205.8	0.042
4.03	50145.4	0.041	4.05	94818.9	0.106	4.06	50213.3	0.040
4.06	50154.7	0.039	4.08	94806.0	0.101	4.09	50220.6	0.039
4.09	50163.8	0.038	4.11	94794.0	0.097	4.12	50227.9	0.037
4.12	50172.8	0.036	4.14	94782.8	0.093	4.15	50235.1	0.036
4.15	50181.7	0.035	4.17	94772.1	0.089	4.18	50242.5	0.034
4.18	50190.4	0.033	4.20	94762.3	0.086	4.21	50249.5	0.033
4.21	50198.9	0.032	4.23	94753.1	0.082	4.24	50256.4	0.032
4.24	50207.2	0.031	4.26	94744.6	0.079	4.27	50263.2	0.030
4.27	50215.4	0.030	4.29	94736.8	0.075	4.30	50269.8	0.029
4.30	50223.4	0.028	4.32	94731.1	0.072	4.33	50276.4	0.028
4.33	50231.3	0.027	4.35	94724.4	0.069	4.36	50282.9	0.027
4.36	50239.0	0.026	4.48	94718.2	0.066	4.39	50289.2	0.026
4.39	50246.5	0.025				4.42	50295.4	0.025
4.42	50253.9	0.024				4.45	50301.5	0.024
4.45	50261.1	0.023				4.48	50307.4	0.023
4.48	50268.2	0.022						

(2) ⁴ Σ ⁻		
R (Å)	E (cm ⁻¹)	μ (a.u.)
1.41	146056.0	0.420
1.44	139664.5	0.427
1.47	134340.4	0.435
1.50	129667.9	0.442
1.53	125877.3	0.448
1.56	122314.4	0.449
1.59	119008.6	0.450
1.62	115680.1	0.448
1.65	113243.9	0.443
1.68	111312.6	0.439
1.71	109740.6	0.433
1.74	108249.9	0.422
1.77	106681.6	0.412
1.79	105595.0	0.403
1.82	104445.0	0.393
1.84	103694.6	0.387
1.88	102401.9	0.372
1.90	101787.4	0.367
1.91	101458.1	0.361
1.97	99829.6	0.341
2.01	99098.8	0.327

2.04	98736.7	0.316
2.06	98385.5	0.308
2.10	97946.5	0.299
2.13	97705.1	0.292
2.16	97441.8	0.285
2.17	97375.9	0.282
2.21	97068.6	0.274
2.24	96890.3	0.268
2.27	96706.5	0.259
2.31	96533.1	0.250
2.34	96410.2	0.240
2.37	96322.4	0.232
2.40	96212.7	0.225
2.43	96138.1	0.218
2.46	96054.7	0.212
2.49	95968.4	0.209
2.52	95890.1	0.204
2.55	95828.3	0.201
2.58	95775.8	0.200
2.61	95736.9	0.202
2.64	95708.1	0.203
2.67	95688.6	0.202
2.70	95677.7	0.205
2.73	95675.0	0.209
2.76	95677.9	0.214
2.79	95685.6	0.219
2.82	95695.6	0.225
2.85	95706.6	0.233
2.88	95683.1	0.235
2.91	95697.4	0.237
2.94	95097.1	0.237
2.97	95073.0	0.233
3.00	95050.6	0.229
3.03	95029.7	0.226
3.06	95010.3	0.223
3.09	94992.2	0.220
3.12	94975.2	0.217
3.15	94958.8	0.214
3.18	94945.9	0.211
3.21	94931.8	0.209
3.24	94918.6	0.207
3.27	94906.2	0.204
3.30	94894.5	0.203
3.33	94883.5	0.201

