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Self-consistent-field potential energies for the ground negative-ion and neutral states of HeH, ArH, and ArCl

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Self-consistent-field (SCF) calculations have been used to determine the ground negative-ion and ground neutral potential-energy curves for HeH, ArH, and ArCl. In the systems studied, the $X\,^1\Sigma$ potential of the negative-ion state is more repulsive at intermediate internuclear separations than the $X\,^2\Sigma$ potential of the neutral partners, leading to a curve crossing of the negative-ion state into the continuum. However, at small internuclear separations the negative-ion potential becomes less repulsive than the neutral potential, leading to a second curve crossing out of the continuum. The calculated potential-energy curves are used to provide estimates of the energy thresholds and cross sections for electron detachment in the collisions $H^- + He$, $H^- + Ar$, and $Cl^- + Ar$. The angular thresholds for electron detachment in differential-scattering measurements are also given and compared to experimental data.

I. INTRODUCTION

In recent years, considerable interest has centered on electron-detachment mechanisms for collisions of negative ions and atoms. A complex-potential model similar to that used in Penning-ionization calculations has been successfully employed by Lam *et al.*[1] to describe electron detachment in a low-energy ($E \leq 100$ eV) H^- +He collisions. However, the complex-potential method is not universally applicable and is known to fail[2] for collisions of H^- and Ar. Another electron-detachment model has been proposed by Devdariani,[3] which has been shown by Esaulov *et al.*[4] to work well for medium-energy ($100 \leq E \leq 1000$ eV) H^-+ He and H^-+ Ar collisions.

However, considerable uncertainties exist in the application of any electron-detachment model because of the lack of information available on the potential-energy curves followed during the collision. It is extremely difficult to test an electron-detachment model against the experimental scattering data when the data must first be inverted to obtain both the negative-ion and the neutral-state potentials, and the coupling width of the electron to the continuum. The uniqueness of the potentials so obtained is questionable.

Hence, we have directed our attention to the *ab initio* calculation of the potential curves needed to analyze the scattering data for three systems where measurements exist: HeH^-, ArH^-, and $ArCl^-$. The self-consistent-field (SCF) method has been used to obtain the adiabatic potentials of the ground negative-ion and ground neutral-molecular states. These potentials are then used to crudely estimate the energy and angular thresholds for electron detachment and the magnitude of the cross sections. The values obtained are compared to the experimental data. Comparisons are also made between our calculated potentials and those obtained from the inversion of experimental scattering data.

II. CALCULATIONAL METHOD

Approximations to the Born-Oppenheimer electronic wave functions and energies were calculated using the SCF method. The calculations were performed using ALCHEMY, a system of programs for the calculation of molecular wave functions developed by Bagus, Liu, McLean, and Yoshimine.

The basis sets employed in the calculations are given in Table I. The He basis set was obtained from the work of Weiss[5] and augmented with the optimized diffuse functions on the 2*s*, 2*p*, 3*p*, and 3*d* orbitals from the paper by McLaughlin and Schaefer.[6] With this basis set the SCF energy of He was calculated to be $-2.861\,678$ hartrees, which is within 1×10^{-6} hartrees of the restricted Hartree-Fock (RHF) value.[7] The calculated SCF polarizability of He was found to be $1.322a_0^3$, which may be compared to the accepted value[8] of $1.383a_0^3$ and the RHF value[9] of $1.32a_0^3$.

The Ar basis set for the filled electron shells was taken from the $(6s/5p)$ basis of Clementi and Roetti.[7] This basis was augmented with the optimized 4*s*, 4*p*, and 3*d* functions given by Saxon and Liu.[10] As obtained by these latter authors, this basis yields a SCF energy for the Ar atom of $-526.816\,620$ hartrees and a SCF dipole polarizability of $10.17a_0^3$. The SCF polarizability may

TABLE I. Slater-orbital exponents for the H, H^- + He, Ar and Cl, Cl^- + Ar calculations.

