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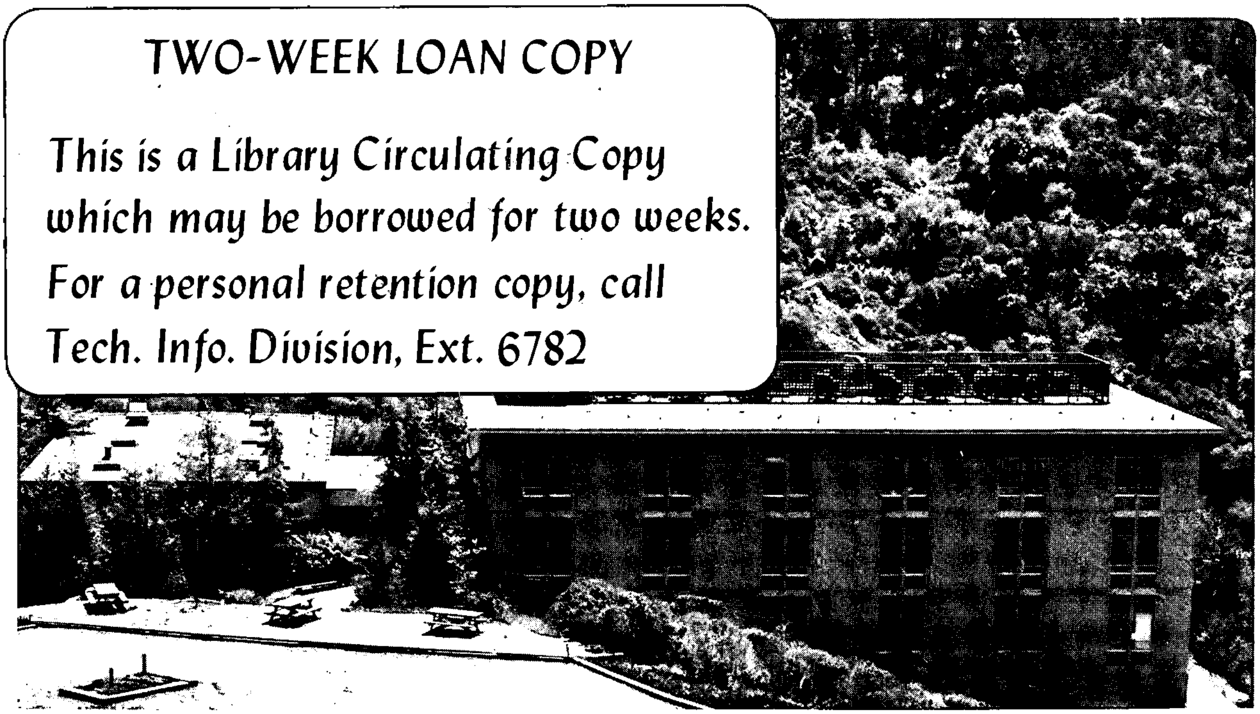

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Improved *Ab Initio* Effective Core Potentials for Molecular Calculations

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ABSTRACT

We have investigated the sources of error in bond lengths and dissociation energies computed from *ab initio* effective potentials derived from Phillips-Kleinman type pseudo-orbitals. We propose an alternate pseudo-orbital, effective potential treatment with the primary objective of agreement with all-electron molecular calculations. This new treatment forces the pseudo-orbitals to match precisely the Hartree-Fock orbitals in the valence region and thereby eliminates the major cause of error in the earlier calculations. Effective core potentials derived from these revised pseudo-orbitals were used to compute potential energy curves for the ground states of F_2, $C\ell_2$ and $LiC\ell$ and the results are compared with previous all-electron and effective potential calculations. Our effective potentials yield dissociation energies and bond lengths which are in excellent agreement with the all-electron values. Furthermore, in contrast to other procedures, our revised effective potentials result in an excellent description of the inner repulsive walls of the dissociation curves.

I. Introduction

Since the pioneering pseudo-potential studies of Phillips and Kleinman[1] and of Weeks and Rice[2] a great deal of effort has gone into the development of *ab initio* effective potential procedures for investigating the valence structure of molecular systems containing large numbers of electrons.[3-12] These procedures are based on the assumptions that, first, the polarization of the core orbitals upon molecular formation is of negligible importance relative to the valence effects (this is the frozen core approximation) and secondly, that the effects that the core electrons do have upon the molecular valence orbitals (including overlap effects) can be well approximated using a potential expressed as a sum of local functions multiplied by projection operators. Although these procedures have tremendously broadened the scope of molecular calculations, inconsistencies relative to all-electron calculations have become apparent in the last few years. The most troublesome of these is the shortening of bond lengths and deepening of potential wells (relative to all-electron results) sometimes seen in potential surface calculations. This problem became discouragingly apparent in the calculations of Kahn et al.[12] on F_2 and in the recent calculations of Hay, Wadt and Kahn[13] on F_2 and $C\ell_2$. The problem has also been observed in calculations on heavier diatomic molecules.[14,15] For $C\ell_2$ Hay et al., using effective potentials developed by Kahn, obtained a bond length that was short by nearly 0.3 bohr and a dissociation energy that was too large be about 70%. They obtained similar results for F_2, though not as exaggerated.

