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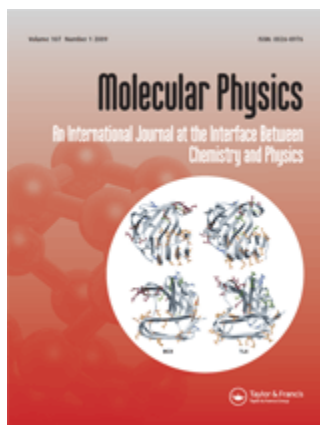
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Interaction Potentials, Spectroscopy and Transport Properties of RG^+ / He ($RG=Ar-Rn$)

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5 **Interaction Potentials, Spectroscopy and Transport Properties of RG^+-He**
6 **($RG=Ar-Rn$)**
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20
21 **Abstract**
22

23 High-level *ab initio* potential energy curves are calculated for the RG^+-He complexes
24 ($RG = Ar-Rn$). RCCSD(T) calculations are employed with large basis sets, and taking
25 account of spin-orbit coupling. The calculated spectroscopic parameters are
26 compared to experimentally-determined values, to other high-level *ab initio* results,
27 and to results from potentials that were obtained by fitting to experimental data. The
28 gas-phase mobilities of RG^+ ions in He are calculated from our potentials and
29 compared, graphically and statistically, to the experimental mobilities as a function of
30 E/n_0 at several temperatures. We conclude that more precise experimental data are
31 required in order to discriminate between potentials with more certainty. In addition,
32 we discuss previously reported, unexpectedly large drops in experimental mobility
33 values for RG^+ in He at 4.35 K as $E/n_0 \rightarrow 0$.
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I. Introduction

Recently, we presented¹ high-quality *ab initio* potential energy curves for the $\text{Ne}^+\text{-He}$ and $\text{He}^+\text{-Ne}$ complexes, and compared calculated spectroscopic parameters and transport coefficients with those previously available and with new experimental mobility data. In general, the agreement was excellent, the only exception being the comparison with some of the experimental spectroscopic data² for $\text{Ne}^+\text{-He}$. In the present study, we extend our work to the heavier rare gas atomic cations interacting with He. As before, we aim to produce high quality *ab initio* curves, to employ these in the derivation of spectroscopic and transport quantities, and to compare them to available experimental values. Mobilities are useful in understanding chemical reactions, such as those in plasmas. In addition, they provide a good experimental test of calculated potentials, over a wider range of internuclear separations than is generally possible using spectroscopic or scattering techniques. The latter is particularly important for open-shell species, which are often difficult to generate experimentally, and additionally there are questions as to which potentials to be used, depending on the spin-orbit states present in the experiment, which can depend on the experimental conditions.¹ Reliable potentials, of course, are useful across a wide range of chemistry, but they are of greater use if their reliability has been tested.

An early report of spectra by Tanaka *et al.*³ was extended by Dabrowski, Herzberg and Yoshino (DHY),⁴ who published a detailed UV absorption spectroscopic study of the $\text{Ar}^+\text{-He}$ complex. Since the ground state of Ar^+ is 2P , interaction with He gives $^2\Pi$ and $^2\Sigma^+$ electronic states in the absence of spin-orbit coupling, with the latter state expected to be lower in energy owing to less electron repulsion along the internuclear axis. Spin-orbit coupling leads to $^2P_{3/2}$ and $^2P_{1/2}$ states of Ar^+ which, upon interaction with He, yield $^2\Sigma_{1/2}^+$, $^2\Pi_{3/2}$ and $^2\Pi_{1/2}$ molecular states; the first two correlate with the lower, $^2P_{3/2} + \text{He}$ asymptote, and the third with the higher, $^2P_{1/2} + \text{He}$ one. The molecular states, according to a Hund's case (a) analysis, are thus $X^2\Sigma_{1/2}^+$, $A_1^2\Pi_{3/2}$ and $A_2^2\Pi_{1/2}$. Emission lines were observed by DHY, giving spectroscopic information on the $A_2^2\Pi_{1/2}$ and $X^2\Sigma_{1/2}^+$ states, as discussed below.

Saito *et al.*⁵ have estimated an $\text{Ar}^+\text{-He}$ binding energy of 37 meV ($\sim 300\text{ cm}^{-1}$) from mobility measurements. Carrington and coworkers⁶ have recorded microwave spectra of $\text{Ar}^+\text{-He}$ at energies close to the dissociation asymptote. These transitions are in regions where the Born-Oppenheimer approximation was found to break down, and a detailed treatment of the energy levels was presented. The transitions observed in that work, together with those from DHY, were employed to generate fitted potential energy curves for all three states mentioned above; this set of potentials was designated MAL1.

In addition to this fitted potential, other theoretical results are available for $\text{Ar}^+\text{-He}$. Early work focused on charge exchange, mainly concerned with nascent He^+ ions in Ar .^{7,8} In 1978, Olson and Liu⁹ calculated CI curves for the $X^2\Sigma^+$ and $A^2\Pi$ states of $\text{Ar}^+\text{-He}$ in the absence of spin-orbit coupling. In 1985, Hausamann and Morgner¹⁰ made use of theoretical and experimental data available at the time and a model to obtain potential energy curves for $\text{Ar}^+\text{-He}$, $\text{Kr}^+\text{-He}$ and $\text{Xe}^+\text{-He}$ that included spin-orbit coupling. Soon afterwards, Siska¹¹ reported the results of a modified Tang-Toennies model for the potential energy curves for $\text{Ar}^+\text{-He}$, but in the absence of spin-orbit coupling. An MRDCI study by Stärk and Peyerimhoff¹² in 1986

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3 considered a number of low-lying states of the $[\text{Ar-He}]^+$ system, with the lowest
4 $^2\Sigma^+$ and $^2\Pi$ states corresponding to Ar^+-He ; owing to emphasis being placed on the
5 excited states, they did not achieve an optimal description of the lower states that are
6 pertinent to the present study. Potential curves were also obtained by Brunetti *et al.*¹³
7 by fitting an expression to the spectroscopic data and assuming the spin-orbit coupling
8 was equal to that of the separated atoms and independent of the internuclear
9 separation. Balasubramanian *et al.*¹⁴ reported non-spin-orbit curves for Ar^+-He .¹⁵ In
10 1990, Staemmler¹⁶ reported ab initio calculations at the SCF and CEPA levels using
11 large Gaussian basis sets for the lowest states of Ar^+-He ; spin-orbit effects were
12 added using a semi-empirical treatment. Gemein and Peyerimhoff¹⁷ used MRD-CI
13 calculations, both with and without spin-orbit coupling, to calculate potential energy
14 curves, reporting equilibrium bond lengths, dissociation energies and harmonic
15 vibrational frequencies. In 1991, Viehland, Viggiano and Mason (VVM)¹⁸ combined
16 the SCF and CI potentials of Olson and Liu⁹ with the known long-range behaviour to
17 obtain potentials (without spin-orbit effects) for the $^2\Sigma^+$ and $^2\Pi$ states of Ar^+-He ; the
18 Siska¹¹ potentials were also employed, but in a modified form. Ionization energies for
19 RG-He and the associated spectroscopic parameters for RG^+-He have been reported
20 by Ma, Li and Ng¹⁹; no spin-orbit coupling was included. In 2001, Murrell *et al.*²⁰
21 reported non-SO and SO potential energy curves for Ar^+-He over a limited range
22 using MRCI+Q energies and an aug-cc-pVQZ basis set. Most recently, to our
23 knowledge, Bera *et al.*²¹ have reported UCCSD(T)/aug-cc-pVTZ spectroscopic and
24 potential parameters for Ar^+-He . In the present work, we shall compare the above
25 results with our potential energy curves, and additionally assess them against other
26 experimental data.
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31 The large body of data on Ar^+-He is not matched for the Kr^+-He ion. Early
32 experimental work comprises the UV emission spectra from Tanaka *et al.*³ where the
33 assignment was only tentative, and scattering studies of He^+ and Kr by Weise.²² The
34 transport studies of Saito *et al.*⁵ suggested that the binding energy of the Kr^+-He
35 ground state was ~ 29 meV (~ 230 cm^{-1}). There are model potential results for Kr^+-He
36 from Hausamann and Morgner¹⁰ and relativistic CI calculations by Balasubramanian
37 *et al.*²³, where spin-orbit coupling was included using basis sets of approximately
38 double- ζ quality.¹⁵ Ma *et al.*¹⁹ also reported spectroscopic and potential parameters
39 for Kr^+-He . The most detailed information, however has come from a joint
40 microwave and theoretical study by Carrington and coworkers.²⁴ At present, the fitted
41 (MAL1) interaction potential reported in that work (similar to that obtained for Ar^+-
42 He , mentioned above) represents most of the information that is known for this
43 species.
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46 To our knowledge, there is no experimental or theoretical spectroscopic information
47 available for Xe^+-He or Rn^+-He , except for the model potential calculations for Xe^+-
48 He , by Hausamann and Morgner.¹⁰
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51 Experimental studies have been performed on the transport of RG^+ ions through He .
52 We have already mentioned our previous work on Ne^+ in He^1 , but all of the other RG^+
53 ions (except Rn) have also been studied. The mobility of Ar^+ through He has been
54 studied at a number of temperatures: at 4.35 K by Saito *et al.*⁵; at 82 K by Koizumi *et*
55 *al.*²⁵; at 92, 170, 293, 428 and 552 K by Viehland *et al.*¹⁸ and at 300 K by Lindinger
56 and Albritton.²⁶ By calculating theoretical transport coefficients and comparing to the
57 experimental data, it is possible to test the potential (or conversely the experimental
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data) over a wide range of internuclear separations.²⁷ Generally, such tests are more stringent than comparison with spectroscopic data, as the latter usually only sample a very small region of internuclear separation. One of the present species is an exception, however, since spectroscopic data close to the minimum,⁴ as well as at very long range⁶ are available for Ar⁺-He.

For Kr⁺ in He, the mobilities having been measured at: 4.35 K by Saito *et al.*⁵; 82 K by Koizumi *et al.*²⁸; 294 K by Jones *et al.*²⁹; and 300 K by two groups, Johnsen *et al.*³⁰ and Kaneko *et al.*³¹ For Xe⁺ in He, only two sets of data have been reported: at 82 K by Koizumi *et al.*²⁸, and at 295 K by Johnsen *et al.*³⁰

II. Calculations

A. *Ab initio* Potentials

The calculations reported here were performed at the RCCSD(T) level of theory, employing d-aug-cc-pV5Z quality basis sets for He-Ar; the frozen core approximation was used throughout. The basis sets were doubly-augmented to allow a good description of the long-range interactions, with the double-diffuse augmentation being achieved by extending the basis set by one set of functions of each angular momentum type; the ζ values were obtained by even-tempered extrapolations of the two most diffuse functions of the same type in the standard basis set. For the heavier atoms, small-core relativistic effective core potentials (ECPs) were employed: ECP10MDF, ECP28MDF and ECP60MDF for Kr, Xe and Rn, respectively; the standard aug-cc-pV5Z valence basis sets³² were then used with these ECPs, again extending the basis set by one diffuse function of each type, as described above. The potential energy curves of the $^2\Sigma^+$ and $^2\Pi$ electronic states were calculated point by point using the MOLPRO³³ suite of programs. A full counterpoise correction was made at each point to correct for basis set superposition error.

Since the interaction between He and RG⁺ is expected to be weak, the spin-orbit coupling is expected to be localized on Ar⁺, as was assumed in ref. 6. We therefore derived the SO potentials analytically, using expressions arising from the well-known atomic model³⁴ that connects the SO-potentials, $X^2\Sigma_{1/2}^+$, $A_1^2\Pi_{3/2}$ and $A_2^2\Pi_{1/2}$ (denoted V_X , V_{A_1} and V_{A_2}), to the $^2\Sigma^+$ and $^2\Pi$ potentials (denoted V_Σ and V_Π). These expressions are

$$V_X = \frac{1}{2}(V_\Sigma + V_\Pi + \Delta - \delta) \quad (1)$$

$$V_{A_1} = V_\Pi \quad (2)$$

and

$$V_{A_2} = \frac{1}{2}(V_\Sigma + V_\Pi + \Delta + \delta), \quad (3)$$

where

$$\delta^2 = (V_{\Sigma} - V_{\Pi})^2 - \frac{2\Delta}{3}(V_{\Sigma} - V_{\Pi}) + \Delta^2 \quad (4)$$

and Δ is the SO splitting between the RG^+ atomic $^2P_{3/2}$ and $^2P_{1/2}$ states. The values of Δ are 1431.41, 5371.0, 10537.01 and 30895.1 cm^{-1} for $\text{RG} = \text{Ar-Rn}$, respectively.³⁵

B. Spectroscopic Constants

Once obtained, the potential energy data set was used as input into the LEVEL program³⁶ in order to obtain spectroscopic and other data, in particular the rovibrational energy levels. From the latter, fits of the lowest few levels to standard spectroscopic formulae were employed to obtain equilibrium values.

C. Transport Properties

To obtain transport coefficients, the calculated potentials were first employed in the QVALUES program^{37,38} to obtain transport cross sections with a precision of 0.1%. Transport coefficients were obtained by employing these cross sections in the GC program,³⁹ a modified version of the older GRAMCHAR program.⁴⁰ The modifications were made to cope with the increased demands when the ion mobility has both a maximum and a minimum (as was the case for systems involving the coinage metal cations moving through the rare gases³⁹), to allow higher-order approximations to be employed, and finally to take advantage of faster, modern computers.