He	1*s*	3.30	Ar	1*s*	19.0285
		1.52			14.0031
	2*s*	3.30		2*s*	7.7115
		1.52			6.1850
		1.00		3*s*	3.21815
	2*p*	4.30			2.0295
		2.40		4*s*	0.8605
		1.50		2*p*	14.502
	3*p*	4.30			8.1291
		1.50		3*p*	6.3957
	3*d*	0.90			2.9048
					1.6099
				4*p*	0.6315
				3*d*	2.2000
					1.1300
H	1*s*	2.00	H^-	1*s*	1.60
		1.00			1.10
		0.50			0.45
		0.33333333		2*s*	1.10
	2*s*	0.50			0.45
		0.33333333		2*p*	1.20
	3*s*	0.33333333			0.85
	2*p*	1.0		3*p*	1.20
		0.5		3*d*	1.70
		0.33333333		4*d*	1.70
	3*p*	0.33333333			
	3*d*	0.33333333			
Cl	1*s*	17.36120	Cl^-	1*s*	17.24050
		28.27580			28.92250
	2*s*	6.84172		2*s*	6.81054
		15.47230			15.17810
	3*s*	2.97140		3*s*	2.87181
		1.85605			1.67233
		5.99804			5.86922
	2*p*	7.67977		2*p*	7.62972
		14.06740			13.76380
	3*p*	2.61823		3*p*	2.92646
		1.45933			1.01565
		5.93136			5.93996
					1.83188

be compared to the accepted value[8] of $11.08a_0^3$.

The H basis set employed in the calculations is the exact basis through the $n=3$ level. The largest exponents on the 1*s* and 2*p* orbitals were added to help describe the strong distortion of the atomic orbitals in the molecular field and yield an improved dipole polarizability. The calculated SCF polarizability of H was found to be $4.454a_0^3$, which may be compared to the true value of $4.500a_0^3$. The SCF energies for H were found to be exact through the $n=3$ excited level.

The H^- basis set is from the work of Liu et al.[11] with the deletion of the 4*f* function which was deemed unnecessary for these calculations. This basis set was chiefly taken from the complete configuration-interaction (CI) wave function of H^- obtained by Weiss.[5] The SCF energy obtained for the H^- ion was -0.487921 hartrees, which is within 1×10^{-6} hartrees of the restricted Hartree-Fock value.[5]

Both the Cl and Cl^- basis sets were taken directly from the tabulations of Clementi and Roetti.[7] The SCF energy of the Cl atom was -459.48181 hartrees, while that of the Cl^- ion was -459.57670 hartrees.

The ionic and neutral-molecular states considered here all arise from interactions between two closed-shell systems, or a closed-shell system and an open-shell system. Therefore, the SCF method is expected to yield realistic interaction potentials for these states. However, the SCF method does not yield accurately the relative positions of the ionic and the neutral potential curves. This is because the electron affinities of H and Cl are underestimated by ~1 eV in the SCF approximation. In particular, H^- is unbound in this approximation, and the resulting potential curves are incorrectly ordered for a large range of internuclear separations. Consequently, in order to obtain realistic estimates of the crossings between the ionic and neutral potentials, it has been necessary to shift the calculated curves relative to one another to yield the correct asymptotic separations. The justification for this procedure lies in the accuracy of the individual interaction potentials. Recent study on LiH^- (Ref. 11) and $LiCl^-$ (Ref. 12) have shown that SCF potential curves of these ions are in near quantitative agreement with accurate potential curves obtained by extended configuration-interaction calculations. The ionic curves reported here are expected to be of comparable accuracy.

III. RESULTS AND DISCUSSION

A. HeH

The numerical results for the HeH calculations are presented in Table II and depicted graphically in Fig. 1. In Fig. 1, the potential curves have been shifted by an amount equal to the electron affinity of H (0.754 eV), so that the curves dissociate to their true limits relative to one another.