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3.36	94873.2	0.199
3.39	94863.4	0.198
3.42	94854.2	0.196
3.45	94845.5	0.195
3.48	94837.2	0.194
3.51	94829.3	0.193
3.54	94821.8	0.192
3.57	94814.7	0.192
3.60	94807.8	0.191
3.63	94801.3	0.190
3.66	94795.0	0.190
3.69	94788.9	0.190
3.72	94783.1	0.189
3.75	94777.5	0.189
3.78	94772.1	0.189
3.81	94766.8	0.189
3.84	94761.7	0.189
3.87	94756.8	0.189
3.90	94752.0	0.189
3.93	94747.3	0.189
3.96	94742.8	0.189
3.99	94738.5	0.189
4.02	94734.2	0.189
4.05	94730.1	0.189
4.08	94726.2	0.189
4.11	94722.3	0.188
4.14	94718.6	0.188
4.17	94715.1	0.188
4.20	94711.7	0.187
4.23	94708.4	0.187
4.26	94705.3	0.186
4.29	94702.4	0.185
4.32	94699.5	0.185
4.35	94697.5	0.184
4.38	94695.0	0.183
4.41	94692.6	0.182
4.44	94690.4	0.181
4.48	94688.4	0.180

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Table (SM.2): Numerical data corresponding to the transition dipole moment (a.u.) some low-lying doublet states:

R (Å)	Transition dipole moment (a.u.)					
	$X^2\Sigma^+-(1)^2\Pi$	$X^2\Sigma^+-(2)^2\Sigma^+$	$(1)^2\Pi-(1)^2\Delta$	$(2)^2\Pi-(1)^2\Delta$	$(1)^2\Pi-(1)^2\Sigma^-$	$(2)^2\Pi-(1)^2\Sigma^-$
1.40	1.466	1.042	-0.247	0.009	-0.280	0.095
1.43	1.465	1.044	-0.248	0.013	-0.279	0.091
1.46	1.461	1.045	-0.249	0.015	-0.278	0.088
1.49	1.454	1.044	-0.250	0.017	-0.275	0.085
1.52	1.446	1.036	-0.249	0.017	-0.272	0.083
1.55	1.435	1.018	-0.249	0.017	-0.269	0.080
1.58	1.420	0.970	-0.248	0.018	-0.265	0.078
1.61	1.400	0.836	-0.246	0.015	-0.260	0.073
1.64	1.372	0.568	-0.244	0.014	-0.253	0.072
1.67	1.329	0.276	-0.240	0.005	-0.244	0.060
1.70	1.261	0.062	-0.233	-0.245	-0.231	-0.260
1.73	1.148	-0.077	-0.220	-0.243	-0.210	-0.254
1.76	0.960	-0.170	-0.196	-0.240	-0.175	-0.248
1.79	0.694	-0.239	-0.158	-0.235	-0.127	-0.239
1.82	0.431	-0.292	-0.118	-0.228	-0.080	-0.226
1.85	0.240	-0.337	-0.088	-0.211	-0.046	-0.198
1.88	0.116	-0.377	-0.068	0.142	-0.024	0.185
1.91	0.035	-0.413	-0.055	-0.202	-0.010	-0.230
1.94	-0.019	-0.448	-0.045	-0.218	-0.001	-0.232
1.97	-0.058	-0.482	-0.039	-0.210	0.005	-0.226
2.00	-0.086	-0.516	-0.034	-0.207	0.009	-0.218
2.03	-0.106	-0.550	-0.030	-0.204	0.012	-0.215
2.06	-0.121	-0.585	-0.027	-0.199	0.014	-0.209
2.09	-0.133	-0.620	-0.025	-0.194	0.015	-0.202
2.12	-0.142	-0.657	-0.022	-0.189	0.016	-0.196
2.15	-0.149	-0.695	-0.021	-0.183	0.016	-0.189
2.18	-0.154	-0.734	-0.019	-0.177	0.016	-0.182
2.21	-0.157	-0.774	-0.018	-0.171	0.016	-0.175
2.24	-0.160	-0.816	-0.017	-0.165	0.016	-0.168
2.27	-0.161	-0.860	-0.015	-0.158	0.016	-0.161
2.30	-0.162	-0.904	-0.014	-0.151	0.015	-0.154
2.33	-0.162	-0.949	-0.013	-0.145	0.015	-0.147
2.36	-0.161	-0.994	-0.013	-0.138	0.014	-0.140
2.39	-0.160	-1.040	-0.012	-0.131	0.014	-0.133
2.42	-0.158	-1.085	-0.011	-0.124	0.013	-0.126
2.45	-0.155	-1.128	-0.010	-0.118	0.013	-0.119
2.48	-0.152	-1.169	-0.010	-0.111	0.012	-0.112
2.51	-0.149	-1.208	-0.009	-0.105	0.011	-0.106
2.54	-0.145	-1.242	-0.008	-0.099	0.011	-0.099
2.57	-0.141	-1.272	-0.008	-0.093	0.010	-0.094
2.60	-0.136	-1.296	-0.007	-0.087	0.010	-0.088
2.63	-0.131	-1.314	-0.007	-0.082	0.009	-0.083
2.66	0.126	1.325	-0.006	-0.077	0.008	-0.077
2.69	0.120	1.330	-0.006	-0.072	0.008	-0.073
2.72	0.114	1.328	-0.005	-0.067	0.007	-0.068
2.75	0.109	1.320	-0.005	-0.063	0.007	-0.064
2.78	0.103	1.307	-0.004	-0.059	0.006	-0.060