The overall precision for the calculated mobilities is 0.1% at small E/n_0 (the ratio of the electric field strength to the gas number density). In the worst cases, it is 1% near and beyond the mobility maximum, but only 3% in the region between the minima and maximum, where the mobility is increasing rapidly with increasing E/n_0 .

Calculated values for the mobilities and other transport coefficients for each one of the naturally-occurring RG^+ isotopes in He have been obtained over wide ranges of E/n_0 at gas temperatures of 100, 200, 300, 400 and 500 K, and for gas temperatures that have been used in transport experiments (see above). All of these results have been entered into the database maintained at Chatham University.⁴¹

III. Results and Discussion

A. Potential Curves and Spectroscopy

In Figure 1, we show our *ab initio* calculated potential energy curves for $\text{Ar}^+\text{-He}$, along with the MAL1 potentials⁶. As may be seen, the two sets of curves are in very good agreement, and although there are differences at the minima, the directions of these differences are not consistent for the three SO states. (The data points for our curves are given as Supplementary Material.)

We start by commenting on the *ab initio* results that did not include SO coupling, although such studies cannot be assessed against experimental data directly. Results prior to the work in ref. 6 have been commented on previously^{6,24}. The more recent work of Murrell *et al.*²⁰ reports the results of MRCI+Q calculations employing an

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aug-cc-pVQZ basis set. We have noted previously¹ that for Ne⁺-He a single-reference method appears to be satisfactory and we assume the same is true for the species considered herein. For Ar⁺-He, this certainly seems to be the case since the derived R_e and D_e values in Table 1 for the MRCI²⁰ and the present RCCSD(T) potentials are very close, both for the $^2\Sigma^+$ and the $^2\Pi$ states. The most recent study by Bera *et al.*²¹ reports CCSD(T) calculations employing aug-cc-pVTZ basis sets for the $^2\Sigma^+$ state. Since the Gaussian program⁴² was employed therein, we assume that unrestricted wave functions were used. A number of calculations were employed, including the DFT hybrid method, B3LYP, as well as MP2 and CCSD(T). The B3LYP values indicated a large overestimate of the interaction, something that has been noted previously by one of us for NO⁺-Ar.⁴³ The MP2 and CCSD(T) results²¹ are much closer to each other, with the CCSD(T) values being closer to the results of the present study (see Table 1). We note that results were also reported where all electrons were correlated, at both the MP2 and CCSD(T) levels; however, since no tight functions were included to describe the core-valence correlation, those results must be viewed with caution. We only include the frozen core CCSD(T) results in Table 1, for which good agreement is seen for R_e , but the well depths are shallower than those found herein.

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Moving on to studies which have included SO coupling, we only consider the most recent and reliable potentials, the key aspects of which are presented in Table 2. (The other potentials are commented upon in refs. 6 and 18.) We first note that the model potential results of Siska¹¹ and a modified version of these¹⁸ were mainly fitted to the UV results of Dabrowski *et al.*⁴, whereas the MAL1 potentials also have input from the microwave spectrum that helps characterize the long-range region better. As noted before,⁶ there are significant differences between the three aforementioned potentials, with the differences being largest for the A_1 state, for which there were no observed transitions in the UV study. Comparing these to the present results and to the MAL1 potential, we see that the present R_e value is slightly larger, with the D_e value being slightly smaller; interestingly the present value falls between the previously determined values. For the A_2 state, we obtain excellent agreement with the D_e value from the MAL1 potential,⁶ and indeed with the value from Siska.¹¹ All of these values lie significantly above those of VVM¹⁸ and the value from DHY.⁴ In the latter case, dissociation energies were obtained from a combination of extrapolation and energy differences, so perhaps it is not surprising that the value is not so accurate. Lastly, the most dramatic differences in D_e values occur for the A_1 state, for which there were no experimental data; however, since the three states here are interconnected *via* spin-orbit coupling, knowing two of them defines the third. It may be seen from Table 2 that the present work is in excellent agreement with the MAL1 potentials for both R_e and D_e . In conclusion, the MAL1 potentials, having included long-range spectroscopic data in the fit, appear to be much more reliable potentials than either of the two earlier ones, which were based purely on the UV spectra. The MAL1 potentials are in very good agreement with the curves obtained in the present work. We note that there is also very good agreement with the SO results reported in ref. 20 for the X and A_2 states (no parameters were reported for the A_1 state).

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For Kr⁺-He, there is no assigned UV spectrum. Hence, all of the information on this species comes from the microwave study of Carrington and coworkers²⁴ on levels that are only a few cm⁻¹ from the dissociation limit. Thus, these experiments sample only

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3 the long-range portion of the interaction potential. Since microwave spectroscopy is
4 such a precise technique, the whole potential curve should be obtainable, in principle,
5 if enough transitions are observed. In fact, sufficient transitions were observed²⁴ to
6 generate MAL1 potentials, similar in type to those for Ar⁺-He, but now having no
7 input from UV spectra. These MAL1 potential are, therefore, *only* defined in terms of
8 transitions between levels very close to the dissociation limits.
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11 As may be seen in Figure 2, the agreement between our Kr⁺-He potentials and the
12 MAL1 potentials looks very good, with the MAL1 potentials being very slightly
13 deeper in all cases, especially for the *X* state. These features are evident in the data
14 presented in Table 2. Given that the MAL1 potentials have been obtained by fitting
15 only to transitions between high-lying levels, the agreement between the two sets of
16 curves is remarkable.
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19 We note in passing that the previous study by Balasubramanian *et al.*¹⁵ has been noted
20 as having an error²⁴, as the ground state is designated $X^2\Pi_{3/2}$, and the dissociation
21 energies are far from those obtained here or from the MAL1 potentials. However, the
22 estimate for the binding energy of 29 meV ($\sim 230\text{ cm}^{-1}$) from mobility studies⁵ is of
23 the correct magnitude.
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26 There are no reliable data to which to compare our results for either Xe⁺-He or Rn⁺-
27 He, although in the former case there are experimental mobility results, and these will
28 be considered below.
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30 31 *B. Transport Results for Ar⁺ in He*

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33 As noted in the Introduction, there have been a number of studies measuring the
34 mobility of Ar⁺ in He at a variety of temperatures. Such studies can, if there are
35 enough data points, and if the accuracy and precision are high enough, provide
36 stringent tests of potentials across a very wide range of internuclear separation.²⁷ To
37 this end, we have calculated mobilities using both the MAL1 and the present
38 potentials, and have compared the results to experimental data. In Figure 3, the
39 results at 300 K are given, both those calculated from the present potentials and the
40 experimental data points.
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43 For the calculations, we have employed a (110) weighting of the cross sections arising
44 from the *X*, *A*₁ and *A*₂ potentials, which is akin to assuming only the $^2P_{3/2}$ atomic state
45 of Ar⁺ is present. We have also used a (001) weighing, which is for the $^2P_{1/2}$ state.
46 We have performed such calculations for both the MAL1 and present potentials.
47 Unfortunately, the cited experimental error bars are large enough that they encompass
48 both of the calculated curves. If it is assumed that the error bars are pessimistic, then
49 by eye it appears that the (110) weighting of the potentials is in better agreement with
50 the actual experimental data points than the (001) one. In agreement with our
51 conclusion for Ne⁺ in He¹, this would suggest that only the $^2P_{3/2}$ ground state of Ar⁺
52 were present in the experiments, i.e., any ions created in the higher SO state were
53 efficiently quenched to the lower state before they reached the drift region of the
54 apparatus.
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3 Another way of comparing data is to employ the statistical quantities δ and χ .³⁸ The
4 dimensionless quantity δ is a measure of the relative differences compared to the
5 combined experimental and calculational errors, while χ is a measure of the relative
6 standard deviation to the sum of the squared error estimates. Values of $|\delta|$ that are
7 substantially lower (alternatively, higher) than 1 indicate that there is substantial
8 agreement (disagreement) between the calculated and measured values, on average.
9 Values of χ that are not much larger than $|\delta|$ indicate that there is little scatter in the
10 experimental data and that the agreement between the calculated and measured values
11 is uniform over all values of E/n_0 , while values of χ substantially greater than $|\delta|$
12 indicate that at least one of these factors is not true. In Table 3, we report these
13 quantities for the present potential and smoothed versions^{44,45,46} of the experimental
14 data for $^{40}\text{Ar}^+$ in He, but not including the experimental values for $E/n_0 < 2$ Td (see
15 below). What is immediately clear is that for the data at the higher temperatures (≥ 293
16 K) there is agreement between calculated and experimental data for either state, which
17 is a result of the large experimental error bars, as can be seen in Figure 3. These
18 statistical quantities also indicate that, with regards to the mobility data, there is no
19 statistical difference between the results obtained using the present potentials and
20 those obtained using the MAL1 potentials.
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24 The mobility data from VVM²³ for RG^+ in He have been suspected^{47,48} for many years
25 of being less accurate than claimed by the experimenters. Hence it is not surprising to
26 find in Table 3 that these data are in significant disagreement with the present
27 calculations, as they are in similar disagreement with results calculated from all of the
28 other available potentials.
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31 The data which have the smallest error bars are those at 4.35 K.⁵ Interestingly, the
32 experimental data show a distinct drop in the mobility of RG^+ in He as $E/n_0 \rightarrow 0$ —
33 see Figure 4. Similar results had been reported previously for He^+ in He,⁴⁹ a system in
34 which resonant charge transfer (RCT) occurs. One explanation that has been put
35 forward⁵ is quantum effects, as previously predicted by Dickinson⁵⁰ and Heiche and
36 Mason.⁵¹ The same unusual mobility behaviour was found in N_2^+ and CO^+ in He by
37 Sanderson *et al.*⁵² in which RCT cannot occur, and in this case orbiting resonances
38 and/or collision-induced rotational excitation were proposed. Other experiments have
39 also observed such unusual low- E/n_0 mobilities, in He for Ne^+ ,^{5,53} O_2^+ ,⁵⁴ NO^+ ,⁵⁵ and
40 other ions.⁵⁶ A first theoretical account of the low E/n_0 anomalous mobilities of
41 N_2^+ and O_2^+ in He at 4.35 K was presented by Ohtsuki *et al.*⁵⁷ They calculated
42 mobilities from MRCI potentials, and demonstrated that the anomalous behavior was
43 due to Feshbach-like resonances, where rotational excitation of the molecular ions
44 occurred as a result of collisions with He. This explanation cannot apply to atomic
45 ions such as RG^+ in He, of course, nor for other atomic ions, O^+ and N^+ ,⁵⁸ for which
46 similar behaviour has been found. The suggestion that quantum effects might be the
47 source of the low E/n_0 behaviour was tested explicitly by Viehland and Hurly in
48 1996⁴⁸ and was found not to explain the observed results. As such, the anomalous
49 low E/n_0 behaviour of atomic ions in He at 4.35 K so far remains unexplained.
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53 The fact that the present results, as was the case for Ne^+ in He,¹ also show that the
54 theoretical mobilities do not show the dramatic fall in values as $E/n_0 \rightarrow 0$ has led us to
55 consider this issue further. We note that, in ref. 5, the ions were provided with a
56 constant injection energy of 20 eV. Consequently, the value of E/n_0 is controlled by
57 varying the pressure, and hence low E/n_0 values are achieved at higher pressures. At
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3 4.35 K, there is a possibility for He₂ (and possibly higher-order clusters) to form, and
4 since the formation would be a termolecular process (with a third body being required
5 to stabilize the He₂ species) it would be highly pressure dependent. The effect of He
6 dimer formation would be to increase the effective reduced mass of collisions, and
7 hence lower the mobility. This hypothesis could be tested by performing
8 measurements at E/n_0 values where both E and the pressure were changed, but
9 yielding the same resulting E/n_0 value.
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11 *B. Other Transport Results*

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14 Figures 5 and 6 compare calculated and experimental mobilities for ⁸⁴Kr⁺ in He at 300
15 and 4.35 K, respectively. In Table 4, we report the statistical quantities from a
16 comparison of the present potential for ⁸⁴Kr⁺ in He and smoothed versions^{40,41,44} of the
17 experimental data in which neither the isotope nor the state was specified. The
18 calculated mobilities for the five naturally occurring isotopes of Kr are very similar.
19 This is consistent with the theoretical prediction (from the first approximation of the
20 two-temperature kinetic theory⁵⁹) that the mobility is inversely proportional to the
21 square root of the reduced mass. Hence any differences between theory and
22 experiment shown in Table 4 are not due to which isotope was used.
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26 Again we note that calculated mobilities involving the MAL1 potentials are not
27 statistically different from those using the present potentials — more evidence for
28 their close agreement. Table 4 shows that at 4.35 K there is agreement between
29 calculated and experimental data for either state. Note that again we do not include
30 the experimental values for $E/n_0 < 2$ Td at 4.35 K, for the reasons we have discussed
31 for Ar⁺ in He above. The data at 82 K are in satisfactory agreement with the
32 calculations for both states, owing to our use of 4% as the experimental accuracy; the
33 experimenters did not state the accuracy of their results, but examination of the raw
34 data²⁸ shows rapid variations by as much as 4%. Finally, the data near room
35 temperature are in good to excellent agreement with the calculations for the ²P_{1/2}
36 excited state but not with those for the ²P_{3/2} ground state.
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40 As shown in Figures 4 and 6, a small mobility minimum occurs at low gas
41 temperatures. Such minima arise frequently with open-shell ions, because the R^{-6}
42 component of their long-range interactions with rare gas atoms is large, compared to
43 the R^{-4} component that dominates at the very largest separations. More extensive
44 comments about mobility minimum have been given previously.³⁹
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47 The calculated mobilities for ¹³²Xe⁺ in He at 300 K are compared with experimental
48 values in Figure 7 and Table 5. As before, the calculated mobilities for different
49 isotopes are very similar, so difference between theory and experiment are not due to
50 which isotope was used. The data at 82 K are in reasonable agreement with the
51 calculations for both states, owing to our choice again to use 4% for the accuracy, a
52 value that was not reported by the experimenters.²⁸ The data near room temperature
53 are not in good agreement with the calculations, suggesting that those data may be
54 even less accurate than the estimate of 5% made by the experimenters²⁷.
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57 There are no experimental values for Rn⁺ in He, and so the quantities calculated here
58 and placed into the database⁴¹ represent the only values available.
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3 A word of caution is in order, however, as we previously^{1,60} noted problems arising
4 from injection effects when a heavy ion is passed into a drift tube containing a light
5 gas; this can lead to a measured mobility that is too high and careful checking of
6 experimental values is required.
7

