PHYSICAL REVIEW A VOLUME 46, NUMBER 5 1 SEPTEMBER 1992

Numerical Hartree-Fock characterization of the metastable $^4\Pi_u$ state of the Ne_2^- ion

John M. Millam and Ludwik Adamowicz
Department of Chemistry, University of Arizona, Tucson, Arizona 85721

(Received 10 February 1992)

The metastable $^4\Pi_u$ state of the Ne_2^- anion is examined with the use of the numerical Hartree-Fock method. The results suggest that due to its similarity to the experimentally discovered $^4\Pi_g$ state of He_2^-, this state should also be long lived.

PACS number(s): 31.20.Di

I. INTRODUCTION

The determination of the interaction energy of two neon atoms has been a problem frequently considered by quantum chemists. Although most attention has been paid to the van der Waals region, there have also been numerous studies of the repulsion portion of the interaction potential [1–6]. There have also been several theoretical [7,8] and experimental [9,10] investigations on Ne_2 excited states. *Ab initio* quantum calculations on the Ne_2 system are very demanding, especially for larger internuclear separations due to small bonding effects. In particular, the basis-set superposition error (BSSE) presents a significant problem, and extended, well-optimized basis sets are usually necessary to obtain meaningful results. Even more challenging than calculations for the neutral neon dimer are calculations of the metastable Ne_2^- anion, which is the topic of the present work. Equally challenging have been experimental studies on metastable anions which started with the discovery of the $^4\Pi_g$ state of He_2^- by Bea, Coggiola, and Peterson [11] and subsequent characterization of this state by Kvale *et al.* [12]. The measurements were accomplished using an experimental technique called "excimer" autodetachment spectroscopy [13,14]. An advantage of this technique is the possibility of accurately measuring the energy of a transition from the vibrational levels of the bound metastable state of the anion into the repulsive continuum of the ground state of the neutral complex.

Theoretical work on metastable states of He_2^- were reported by Michels [15,16] and by one of us with coworkers [17–20]. These studies show that the principle of the formation of the anion rests in a two-electron attachment to the He_2^+ core with both electrons going to very diffused Rydberg orbitals and forming a high-spin state.

The present work is a continuation of our theoretical interest in long-lived metastable anions of the rare-gas dimers and focuses on theoretical characterization of a metastable state of Ne_2^-. The following characterization of metastable states emerged from our previous investigations.

(i) The electronic structure of these states can be described as the positively charged core with two valence electrons located on diffused orbits forming a quartet state.

(ii) Both valence electrons are bound if the valence shells that they occupy have bonding character (i.e., no nodes in the perpendicular symmetry plane) and their angular quantum numbers do not differ by more than 1.

(iii) Both valence shells have a similar level of diffuseness. In effect, the attractive forces toward the core felt by each electron are similar.

Several metastable states possessing the above features have been calculated for He_2^-. Following these studies, a question was raised as to whether a similar pattern of metastable anionic states would exist for Ne_2^-. In this work we provide an affirmative answer to this question based on *ab initio* quantum-chemical calculations performed with the use of the numerical Hartree-Fock method, which will be shortly reviewed in Sec. II.

The paper is organized as follows: Section II contains some details about the computational method and a rationale for its selection; in Sec. III we present numerical results. The work is summarized in Sec. IV.

II. DESCRIPTION OF THE METHOD

There have been several attempts in the past to develop a procedure for solving numerically the Hartree-Fock and multiconfiguration self-consistent-field (MCSCF) equations for diatomic molecules, starting with the early work of Kimball and Shortly [21]. Particularly successful were the approaches advanced by Laaksonen, Pyykkö, and Sundholm [22] and by McCullough and co-workers [23]. For lighter molecular systems, the above two methods provide a similar level of accuracy, with the latter being two to three orders of magnitude faster. One needs to mention also some more recent work on the numerical approach of Heinemann *et al.* [24] and an interesting numerical relativistic treatment by Yang, Heinemann, and Kolb [25].