Our SCF calculations for H + He do not include dispersion forces ($-C_{ab}/R^6$), hence we do not obtain a Van der Waals well depth which can be considered accurate. The repulsive wall of the potential, however, should be reasonably represented by the SCF calculations. As a test, we can compare our SCF potential for the $X^2\Sigma$ state of H + He to the CI calculations of Miller and Schaefer.[13] Representative points where the two calculations overlap are $R=2a_0$, $V(\mathrm{SCF})=70.228$

TABLE II. Self-consistent-field interaction potential energies for H, $H^- +$ He, $E(R)-E(\infty)$ (units of 10^{-3} hartrees).

$R(a_0)$	$X\,^2\Sigma$ (H + He)	$X\,^1\Sigma$ (H^- + He)
0.75	543.575	538.931
1.0	306.999	318.794
1.25	203.308	240.040
1.4	163.681	210.922
1.5	142.236	193.919
1.75	100.277	155.485
2.0	70.228	121.922
2.25	48.683	93.777
2.5	33.390	71.202
3.0	15.244	40.313
3.5	6.721	22.744
4.0	2.877	12.932
6.0	0.078	1.493
8.0	0.001	0.163
10.0	−0.001	−0.006
15.0	0	−0.011
20.0	0	−0.032
25.0	0	−0.011
Asymptotic total energies (hartrees)		
	−3.361 678	−3.349 600

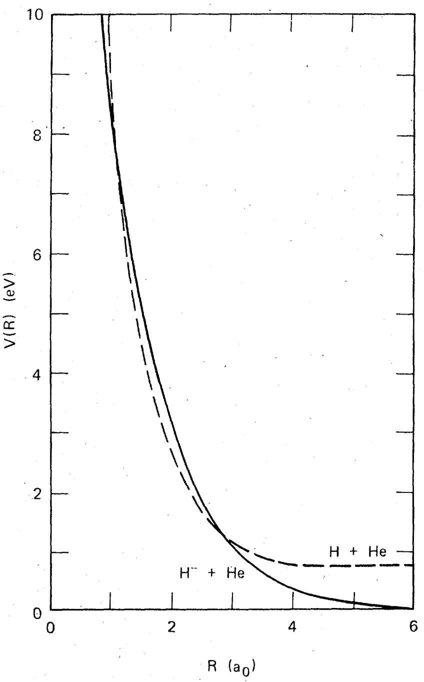

FIG. 1. Self-consistent-field potential-energy curves for the $X\,^1\Sigma$ state of HeH^- and the $X\,^2\Sigma$ state of HeH. The curves have been shifted relative to one another to yield the correct separation at large distances (0.754 eV).

mH (millihartrees) and $V(\mathrm{CI}) = 66.382$ mH; and $R = 4a_0$, $V(\mathrm{SCF}) = 2.877$ mH and $V(\mathrm{CI}) = 2.484$ mH. Hence, even at $2a_0$, the SCF values are only too high by 3.846 mH or 0.105 eV. For the $X\,^1\Sigma$ state of H^- +He, we could find no other calculations to compare with our values for the repulsive wall.

An interesting feature of the HeH potentials is that the $X\,^1\Sigma$ state of H^- +He crosses the $X\,^2\Sigma$ state of H+He twice. At intermediate internuclear separations the negative-ion potential is more repulsive than the neutral potential due to the fact that there is an extra electron between the two nuclei. However, as the internuclear separation further decreases, the negative-ion potential becomes less repulsive than the neutral potential. This is expected since we are calculating adiabatic potentials and the neutral state correlates at the united-atom limit to the ground state of Li, while the negative-ion state correlates to Li^- which is bound by 0.620 eV.[14]

In Fig. 2 we have plotted the difference in potential energy between the negative ion and neutral state as a function of internuclear separation R. From this graph, we can see that there is good penetration of the negative-ion state into the continuum. Hence, we would expect that the complex-potential model proposed by Lam *et al.*[1] for electron detachment would be appropriate for this