8 9 **IV. Conclusions**

10 The favourable comparison of the present, completely *ab initio*, potentials with
11 previous experimental (DHY⁴) results and fitted MAL1^{6,24} results for Ar⁺-He and
12 Kr⁺-He, suggests that the present results are reliable. It is noteworthy that, for the
13 most part, there is agreement with the MAL1 potentials of Carrington *et al.*^{6,24} and the
14 non-SO potentials of Siska¹¹ and VVM.¹⁸ The discrepancies between those results and
15 ours are likely in part attributable to different parameterizations and the different
16 experimental data sets employed. The good agreement with the Kr⁺-He MAL1
17 potentials²⁴ is particularly noteworthy, since the latter was obtained by fitting only to
18 experimental spectroscopic data obtained from transitions between levels within a few
19 cm⁻¹ of the dissociation limit.
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23 The agreement in Table 2 of our calculated spectroscopic quantities with those
24 obtained from UV absorption spectra⁴ is good, in the main. However, independent
25 checking of some values is desirable, particularly for the dissociation energies.
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28 Transport coefficients are known to be good tests of interaction potentials across a
29 very wide range of interatomic (or intermolecular) separation, but such tests are
30 reliant on the experimental precision being sufficiently good. The results above have
31 shown that, near room temperature, the experimental errors of 5–7% are too large to
32 be discriminatory for Ar⁺ in He. We noted, however, that there appears to be a better
33 agreement between the reported data points and the values calculated by assuming
34 only Ar⁺ (²P_{3/2}) was present—a conclusion that would be consistent with our previous
35 findings for Ne⁺ in He¹, but somewhat contrary to comments made previously⁵
36 regarding populations of the spin-orbit states. We have also noted that the distinct fall
37 in the mobility values as $E/n_0 \rightarrow 0$ at 4.35 K is not in agreement with the theoretical
38 predictions; this has been discussed previously,⁴⁸ where quantum chemical effects
39 were ruled out. Since constant injection energies were employed in the mobility
40 measurements and the low E/n_0 values were determined by increases in the pressure,
41 we have conjectured that the presence of dimers (and other clusters) at 4.35 K could
42 be the cause of the anomalous experimental results. We have suggested that these
43 results should be independently checked in experiments where both E and n_0 are
44 varied.
45
46

47 Finally, we note that the comments above regarding Ar⁺-He and Kr⁺-He suggest that
48 the Xe⁺-He and Rn⁺-He potentials should also be reliable. In these cases, however,
49 higher precision experimental results are required in order to test our potentials more
50 definitively.
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53 **Acknowledgements**

54
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3 Nottingham for an EPSRC DTA studentship. Dr. Mark Law (Aberdeen) and Prof.
4 Jeremy Hutson (Durham) are thanked for providing the MAL1 potentials.
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Table 1: Spectroscopic Parameters for He–RG⁺ — Non-Spin-Orbit Curves. Isotopes employed are: ⁴He, ⁴⁰Ar, ⁸⁴Kr, ¹³¹Xe and ²²²Rn. Here, the symbols represent the usual spectroscopic quantities: R_e is the equilibrium bond length, D_e is the depth of the potential, D_0 is the energy between the zero-point and the asymptote, ω_e is the harmonic vibrational frequency, $\omega_e x_e$ is the anharmonicity constant, B_0 is the equilibrium rotational constant of the $v = 0$ level, D_{0J} is the first distortion constant for the $v = 0$ level, σ is the crossing point of the potential, when the potential = 0, and $\Delta G_{1/2}$ and $\Delta G_{3/2}$ are the first two vibrational term values.

System	State [Ref]	$\sigma/\text{\AA}$	$R_e/\text{\AA}$	D_e/cm^{-1}	D_0/cm^{-1}	ω_e/cm^{-1}	$\omega_e x_e/\text{cm}^{-1}$	B_0/cm^{-1}	$D_{0J}/10^{-5}\text{cm}^{-1}$	$\Delta G_{1/2}/\text{cm}^{-1}$	$\Delta G_{3/2}/\text{cm}^{-1}$
He–Ar ⁺ ² Σ^+	This Work	2.05	2.41	420.1	341.2	164.3	17.31	0.754	8.33	130.2	94.1
	BBD ^{21 a}		2.45	331		155.7	32.44		7.50	97.86	50.30
	GP ¹⁷		2.47	274		186					
² Π	MNG ²⁰		2.42	403							
	This Work	2.52	3.00	142.0	102.0	75.6	10.79	0.468	9.22	55.6	29.3
	GP ¹⁷		3.12	113		140					
He–Kr ⁺ ² Σ^+	MNG ²⁰		3.02	137							
	This Work	2.30	2.68	301.7	240.0	127.9	14.57	0.578	6.28	99.4	68.4
	² Π	This Work	2.82	3.22	115.6	81.8	63.2	9.23	0.387	7.42	46.2
He–Xe ⁺ ² Σ^+	This Work	2.63	3.03	203.6	156.9	95.6	11.97	0.441	5.07	72.4	46.1
	² Π	This Work	3.11	3.52	87.8	60.2	58.0	9.31	0.316	5.87	39.4
He–Rn ⁺ ² Σ^+	This Work	2.73	3.15	184.0	141.0	87.7	11.15	0.406	4.71	66.2	41.6
	² Π	This Work	3.22	3.65	79.2	53.9	44.8	6.71	0.291	5.93	32.9

^a CCSD(T)/FC values only cited from that work.

Table 2: Spectroscopic Parameters for He–RG⁺ —Spin-Orbit Curves. Isotopes employed are: ⁴He, ⁴⁰Ar, ⁸⁴Kr, ¹³¹Xe and ²²²Rn. Quantities are defined in Table 1.

System	Ref	$\sigma/\text{\AA}$	$R_e/\text{\AA}$	D_e/cm^{-1}	D_0/cm^{-1}	ω_e/cm^{-1}	$\omega_e x_e/\text{cm}^{-1}$	B_0/cm^{-1}	$D_0/10^{-5}/\text{cm}^{-1}$	$\Delta G_{1/2}/\text{cm}^{-1}$	$\Delta G_{3/2}/\text{cm}^{-1}$
He–Ar ⁺ ² $\Sigma_{1/2}^+$	This work	2.18	2.60	271.1	215.5	117.6	13.60	0.643	10.4	90.9	62.3
	DHY ⁴		2.585	262		120.3	13.60	0.659			
	Sis ¹¹	2.19	2.564	282.6							
	Sta ¹⁶		2.66	242	190	116.9	17.7			83.9	55.2
	GP ¹⁷		2.77	177		105					
	MNG ²⁰		2.62	258							
	MAL1 ⁶		2.573	281.6				0.651		93.2	64.1
² $\Pi_{3/2}$	This Work	2.17	2.65	269.4	215.3						
	This Work	2.52	3.00	142.0	102.0	75.6	10.79	0.468	9.22	55.6	29.3
	Sta ¹⁶		3.03	133	94	89.3	21.2			52.9	26.9
	GP ¹⁷		3.10	105		80					
	MAL1 ⁶		2.98	143.4							
² $\Pi_{1/2}$	HM ¹⁰	2.59	2.96	161.3	114.5						
	This Work	2.52	2.88	178.1	131.7	91.6	12.58	0.512	8.33	68.0	38.2
	Sta ¹⁶		2.91	166	121	102.2	21.7			64.0	35.1
	GP ¹⁷		3.00	137		93					
	MNG ²⁰		2.89	169							
	DHY ⁴		2.872	154				0.5146		69.2	
	Sis ¹¹	2.48	2.872	185.4							
	MAL1 ⁶		2.863	181.6				0.5160		68.9	
HM ¹⁰	2.51	2.86	192.8	140.3							

He-Kr ⁺ $^2\Sigma_{1/2}^+$	This Work	2.51	2.90	199.8	152.4	96.0	12.33	0.487	6.75	72.3	44.7
	HM ¹⁰	2.51	2.91	240.4	183.1						
	MAL1 ⁶		2.87	208							
$^2\Pi_{3/2}$	This Work	2.82	3.22	115.6	81.8	63.2	9.23	0.387	7.42	46.2	23.3
	HM ¹⁰	2.78	3.18	161.3							
	MAL1 ⁶		3.20	116							
$^2\Pi_{1/2}$	This Work	2.70	3.09	145.9	106.4	76.4	10.68	0.424	6.87	56.4	30.9
	HM ¹⁰	2.65	3.04	192.8	140.3						
	MAL1 ⁶		3.06	149							
He-Xe ⁺ $^2\Sigma_{1/2}^+$	This Work	2.83	3.24	143.5	106.0	75.8	10.59	0.383	5.45	55.1	32.5
	HM ¹⁰	2.25	2.65	403.3	327.5						
$^2\Pi_{3/2}$	This Work	3.11	3.52	87.8	60.1	58.0	9.31	0.316	5.87	39.4	20.8
	HM ¹⁰	2.78	3.18	149.2	104.9						
$^2\Pi_{1/2}$	This Work	2.98	3.40	109.3	77.5	62.6	9.38	0.343	5.71	45.1	22.7
	HM ¹⁰	2.59	2.59	22.6	167.8						
He-Rn ⁺ $^2\Sigma_{1/2}^+$	This Work	2.93	3.35	129.2	94.7	67.9	9.46	0.352	5.08	50.0	27.9
$^2\Pi_{3/2}$	This Work	3.22	3.65	79.2	53.9	44.8	6.71	0.291	5.93	32.9	14.8
$^2\Pi_{1/2}$	This Work	3.09	3.52	98.6	69.5	55.0	8.11	0.316	5.45	40.0	19.9

Table 3: Statistical Comparison between Calculated and Experimental Mobility Data for Ar^+ in He. See text for definitions of δ and χ . N is the number of data points, and %Expt and %Calc are the experimental and calculational precisions. When N is small, over-interpretation of the results should be avoided.

T/K	Data Source	State	E/n_0 Td	N	%Expt	%Calc	δ	χ
4.35	Ref. 39	$^2P_{3/2}$	2.0–11.5	7	2.0	0.1	0.25	0.34
			115–35.5	6	2.0	0.1	-1.23	1.39
		$^2P_{1/2}$	2.0–11.4	7	2.0	0.1	-0.16	0.22
			12.4–50.0	6	2.0	1.0	-0.79	1.33
82	Ref. 40	$^2P_{3/2}$	5.0–32.0	5	4.0	0.1	1.45	1.47
			32.0–70.0	4	4.0	0.5	0.79	1.05
		$^2P_{1/2}$	5.0–32.0	5	4.0	0.1	1.58	1.70
			32.0–70.0	4	4.0	0.5	2.30	2.38
92	Ref. 39	$^2P_{3/2}$	1.0–15.0	10	5.0	0.1	1.73	1.75
		$^2P_{1/2}$	1.0–15.0	10	5.0	0.1	1.62	1.65
170	Ref. 39	$^2P_{3/2}$	4.0–30.0	10	5.0	0.1	1.09	1.10
		$^2P_{1/2}$	4.0–30.0	10	5.0	0.1	1.29	1.35
293	Ref. 39	$^2P_{3/2}$	6.0–40.0	10	5.0	0.1	-0.62	0.62
		$^2P_{1/2}$	6.0–40.0	10	5.0	0.1	0.14	0.33
300	Ref. 41	$^2P_{3/2}$	5.0–50.0	10	7.0	0.1	-0.03	0.11
			50.0–130.0	8	7.0	0.1	-0.57	0.62
		$^2P_{1/2}$	5.0–50.0	10	7.0	0.1	0.67	0.70
			50.0–130.0	8	7.0	0.5	0.58	0.61
428	Ref. 39	$^2P_{3/2}$	8.0–50.0	10	5.0	0.1	-0.64	0.72
		$^2P_{1/2}$	8.0–50.0	10	5.0	0.1	0.48	0.75
552	Ref. 39	$^2P_{3/2}$	10.0–50.0	9	5.0	0.1	-0.46	0.53
		$^2P_{1/2}$	10.0–50.0	9	5.0	0.1	0.88	0.97

Table 4: Statistical Comparison between Calculated and Experimental Mobility Data for $^{84}\text{Kr}^+$ in He. See text for definitions of δ and χ . N is the number of data points, and %Expt and %Calc are the experimental and calculational precisions. When N is small, over-interpretation of the results should be avoided.