2.81	0.098	1.290	-0.004	-0.055	0.006	-0.056
2.84	0.092	1.268	-0.004	-0.051	0.005	-0.053
2.87	0.087	1.242	-0.003	-0.048	0.005	-0.050
2.90	0.082	1.214	-0.003	-0.045	0.005	-0.047
2.93	0.078	1.184	-0.003	-0.041	0.004	-0.044
2.96	0.074	1.152	-0.003	-0.038	0.004	-0.042
2.99	0.069	1.119	-0.002	-0.035	0.004	-0.040
3.02	0.066	1.086	-0.002	-0.032	0.003	-0.038
3.05	0.062	1.052	-0.002	-0.027	0.003	-0.037
3.08	0.059	1.019	-0.002	-0.022	0.003	-0.035
3.11	0.055	0.986	-0.002	-0.015	0.002	-0.032
3.14	0.053	0.953	-0.001	-0.009	0.002	-0.029
3.17	0.050	0.921	-0.001	-0.004	0.002	-0.026
3.20	0.047	0.890	-0.001	0.000	0.002	-0.024
3.23	0.045	0.860	-0.001	0.003	0.002	-0.023
3.26	0.042	0.830	-0.001	0.005	0.001	-0.022
3.29	0.040	0.802	-0.001	0.007	0.001	-0.021
3.32	0.038	0.774	-0.001	0.009	0.001	-0.020
3.35	0.036	0.746	-0.001	0.010	0.001	-0.020
3.38	0.035	0.720	-0.001	0.011	0.001	-0.020
3.41	0.033	0.694	-0.001	0.012	0.001	-0.020
3.44	0.032	0.670	0.000	0.012	0.001	-0.019
3.47	0.030	0.645	0.000	0.013	0.001	-0.019
3.50	0.029	0.622	0.000	0.013	0.000	-0.019
3.53	0.027	0.599	0.000	0.013	0.000	-0.019
3.56	0.026	0.576	0.000	0.014	0.000	-0.018
3.59	0.025	0.555	0.000	0.014	0.000	-0.018
3.62	0.024	0.533	0.000	0.014	0.000	-0.018
3.65	0.023	0.513	0.000	0.014	0.000	-0.017
3.68	0.022	0.492	0.000	0.014	0.000	-0.017
3.71	0.021	0.472	0.000	0.014	0.000	-0.017
3.74	0.020	0.453	0.000	0.013	0.000	-0.016
3.77	0.020	0.434	0.000	0.013	0.000	-0.016
3.80	0.019	0.415	0.000	0.013	0.000	-0.016
3.83	0.018	0.397	0.000	0.013	0.000	-0.015
3.86	0.017	0.379	0.000	0.013	0.000	-0.015
3.89	0.017	0.361	0.000	0.012	0.000	-0.014
3.92	0.016	0.344	0.000	0.012	0.000	-0.014
3.95	0.016	0.327	0.000	0.012	0.000	-0.014
3.98	0.015	0.310	0.000	0.011	0.000	-0.013
4.01	0.015	0.293	0.000	0.011	0.000	-0.013
4.04	0.014	0.277	0.000	0.011	0.000	-0.012
4.07	0.014	0.261	0.000	0.010	0.000	-0.012
4.10	0.013	0.245	0.000	0.010	0.000	-0.011
4.13	0.013	0.230	0.000	0.010	0.000	-0.011
4.16	0.012	0.215	0.000	0.009	0.000	-0.011
4.19	0.012	0.200	0.000	0.009	0.000	-0.010
4.22	0.012	0.186	0.000	0.009	0.000	-0.010
4.25	0.011	-0.172	0.000	0.008	0.000	-0.010
4.28	0.011	-0.159	0.000	0.008	0.000	-0.009
4.31	0.011	-0.147	0.000	0.008	0.000	-0.009
4.34	0.010	-0.135	0.000	0.007	0.000	-0.008