SCF calculations for F_2 and $C\ell_2$ in which only the valence orbitals were optimized (the core orbitals having been obtained from atomic calculations) indicated that, for the bond lengths employed in the studies by Kahn et al. and Hay et al., the error in the potential curves due to the frozen core approximation was relatively small.[16]

During the course of their study, Hay, Wadt and Kahn concluded that the error in their $C\ell_2$ and F_2 calculations arose from long-range negative tails in their chlorine 3d and fluorine 2p effective potentials and suggested ad hoc procedures for eliminating them. Using their revised potentials they obtained greatly improved dissociation curves for F_2 and $C\ell_2$, but errors in the neighborhood of 0.1 bohr still remained in their computed bond lengths for $C\ell_2$ and LiCℓ. This error, along with the somewhat inconsistent nature of their corrections (relative to their effective potential formalism) indicated to us that the problem needed to be investigated in a more fundamental manner.

In the present paper we have investigated the origins of the difficulties discussed by Hay et al. in terms of their effective potential formalism. We then suggest an alternative effective potential (EP) procedure which is formally more satisfactory than the corrections of Hay et al. and which in practice yields dissociation curves for F_2, $C\ell_2$ and LiCℓ which are in excellent agreement with all-electron (AE) calculations, even for relatively small internuclear separations.

Although our discussion is based primarily on the Kahn procedure, most of our findings are equally applicable to other formalisms in which the EP's are defined in terms of Phillips-Kleinman type pseudo-orbitals.

II. Long Range Effective-Potential Behavior

In the Kahn formalism,[12] the first step is to solve[17] numerically the atomic Hartree-Fock (HF) equations for accurate representations of the HF orbitals and orbital energies. The normalized valence pseudo-orbitals χ_v are then defined as linear combinations of the valence and core HF orbitals ϕ_v, ϕ_c of a given ℓ quantum number (as in Phillips and Kleinman),

$$\chi_v = C_v\phi_v + \sum_c^{\text{core}} C_c\phi_c. \qquad (1)$$

The expansion coefficients in (1) are chosen such that χ_v is smooth and nodeless near the origin. Note that, since χ_v must be normalized and the ϕ_v and ϕ_c are all orthonormal orbitals, the coefficient C_v must be smaller than unity unless all of the C_c are zero - a situation which arises only when there are no core orbitals of the same symmetry as ϕ_v.

The effective potential U^{EP} is obtained by requiring that it reproduce the pseudo-orbital χ_v and the true eigenvalue ε_v of the Hartree-Fock orbital,

$$(-\frac{1}{2}\nabla^2 - \frac{Z}{r} + U^{EP} + W_{val}^{PS})\,\chi_v = \varepsilon_v\chi_v, \qquad (2)$$

where Z is the atomic number and W_{val}^{PS} is the potential (comprising the usual coulomb and exchange terms) due to the interaction of an electron in χ_v with the other electrons in the occupied pseudo-orbitals. The local potential is then given by

$$U^{EP}(r) = \{(\varepsilon_v + \frac{1}{2}\nabla^2 + \frac{Z}{r} - W_{val}^{PS})\ \chi_v\}/\chi_v. \tag{3}$$

If we keep in mind that the core orbitals become negligible in the outer valence region and if C_v is less than unity, then it is apparent from equation (1) that the amplitude of the pseudo-orbital in the tail region must be smaller than that of the corresponding HF orbital. If r_c is the radius at which the most diffuse core orbital becomes negligibly small, then, for r larger than r_c, the pseudo-orbital is given by

$$\chi_v(r) \approx C_v\phi_v(r). \tag{4}$$

If we substitute (4) into equation (2) we see that U^{EP} becomes

$$U^{EP} \approx W_{core}^{HF} + W_{val}^{HF} - W_{val}^{PS}, \qquad r>r_c, \tag{5}$$

where W_{core}^{HF} and W_{val}^{HF} are the sums of the coulomb and exchange potentials arising from the HF core and valence orbitals respectively. However, for large values of r, W_{core}^{HF} must have the form

$$W_{core}^{HF} \approx \frac{N_c}{r}, \tag{6}$$

where N_c is the number of core electrons. Thus, any explanation for the excessive long-range negative tails in the fluorine and chlorine EP's must be in terms of W_{val}^{HF} and W_{val}^{PS}. (Hay et al. eliminated the long-range tail in their chlorine d potential by replacing the s and p pseudo-orbitals in W_{val}^{PS} with HF orbitals, in which case $W_{val}^{PS} = W_{val}^{HF}$. However the d potential, though it decays as N_c/r for large r, is then inconsistent with the s and p potentials.)