T/K	Data Source	State	E/n_0 Td	N	%Expt	%Calc	δ	χ
4.35	Ref. 39	$^2P_{3/2}$	2.0–11.5	7	2.0	0.1	0.07	0.19
			11.5–35.5	8	2.0	0.1	-0.34	0.54
		$^2P_{1/2}$	2.0–11.5	7	2.0	0.1	0.23	0.28
			11.5–50.0	6	2.0	0.3	-0.27	0.63
82	Ref. 39	$^2P_{3/2}$	4.0–32.0	10	4.0	0.1	0.64	0.65
			32.0–70.0	4	4.0	0.1	0.46	0.47
		$^2P_{1/2}$	4.0–32.0	10	4.0	0.1	0.54	0.57
			32.0–70.0	4	4.0	0.1	0.82	0.82
294	Ref. 40	$^2P_{3/2}$	3.0–45.0	5	4.0	0.1	-0.79	0.87
			45.0–250.0	5	4.0	0.1	-0.89	0.91
		$^2P_{1/2}$	3.0–45.0	5	4.0	0.1	-0.66	0.71
			45.0–250.0	5	4.0	0.1	0.02	0.53
300	Ref. 41	$^2P_{3/2}$	5.0–35.0	9	7.0	0.1	-1.87	1.93
			35.0–100.0	5	7.0	0.1	-1.73	1.87
		$^2P_{1/2}$	5.0–35.0	9	7.0	0.1	-0.49	0.53
			35.0–100.0	5	7.0	0.1	-0.09	0.25

Table 5: Statistical Comparison between Calculated and Experimental Mobility Data for $^{132}\text{Xe}^+$ in He. See text for definitions of δ and χ . N is the number of data points, and %Expt and %Calc are the experimental and calculational precisions. When N is small, over-interpretation of the results should be avoided.

T/K	Data Source	State	E/n_0 Td	N	%Expt	%Calc	δ	χ
82	Ref. 39	$^2P_{3/2}$	17.0–32.0	3	4.0	0.1	0.55	0.56
			32.0–70.0	5	4.0	0.1	0.20	0.43
		$^2P_{1/2}$	17.0–32.0	3	4.0	0.1	0.41	0.44
			32.0–70.0	4	4.0	0.1	0.33	0.46
295	Ref. 55	$^2P_{3/2}$	3.0–32.0	11	5.0	0.1	-1.24	1.28
			32.0–80.0	4	5.0	0.1	0.54	1.04
		$^2P_{1/2}$	3.0–32.0	11	5.0	0.1	-1.24	1.30
			32.0–80.0	4	5.0	0.1	-0.72	1.27

Figure Captions

Figure 1

Calculated potential energy curves for $\text{Ar}^+\text{-He}$. The solid black curves represent the present potential, calculated at the RCCSD(T)/d-aug-cc-pV5Z level of theory, while the red dashed ones represent the MAL1 potentials from ref. 6.

Figure 2

Calculated interaction energy curves for $\text{Kr}^+\text{-He}$. The black curves are the present ones, calculated at the RCCSD(T)/d-aug-cc-pV5Z level of theory — see text for details. The red dashed ones are the MAL1 potentials from ref. 24.

Figure 3

Standard mobilities for Ar^+ in He at 300 K. The points, with error bars are the experimental (smoothed) data points from refs. 44, 45, 46. The solid line is the calculated mobility curve assuming the $^2P_{3/2}$ state only is present; the dashed line is the calculated mobility curve assuming the $^2P_{1/2}$ state only is present. The ordinate is the standard mobility in $\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$, and the abscissa is the ratio of the electric field to the number density, in units of Townsend (Td).

Figure 4

Standard mobilities for Ar^+ in He at 4.35 K. The points, with error bars are the experimental data points from ref. 5. The solid line is the calculated mobility curve assuming the $^2P_{3/2}$ state only is present; the dashed line is the calculated mobility curve assuming the $^2P_{1/2}$ state only is present. The ordinate is the standard mobility in $\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$, and the abscissa is the ratio of the electric field to the number density, in units of Townsend (Td).

Figure 5

Standard mobilities for Kr^+ in He at 300 K. The points, with error bars are the experimental (smoothed) data points from refs. 44, 45, 46. The solid line is the calculated mobility curve assuming the $^2P_{3/2}$ state only is present; the dashed line is the calculated mobility curve assuming the $^2P_{1/2}$ state only is present. The ordinate is the standard mobility in $\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$, and the abscissa is the ratio of the electric field to the number density, in units of Townsend (Td).

Figure 6

Standard mobilities for Kr^+ in He at 4.35 K. The points, with error bars are the experimental data points from ref. 5. The solid line is the calculated mobility curve assuming the $^2P_{3/2}$ state only is present; the dashed line is the calculated mobility curve assuming the $^2P_{1/2}$ state only is present. The ordinate is the standard mobility in

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3 $\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$, and the abscissa is the ratio of the electric field to the number density, in
4 units of townsend (Td).
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6 **Figure 7**
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8 Standard mobilities for Xe^+ in He at 300 K. The points, with error bars are the
9 experimental (smoothed) data points from refs. 44, 45, 46. The solid line is the
10 calculated mobility curve assuming the $^2P_{3/2}$ state only is present; the dashed line is
11 the calculated mobility curve assuming the $^2P_{1/2}$ state only is present. The ordinate is
12 the standard mobility in $\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$, and the abscissa is the ratio of the electric field to
13 the number density, in units of townsend (Td).
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Figure 1