4.37	0.010	-0.124	0.000	0.007	0.000	-0.008
4.40	0.010	-0.113	0.000	0.007	0.000	-0.008
4.43	0.009	-0.104	0.000	0.007	0.000	-0.007
4.46	0.009	-0.094	0.000	0.006	0.000	-0.007
4.49	0.009	-0.086	0.000	0.006	0.000	-0.007
4.52	0.009	-0.078	0.000	0.006	0.000	-0.007
4.55	0.008	-0.071	0.000	0.006	0.000	-0.006

R (Å)	Transition dipole moment (a.u.)				
	(1) ² Π-(2) ² Π	X ² Σ ⁺ -(2) ² Π	X ² Σ ⁺ -(3) ² Σ ⁺	X ² Σ ⁺ -(4) ² Σ ⁺	(2) ² Σ ⁺ -(3) ² Σ ⁺
1.40	0.206	-0.395	0.010	-0.447	-0.713
1.42	0.210	-0.395	-0.016	-0.442	-0.672
1.43	0.215	-0.399	-0.050	-0.444	-0.595
1.45	0.220	-0.399	-0.111	-0.441	-0.481
1.48	0.229	-0.400	-0.197	-0.427	-0.299
1.49	0.234	-0.400	-0.238	-0.408	-0.252
1.52	0.247	-0.400	-0.224	-0.360	-0.247
1.54	0.253	-0.400	-0.182	-0.334	-0.318
1.55	0.261	-0.397	-0.061	-0.284	-0.456
1.57	0.269	-0.397	0.452	1.123	-0.971
1.58	0.276	-0.397	1.137	0.196	-1.695
1.60	0.287	-0.397	1.152	-0.968	-1.714
1.61	0.300	-0.386	1.153	-0.957	-1.689
1.63	0.321	-0.386	1.151	-0.757	-1.596
1.64	0.342	-0.377	1.143	0.038	-1.442
1.67	0.355	-0.323	1.127	0.419	-1.092
1.68	-1.482	0.162	1.121	-0.952	-0.978
1.69	-1.471	0.742	1.113	-0.949	-0.864
1.70	-1.455	1.426	1.101	-0.824	-0.743
1.71	-1.433	1.420	1.091	-0.734	-0.645
1.72	-1.404	1.413	1.077	-0.636	-0.544
1.73	-1.366	1.406	1.054	-0.543	-0.432
1.74	-1.317	1.398	1.034	-0.472	-0.309
1.75	-1.256	1.389	0.993	-0.437	-0.200
1.76	-1.181	1.379	0.942	-0.342	-0.087
1.77	-1.091	1.368	0.844	-0.284	0.033
1.78	-0.988	1.356	0.723	-0.254	0.128
1.79	-0.874	1.341	0.647	-0.181	0.208
1.80	-0.753	1.323	0.654	-0.135	0.220
1.81	-0.629	1.302	0.694	-0.108	0.208
1.82	-0.503	1.275	0.767	-0.032	0.146
1.83	-0.374	1.239	0.893	0.014	-0.007
1.84	-0.239	1.190	1.054	0.035	-0.402
1.85	-0.095	1.123	1.217	0.104	-0.683
1.86	0.061	1.047	1.221	0.152	-0.695
1.87	0.314	0.991	1.216	0.171	-0.627
1.88	1.044	-1.067	1.208	0.240	-0.554
1.89	-0.140	1.313	1.199	0.282	-0.517
1.90	-0.331	1.367	1.186	0.308	-0.492
1.91	-0.726	1.375	1.174	-0.372	-0.476
1.92	-0.587	1.374	1.156	-0.435	-0.445