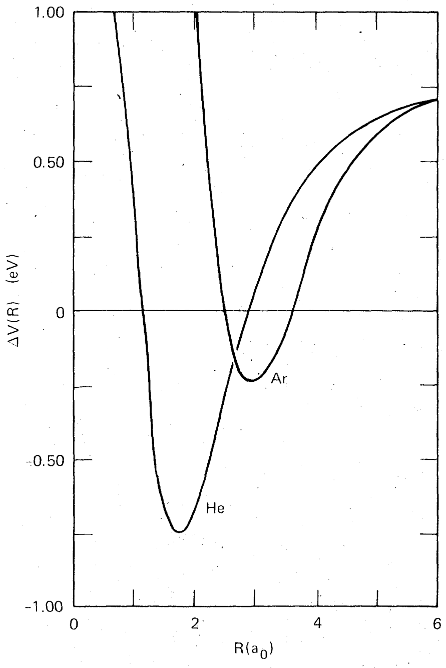

FIG. 2. Difference in potential energies between the negative-ion state and the neutral state for the HeH and ArH systems.

TABLE III. Electron-detachment characteristics.

System	$R_x(a_0)$	$V(R_x)$ (eV)	πR_x^2 (cm^2)	$\tau_{\rm el}$ (eV deg)	$\tau_{\rm inel}$ (eV deg)
H^- + He	2.90	1.23	7.4(−16)	150	110
H^- + Ar	3.65	1.39	1.2(−15)	190	150
Cl^- + Ar	3.45	10.1	1.0(−15)	1470	1280

system.

Critical parameters for estimating the electron-detachment cross sections and thresholds are the location of the outer crossing into the continuum and the collision energy required to reach it. In Table III we have summarized these parameters.

Our calculations indicate that the outer crossing into the continuum is located at $2.90a_0$. This value may be compared to the estimate of Browne and Dalgarno[15] of $3a_0$ and to the value of $2.1a_0$ obtained by Lam *et al.*[1] from the inversion of the scattering data. The crossing into the continuum is found to be located 1.23 eV above the asymptotic limit of the negative-ion state. Hence, barring appreciable quantum-mechanical tunneling into the continuum, this value should be a lower limit to the threshold for electron detachment. Lam *et al.*[1] obtain a value of 1.57 eV for the threshold. An upper limit to the electron-detachment cross section, neglecting tunneling, which should be unimportant for this system, is πR_x^2, where R_x is the outer-curve crossing distance into the continuum. For the HeH system, we obtain an upper-limit value of 7.4×10^{-16} cm^2 for the electron-detachment cross section which is appropriate at collision energies when a molecular representation is valid. For electron detachment from H^-, this would correspond to collision velocities less than that of the electrons on H^- or $v \ll 0.24$ a.u. or energies $E \ll 1.4$ keV. Experimental measurements by Champion *et al.*[2] and Risley and Geballe[16] indicate a maximum cross section for electron detachment of ~ 3.5–5.0×10^{-16} cm^2. Combining the experimental and theoretical results, leads us to estimate an average probability for electron detachment of ~60% for collisions with impact parameters less than R_x, leaving 40% of the collisions available for elastic scattering and inelastic processes to higher-lying states such as have been observed experimentally.[16]

We have also used the potentials to estimate the angular thresholds for electron detachment. The calculations employ the classical deflection functions for scattering on both the negative-ion and neutral potential-energy curves. For the onset of the electron detachment in the elastic differential scattering, we have used a high-energy-limit approximation[17] and evaluated the deflection function at an impact parameter $b = R_x$ for scattering on the negative-ion potential. This leads to a predicted threshold of 150 eV deg which may be compared to the estimate of Lam *et al.*[1] of 200 eV deg.

For the prediction of the onset of the detachment channel, that is

$$H^- + He \rightarrow H + He + e ,$$

we have used the average of the deflection functions for the negative-ion and neutral states evaluated at $b = R_x$. We obtain a threshold angle of 110 eV deg, Table III, a value somewhat less than that for the elastic scattering threshold since the outgoing neutral channel is less repulsive than the initial negative-ion channel. Esaulov *et al.*[4] measure an inelastic angular threshold of ~125 eV deg for the value where the cross section first reaches the magnitude equal to one-half the first Stückelberg oscillation.

TABLE IV. Self-consistent-field interaction potential energies for H, H^- + Ar, $E(R)-E(\infty)$ (units of 10^{-3} hartrees).