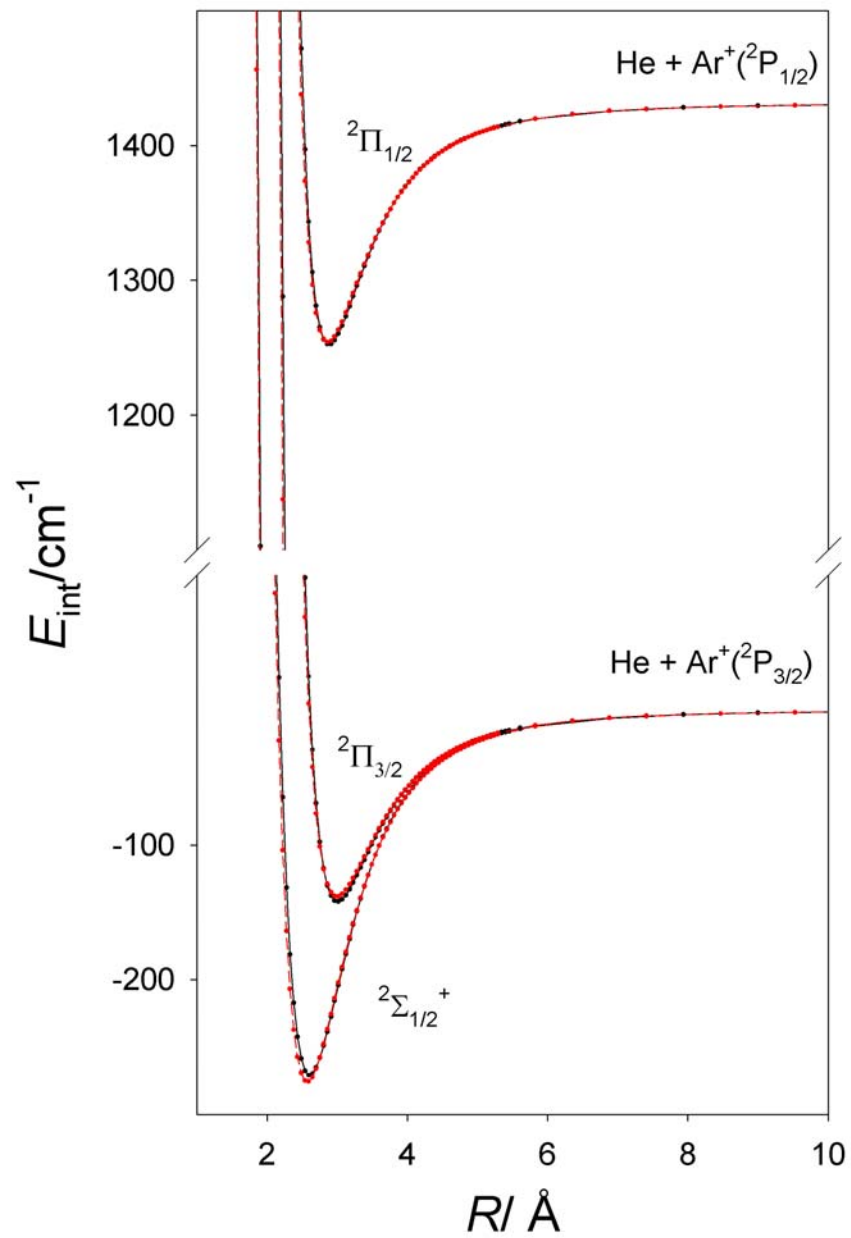


Figure 2

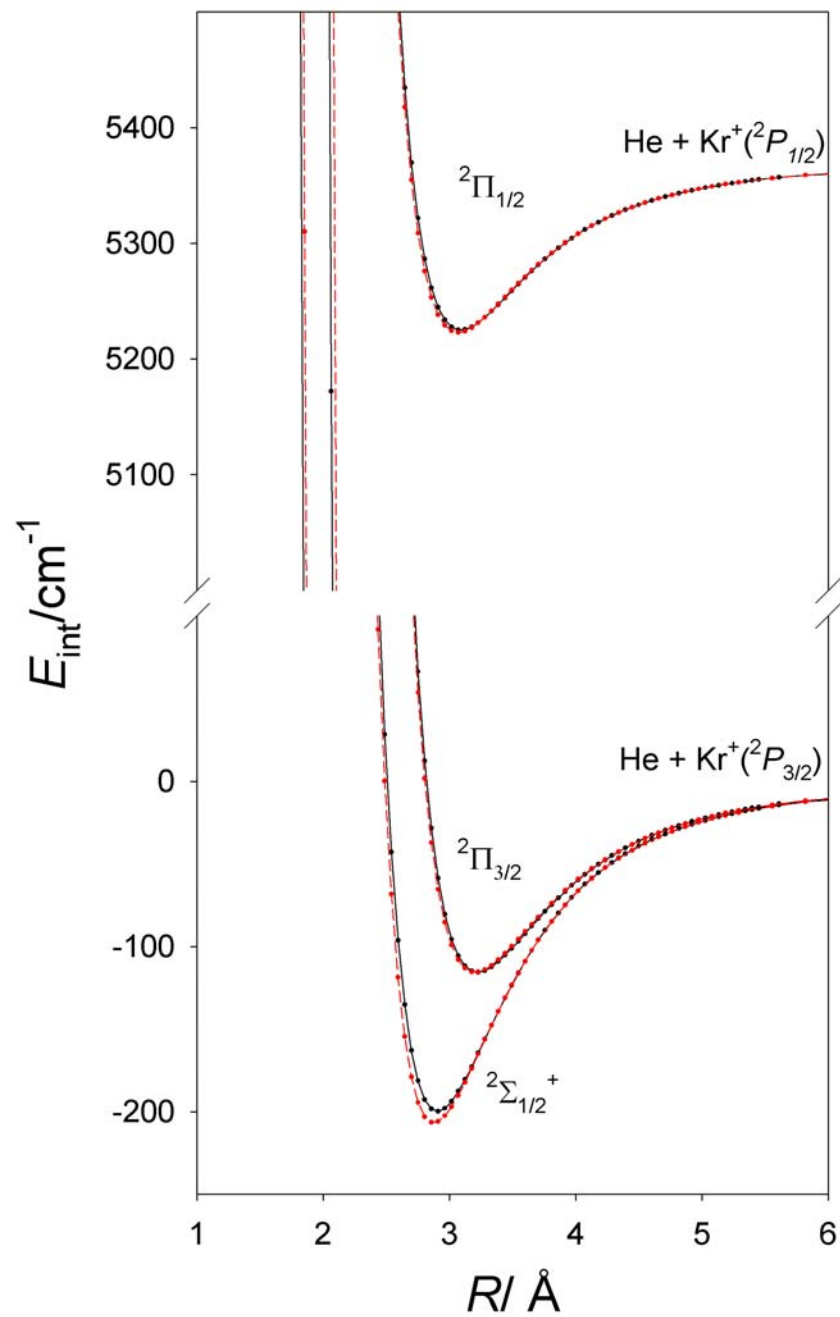


Figure 3

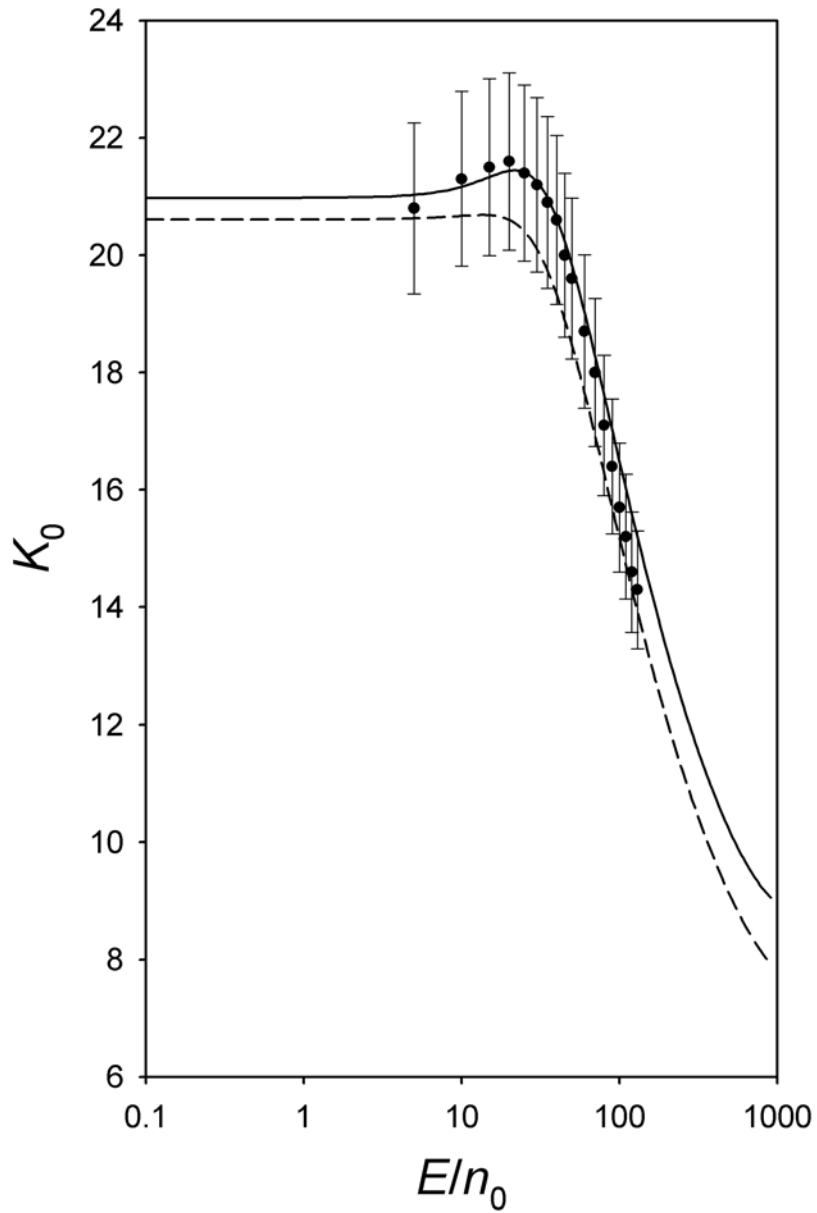
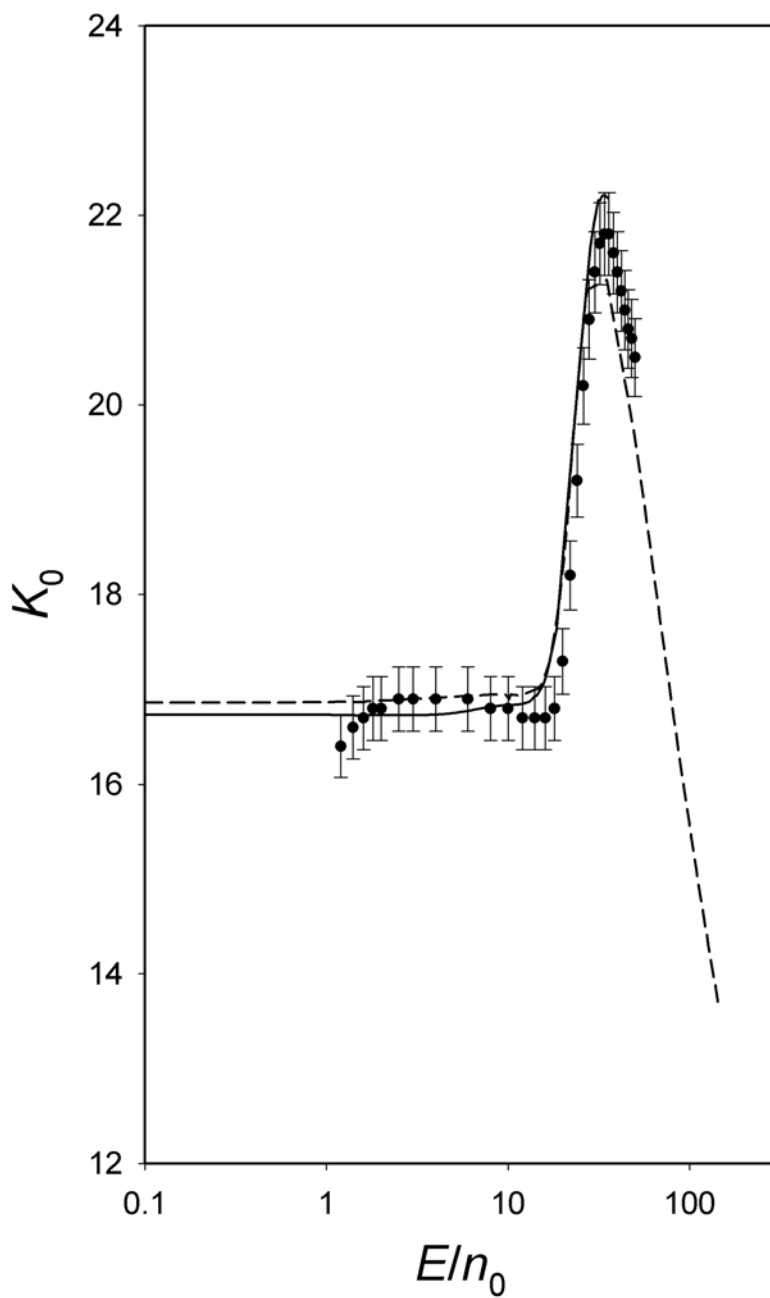


Figure 4



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Figure 5

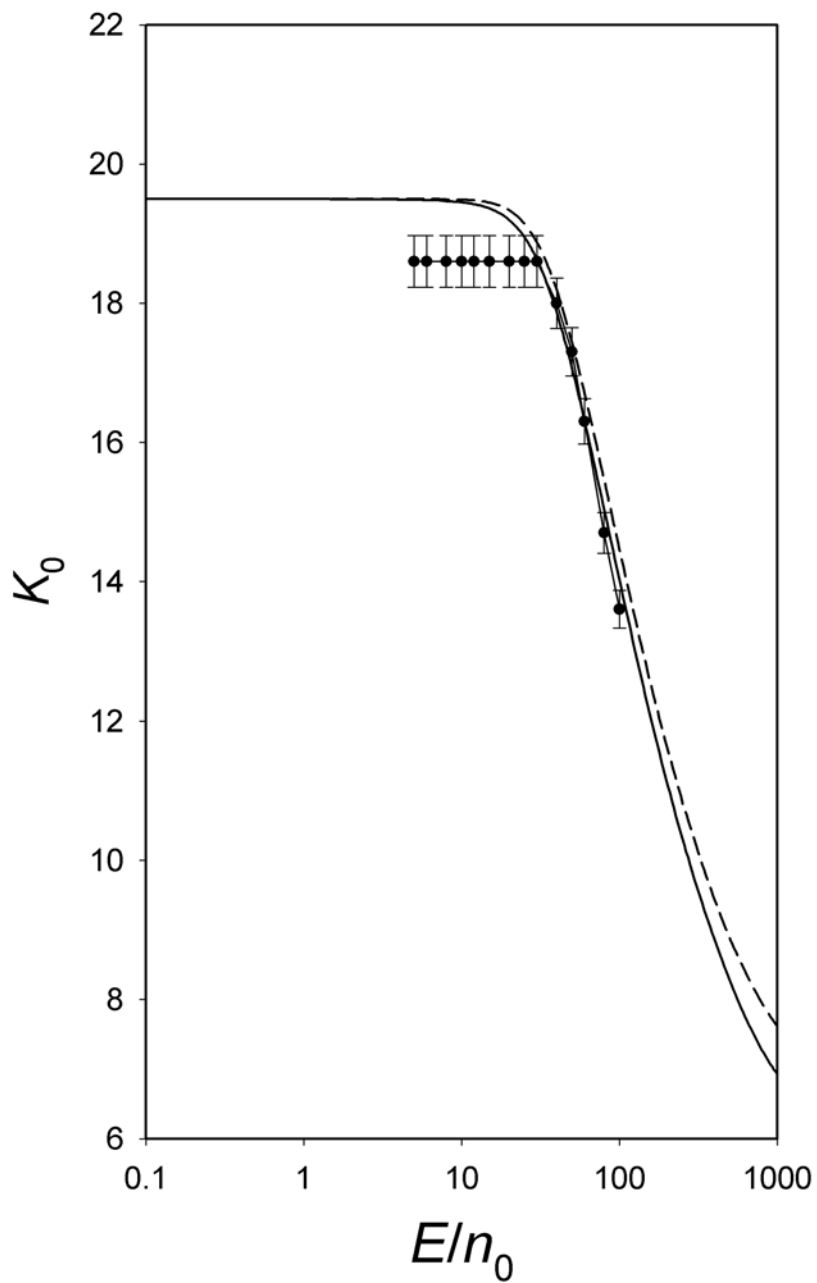
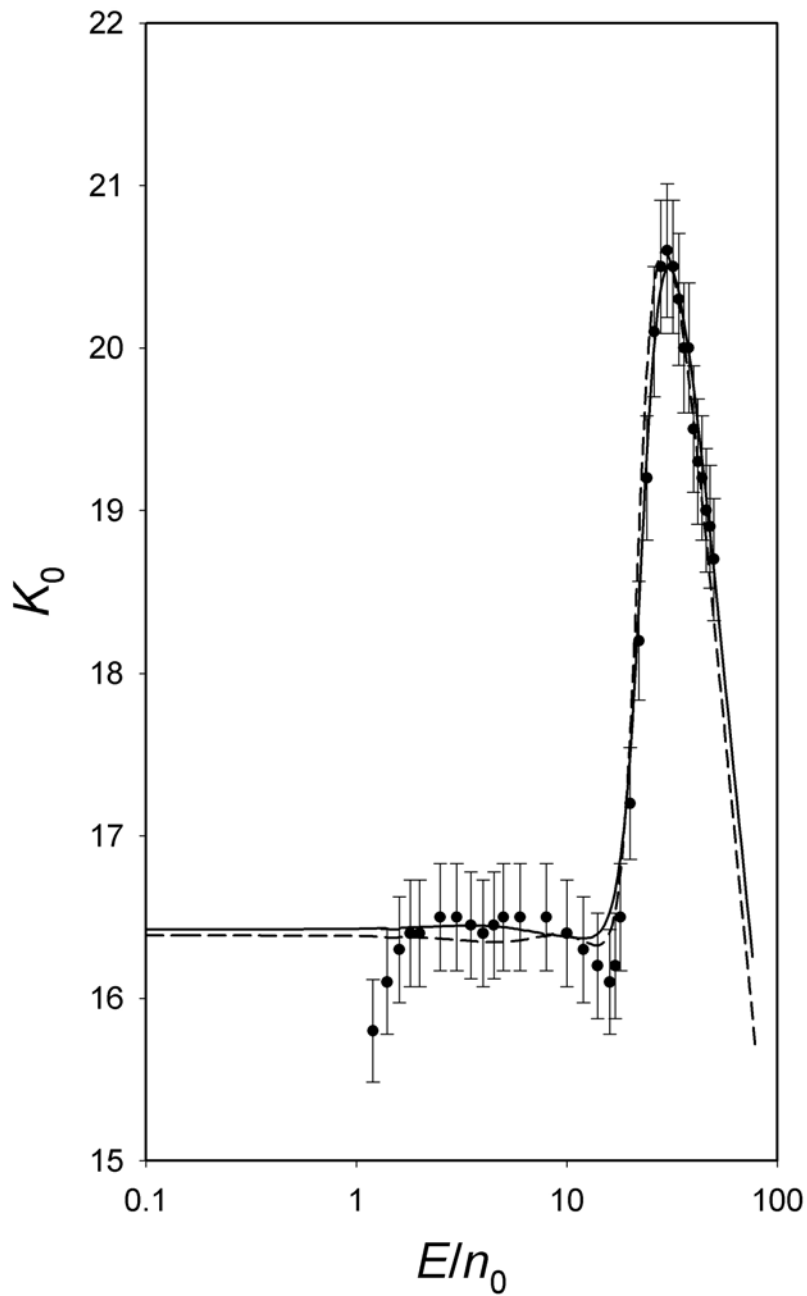
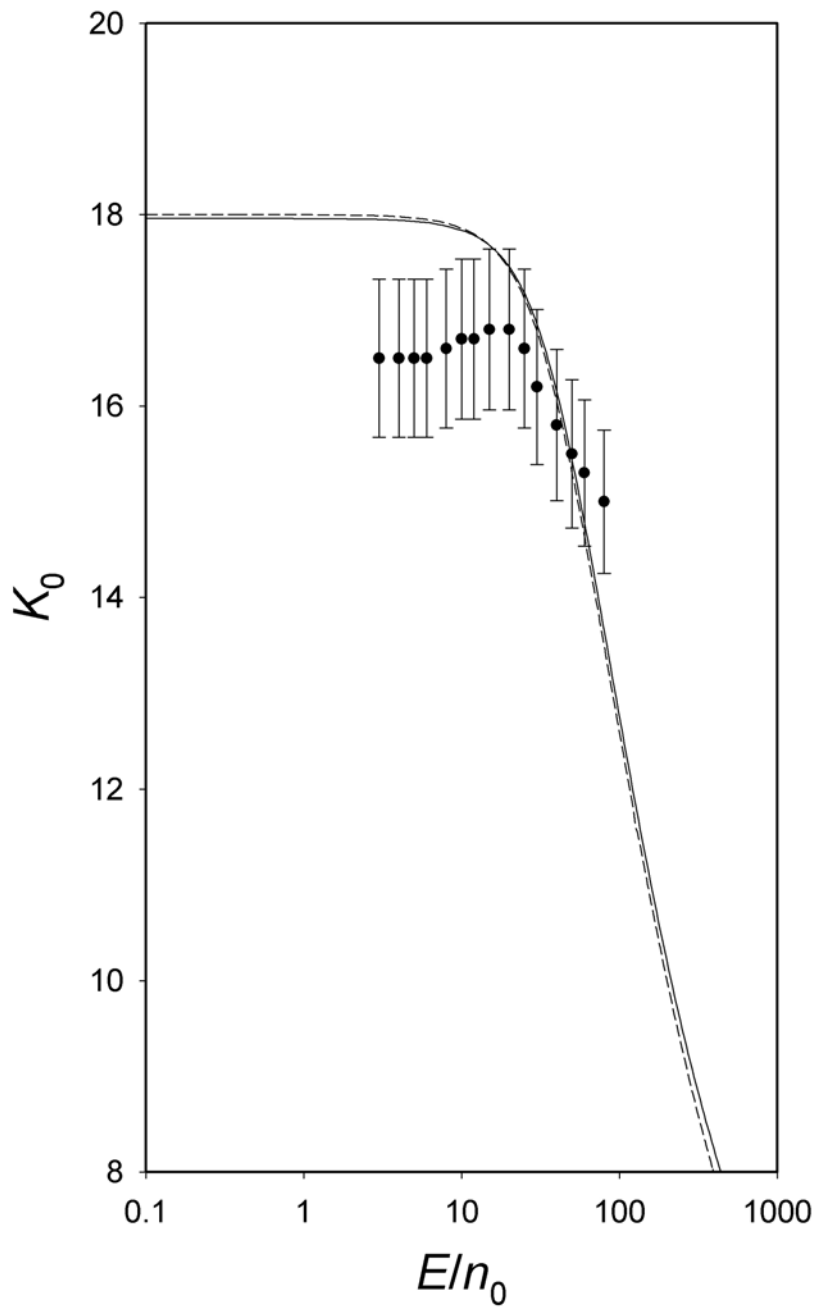