1.94	-0.515	1.362	1.132	-0.496	-0.415
1.96	-0.435	1.347	1.099	-0.557	-0.385
1.97	-0.397	1.339	1.075	-0.619	-0.368
1.98	-0.362	1.330	1.052	-0.652	-0.354
1.99	-0.338	1.322	1.029	-0.682	-0.340
2.00	-0.322	1.315	1.000	-0.746	-0.326
2.01	-0.306	1.307	0.971	-0.800	-0.313
2.02	-0.294	1.300	0.944	-0.847	-0.301
2.03	-0.278	1.290	0.907	-0.890	-0.289
2.05	-0.263	1.277	0.864	-0.971	-0.266
2.06	-0.256	1.268	0.829	-1.010	-0.255
2.07	-0.248	1.259	0.802	-1.053	-0.244
2.08	-0.238	1.249	0.770	-1.096	-0.234
2.09	-0.231	1.240	0.736	-1.139	-0.225
2.10	-0.221	1.232	0.707	-1.177	-0.215
2.11	-0.212	1.221	0.676	-1.197	-0.207
2.12	-0.204	1.211	0.642	-1.267	-0.198
2.13	-0.196	1.200	0.614	-1.306	-0.190
2.14	-0.189	1.189	0.588	-1.324	-0.182
2.15	-0.182	1.179	0.553	-1.373	-0.175
2.16	-0.175	1.169	0.520	-1.407	-0.168
2.18	-0.163	1.148	0.470	-1.435	-0.156
2.20	-0.150	1.126	0.420	1.518	-0.144
2.21	-0.145	1.114	0.395	1.569	-0.139
2.23	-0.136	1.091	0.350	1.592	-0.130
2.24	-0.132	1.079	0.328	1.606	-0.122
2.26	-0.124	1.055	0.298	1.607	-0.119
2.27	-0.120	1.042	0.269	1.257	-0.116
2.29	-0.110	1.010	0.227	-1.447	-0.110
2.31	-0.110	0.990	0.195	-1.482	-0.105
2.34	-0.100	0.949	0.154	-1.441	-0.099
2.36	-0.089	0.919	0.133	-1.390	-0.096
2.39	-0.081	0.877	0.099	-1.138	-0.093
2.41	-0.075	0.849	0.080	1.280	-0.091
2.42	-0.074	0.833	0.070	1.417	-0.091
2.44	-0.068	0.801	0.052	1.523	-0.090
2.47	-0.062	0.760	0.029	1.592	-0.090
2.48	-0.060	0.743	0.023	1.604	-0.090
2.51	-0.055	0.698	0.004	1.589	-0.090
2.54	-0.050	0.653	-0.011	1.569	-0.092
2.57	-0.045	0.608	-0.024	1.541	-0.094
2.60	-0.040	0.563	-0.035	1.506	-0.097
2.63	-0.036	0.520	-0.043	1.480	-0.100
2.65	-0.034	0.478	-0.040	1.453	-0.102
2.66	-0.033	-0.479	0.050	-1.446	-0.103
2.69	-0.029	-0.438	0.057	-1.419	-0.106
2.72	-0.026	-0.400	0.058	-1.392	-0.109
2.75	-0.023	-0.364	0.059	-1.366	-0.112
2.78	-0.021	-0.331	0.060	-1.339	-0.115
2.81	-0.018	-0.299	0.059	-1.306	-0.117
2.84	-0.016	-0.271	0.057	-1.270	-0.118
2.87	-0.014	-0.244	0.055	-1.244	-0.118