In the present numerical Hartree-Fock (NHF) study we used the numerical MCSCF program of McCullough *et al.* [23]. The molecular orbitals with angular momentum m (for $m=0$ the orbital has σ symmetry, for $m=1$ the orbital has π symmetry, etc.) and m_p ($m_p=\pm m$) in this method are represented as partial-wave expansions in elliptic coordinates with numerical radial components X:

$$\Psi_m^{m_p}(\zeta,\eta,\phi)=\sum_{L=m} X_L^m(\zeta)Y_L^{m_p}(\eta,\phi)\ , \tag{1}$$

where

$$\xi=(r_a+r_b)/R, \quad 1\le\xi\le\infty$$

$$\eta=(r_a-r_b)/R, \quad -1\le\eta\le 1$$

$$\phi, \quad 0\le\phi\le 2\pi$$

r_a and r_b are the scalar distances of the point in space from the nuclei a and b, respectively; ϕ is the angle of rotation about the internuclear axis; and R is the internuclear separation.

In the conventional molecular-orbital (MO) approach, MO's are represented by truncated basis-set expansions. The error introduced by the truncation can be serious if an improper basis set is chosen. The NHF method avoids this deficiency by solving the Fock equations for the radial function, X, on a grid of points. The resulting molecular orbitals are essentially exact because the monotonic convergence of the partial-wave expansion (1) enables one to control the truncation error. Besides the length of the partial-wave expansion, the numerical grid-point spacing is also a critical accuracy-determining factor. In practice, one needs to experiment with different grid spacings and lengths of the partial-wave expansions to achieve the desired convergence of the results. This has been the approach taken in the present study.

Use of the NHF method practically eliminates both the basis-set superposition error and the basis-set incompleteness problem. These features are particularly important in calculations on diffused anionic states such as the ones considered in this work. In addition, in the NHF method, the tendency for an electron to leave the system and escape to the continuum is clearly manifested by the increasing size or the orbitals, which the electron occupies, and the orbital energy rising and approaching zero. This feature was particularly instrumental in determining if the metastable anionic state under consideration tends to be a spatially bound state or a resonance state.

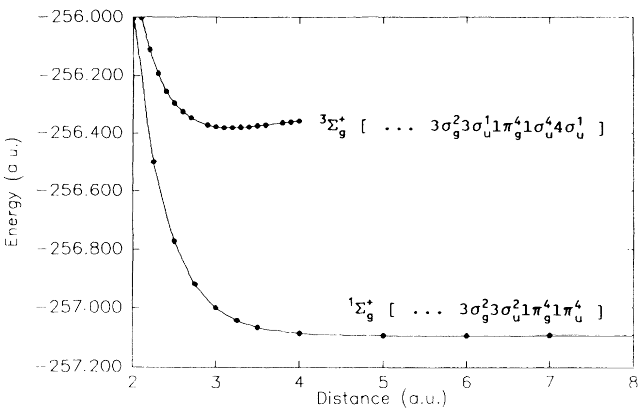

FIG. 1. Energy curves for the $^1\Sigma_g^+$ $(\cdots 3\sigma_g^2 3\sigma_u^2 1\pi_g^4 1\pi_u^4)$ ground state and the $^3\Sigma_g^+$ $(\cdots 3\sigma_g^2 3\sigma_u^1 1\pi_g^4 1\pi_u^4 4\sigma_u^1)$ excited state of the Ne_2 dimer.

III. RESULTS AND DISCUSSION

As mentioned above, two electrons should remain bound to the Ne_2^+ core if they are kept sufficiently diffused and none of them has a greater tendency to contract towards the nuclei. Therefore, a search was conducted with the use of the NHF method for two Rydberg triplet states of Ne_2, which exhibit similar levels of diffuseness and posses similar energies over a more extended range of internuclear separations. Two states,

$$^3\Sigma_g^+(\cdots 3\sigma_g^2 3\sigma_u^1 1\pi_u^4 1\pi_g^4 4\sigma_u^1)$$

and

$$^3\Pi_g(\cdots 3\sigma_g^2 3\sigma_u^1 1\pi_u^4 1\pi_g^4 2\pi_u^1),$$

TABLE I. HF energy, $4\sigma_u$ orbital energy, and expectation value of the squared distance (R^2) for the $4\sigma_u$ electron measured from the middle of the molecule for Ne_2 $[^3\Sigma_g(\cdots 3\sigma_g^2 3\sigma_u^1 \pi_u^4 1\pi_g^4 4\sigma_u^1)]$ at different bond lengths.