Figure 6



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Figure 7



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6 The Supplementary Material consists of an Excel spreadsheet with four worksheets.
7 There is one sheet for each of Ar⁺-He, Kr⁺-He, Xe⁺-He and Rn⁺-He. In each sheet,
8 the non-spin-orbit curves for the ²Π and ²Σ⁺ states are given, as well as the three spin
9 orbit potentials (see text). Note the units given at the tops of the columns!
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R (Bohr)	SIGMA (H ₂ PI (Hartree	SIGMA (cn PI (cm-1)	R (Bohr)	X (cm-1)	V1 (cm-1)	V2 (cm-1)
1.5	0.971199		1.5			
1.6	0.773494		1.6			
1.7	0.620759	1.04432	1.7	136713	229201.7	230160.8
1.8	0.500106	0.879911	1.8	110232.3	193118.2	194077.9
1.9	0.403194	0.759758	1.9	88962.11	166747.6	167707.7
2	0.324521	0.645709	2	71694.86	141716.7	142677.4
2.1	0.260337	0.546381	2.1	57607.32	119916.7	120878.2
2.2	0.207943	0.460252	2.2	46107.3	101013.7	101976.1
2.3	0.165275	0.385949	2.3	36741.46	84705.97	85669.55
2.4	0.130665	0.322222	2.4	29144.11	70719.46	71684.44
2.5	0.102725	0.267891	2.5	23010.29	58795.17	59761.83
2.6	0.080281	0.221833	2.6	18082.34	48686.74	49655.44
2.7	0.062339	0.182994	2.7	14142.09	40162.48	41133.64
2.8	0.048062	0.150397	2.8	11005.78	33008.36	33982.47
2.9	0.036752	0.123159	2.9	8519.87	27030.19	28007.85
3	0.027828	0.100488	3	6557.064	22054.57	23036.52
3.1	0.020816	0.081689	3.1	5012.838	17928.69	18915.79
3.2	0.015327	0.066155	3.2	3802.016	14519.31	15512.6
3.3	0.011049	0.053361	3.3	2855.687	11711.4	12712.08
3.4	0.00773	0.042858	3.4	2118.426	9406.266	10415.78
3.5	0.005169	0.034263	3.5	1545.874	7519.894	8539.886
3.6	0.003206	0.027252	3.6	1102.668	5981.096	7013.433
3.7	0.001713	0.021551	3.7	760.6937	4729.858	5776.611
3.8	0.000591	0.01693	3.8	497.6672	3715.798	4779.197
3.9	-0.000242	0.013199	3.9	295.9834	2896.791	3979.14
4	-0.000848	0.010196	4	141.805	2237.748	3341.296
4.1	-0.001277	0.007789	4.1	24.35397	1709.536	2836.314
4.2	-0.001569	0.005869	4.2	-64.6902	1288.015	2439.655
4.3	-0.001757	0.004343	4.3	-131.6633	953.2551	2130.812
4.4	-0.001863	0.003138	4.4	-181.3439	688.8058	1892.648
4.5	-0.001909	0.002192	4.5	-217.3291	481.152	1710.916
4.6	-0.00191	0.001454	4.6	-242.3557	319.2061	1573.854
4.7	-0.001877	0.000884	4.7	-258.555	193.9102	1471.853
4.8	-0.001822	0.000446	4.8	-267.6479	97.87471	1397.14
4.9	-0.00175	0.000114	4.9	-271.0465	25.1057	1343.51
5	-0.001668	-0.000133	5	-269.9408	-29.24938	1306.055
5.1	-0.00158	-0.000315	5.1	-265.3687	-69.10378	1280.914
5.2	-0.001489	-0.000445	5.2	-258.1769	-97.60037	1265.086
5.3	-0.001399	-0.000534	5.3	-249.0905	-117.2587	1256.236
5.4	-0.00131	-0.000593	5.4	-238.7008	-130.0848	1252.567
5.5	-0.001224	-0.000627	5.5	-227.4902	-137.672	1252.692
5.6	-0.001141	-0.000644	5.6	-215.8445	-141.2846	1255.547
5.7	-0.001063	-0.000647	5.7	-204.0617	-141.9189	1260.319
5.8	-0.000989	-0.00064	5.8	-192.3703	-140.354	1266.392
5.9	-0.00092	-0.000625	5.9	-180.9417	-137.2068	1273.294
6	-0.000855	-0.000606	6	-169.8956	-132.9511	1280.675
6.1	-0.000795	-0.000583	6.1	-159.3134	-127.9559	1288.274
6.2	-0.000739	-0.000558	6.2	-149.2503	-122.502	1295.899
6.3	-0.000688	-0.000532	6.3	-139.7367	-116.8066	1303.407
6.4	-0.00064	-0.000506	6.4	-130.7847	-111.0256	1310.705
6.5	-0.000596	-0.00048	6.5	-122.3895	-105.2798	1317.726

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3	6.6	-0.000555	-0.000454	-121.8721	-99.65246	6.6	-114.5418	-99.65246	1324.427
4	6.7	-0.000518	-0.000429	-113.6396	-94.2029	6.7	-107.2191	-94.2029	1330.787
5	6.8	-0.000483	-0.000405	-106.0633	-88.97063	6.8	-100.4109	-88.97063	1336.787
6	6.9	-0.000451	-0.000383	-99.05987	-83.97977	6.9	-94.06835	-83.97977	1342.439
7	7	-0.000422	-0.000361	-92.60732	-79.24132	7	-88.17963	-79.24132	1347.741
8	7.1	-0.000395	-0.000341	-86.65297	-74.75964	7.1	-82.71043	-74.75964	1352.708
9	7.2	-0.00037	-0.000321	-81.15513	-70.53256	7.2	-77.63175	-70.53256	1357.354
10	7.3	-0.000347	-0.000303	-76.07649	-66.55349	7.3	-72.9162	-66.55349	1361.696
11	7.4	-0.000325	-0.000286	-71.38632	-62.81583	7.4	-68.54087	-62.81583	1365.749
12	7.5	-0.000305	-0.00027	-67.04511	-59.30643	7.5	-64.47483	-59.30643	1369.533
13	7.6	-0.000287	-0.000255	-63.03311	-56.01651	7.6	-60.70188	-56.01651	1373.062
14	7.7	-0.00027	-0.000241	-59.31082	-52.93509	7.7	-57.19188	-52.93509	1376.356
15	7.8	-0.000255	-0.000228	-55.86727	-50.0468	7.8	-53.93236	-50.0468	1379.428
16	7.9	-0.00024	-0.000216	-52.66733	-47.34068	7.9	-50.89618	-47.34068	1382.298
17	8	-0.000226	-0.000204	-49.69784	-44.80794	8	-48.07158	-44.80794	1384.976
18	8.1	-0.000214	-0.000193	-46.93684	-42.43761	8.1	-45.44024	-42.43761	1387.476
19	8.2	-0.000202	-0.000183	-44.3668	-40.21653	8.2	-42.98605	-40.21653	1389.813
20	8.3	-0.000191	-0.000174	-41.97233	-38.13811	8.3	-40.69653	-38.13811	1391.996
21	8.5	-0.000172	-0.000157	-37.65965	-34.36095	8.5	-36.56177	-34.36095	1395.951
22	8.6	-0.000163	-0.000149	-35.71291	-32.64905	8.6	-34.69308	-32.64905	1397.741
23	8.7	-0.000154	-0.000141	-33.89347	-31.0403	8.7	-32.94367	-31.0403	1399.42
24	8.9	-0.000139	-0.000128	-30.58868	-28.11199	8.9	-29.76407	-28.11199	1402.473
25	9	-0.000133	-0.000122	-29.09874	-26.77769	9	-28.3259	-26.77769	1403.859
26	9.1	-0.000126	-0.000116	-27.69588	-25.5221	9.1	-26.97202	-25.5221	1405.164
27	9.3	-0.000115	-0.000106	-25.13737	-23.22511	9.3	-24.50052	-23.22511	1407.548
28	9.4	-0.000109	-0.000101	-23.97063	-22.17405	9.4	-23.37227	-22.17405	1408.638
29	9.5	-0.000104	-9.65E-05	-22.87042	-21.18226	9.5	-22.30814	-21.18226	1409.665
30	9.7	-9.5E-05	-8.82E-05	-20.85945	-19.36094	9.7	-20.3603	-19.36094	1411.55
31	9.8	-9.08E-05	-8.44E-05	-19.93276	-18.52451	9.8	-19.46365	-18.52451	1412.416
32	9.9	-8.69E-05	-8.08E-05	-19.06834	-17.73361	9.9	-18.62371	-17.73361	1413.232
33	10.1	-7.95E-05	-7.42E-05	-17.45437	-16.27675	10.1	-17.06205	-16.27675	1414.741
34	10.2	-7.62E-05	-7.11E-05	-16.72981	-15.60581	10.2	-16.35534	-15.60581	1415.43
35	10.3	-7.3E-05	-6.82E-05	-16.02108	-14.97019	10.3	-15.67095	-14.97019	1416.09
36	10.6	-6.45E-05	-6.04E-05	-14.15249	-13.25399	10.6	-13.85312	-13.25399	1417.857
37	11	-5.49E-05	-5.17E-05	-12.05844	-11.34338	11	-11.82016	-11.34338	1419.828
38	13	-2.7E-05	-2.59E-05	-5.922238	-5.688253	13	-5.844251	-5.688253	1425.644
39	15	-1.48E-05	-1.44E-05	-3.243847	-3.154161	15	-3.213953	-3.154161	1428.226
40	17	-8.86E-06	-8.6E-06	-1.945034	-1.888348	17	-1.926139	-1.888348	1429.503
41	20	-4.57E-06	-4.44E-06	-1.003242	-0.975325	20	-0.993936	-0.975325	1430.425
42	25	-1.84E-06	-1.81E-06	-0.403401	-0.397678	25	-0.401494	-0.397678	1431.01
43	30	-8.65E-07	-8.79E-07	-0.189884	-0.192901	30	-0.190889	-0.192901	1431.218
44	40	-3.3E-07	-2.89E-07	-0.072404	-0.063373	40	-0.069393	-0.063373	1431.344
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R (Bohr)	SIGMA (H ₂ PI (Hartree	SIGMA (cn PI (cm-1)	R (Bohr)	X (cm-1)	V1 (cm-1)	V2 (cm-1)
1.5	1.53087		1.5			
1.6	1.206861		1.6			
1.7	0.95986		1.7			
1.8	0.768867	0.984674	1.8	170407.1	216111	219821.8
1.9	0.619182		1.9			
2	0.500441	0.824559	2	111536.6	180969.8	184638.2
2.1	0.405279	0.700283	2.1	90642.64	153694.3	157371.2
2.2	0.328413	0.594032	2.2	73762.18	130375	134062.1
2.3	0.265989	0.503048	2.3	60049.36	110406.2	114105.8
2.4	0.215135	0.425042	2.4	48873.44	93285.89	97000.12
2.5	0.173653	0.358196	2.5	39751.67	78614.97	82346.68
2.6	0.139818	0.301016	2.6	32305.17	66065.28	69817.63
2.7	0.112249	0.252227	2.7	26230.05	55357.41	59134.08
2.8	0.08982	0.210721	2.8	21278.95	46247.97	50053.18
2.9	0.071608	0.175521	2.9	17248.44	38522.48	42361.07
3	0.05685	0.145763	3	13970.59	31991.28	35868.71
3.1	0.044916	0.120683	3.1	11306.55	26486.86	30409.22
3.2	0.035288	0.09961	3.2	9141.777	21861.95	25835.88
3.3	0.027536	0.081957	3.3	7381.988	17987.54	22020.09
3.4	0.021312	0.067212	3.4	5949.985	14751.37	18849.77
3.5	0.016326	0.054931	3.5	4782.829	12056.02	16227.32
3.6	0.012344	0.044732	3.6	3829.627	9817.506	14068.14
3.7	0.009175	0.036285	3.7	3049.47	7963.655	12298.97
3.8	0.006664	0.02931	3.8	2409.774	6432.731	10856.49
3.9	0.004683	0.023566	3.9	1884.678	5172.152	9686.199
4	0.003129	0.018851	4	1453.754	4137.261	8741.301
4.1	0.00192	0.014992	4.1	1100.755	3290.259	7981.913
4.2	0.000987	0.011843	4.2	812.6317	2599.227	7374.281
4.3	0.000276	0.009283	4.3	578.7552	2037.365	6890.156
4.4	-0.000259	0.007209	4.4	390.2849	1582.116	6506.018
4.5	-0.000653	0.005534	4.5	239.7856	1214.681	6202.548
4.6	-0.000936	0.004189	4.6	120.92	919.3112	5963.897
4.7	-0.001132	0.003112	4.7	28.27831	682.964	5777.221
4.8	-0.00126	0.002254	4.8	-42.78013	494.7704	5632.078
4.9	-0.001335	0.001576	4.9	-96.19083	345.7833	5520.076
5	-0.001369	0.001042	5	-135.3051	228.5894	5434.427
5.1	-0.001373	0.000625	5.1	-162.9259	137.1255	5369.7
5.2	-0.001355	0.000302	5.2	-181.4041	66.38669	5321.51
5.3	-0.00132	5.6E-05	5.3	-192.681	12.29758	5286.358
5.4	-0.001273	-0.00013	5.4	-198.3567	-28.47903	5261.429
5.5	-0.001219	-0.000267	5.5	-199.7397	-58.66518	5244.471
5.6	-0.001161	-0.000367	5.6	-197.8876	-80.46818	5233.686
5.7	-0.0011	-0.000436	5.7	-193.6526	-95.68004	5227.638
5.8	-0.001038	-0.000482	5.8	-187.7143	-105.7451	5225.188
5.9	-0.000977	-0.00051	5.9	-180.6092	-111.8272	5225.43
6	-0.000917	-0.000523	6	-172.7571	-114.8555	5227.654
6.1	-0.000859	-0.000527	6.1	-164.482	-115.5715	5231.303
6.2	-0.000804	-0.000522	6.2	-156.0387	-114.5636	5235.936
6.3	-0.000752	-0.000512	6.3	-147.5925	-112.2902	5241.231
6.4	-0.000703	-0.000497	6.4	-139.2924	-109.1184	5246.921
6.5	-0.000657	-0.00048	6.5	-131.2324	-105.3279	5252.813