From equation (4) one can see that, in effect, by forming Phillips-Kleinman pseudo-orbitals one transfers valence electron density from the valence region into the core. For this reason the Phillips-Kleinman pseudo-orbitals alone cannot accurately account for the interaction of electrons in the valence region. This deficiency introduces, through equation (3), a long range tail in the EP. One can see this effect, in part, in the coulomb potential arising from a Phillips-Kleinman pseudo-orbital. From (4) it can be easily shown that the difference of the spherically averaged coulomb potentials[18] for corresponding HF orbitals and Phillips-Kleinman pseudo-orbitals is given by

$$J_v^{HF}(r) - J_v^{PS}(r) \approx \frac{1}{r}(C_v^2-1)\int_r^\infty |\phi_v(t)|^2(t^2-rt)dt, \quad r>r_c. \qquad (7)$$

The expression in equation (5) $(W_{val}^{HF} - W_{val}^{PS})$ is given by the sum of terms $(J_v^{HF} - J_v^{PS})$ over all other occupied valence orbitals together with corresponding aspherical coulomb and exchange terms. Since the integral in equation (7) is necessarily positive and the factor (C_v^2-1) is negative, all of the $(J_v^{HF} - J_v^{PS})$ terms are negative. Thus, from equation (5), one sees that these terms introduce a negative contribution to the effective potential arising from the difference between the pseudo- and HF orbitals in the outer part of the atom. These terms account for a large fraction of the excessive negative potential that Hay et al. found in the Kahn EP for chlorine. The fact that the tail is at least partially coulombic implies that, in general, it cannot be ignored as an artifact of the local potential approximation. Furthermore, since the expansions for the corresponding exchange and aspherical coulomb potentials will, for most cases, contain powers of r which are different from those that occur in the spherical coulomb potential, it appears that perfect cancellation with equation (7) is unlikely.

From equations (2) and (3) it is clear that the negative tail in the EP is a necessary part of its long-range behavior if the EP is to accurately reproduce the Hartree-Fock atomic orbital energies. However, for orbitals other than those from which it was derived, the potential is only an approximation and may lead to erroneous results. One would expect this to be particularly true in molecular calculations where the tail of the potential extends into the bonding region and into the space of other atoms.

The above discussion suggests that there are fundamental problems associated with the use of Phillips-Kleinman type pseudo-orbitals for generating effective potentials for molecular calculations. These problems are due to the deviation of the tail behavior of the EP's relative to the "point charge" potential one would expect from the HF core orbitals. From equation (4) and (7) it is clear that at least part of this deviation is due to the mismatch of the pseudo and HF orbitals in the valence region and can in general be eliminated only if χ_v and ϕ_v are required to be identical in that region.

For these reasons, we abandon the Phillips-Kleinman method of generating pseudo-orbitals and adopt the simple objective of close agreement with all-electron molecular calculations for a system of pseudo-orbitals and effective potentials. We retain equation (3) and subsequent portions of the usual EP treatment, e.g., Kahn et al.,[12] but abandon equation (1) and require instead that the pseudo-orbital match exactly the HF valence orbital outside the core region. Thus we define

$$\chi_v = \phi_v + f_v \tag{8}$$

where the function f_v is zero outside the core region and is otherwise chosen to cancel the oscillations of ϕ_v in the core region so that χ_v will be smooth and have no radial nodes. Thus we effectively partition ϕ_v into core and valence terms. For molecular calculations one directly optimizes only the molecular counterpart of the valence term, χ_v.

Although there are no explicit core-valence orthogonality conditions which the orbitals, χ_v, must satisfy, the partitioning in equation (8) suggests that there are implicit overlap requirements. In the EP approximation one assumes that these requirements are enforced by the shape of the potential in the core region. However, for molecular calculations, if the potential is not sufficiently large, one might expect perturbations from other centers to alter the form of the molecular orbitals in the core region such that a breakdown in the implied overlap conditions might occur. Since the magnitude of the potential depends roughly on the reciprocal of χ_v, one can force the EP to be large in the core region by choosing χ_v to be small near the origin. Furthermore, if χ_v were large near the origin or contained unnecessary oscillations then one would need a significantly larger basis set for molecular calculations. For these reasons, in addition to the requirement that χ_v and ϕ_v be identical in the valence region, we also wish χ_v to be smooth and as small as possible in the core region.