R	E_{HF}	$\varepsilon\ (4\sigma_u)$	$\langle R^2\rangle\ (4\sigma_u)$
1.75	−255.241 72	−0.017 51	1972
1.90	−255.657 90	−0.017 65	1943
2.00	−255.853 86	−0.017 67	1939
2.10	−256.001 15	−0.017 67	1939
2.20	−256.111 11	−0.017 67	1940
2.30	−256.192 60	−0.017 66	1942
2.60	−256.326 67	−0.017 61	1953
2.70	−256.348 17	−0.017 59	1958
2.80	−256.362 61	−0.017 58	1963
2.90	−256.371 77	−0.017 55	1968
3.00	−256.377 04	−0.017 53	1973
3.10	−256.379 44	−0.017 51	1978
3.20	−256.379 78	−0.017 49	1983
3.30	−256.378 67	−0.017 47	1989
3.40	−256.376 54	−0.017 45	1994
3.50	−256.373 76	−0.017 42	2000
3.60	−256.370 58	−0.017 40	2005
3.80	−256.363 71	−0.017 35	2016
3.90	−256.360 27	−0.017 33	2022
4.00	−256.356 93	−0.017 31	2028

TABLE II. HF energy, $2\pi_u$ orbital energy, and expectation value of the squared distance (R^2) for the $2\pi_u$ electron measured from the middle of the molecule for Ne_2 $[{}^3\Pi_g(\cdots 3\sigma_g^2 3\sigma_u^1 1\pi_u^4 1\pi_g^4 2\pi_u^1)]$ at different bond lengths. All entries in atomic units.

R	E_{HF}	ε $(2\pi_u)$	$\langle R^2 \rangle$ $(2\pi_u)$
1.75	−255.242 58	−0.018 42	1777
2.00	−255.854 33	−0.018 17	1827
2.25	−256.155 30	−0.018 04	1854
2.50	−256.296 04	−0.017 95	1873
2.75	−256.356 41	−0.017 89	1886
2.90	−256.372 08	−0.017 86	1892
3.00	−256.377 34	−0.017 84	1895
3.10	−256.379 75	−0.017 82	1898
3.20	−256.380 10	−0.017 81	1901
3.25	−256.379 70	−0.017 80	1902
3.30	−256.378 99	−0.017 80	1903
3.35	−256.378 04	−0.017 79	1905
3.40	−256.376 88	−0.017 78	1906
3.50	−256.374 11	−0.017 77	1908
3.60	−256.370 84	−0.017 76	1910
3.70	−256.367 55	−0.017 75	1912
3.80	−256.364 09	−0.017 74	1914
3.9	−256.360 66	−0.017 73	1916
4.00	−256.357 33	−0.017 72	1918

were found to belong to the desired category. In Tables I and II we present the total HF molecular energies of the states along with the orbital energies of the Rydberg orbital and the expectation value of the square of the separation of an electron occupying this orbital from the middle of the molecular bond. Upon examining the results, one can notice the similarities mentioned above. In conclusion, one may expect the $4\sigma_u$ and $2\pi_u$ orbitals to support a two-electron attachment to the $Ne_2{}^+$ core.

In order to illustrate the position of the ${}^3\Sigma_g^+$ and ${}^3\Pi_g$ states with respect to the potential curve for the ground electronic state of the Ne_2 cluster, we included a comparison presented in Fig. 1. In Table III we also included total HF energies and orbital energies for selected internuclear distances for the Ne_2 ground state. This information might provide a valuable reference for studies performed with finite basis sets. Worth noticing in the ground-state potential curve is a very shallow minimum appearing at about 6 a.u. For the excited states, the minima are more pronounced and appear at significantly shorter internuclear distances—an obvious result of removing an antibonding electron and placing it into a diffused orbit with a marginal bonding effect.

In the next step an attempt has been made to converge

TABLE III. Hartree-Fock energy and orbital energies for the ground state of the Ne_2 dimer at different bond lengths. All entries in atomic units.