$R(a_0)$	$X\,^2\Sigma$ (H + Ar)	$X\,^1\Sigma$ (H^- + Ar)
1.5	596.490	576.954
1.75	360.237	342.814
2.0	248.378	237.934
2.25	180.721	188.591
2.5	131.314	157.544
2.75	94.890	130.299
3.0	68.061	104.517
3.25	48.394	81.443
3.5	34.098	62.106
3.75	23.808	46.653
4.0	16.478	34.671
4.5	7.701	18.705
5.0	3.491	9.803
6.0	0.660	2.309
7.0	0.108	0.177
8.0	0.009	−0.355
10.0	−0.008	−0.362
12.0	−0.007	−0.219
15.0	−0.005	−0.099
20.0	−0.002	−0.033
25.0	−0.001	−0.016
Asymptotic total energies (hartrees)		
	−527.316 620	−527.304 542

B. ArH

The calculated potential-energy points for the ArH system are given in Table IV and presented graphically in Fig. 3. The general shapes of the potential curves are very similar to the curves for the HeH system with crossings of the negative-ion state into and out of the continuum. As in the HeH system, the outer crossing is caused by the extra repulsion of the negative-ion state due to its closed-shell structure. The inner crossing is caused by the negative-ion state correlating to the K^- united-atom limit which is bound by 0.501 eV[14] when compared to the ground state of K.

Probably of most interest, however, is the fact that the negative-ion state does not penetrate deeply into the continuum when compared to the HeH system (Fig. 2). This lack of penetration probably explains why the complex-potential model used for the HeH system[1] fails to explain the unexpected behavior[2] of the electron-detachment cross section for Ar upon isotopic substitution of H^- with D^-.

In Table III we list some of the predicted electron-detachment characteristics for the ArH system. The outer crossing is calculated to be located at $3.65a_0$. This crossing distance is in disagreement with the value of $2.38a_0$ which was found by Esaulov *et al.*[4] to yield good agreement with their experimental data. From the theoretical curves we predict that the onset of electron detachment will require a collision energy of 1.39 eV.

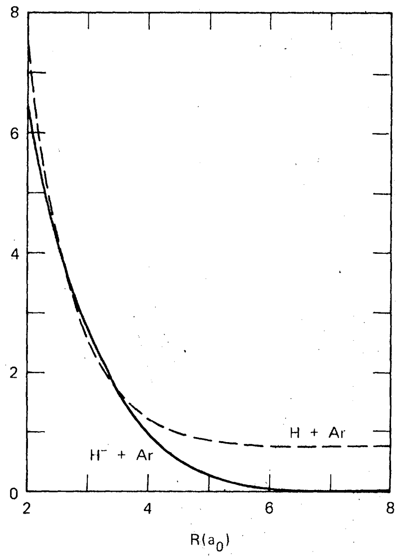

FIG. 3. Self-consistent-field potential-energy curves for the $X\,^1\Sigma$ state of ArH^- and the $X\,^2\Sigma$ state of ArH. The curves have been shifted relative to one another to yield the correct separation at large distances (0.754 eV).

By using the theoretical value for the outer crossing into the continuum, we arrive at a maximum value for the electron-detachment cross section of 1.2×10^{-15} cm^2 for energies $E<1.4$ keV. The experimental measurements of Champion *et al.*[2] and Risley and Geballe[16] yield a maximum cross-section value of $\sim7\times10^{-16}$ cm^2. Hence, as in the HeH system, we obtain an average probability for electron detachment of ~60% for intermediate-energy collisions with impact parameters less than R_x.

The angular thresholds for electron detachment have also been calculated in the same manner as for the HeH system. Here, we find an angular threshold of 190 eV deg for electron detachment in the elastic scattering of H^- by Ar. Champion *et al.*[2] report a value of 150 eV deg. The threshold for the inelastic scattering is predicted to be 150 eV deg, which may be compared to the measured value[4] of ~200 eV deg.