Although pseudo-orbitals of the above form have been proposed in the past,[19,20] the advantages for molecular calculations have not been well documented.

III. Improved pseudo-orbitals and potentials

In this section we will describe a procedure for generating pseudo-orbitals which retain exactly the behavior of the HF valence orbitals in the valence region, but are smooth and nodeless, with $\chi_v(r)/r^\ell$ going to zero at the origin. We will also discuss the long-range behavior of the resulting effective potentials.

We generate the radial factor for our pseudo-orbitals in two sections. The outer one, which spans the region from some matching point, r_{match}, to infinity is just the numerical HF valence orbital in that region. In the inner region (from zero to r_{match}) we define our pseudo-orbital by a five term polynomial expansion in r with a leading power of $\ell+2$. The expansion coefficients are chosen so as to match the amplitude and first three derivatives of the two sections at r_{match} and also to make the total pseudo-orbital normalized. r_{match} is chosen to be the innermost point at which the matching results in a nodeless radial pseudo-orbital with no more than two inflexions in its entire range. This procedure gives our pseudo-orbitals a unique definition which limits the deviation from the exact HF orbital to as small a region around the origin as possible.

It is clear from this definition of the pseudo-orbital that for r values greater than r_{match}, the C_v and r_c in equations (4) and (7) must be replaced by unity and r_{match} respectively. Therefore for r greater than r_{match}, the difference between the spherical parts of the pseudo- and HF coulombic potentials will be zero.

The calculation of the corresponding quantities for the exchange and aspherical coulomb potentials is not nearly so simple. However for the cases we have examined, these terms are very small for values of r that are much greater than r_{match}.

IV. Calculations and Results

We have used the pseudo-orbital selection procedure described in the last section along with the EP generating programs of Kahn et al.[12] to compute revised EP's for fluorine and chlorine. We used these potentials, expanded in terms of gaussian functions, along with gaussian basis sets to compute potential curves for F_2, $C\ell_2$ and $LiC\ell$ and compare our results with other EP calculations.[12,13] We assess the reliability of our potentials by comparison with AE calculations.[13]

Our s and p atomic orbitals (and indirectly pseudo-orbitals) for fluorine and chlorine were obtained from numerical HF calculations[17] on the ground states of the neutral atoms. The chlorine 3d orbital was obtained from a similar calculation using the ^4P multiplet of the configuration (Ne, 3s $3p^5$ 3d).

Our s and p basis sets were obtained by a least-squares fitting of our atomic pseudo-orbitals with three or four primitive gaussian functions. For F and Cℓ we included a single set of primitive d functions with exponents of 0.9 and 0.837 respectively.[13] In addition, for calculations on LiCℓ we added a set of diffuse p functions (the exponent was 0.049[21]) for the chlorine atom. For Li we used the (3s2p) contracted gaussian basis set of Dunning and Hay.[21] Although our fluorine and chlorine s and p basis sets differ considerably from those employed by Hay et al.[13] the more diffuse functions are similar enough that we believe a comparison of molecular results is valid. All of our calculations were carried out in terms of two configuration MCSCF wavefunctions identical in form to those used by Hay[13] and Kahn.[12]

In Table I we list our calculated equilibrium bond lengths and dissociation energies for F_2, $C\ell_2$ and LiCℓ along with all-electron (AE) and EP results from references 12 and 13. For F_2 our bond length differs from the AE value by about the same amount as did that of Hay et al., 0.02 bohr, but in the opposite direction. Both values are in much better agreement with the AE results than are those based on the EP of Kahn et al. (The fluorine EP's of Hay and Kahn differ only in that Hay et al.

truncated the tail behavior of the potential.) Our value for D_e for F_2 is considerably better than those computed from the EP's of either Hay or Kahn.

For $C\ell_2$ and $LiC\ell$ we obtained significantly better bond lengths than did Hay et al. For both cases our errors, relative to the AE values, were around 0.01 bohr or smaller (Hay's values were in error by close to 0.1 bohr). Also for both $C\ell_2$ and $LiC\ell$ our values for the dissociation energy differ from the AE value by about half as much as do those of Hay et al. (The value for D_e for $C\ell_2$ derived from the Kahn EP is too large by nearly a factor of two.)