		Orbital energies							
R	E_{HF}	$1\sigma_g$	$1\sigma_u$	$2\sigma_g$	$2\sigma_u$	$3\sigma_g$	$3\sigma_u$	$1\pi_g$	$1\pi_u$
2.00	−256.003 56	−32.722 90	−32.722 98	−2.353 93	−1.761 36	−1.144 02	−0.280 44	−0.736 94	−1.059 67
2.25	−256.498 58	−32.698 34	−32.698 47	−2.165 74	−1.786 81	−1.072 49	−0.464 45	−0.744 57	−0.958 52
2.50	−256.770 87	−32.714 49	−32.714 60	−2.069 17	−1.826 89	−1.026 55	−0.587 17	−0.771 37	−0.914 36
2.75	−256.918 54	−32.730 89	−32.730 96	−2.013 05	−1.858 42	−0.988 09	−0.669 24	−0.793 45	−0.889 64
3.00	−256.998 60	−32.743 67	−32.743 72	−1.979 87	−1.881 17	−0.956 98	−0.727 75	−0.809 88	−0.874 94
3.25	−257.042 12	−32.754 32	−32.754 36	−1.960 75	−1.897 75	−0.931 83	−0.754 33	−0.822 46	−0.866 69
3.50	−257.065 45	−32.755 35	−32.755 37	−1.946 96	−1.906 60	−0.944 10	−0.782 99	−0.828 60	−0.858 97
4.00[a]	−257.085 64	−32.764 41	−32.772 07	−1.929 30	−1.930 03	−0.882 64	−0.817 49	−0.847 80	−0.849 46
5.00[a]	−257.093 44	−32.770 54	−32.773 24	−1.929 62	−1.930 75	−0.857 70	−0.843 16	−0.849 55	−0.850 71
6.00	−257.094 04	−32.772 30	−32.772 33	−1.930 57	−1.930 12	−0.853 46	−0.847 33	−0.849 96	−0.850 76
7.00	−257.093 57	−32.772 11	−32.772 25	−1.930 42	−1.930 34	−0.851 29	−0.849 52	−0.850 31	−0.850 51
8.00	−257.091 46	−32.771 09	−32.771 61	−1.930 37	−1.930 36	−0.850 66	−0.850 15	−0.850 40	−0.850 45

[a] Numerical HF calculations at this point were performed without imposing the gerade-upgerade symmetry on orbitals due to the lack of convergence of the numerical HF procedure with the *g-u* symmetry explicitly enforced. Both approaches should give virtually identical values of the total energy.

TABLE IV. HF energy, orbital energies of $4\sigma_u$ and $2\pi_u$ orbitals, and expectation values of R^2 (i.e., the distance between the middle of the molecule and the electron) for the $4\sigma_u$ and $2\pi_u$ orbitals for $\mathrm{Ne_2}^-$ [$^4\Pi_u(\cdots 3\sigma_g^2 3\sigma_u^1 1\pi_u^4 1\pi_g^4 4\sigma_u^1 2\pi_u^1)$] at different internuclear separations. All entries in atomic units.

		ε		$\langle R^2 \rangle$	
R	E_{HF}	$4\sigma_u$	$2\pi_u$	$4\sigma_u$	$2\pi_u$
2.00	−255.854 83	−0.001 81	−0.001 70	3062	3203
2.25	−256.155 87	−0.001 86	−0.001 84	3059	3251
2.50	−256.296 67	−0.001 89	−0.001 57	3050	3298
2.75	−256.357 05	−0.001 94	−0.001 50	3033	3346
3.00	−256.377 95	−0.001 98	−0.001 40	3001	3408
3.25	−256.380 31	−0.002 07	−0.001 24	2933	3518
3.30	−256.379 61	−0.002 09	−0.001 20	2914	3547
3.31	−256.379 43	−0.002 10	−0.001 19	2907	3557
3.32	−256.379 25	−0.002 11	−0.001 17	2900	3568
3.33	−256.379 06	−0.002 12	−0.001 16	2891	3582
3.34	−256.378 86	−0.002 14	−0.001 13	2879	3600
3.35	−256.378 65	−0.002 15	−0.001 12	2871	3615
3.355	−256.378 55	−0.002 19	−0.001 06	2839	3661
3.3555	−256.378 53	−0.002 20	−0.001 03	2826	3681

the NHF procedure for the $^4\Pi_u$ metastable state of the $\mathrm{Ne_2}^-$ anion corresponding to the following electronic configuration:

$$(\cdots 3\sigma_g^2 3\sigma_u^1 1\pi_u^4 1\pi_g^4 4\sigma_u^1 2\pi_u^1) .$$

The attempt was successfully, and converged results have been obtained for several internuclear separations. The results of the calculations, i.e., the total HF energy, the orbital energies of the $4\sigma_u$ and $2\pi_u$ orbitals, are presented in Table IV. Upon examining the results, one notices that at shorter internuclear separations, both Rydberg electrons are almost isoenergetic; however, with an increasing distance, the $4\sigma_u$ orbital noticeably contracts (as shown by the decreasing magnitude of the orbital energy and the increasing expectation value of R^2) and the $2\pi_u$ orbital expands, indicating a weakening bonding. At the internuclear distance of 3.35 a.u.—this is past the minima on both curves corresponding to the "parent" excited states of the neutral system—the $2\pi_u$ electron is spontaneously ejected from the molecule. This can be noticed by examining the expectation values of R^2 at 3.35, 3.355, and 3.3555 a.u. Beyond this point, the NHF calculation for $\mathrm{Ne_2}^-$ could not be converged.