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6.6	-0.000613	-0.000461	-134.5796	-101.1383	6.6	-123.4787	-101.1383	5258.761
6.7	-0.000573	-0.000441	-125.7019	-96.71571	6.7	-116.0745	-96.71571	5264.657
6.8	-0.000535	-0.00042	-117.4365	-92.18812	6.8	-109.0467	-92.18812	5270.422
6.9	-0.0005	-0.000399	-109.7505	-87.65122	6.9	-102.4042	-87.65122	5276.003
7	-0.000468	-0.000379	-102.6154	-83.1743	7	-96.15063	-83.1743	5281.361
7.1	-0.000437	-0.000359	-95.99381	-78.80966	7.1	-90.27797	-78.80966	5286.474
7.2	-0.000409	-0.00034	-89.8595	-74.59284	7.2	-84.78025	-74.59284	5291.328
7.3	-0.000384	-0.000321	-84.17291	-70.54542	7.3	-79.63809	-70.54542	5295.92
7.4	-0.00036	-0.000304	-78.90113	-66.68517	7.4	-74.83531	-66.68517	5300.249
7.5	-0.000337	-0.000287	-74.02001	-63.01775	7.5	-70.3576	-63.01775	5304.32
7.6	-0.000317	-0.000271	-69.49225	-59.54786	7.6	-66.18154	-59.54786	5308.141
7.7	-0.000298	-0.000256	-65.2959	-56.27549	7.7	-62.29246	-56.27549	5311.721
7.8	-0.00028	-0.000242	-61.40461	-53.19187	7.8	-58.66982	-53.19187	5315.073
7.9	-0.000263	-0.000229	-57.79206	-50.29481	7.9	-55.2953	-50.29481	5318.208
8	-0.000248	-0.000217	-54.43849	-47.57552	8	-52.15278	-47.57552	5321.139
8.1	-0.000234	-0.000205	-51.32195	-45.02522	8.1	-49.22468	-45.02522	5323.878
8.2	-0.000221	-0.000194	-48.42488	-42.63514	8.2	-46.49636	-42.63514	5326.436
8.3	-0.000208	-0.000184	-45.72973	-40.39431	8.3	-43.95244	-40.39431	5328.828
8.5	-0.000186	-0.000166	-40.87934	-36.33183	8.5	-39.36436	-36.33183	5333.153
8.6	-0.000176	-0.000157	-38.69777	-34.48824	8.6	-37.29533	-34.48824	5335.109
8.7	-0.000167	-0.000149	-36.66324	-32.75878	8.7	-35.36238	-32.75878	5336.94
8.8	-0.000158	-0.000142	-34.76039	-31.13687	8.8	-33.55309	-31.13687	5338.656
8.9	-0.00015	-0.000135	-32.98202	-29.61468	8.9	-31.86004	-29.61468	5340.263
9	-0.000143	-0.000128	-31.31858	-28.18304	9	-30.27381	-28.18304	5341.772
9.1	-0.000136	-0.000122	-29.75857	-26.83698	9.1	-28.78506	-26.83698	5343.19
9.3	-0.000123	-0.000111	-26.92826	-24.37648	9.3	-26.07793	-24.37648	5345.773
9.4	-0.000117	-0.000106	-25.64143	-23.25118	9.4	-24.84492	-23.25118	5346.952
9.5	-0.000111	-0.000101	-24.43234	-22.1909	9.5	-23.6854	-22.1909	5348.062
9.7	-0.000101	-9.22E-05	-22.22482	-20.24481	9.7	-21.56498	-20.24481	5350.095
9.8	-9.67E-05	-8.82E-05	-21.21598	-19.35168	9.8	-20.59469	-19.35168	5351.027
9.9	-9.23E-05	-8.43E-05	-20.26603	-18.50816	9.9	-19.6802	-18.50816	5351.906
10.1	-8.44E-05	-7.73E-05	-18.52235	-16.95562	10.1	-18.00021	-16.95562	5353.522
10.2	-8.07E-05	-7.4E-05	-17.72206	-16.24097	10.2	-17.22845	-16.24097	5354.265
10.3	-7.73E-05	-7.09E-05	-16.96646	-15.56471	10.3	-16.49929	-15.56471	5354.968
10.6	-6.8E-05	-6.26E-05	-14.92992	-13.7406	10.6	-14.53354	-13.7406	5356.863
11	-5.77E-05	-5.34E-05	-12.6743	-11.71487	11	-12.35453	-11.71487	5358.965
13	-2.8E-05	-2.64E-05	-6.135025	-5.799921	13	-6.023328	-5.799921	5365.088
15	-1.52E-05	-1.46E-05	-3.340628	-3.20365	15	-3.294969	-3.20365	5367.751
17	-9.02E-06	-8.73E-06	-1.979413	-1.914992	17	-1.95794	-1.914992	5369.064
20	-4.61E-06	-4.51E-06	-1.012619	-0.988985	20	-1.004741	-0.988985	5370.003
25	-1.87E-06	-1.83E-06	-0.409457	-0.402579	25	-0.407164	-0.402579	5370.595
30	-9.03E-07	-8.92E-07	-0.198253	-0.195697	30	-0.197401	-0.195697	5370.803
40	-3.01E-07	-2.99E-07	-0.066036	-0.065542	40	-0.065871	-0.065542	5370.934

R (Bohr)	SIGMA (H ₂ PI (Hartree	SIGMA (cn PI (cm-1)	R (Bohr)	X (cm-1)	V1 (cm-1)	V2 (cm-1)
2	1.027011	225402.9	0			
2.1	0.835373	1.0853	183343.2	238195.7	2.1	190534.1 238195.7 261899.9
2.2	0.681153	0.889625	149495.8	195250	2.2	156235.9 195250 219405
2.3	0.556505	0.781772	122138.7	171579	2.3	129075.5 171579 195537.3
2.4	0.455442	0.664318	99957.9	145801.1	2.4	106703 145801.1 169951.1
2.5	0.373281	0.565291	81925.79	124067.1	2.5	88450.78 124067.1 148437.2
2.6	0.306301	0.48144	67225.22	105663.9	2.6	73503.07 105663.9 130281.2
2.7	0.251533	0.410143	55205.1	90015.97	2.7	61209.93 90015.97 114906.2
2.8	0.206624	0.349311	45348.76	76664.83	2.8	51056.45 76664.83 101852.2
2.9	0.169712	0.297283	37247.56	65245.98	2.9	42636.6 65245.98 90752.04
3	0.139321	0.252725	30577.32	55466.71	3	35629.74 55466.71 81309.38
3.1	0.114268	0.214548	25078.92	47087.81	3.1	29781.15 47087.81 73280.69
3.2	0.093603	0.181845	20543.49	39910.33	3.2	24887 39910.33 66461.93
3.3	0.076552	0.153851	16801.31	33766.37	3.3	20783.05 33766.37 60679.73
3.4	0.062485	0.129914	13713.78	28512.82	3.4	17336.32 28512.82 55785.39
3.5	0.050881	0.109474	11167.15	24026.83	3.5	14438.45 24026.83 51650.63
3.6		0.092049	0	20202.36		
3.7	0.033437	0.077219	7338.626	16947.63	3.7	9950.14 16947.63 45231.21
3.8	0.026954	0.064622	5915.675	14182.96	3.8	8225.98 14182.96 42767.76
3.9	0.021625	0.053944	4746.156	11839.26	3.9	6777.697 11839.26 40702.82
4	0.017252	0.044909	3786.352	9856.492	4	5562.844 9856.492 38975.1
4.1	0.013669	0.037283	3000.018	8182.594	4.1	4545.597 8182.594 37532.12
4.2	0.01074	0.030858	2357.131	6772.491	4.2	3695.617 6772.491 36329.11
4.3	0.008351	0.025457	1832.806	5587.236	4.3	2987.136 5587.236 35328.01
4.4	0.006408	0.020928	1406.391	4593.227	4.4	2398.204 4593.227 34496.51
4.5	0.004833	0.017139	1060.813	3761.563	4.5	1910.165 3761.563 33807.31
4.6	0.003562	0.013976	781.8476	3067.408	4.6	1507.074 3067.408 33237.28
4.7	0.002541	0.011343	557.7772	2489.499	4.7	1175.414 2489.499 32766.96
4.8	0.001726	0.009157	378.7825	2009.635	4.8	903.6114 2009.635 32379.91
4.9	0.001079	0.007346	236.8043	1612.3	4.9	681.899 1612.3 32062.31
5	0.00057	0.005851	125.094	1284.24	5	501.934 1284.24 31802.5
5.1	0.000174	0.004621	38.0986	1014.269	5.1	356.7076 1014.269 31590.76
5.2	-0.000131	0.003612	-28.79946	792.8104	5.2	240.2585 792.8104 31418.85
5.3	-0.000362	0.002788	-79.45201	611.825	5.3	147.5623 611.825 31279.91
5.4	-0.000533	0.002116	-116.9493	464.4895	5.4	74.44734 464.4895 31168.19
5.5	-0.000656	0.001572	-143.9183	345.0887	5.5	17.37317 345.0887 31078.9
5.6	-0.00074	0.001134	-162.4968	248.7921	5.6	-26.61183 248.7921 31008.01
5.7	-0.000795	0.000782	-174.434	171.5685	5.7	-59.95773 171.5685 30952.19
5.8	-0.000825	0.000501	-181.1631	110.038	5.8	-84.70411 110.038 30908.68
5.9	-0.000838	0.00028	-183.8495	61.37461	5.9	-102.5395 61.37461 30875.16
6	-0.000836	0.000106	-183.4391	23.24017	6	-114.8526 23.24017 30849.75
6.1	-0.000823	-2.88E-05	-180.6913	-6.31656	6.1	-122.7847 -6.31656 30830.88
6.2	-0.000803	-0.000132	-176.225	-28.90481	6.2	-127.2741 -28.90481 30817.24
6.3	-0.000777	-0.000209	-170.5274	-45.8733	6.3	-129.0876 -45.8733 30807.79
6.4	-0.000747	-0.000266	-163.9871	-58.30782	6.4	-128.8409 -58.30782 30801.65
6.5	-0.000715	-0.000306	-156.9112	-67.13289	6.5	-127.043 -67.13289 30798.1
6.6	-0.000681	-0.000333	-149.5346	-73.07188	6.6	-124.0891 -73.07188 30796.58
6.7	-0.000647	-0.00035	-142.0418	-76.75128	6.7	-120.3089 -76.75128 30796.62
6.8	-0.000613	-0.000358	-134.5731	-78.64873	6.8	-115.9541 -78.64873 30797.83
6.9	-0.00058	-0.000361	-127.2316	-79.18001	6.9	-111.231 -79.18001 30799.92
7	-0.000547	-0.000358	-120.0943	-78.65751	7	-106.2944 -78.65751 30802.64