The difference between our calculations and the previous EP calculations becomes most apparent at small internuclear separations. In Tables II through IV we list the dissociation potential energy curves (relative to separated atoms) for F_2, $C\ell_2$ and $LiC\ell$. Although Hay et al. obtained reasonable bond lengths and dissociation energies for F_2, as can be seen in Table II, their curve deviates considerably from the AE curve for bond distances shorter than about 2.6 bohr. At 2.2 bohr the Hay EP underestimates the energy by about 0.007 hartrees. The problem is much more serious for $C\ell_2$ where at 3.0 bohr the Hay EP underestimates the energy by more than 0.03 hartree. This is contrary to what one would expect from the original frozen core approximation since core polarization should reduce the energy. By comparison, for both $C\ell_2$ and F_2 our EP overestimates the energy by about 0.002 hartree at the shortest bond lengths tested - a very small error in the expected direction. Not only do we get better behavior in the equilibrium region but we also get a much better representation of the inner repulsive wall of the potential curve.

In figures 1 through 3 we have plotted the EP and AE dissociations curves for F_2, $C\ell_2$ and $LiC\ell$. Clearly, in all cases, our dissociation curves match more uniformly the AE curves than do the EP dissociation curves of either Hay or Kahn.

V. Summary

We have shown that effective potential calculations of molecular properties can reliably yield results in close agreement with all-electron calculations only if the atomic pseudo-orbitals retain the correct radial distribution of charge in the valence region given by all-electron atomic calculations.

Pseudo-orbitals obtained by the Phillips-Kleinman method move some electron density from the valence to the core region (if there are core orbitals of the same symmetry) and this shift of charge leads to excessive long-range negative tails in the resulting effective potentials. In turn in molecular calculations, the interatomic potential curve is too low at short distances leading to an excessive dissociation energy and too short an equilibrium bond distance.

With the objective that calculations of "valence level" molecular properties based on effective potentials should lead, as nearly as possible, to the same results as all-electron calculations, we adopt a simple, unambiguous procedure for generating pseudo-orbitals from HF atomic orbitals in a manner that retains exact equality in the outer portion of the atom. The usual equation is retained for the generation of effective potentials from pseudo-orbitals, orbital energies, etc. The use of our pseudo-orbitals with Kahn's effective potential formalism in molecular calculations results in potential energy curves which are in excellent agreement with all-electron calculations. The most noticeable improvement relative to recent results of Hay et al and Kahn et al is in the region of short inter-nuclear separation.

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Table I. Bond Lengths (bohr) and Dissociation Energies (kcal/mole) for the Ground States of F_2, $C\ell_2$ and $LiC\ell$ from 2-configurations MCSCF wavefunctions

Potential	F_2		$C\ell_2$		$LiC\ell$	
	R_e	D_e	R_e	D_e	R_e	D_e
All Electron[a]	2.84	14.8	4.04	27.0	4.02	86.6
Hay EP[a]	2.82	16.1	3.94	24.6	3.95	87.1
Kahn EP[b]	2.70	21.2	3.76	45.7	4.00	85.7
Present	2.86	14.6	4.04	25.7	4.03	86.9

[a] Values were taken from Hay et al., reference 13.

[b] Values were computed by Hay et al. using potentials from Kahn et al., reference 12.

Table II. Potential Energy Curves for the Ground State of F_2 from 2-configuration MCSCF Wavefunctions

R(bohr)	Energies (hartrees)		
	All-electron[a]	Hay[a]	Present
2.2	0.0570	0.0501	0.0592
2.4	0.0031	-0.0018	0.0052
2.6	-0.0183	-0.0215	-0.0170
2.8	-0.0234	-0.0256	-0.0230
3.0	-0.0215	-0.0228	-0.0213
3.4	-0.0124	-0.0129	-0.0124
20.0	0.0	0.0	0.0

[a] Values taken from Hay et al., reference 13.

Table III. Potential Energy Curves for the Ground State of Cl_2 from 2-configuration MCSCF Wavefunctions

R(bohr)	Energies (hartrees)			
	All-Electron[a]	Hay[a]	Kahn[b]	Present
3.0	0.1147	0.0813	0.0247	0.1166
3.5	-0.0210	-0.0260	-0.0676	-0.0199
3.756	-0.0387	-0.0378	-0.0729	-0.0369
4.0	-0.0430	-0.0391	-0.0687	-0.0408
4.25	-0.0408	-0.0353	-0.0603	-0.0388
4.5	-0.0353	-0.0292	-0.0503	-0.0336
5.0	-0.0217	-0.0165	-0.0315	-0.0208
6.0	-0.0045	-0.0029	-0.0098	-0.0042
20.0	0.0	0.0	0.0	0.0

[a] Values were taken from Hay et al., reference 13.