The potential curves for the anion and for its "parent" excited states of the neutral system lie above the curve of the neutral ground state. Therefore, all those states are metastable. However, the anion near the equilibrium internuclear separation appears to be bound with respect to both "parent" states. At 3.0 a.u., the energy of the $\mathrm{Ne_2}^-$ $^4\Pi_u$ state is lower by 0.000 61 a.u. than the energy of the $^3\Pi_g$ state of $\mathrm{Ne_2}$, and lower by 0.000 91 a.u. than the energy of the $^3\Sigma_g$ state. At 3.3 a.u., the respective differences are similar and are equal to 0.000 62 and 0.000 94 a.u. The positive electron affinities of $\mathrm{Ne_2^-}$ with respect to the "parent" state should certainly enhance its lifetime.

In order to examine the electronic structure of the $\mathrm{Ne_2}^-$ anion, we present a comparison of the orbital energies and the R^2 expectation values for $\mathrm{Ne_2}$(g.s.), $\mathrm{Ne_2}^+$(g.s.), and $\mathrm{Ne_2}^-(^4\Pi_u)$ in Table V. One can make the following observations upon examining the results: First, the Rydberg electrons in $\mathrm{Ne_2}^-$ occupy orbitals

TABLE V. Comparison or orbital energies and mean values of R^2 (R being the distance between the electron and the middle of the molecular bond) for all occupied orbitals of $\mathrm{Ne_2}$, $\mathrm{Ne_2}^+$, and $\mathrm{Ne_2}^-$ for the internuclear distance of 3.25 a.u. All entries in atomic units.

	$\mathrm{Ne_2}$		$\mathrm{Ne_2}^+$		$\mathrm{Ne_2}^-$	
Orbital	ε	$\langle R^2 \rangle$	ε	$\langle R^2 \rangle$	ε	$\langle R^2 \rangle$
$1\sigma_g$	−32.7543	2.6742	−33.3408	2.6739	−33.2906	2.6739
$1\sigma_u$	−32.7544	2.6741	−33.3407	2.6739	−33.2906	2.6739
$2\sigma_g$	−1.9607	3.4265	−2.4596	3.3494	−2.4095	3.3495
$2\sigma_u$	−1.8977	3.7393	−2.3895	3.7426	−2.3394	3.7429
$3\sigma_g$	−0.9318	3.9211	−1.3192	3.7824	−1.2691	3.7825
$3\sigma_u$	−0.7543	3.9500	−1.3477	3.6194	−1.2976	3.6194
$1\pi_u$	−0.8667	3.8453	−1.3774	3.6681	−1.3273	3.6682
$1\pi_g$	−0.8224	3.9994	−1.3385	3.7242	−1.2884	3.7244
$4\sigma_u$					−0.0021	2933.4704
$2\pi_u$					−0.0012	3517.9897

which are considerably different from the core orbitals. The average distance of the Rydberg electrons from the middle of the molecule is about 30 times larger than for the core electrons. Secondly, the electronic structure of the core for the anion resembles, as expected, the electronic structure of the Ne_2^+ cation, as can be seen by comparing both the values for orbital energies and $\langle R^2 \rangle$.

IV. CONCLUSIONS

The aim of the present work is to examine the stability of the metastable Ne_2^- dimer with the numerical Hartree-Fock method. This method provides a single-configuration solution of the Schrödinger equation, which is basis-set error free—an essential feature in calculations on auto-detaching states. The characteristic features of the $^4\Pi_u$ state of Ne_2^- determined in this study are similar to those of metastable states of He_2^- examined in our previous papers [19,20]. Our calculations indicate that the anion should be long lived due to its energy being lower near the equilibrium separation with respect to the states of the neutral dimer, to which it will dissociate upon an electron ejection.