C. ArCl

Calculations were also performed on the ArCl system to see if there are major changes in shapes of the potential curves when Cl^- is used as an anion instead of H^-. The calculated potential energies are presented in Table V and shown graphically in Fig. 4. As in the HeH and ArH systems, the $X\,^1\Sigma$ negative-ion state is found to cross twice the $X\,^2\Sigma$ state of the neutral products. As before, the inner crossing is expected since the negative ion formed at the united atom, Br^-, is known[14] to be bound by 3.364 eV relative to the ground-state neutral Br. Of interest is that we found the $A\,^2\Pi$ state of ArCl to be more repulsive than the $X\,^1\Sigma$ state of the negative ion. Hence, we would conclude there would be a low probability for electron detachment to produce this state. This conclusion is in contradiction with that drawn by de Vreugd *et al.*[18] from the analysis of the threshold behavior of their differential cross sections.

The characteristics of the outer crossing of the negative-ion state into the continuum are presented in Table III. For the outer-crossing distance, our value of $3.45a_0$ is in good agreement with the value of $3.39a_0$ obtained by Champion and Doverspike[19] from the analysis of their experimental data. However, we do predict a higher threshold for electron detachment, 10.1 eV, than that obtained from the analysis[19] of the experimental data, 7.2 eV. Since we do have a relatively small basis set to describe the ArCl systems, it is possible that the theoretical potentials may overestimate the energy at the crossing by 1–2 eV.

Another possible explanation for this large dif-

TABLE V. Self-consistent-field for Cl, $Cl^- + Ar$, $E(R) - E(\infty)$ (units of 10^{-3} hartrees).

$R(a_0)$	$X\,^2\Sigma$ (Cl + Ar)	$A\,^2\Pi$ (Cl + Ar)	$X\,^1\Sigma$ (Cl^- + Ar)
2.5	1118.019	1407.077	1228.107
2.75	751.527	1062.547	892.470
2.9	593.604	877.059	747.275
3.0	505.460	765.108	665.490
3.1	429.351	664.757	591.449
3.25	335.121	534.878	490.781
3.4	260.958	427.559	401.106
3.5	220.666	367.115	347.798
3.75	144.696	248.514	238.551
4.0	94.510	166.436	160.604
4.5	39.757	72.890	70.399
5.0	16.365	31.182	29.665
5.5	6.573	13.102	11.776
6.0	2.563	5.417	4.090
6.5	0.958	2.200	0.888
7.0	0.333	0.870	−0.367
7.5	0.096	0.327	−0.788
8.0	0.012	0.108	−0.865
8.5	−0.016	0.021	−0.809
9.0	−0.023	−0.012	−0.712
9.5	−0.023	−0.023	−0.609
10.0	−0.021	−0.026	−0.515
12.0	−0.013	−0.019	−0.264
15.0	−0.009	−0.010	−0.112
20.0	−0.006	−0.006	−0.041
25.0	−0.004	−0.003	−0.016
Asymptotic total energies (hartrees)			
	−986.298 791	−986.298 492	−986.393 322

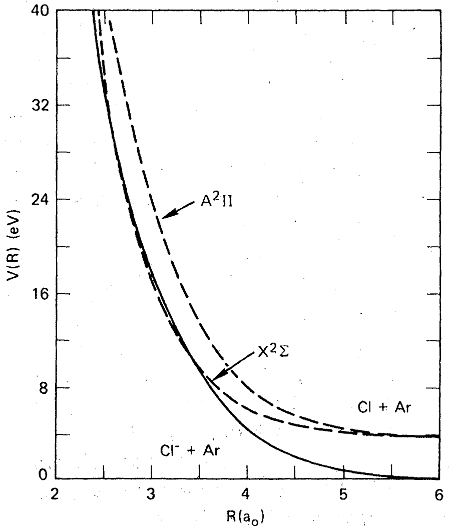

FIG. 4. Self-consistent-field potential-energy curves for the $X\,^1\Sigma$ state of $ArCl^-$ and the $X\,^2\Sigma$ and $A\,^2\Pi$ states of ArCl. The curves have been shifted relative to one another to yield the correct separation at large distances (3.615 eV).