[b] Values were computed by Hay et al. using potentials from Kahn et al., reference 12.

Table IV. Potential Energy Curves for the Ground State of LiCℓ from 2-configuration MCSCF Wavefunctions

R(bohr)	Energies (hartrees)			
	All-Electron[a]	Hay[a]	Kahn[b]	Present
3.75	-0.1351	-0.1375	-0.1330	-0.1353
4.00	-0.1380	-0.1387	-0.1365	-0.1385
4.25	-0.1360	-0.1356	-0.1330	-0.1366
20.0	0.0	0.0	0.0	0.0

[a] Values were taken from Hay et al., reference 13.

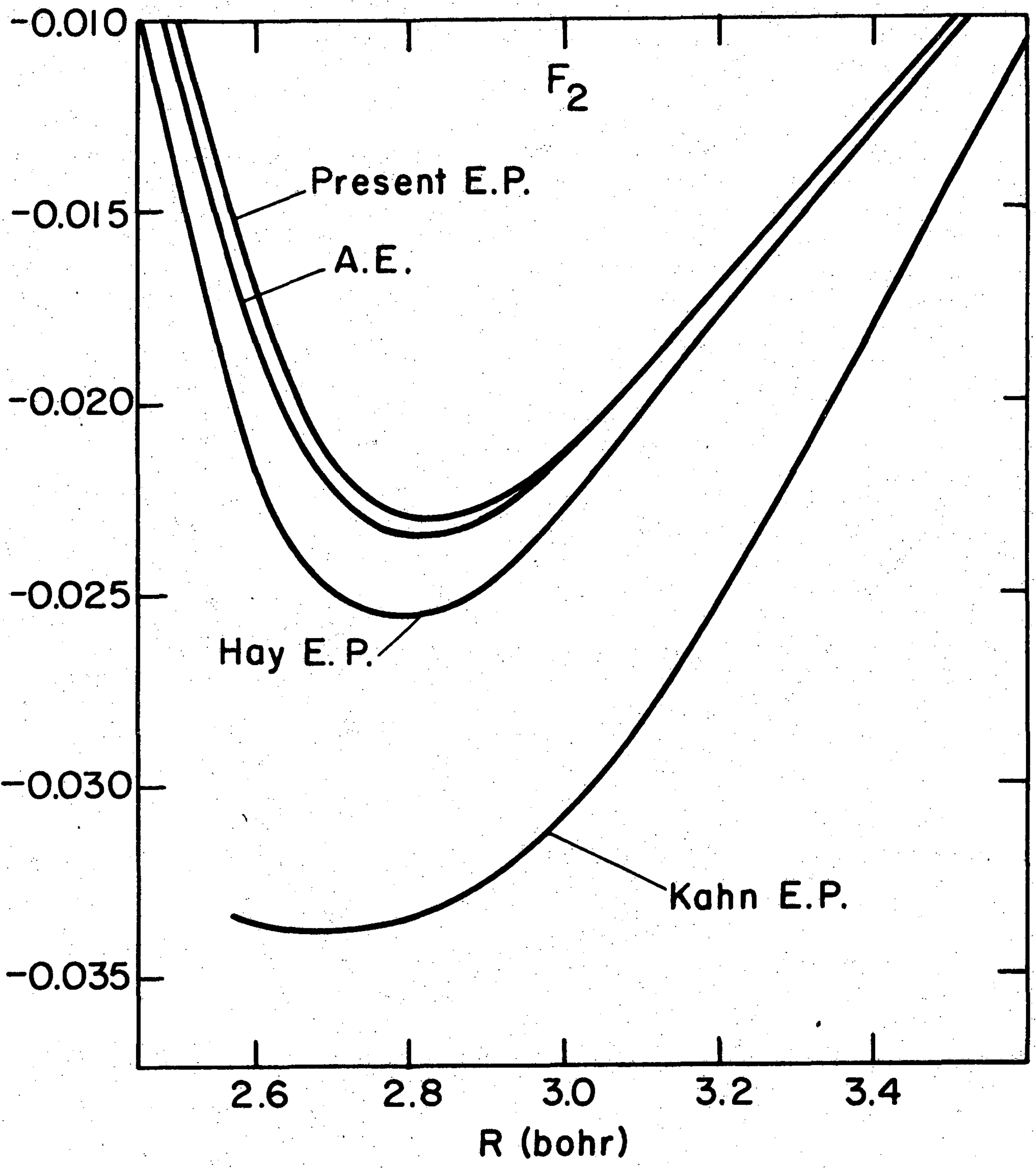
[b] Values were computed by Hay et al., using potentials from Kahn et al., reference 12.