2.90	-0.012	-0.219	0.053	-1.217	-0.118
2.93	-0.010	-0.197	0.050	-1.189	-0.117
2.96	-0.008	-0.176	0.046	-1.158	-0.114
2.99	-0.006	-0.156	0.042	-1.121	-0.111
3.02	-0.004	-0.136	0.037	-1.083	-0.106
3.05	-0.001	-0.115	0.033	-1.045	-0.099
3.08	0.003	-0.090	0.028	-1.009	-0.091
3.11	0.007	-0.064	0.023	-0.971	-0.082
3.14	0.010	-0.043	0.018	-0.941	-0.071
3.17	0.012	-0.027	0.012	-0.913	-0.059
3.20	0.013	-0.016	0.007	-0.885	-0.045
3.23	0.014	-0.009	0.001	-0.856	-0.029
3.26	0.014	-0.004	-0.005	-0.825	-0.011
3.29	0.014	-0.001	-0.011	-0.795	0.010
3.32	0.014	0.002	-0.019	-0.772	0.032
3.35	0.014	0.003	-0.026	-0.746	0.058
3.38	0.013	0.004	-0.033	-0.720	0.084
3.41	0.013	0.004	-0.039	-0.694	0.113
3.44	0.013	0.005	-0.045	-0.670	0.146
3.47	0.012	0.005	-0.052	-0.645	0.182
3.50	0.012	0.005	-0.057	-0.622	0.220
3.53	0.011	0.005	-0.064	-0.599	0.261
3.56	0.011	0.005	-0.072	-0.576	0.306
3.59	0.011	0.005	-0.079	-0.555	1.036
3.62	0.010	0.004	-0.086	-0.533	0.977
3.64	0.010	0.004	-0.089	-0.522	0.019
3.65	0.010	0.004	-0.093	-0.513	0.084
3.68	0.010	0.004	-0.101	-0.492	0.237
3.71	0.009	0.004	-0.110	-0.472	0.343
3.74	0.009	0.003	-0.119	-0.453	0.423
3.77	0.009	0.003	-0.127	-0.434	0.484
3.80	0.008	0.003	-0.135	-0.415	0.535
3.83	0.008	0.003	-0.157	-0.397	0.958
3.86	0.008	0.003	-0.304	-0.379	0.837
3.88	0.008	0.003	-0.304	-0.368	-0.132
3.89	0.007	0.003	0.383	-0.361	0.111
3.92	0.007	0.002	0.385	-0.344	0.530
3.93	0.007	0.002	0.376	-0.344	0.898
3.94	0.007	0.002	0.357	-0.340	-2.238
3.95	0.007	0.002	0.350	-0.327	-2.177
3.98	0.006	0.002	0.327	-0.310	-2.093
4.01	0.006	0.002	0.310	-0.293	-1.982
4.05	0.006	0.002	0.280	-0.270	-1.832
4.08	0.006	0.002	0.262	-0.256	-1.720
4.10	0.006	0.002	0.258	-0.245	-1.647
4.13	0.005	0.001	0.241	-0.230	-1.538
4.16	0.005	0.001	0.225	-0.215	-1.432
4.19	0.005	0.001	0.211	-0.200	-1.329
4.22	0.005	0.001	0.197	-0.186	-1.218
4.25	0.004	0.001	0.184	0.172	1.135
4.28	0.004	0.001	0.173	0.159	1.044
4.31	0.004	0.001	0.161	0.147	0.958

4.34	0.004	0.001	0.151	0.135	0.876
4.37	0.004	0.001	0.141	0.124	0.800
4.40	0.004	0.001	0.132	0.113	0.729
4.43	0.003	0.001	0.124	0.104	0.664
4.46	0.003	0.001	0.116	0.094	0.603
4.49	0.003	0.001	0.108	0.086	0.548
4.52	0.003	0.001	0.101	0.078	0.497
4.55	0.003	0.000	0.095	0.071	0.450

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C. Vibrational levels of some shallow states:

Table (SM.3): The eigenvalues E_v , the rotational constants B_v , the centrifugal distortion constants D_v , the abscissas of the turning points $R_{\min}$ and $R_{\max}$ and some calculated wavelengths of possible vibronic transitions of different shallow states of the ZnF molecule.