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4	7.1	-0.000516	-0.000352	-113.216	-77.35134	7.1	-101.2704	-77.35134	30805.8
5	7.2	-0.000486	-0.000344	-106.6296	-75.46635	7.2	-96.2488	-75.46635	30809.25
6	7.3	-0.000457	-0.000333	-100.3592	-73.1702	7.3	-91.30149	-73.1702	30812.87
7	7.4	-0.00043	-0.000322	-94.4136	-70.59401	7.4	-86.47782	-70.59401	30816.57
8	7.5	-0.000405	-0.000309	-88.79944	-67.83833	7.5	-81.81556	-67.83833	30820.28
9	7.6	-0.000381	-0.000296	-83.5101	-64.98644	7.6	-77.33801	-64.98644	30823.94
10	7.7	-0.000358	-0.000283	-78.539	-62.09781	7.7	-73.06054	-62.09781	30827.52
11	7.8	-0.000337	-0.00027	-73.87736	-59.22084	7.8	-68.99339	-59.22084	30831
12	7.9	-0.000317	-0.000257	-69.50981	-56.38781	7.9	-65.13705	-56.38781	30834.34
13	8	-0.000298	-0.000244	-65.42539	-53.62643	8	-61.4934	-53.62643	30837.54
14	8.1	-0.000281	-0.000232	-61.60653	-50.95542	8.1	-58.05698	-50.95542	30840.6
15	8.2	-0.000264	-0.00022	-58.04007	-48.38757	8.2	-54.82324	-48.38757	30843.5
16	8.3	-0.000249	-0.000209	-54.70844	-45.92726	8.3	-51.78194	-45.92726	30846.25
17	8.5	-0.000222	-0.000188	-48.69703	-41.34902	8.5	-46.24808	-41.34902	30851.3
18	8.6	-0.00021	-0.000179	-45.98652	-39.23548	8.6	-43.7365	-39.23548	30853.61
19	8.7	-0.000198	-0.00017	-43.45598	-37.23168	8.7	-41.38149	-37.23168	30855.79
20	8.9	-0.000177	-0.000153	-38.88663	-33.55652	8.9	-37.11013	-33.55652	30859.77
21	9	-0.000168	-0.000145	-36.82221	-31.87047	9	-35.17181	-31.87047	30861.58
22	9.1		-0.000138	0	-30.28544	9.1			
23	9.3	-0.000143	-0.000125	-31.39849	-27.38375	9.3	-30.06036	-27.38375	30866.38
24	9.4	-0.000136	-0.000119	-29.81403	-26.05726	9.4	-28.56187	-26.05726	30867.79
25	9.5	-0.000129	-0.000113	-28.33109	-24.81229	9.5	-27.15825	-24.81229	30869.11
26	9.8	-0.000111	-0.000103	-24.40349	-22.53321	9.8	-23.78009	-22.53321	30871.94
27	9.9	-0.000106	-9.35E-05	-23.25056	-20.51112	9.9	-22.33746	-20.51112	30873.68
28	10.1	-9.63E-05	-8.53E-05	-21.14294	-18.7137	10.1	-20.33323	-18.7137	30875.58
29	10.2	-9.19E-05	-8.15E-05	-20.18049	-17.8889	10.2	-19.41667	-17.8889	30876.45
30	10.3	-8.78E-05	-7.8E-05	-19.27317	-17.1128	10.3	-18.55308	-17.1128	30877.27
31	10.6	-7.68E-05	-6.85E-05	-16.84621	-15.02519	10.6	-16.23923	-15.02519	30879.47
32	11	-6.46E-05	-5.8E-05	-14.18441	-12.72261	11	-13.69716	-12.72261	30881.89
33	13	-3.03E-05	-2.79E-05	-6.65946	-6.113761	13	-6.477563	-6.113761	30888.8
34	15	-1.62E-05	-1.52E-05	-3.556331	-3.337808	15	-3.48349	-3.337808	30891.69
35	17	-9.48E-06	-9.02E-06	-2.080157	-1.980562	17	-2.046959	-1.980562	30893.09
36	20	-4.79E-06	-4.62E-06	-1.051391	-1.014397	20	-1.039059	-1.014397	30894.07
37	25	-1.92E-06	-1.87E-06	-0.421503	-0.411398	25	-0.418135	-0.411398	30894.69
38	30	-9.3E-07	-9.13E-07	-0.204094	-0.200303	30	-0.20283	-0.200303	30894.9
39	40	-3.15E-07	-3.12E-07	-0.069182	-0.068469	40	-0.068944	-0.068469	30895.03
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R (Bohr)	SIGMA (H ₂ PI (Hartree	SIGMA (cn PI (cm-1)	R (Bohr)	X (cm-1)	V1 (cm-1)	V2 (cm-1)
1.9	0.99675	218761.2	0			
2	0.804579	0.998666	176584.8	219181.8	2	179568.1 219181.8 226735.5
2.1	0.652882	0.91379	143291	200553.8	2.1	146400 200553.8 207981.8
2.2	0.532183	0.755944	116800.7	165910.6	2.2	119848.3 165910.6 173400.1
2.3	0.435403	0.663809	95560.02	145689.3	2.3	98616.27 145689.3 153170
2.4	0.357231	0.567218	78403.05	124489.9	2.4	81422.83 124489.9 132007.1
2.5	0.293662	0.484993	64451.4	106443.7	2.5	67427.84 106443.7 114004.2
2.6	0.241669	0.414581	53040.32	90989.98	2.6	55965.88 90989.98 98601.42
2.7	0.198946	0.354039	43663.6	77702.48	2.7	46530 77702.48 85373.09
2.8	0.16372	0.301868	35932.31	66252.33	2.8	38730.45 66252.33 73991.2
2.9	0.13461	0.256884	29543.51	56379.42	2.9	32263.53 56379.42 64196.41
3	0.110526	0.218119	24257.64	47871.52	3	26889.03 47871.52 55777.15
3.1	0.09059	0.184761	19882.25	40550.24	3.1	22413.98 40550.24 48555.53
3.2	0.07409	0.15611	16260.86	34262.22	3.2	18681.72 34262.22 42378.37
3.3	0.060439	0.131558	13264.82	28873.74	3.3	15563.81 28873.74 37111.76
3.4	0.049155	0.11057	10788.17	24267.37	3.4	12954.98 24267.37 32637.57
3.5	0.039836	0.092675	8742.893	20339.72	3.5	10768.53 20339.72 28851.09
3.6	0.03215	0.077456	7056.107	16999.6	3.6	8933.474 16999.6 25659.25
3.7	0.025821	0.064548	5667.063	14166.73	3.7	7391.488 14166.73 22979.31
3.8	0.020619	0.05363	4525.301	11770.45	3.8	6094.912 11770.45 20737.85
3.9	0.016351	0.044419	3588.689	9748.929	3.9	5004.587 9748.929 18870.04
4	0.012859	0.03667	2822.237	8048.078	4	4088.381 8048.078 17318.94
4.1	0.010009	0.030167	2196.744	6620.83	4.1	3319.641 6620.83 16034.94
4.2	0.007691	0.024724	1687.935	5426.372	4.2	2676.151 5426.372 14975.17
4.3	0.005812	0.020182	1275.567	4429.426	4.3	2139.149 4429.426 14102.85
4.4	0.004296	0.016401	942.8367	3599.612	4.4	1692.721 3599.612 13386.74
4.5	0.003079	0.013263	675.7141	2910.855	4.5	1323.201 2910.855 12800.38
4.6	0.002108	0.010666	462.5603	2340.833	4.6	1018.858 2340.833 12321.55
4.7	0.001338	0.008523	293.6746	1870.523	4.7	769.5673 1870.523 11931.64
4.8	0.000734	0.00676	161.0044	1483.695	4.8	566.5999 1483.695 11615.11
4.9	0.000264	0.005316	57.86449	1166.639	4.9	402.4647 1166.639 11359.05
5	-9.7E-05	0.004136	-21.29089	907.6746	5	270.7127 907.6746 11152.68
5.1	-0.000369	0.003176	-81.04759	697.0075	5.1	165.8581 697.0075 10987.11
5.2	-0.00057	0.002398	-125.1927	526.3287	5.2	83.21686 526.3287 10854.93
5.3	-0.000715	0.001771	-156.8585	388.7005	5.3	18.82752 388.7005 10750.02
5.4	-0.000814	0.001268	-178.5975	278.2851	5.4	-30.64112 278.2851 10667.34
5.5	-0.000877	0.000867	-192.5319	190.2296	5.5	-67.99667 190.2296 10602.7
5.6	-0.000913	0.000549	-200.3386	120.4718	5.6	-95.55011 120.4718 10552.69
5.7	-0.000927	0.000299	-203.4201	65.65024	5.7	-115.2437 65.65024 10514.48
5.8	-0.000925	0.000105	-202.9065	22.9746	5.8	-128.6811 22.9746 10485.76
5.9	-0.00091	-4.49E-05	-199.6978	-9.864025	5.9	-137.1753 -9.864025 10464.62
6	-0.000886	-0.000158	-194.5226	-34.75161	6	-141.8012 -34.75161 10449.54
6.1	-0.000856	-0.000243	-187.9537	-53.26328	6.1	-143.4378 -53.26328 10439.23
6.2	-0.000822	-0.000304	-180.4411	-66.66761	6.2	-142.7886 -66.66761 10432.69
6.3	-0.000785	-0.000346	-172.3425	-76.02079	6.3	-140.4303 -76.02079 10429.08
6.4	-0.000747	-0.000374	-163.9322	-82.1713	6.4	-136.8192 -82.1713 10427.73
6.5	-0.000708	-0.000391	-155.421	-85.81822	6.5	-132.322 -85.81822 10428.09
6.6	-0.00067	-0.000399	-146.9646	-87.52209	6.6	-127.2248 -87.52209 10429.75
6.7	-0.000632	-0.0004	-138.6794	-87.73975	6.7	-121.7542 -87.73975 10432.34
6.8	-0.000595	-0.000396	-130.6511	-86.83514	6.8	-116.0862 -86.83514 10435.61
6.9	-0.00056	-0.000388	-122.9387	-85.09981	6.9	-110.3559 -85.09981 10439.33

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7	-0.000527	-0.000377	-115.5753	-82.76608	7	-104.6616	-82.76608	10443.33
7.1	-0.000495	-0.000365	-108.5873	-80.01674	7.1	-99.08096	-80.01674	10447.49
7.2	-0.000465	-0.000351	-101.9811	-76.99389	7.2	-93.66518	-76.99389	10451.7
7.3	-0.000436	-0.000336	-95.75678	-73.80932	7.3	-88.45111	-73.80932	10455.9
7.4	-0.00041	-0.000321	-89.91217	-70.54793	7.4	-83.46533	-70.54793	10460.02
7.5	-0.000385	-0.000307	-84.43408	-67.27556	7.5	-78.72078	-67.27556	10464.02
7.6	-0.000361	-0.000292	-79.30935	-64.03611	7.6	-74.22319	-64.03611	10467.89
7.7	-0.00034	-0.000277	-74.51822	-60.86632	7.7	-69.97152	-60.86632	10471.6
7.8	-0.000319	-0.000263	-70.04972	-57.79206	7.8	-65.967	-57.79206	10475.14
7.9	-0.0003	-0.00025	-65.8797	-54.83135	7.9	-62.19949	-54.83135	10478.5
8	-0.000282	-0.000237	-61.9928	-51.99354	8	-58.66182	-51.99354	10481.69
8.1	-0.000266	-0.000225	-58.36928	-49.28522	8.1	-55.343	-49.28522	10484.7
8.2	-0.000251	-0.000213	-54.99376	-46.70859	8.2	-52.23348	-46.70859	10487.54
8.3	-0.000236	-0.000202	-51.84869	-44.26803	8.3	-49.32301	-44.26803	10490.22
8.5	-0.00021	-0.000181	-46.18185	-39.77758	8.5	-44.04796	-39.77758	10495.1
8.6	-0.000199	-0.000172	-43.63375	-37.7211	8.6	-41.66361	-37.7211	10497.32
8.7	-0.000188	-0.000163	-41.25465	-35.78534	8.7	-39.43217	-35.78534	10499.4
8.9	-0.000168		-36.9625	0	8.9	-24.67045	0	10524.72
9	-0.00016	-0.00014	-35.02376	-30.63646	9	-33.56173	-30.63646	10504.91
9.1	-0.000151	-0.000133	-33.21324	-29.11989	9.1	-31.84914	-29.11989	10506.53
9.3	-0.000136	-0.00012	-29.93007	-26.3589	9.3	-28.73995	-26.3589	10509.46
9.4	-0.00013	-0.000114	-28.44178	-25.09994	9.4	-27.32807	-25.09994	10510.8
9.7	-0.000112		-24.50737	0	9.7	-16.3509	0	10528.85
9.8	-0.000106	-9.46E-05	-23.35099	-20.7647	9.8	-22.48903	-20.7647	10515.38
9.9	-0.000101	-9.04E-05	-22.26387	-19.83246	9.9	-21.45353	-19.83246	10516.37
10.1	-9.24E-05	-8.26E-05	-20.27583	-18.12317	10.1	-19.55837	-18.12317	10518.17
10.2	-8.82E-05	-7.9E-05	-19.36693	-17.33908	10.2	-18.69107	-17.33908	10519
10.3	-8.43E-05	-7.56E-05	-18.5094	-16.59691	10.3	-17.87198	-16.59691	10519.78
10.6	-7.39E-05	-6.65E-05	-16.2118	-14.60033	10.6	-15.6747	-14.60033	10521.87
11	-6.23E-05	-5.64E-05	-13.68413	-12.38556	11	-13.25131	-12.38556	10524.19
13	-2.95E-05	-2.73E-05	-6.484545	-5.982144	13	-6.317083	-5.982144	10530.86
15	-1.59E-05	-1.49E-05	-3.48376	-3.279535	15	-3.415686	-3.279535	10533.66
17	-9.32E-06	-8.89E-06	-2.045469	-1.951725	17	-2.014221	-1.951725	10535.03
20	-4.73E-06	-4.58E-06	-1.037196	-1.004546	20	-1.026313	-1.004546	10535.99
25	-1.9E-06	-1.86E-06	-0.416213	-0.407331	25	-0.413252	-0.407331	10536.6
30	-9.15E-07	-8.99E-07	-0.200726	-0.197343	30	-0.199598	-0.197343	10536.81
40	-3.04E-07	-3.01E-07	-0.066779	-0.066163	40	-0.066574	-0.066163	10536.94