Figure Captions

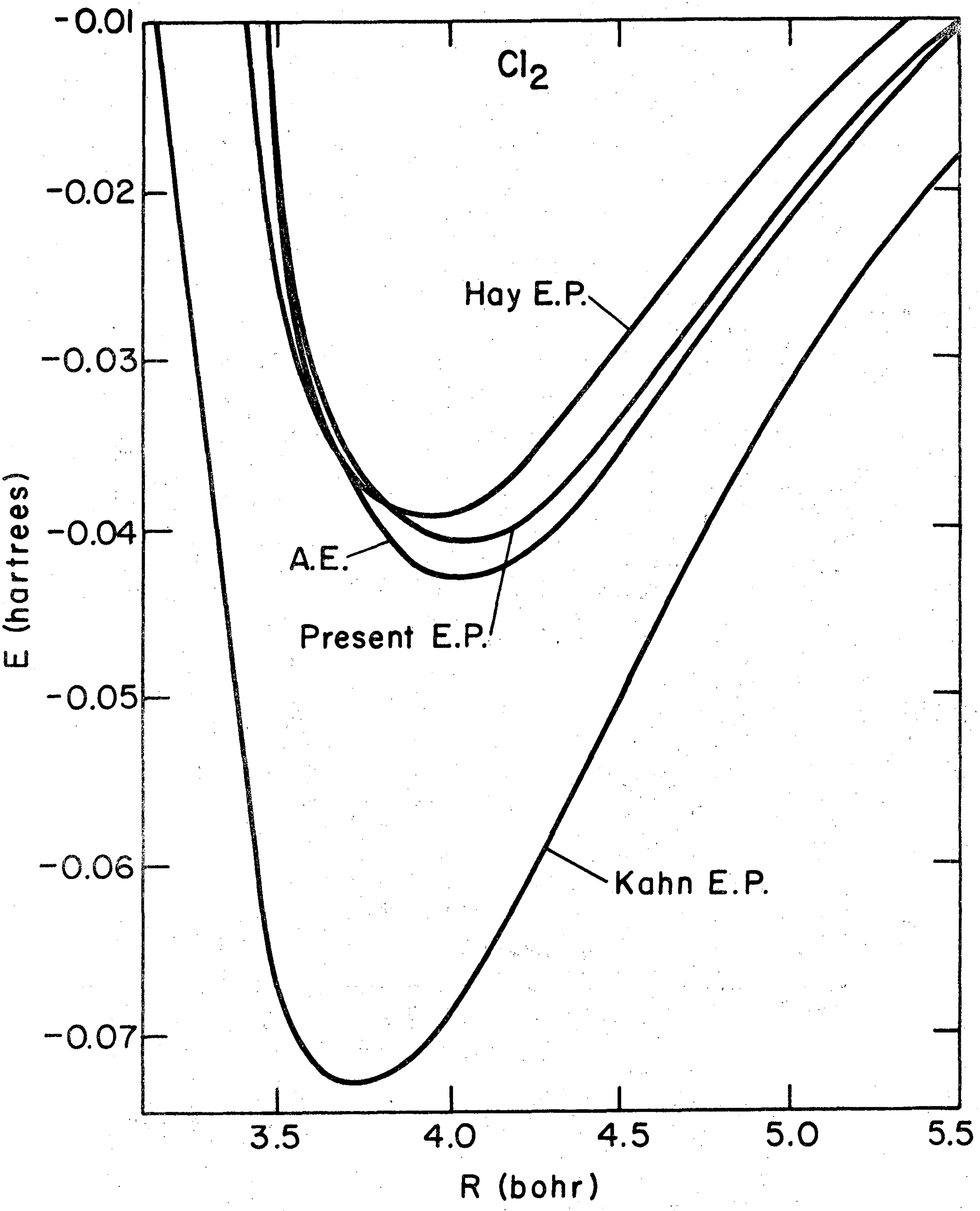
Figure 1. Potential energy curves for the ground state of F_2 from all-electron (AE) and effective potential (EP) calculations using 2-configuration MCSCF wavefunctions.

Figure 2. Potential energy curves for the ground state of $C\ell_2$ from all-electron (AE) and effective potential (EP) calculations using 2-configuration MCSCF wavefunctions.