state	ν	$R_{\min}$ (Å)	$R_{\max}$ (Å)	E_v (cm ⁻¹)	$B_v \times 10^2$ (cm ⁻¹)	$D_v \times 10^6$ (cm ⁻¹)	$\lambda_{v' \leftrightarrow v''}$ (μm)
(1) ² Π	0	3.607	4.116	17.96	7.668	1.465	$\lambda_{1 \leftrightarrow 0} = 292.6$
	1	3.476	4.380	52.14	7.375	1.549	$\lambda_{2 \leftrightarrow 1} = 314.8$
	2	3.399	4.604	83.91	7.062	1.685	$\lambda_{2 \leftrightarrow 0} = 151.6$
(1) ⁴ Σ ⁺	0	2.611	2.936	41.92	14.827	1.922	$\lambda_{1 \leftrightarrow 0} = 124.3$ $\lambda_{2 \leftrightarrow 1} = 134.2$ $\lambda_{2 \leftrightarrow 0} = 64.5$
	1	2.522	3.116	122.37	14.324	2.124	
	2	2.472	3.254	196.90	13.836	1.894	
	3	2.434	3.380	268.67	13.367	2.109	
	4	2.405	3.500	336.43	12.926	2.033	
	5	2.381	3.619	400.76	12.445	2.039	
(1) ⁴ Δ	0	2.777	3.168	30.08	12.934	2.306	$\lambda_{1 \leftrightarrow 0} = 167.1$ $\lambda_{2 \leftrightarrow 1} = 172.6$ $\lambda_{2 \leftrightarrow 0} = 84.9$
	1	2.683	3.360	89.92	12.493	2.132	
	2	2.624	3.517	147.85	12.025	2.232	
	3	2.582	3.663	202.71	11.589	2.407	
(1) ⁴ Σ ⁻	0	2.950	3.368	25.51	11.478	2.377	$\lambda_{1 \leftrightarrow 0} = 202.2$
	1	2.824	3.581	74.98	11.127	2.530	
(3) ⁴ Π	0	2.561	2.848	56.11	15.646	1.230	$\lambda_{1 \leftrightarrow 0} = 91.0$ $\lambda_{2 \leftrightarrow 1} = 94.4$ $\lambda_{2 \leftrightarrow 0} = 46.3$
	1	2.482	2.984	166.01	15.287	1.244	
	2	2.433	3.092	271.92	14.916	1.254	
	3	2.397	3.188	374.05	14.573	1.245	
	4	2.369	3.279	472.76	14.218	1.265	
	5	2.345	3.366	567.92	13.875	1.283	
	6	2.324	3.452	659.56	13.528	1.272	
	7	2.306	3.537	747.87	13.189	1.315	
	8	2.291	3.622	832.77	12.850	1.323	
	9	2.277	3.708	914.26	12.497	1.357	
	10	2.264	3.795	992.31	12.156	1.375	
(4) ⁴ Π	0	2.392	2.639	74.92	18.074	1.104	$\lambda_{1 \leftrightarrow 0} = 69.9$ $\lambda_{2 \leftrightarrow 1} = 76.2$ $\lambda_{2 \leftrightarrow 0} = 36.5$
	1	2.324	2.767	217.99	17.532	1.266	
	2	2.286	2.870	349.19	16.911	1.408	
	3	2.260	2.990	468.90	16.198	1.830	
(5) ⁴ Π	0	2.182	2.393	103.56	21.849	1.005	$\lambda_{1 \leftrightarrow 0} = 49.9$ $\lambda_{2 \leftrightarrow 1} = 52.3$ $\lambda_{2 \leftrightarrow 0} = 25.5$
	1	2.124	2.497	303.91	21.340	1.052	
	2	2.089	2.580	494.99	20.821	1.106	
	3	2.063	2.656	676.79	20.291	1.162	
	4	2.043	2.730	849.42	19.754	1.219	
	5	2.026	2.802	1013.06	19.208	1.283	
	6	2.012	2.874	1167.86	18.657	1.338	
	7	1.999	2.949	1314.12	18.101	1.430	

	8	1.988	3.025	1451.64	17.510	1.539	
	9	1.979	3.104	1580.34	16.934	1.543	
	10	1.971	3.185	1701.18	16.356	1.690	
	11	1.963	3.269	1813.93	15.769	1.704	
	12	1.956	3.357	1919.26	15.185	1.855	
	13	1.951	3.449	2017.16	14.598	1.902	
	14	1.945	3.545	2107.99	13.998	2.005	

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