ference is that unlike in the HeH or ArH systems, the negative-ion and neutral potential curves approach each other with a gentle slope. Hence, it is quite possible there will be significant electron detachment at internuclear separations greater than R_x due to increased tunneling to the continuum. An increase in tunneling may also partially explain why the average electron-detachment probability for intermediate-energy collisions rises to ~ 85% for this system. This value is obtained by dividing the cross section measured by Champion and Doverspike,[19] $\sim 8.5 \times 10^{-16}$ cm^2, by our maximum value $\sim 1.0 \times 10^{-15}$ cm^2. We should note that for systems where the negative-ion potential crosses the neutral state with a very small slope, an estimated upper-limit electron-detachment cross-section value of πR_x^2 may underestimate the true value because it neglects the possibility for tunneling into the continuum. This same potential characteristic may also allow an increasing tunneling to the continuum at higher collision energies, leading to a shift in angular threshold on differential data not unlike that seen for processes induced by rotational coupling, and may explain the observations of Vreugd *et al.*[18]

In Fig. 5 we present the differences in potential energy between the negative-ion and neutral states. If we may draw the analogy to the HeH and ArH systems, it appears that an analysis of the electron detachment based on the complex-poten-

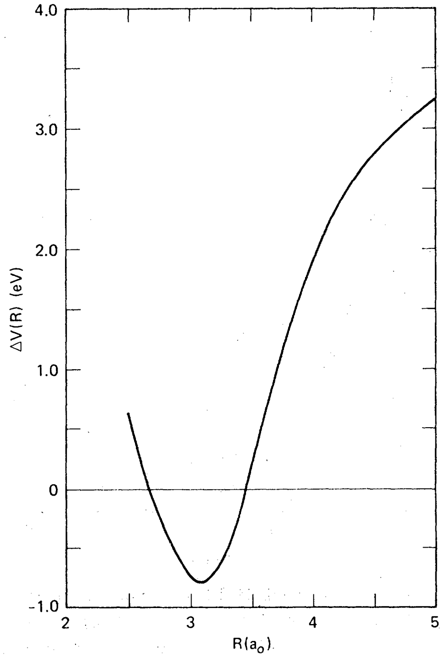

FIG. 5. Difference in potential energies between the $X\,^1\Sigma$ negative-ion state and the $X\,^2\Sigma$ neutral state for the ArCl system.

tial model should be applicable for the ArCl system.

In Table III we also present our estimates of the angular thresholds for electron detachment. Our calculated values for the elastic scattering angular threshold for electron detachment of 1470 eV deg is in reasonable agreement with the measurements of Champion and Doverspike[19] which indicate ~ 1200 eV deg and the measurements of Fayeton *et al.*[20] which indicate ~ 1500 eV deg. The calculated value for the inelastic scattering threshold of 1280 eV deg is also in reasonable agreement with the experimental results of Fayeton *et al.*[20] which indicate ~ 1200 eV deg.

IV. CONCLUDING REMARKS

Self-consistent-field potential-energy curves have been calculated for the ground negative-ion and neutral-molecular states of HeH, ArH, and ArCl. For these three systems the potential curve for the $X^1\Sigma$ state of the negative ion is found to cross twice the $X^2\Sigma$ state of the neutral system, the inner crossing being due to the fact that the negative-ion curve adiabatically correlates to a bound state in the united-atom limit.

Of the three systems studied, ArH is anomalous in that the negative-ion state only penetrates very slightly into the continuum. This potential-energy behavior very probably explains the reason why the complex-potential model for electron detachment was found to be inapplicable for this system. Further study, however, is warranted. Of interest also is the observation that the $X^1\Sigma$ potential of ArCl$^-$ only crosses the $X^2\Sigma$ state of the neutral system and is less repulsive than the $A^2\Pi$ state.

It is hoped that potential-energy calculations such as these will make it possible to more accurately test electron-detachment models by providing two (the negative-ion and neutral-state potentials) of the three ingredients (the third is the coupling matrix to the continuum) necessary to perform electron-detachment calculations.

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