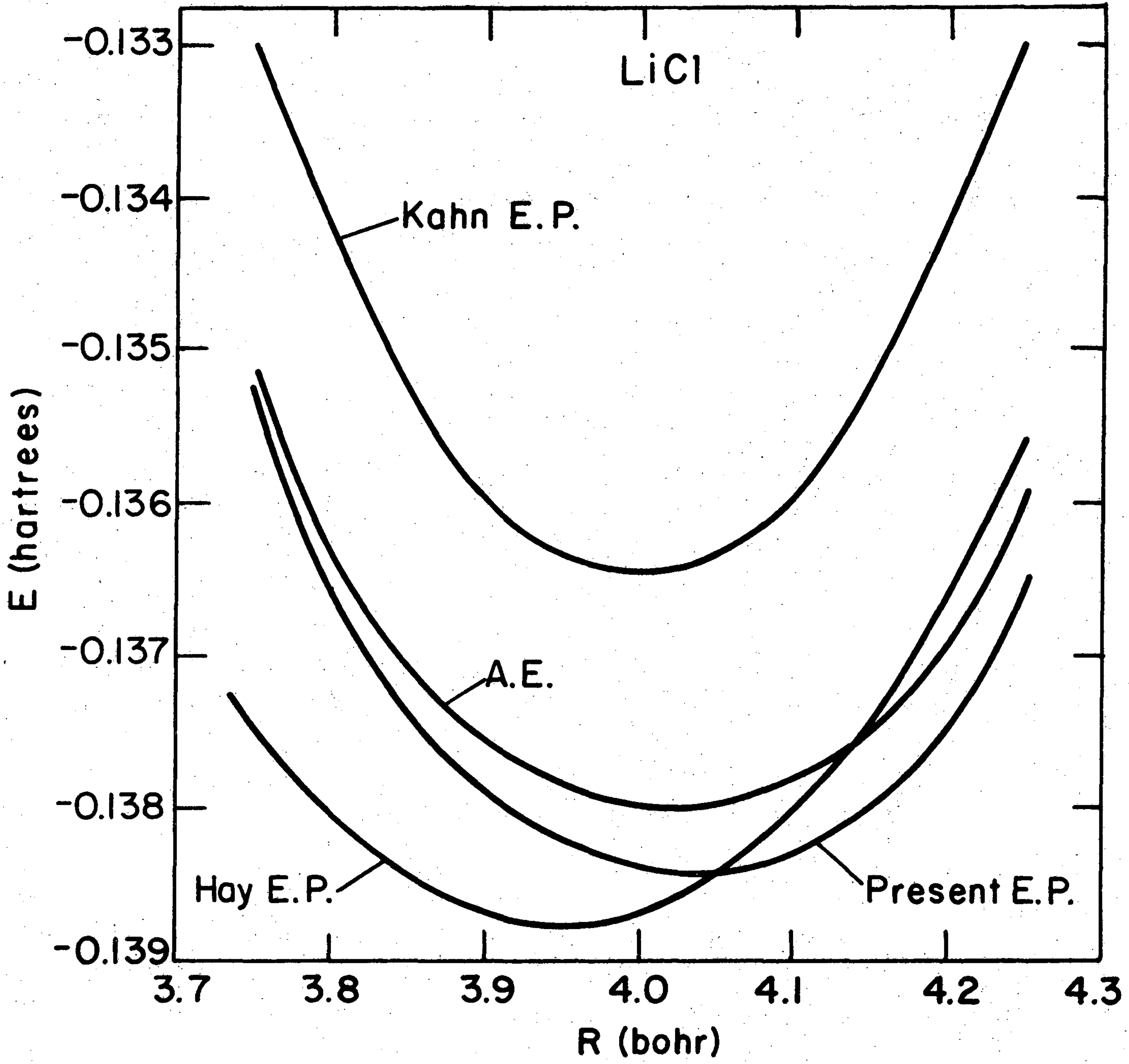
Figure 3. Potential energy curves for the ground state of LiCℓ from all-electron (AE) and effective potential (EP) calculations using 2-configuration MCSCF wavefunctions.


F$_2$
Present E.P.
A.E.
Hay E.P.
Kahn E.P.
E (hartrees)
-0.010
-0.015
-0.020
-0.025
-0.030
-0.035
R (bohr)
2.6
2.8
3.0
3.2
3.4

XBL 794-6126


Cl$_2$
Hay E.P.
A.E.
Present E.P.
Kahn E.P.
E (hartrees)
-0.01
-0.02
-0.03
-0.04
-0.05
-0.06
-0.07
R (bohr)
3.5
4.0
4.5
5.0
5.5

XBL 794-6127


LiCl
Kahn E.P.
A.E.
Hay E.P.
Present E.P.
E (hartrees)
-0.133
-0.134
-0.135
-0.136
-0.137
-0.138
-0.139
3.7
3.8
3.9
4.0
4.1
4.2
4.3
R (bohr)

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