There are two effects that are not accounted for in the present calculations, i.e., the relativistic and electron correlation effects. Although one would expect some relativistic contraction of the core shells and some expansion of the valence shells, this should not alter the picture obtained from the nonrelativistic treatment. A more significant contribution can originate from the electronic correlation effects. In our recent work [18] we studied this contribution for the $^4\Pi_g$ metastable state of He_2^- with the use of high-level coupled-cluster methods and hybrid numerical and Slater-orbital basis sets. The results show that for the interatomic distances where the Hartree-Fock solution is adequate (near the equilibrium), the correlation effects do not change the stability of the anion, although the total energy obtained from the correlated treatment is noticeably lower than the Hartree-Fock energy.

An interesting question that one may ask pertains to the predicted lifetime of metastable Ne_2^-. Decay-rate measurements by Bea *et al.* [14] on He_2^- indicate that the He_2^- beam contained several states with different lifetimes, ranging from less than 10^{-5} s to more than 10^{-4} s, similar to those of the $J=\frac{1}{2}$, $\frac{3}{2}$, and $\frac{5}{2}$ fine-structure states of He^- $^4\Pi$. It is reasonable to assume that because of the similarity of the state calculated here for Ne_2^- to that of He_2^-, the lifetime of this state will be similar.

[1] H. H. Michaels, R. H. Hobbs, and L. A. Wright, Int. J. Quantum Chem. Symp. **12**, 257 (1978).
[2] G. Chalasinski, Mol. Phys. **49**, 1353 (1983).
[3] W. Rijks, M. Gerritsen, and P. E. S. Wormer, Mol. Phys. **66**, 929 (1989).
[4] J. Dias de Silva, J. Brandao, and A. J. C. Varandas, J. Chem. Soc., Faraday Trans. 2 **85**, 1851 (1989).
[5] E. Kapuy and C. Kozmutza, J. Chem. Phys. **94**, 5565 (1991).
[6] F. M. Tao and Y. K. Pan, J. Phys. Chem. **95**, 9811 (1991).
[7] F. Grein, S. D. Peyerimhoff, and R. J. Buenker, J. Chem. Phys. **82**, 353 (1985); **87**, 4684 (1987).
[8] F. Grein, S. D. Peyerimhoff, and R. Klotz, Theor. Chim. Acta **72**, 403 (1987).
[9] D. J. Kane, Diss. Abstr. Int. B1990 **50**, 5133 (1989).
[10] W. Giessl, C. Voelkner, S. Czer, M. Zoeger, and H. Langhoff, J. Phys. B **24**, 4203 (1991).
[11] Y. K. Bea, M. J. Coggiola, and J. R. Peterson, Phys. Rev. Lett. **52**, 747 (1984).
[12] T. J. Kvale, R. N. Compton, G. D. Alton, J. S. Thompson, and D. J. Pegg, Phys. Rev. Lett. **56**, 582 (1986).
[13] P. S. Drzaic, J. Marks, and J. I. Brauman, in *Gas Phase Ion Chemistry,* edited by M. T. Bowers (Academic, New York, 1984).
[14] Y. K. Bea, J. R. Peterson, H. H. Michels, and R. H. Hobbs, Phys. Rev. A **37**, 2778 (1988).
[15] H. H. Michels, Chem. Phys. Lett. **126**, 537 (1986).
[16] H. H. Michels, Phys. Rev. Lett. **52**, 1413 (1984).
[17] T. Pluta, R. J. Bartlett, and L. Adamowicz, Int. J. Quantum Chem. Symp. **22**, 225 (1988).
[18] T. Pluta, R. J. Bartlett, and L. Adamowicz, Phys. Rev. A **40**, 2253 (1989).
[19] L. Adamowicz and T. Pluta, Chem. Phys. Lett. **179**, 517 (1991).
[20] L. Adamowicz and T. Pluta, Phys. Rev. A **44**, 2860 (1991).
[21] G. E. Kimball and G. H. Shortly, Phys. Rev. **45**, 815 (1934).
[22] L. Laaksonen, P. Pyykkö, and D. Sundholm, Comput. Phys. Rep. **4**, 313 (1986).
[23] E. A. McCullough, Jr., Chem. Phys. Lett. **24**, 55 (1974); J. Chem. Phys. **62**, 3991 (1975); **63**, 5050 (1975); P. A. Christiansen and E. A. McCollough, Jr., *ibid.* **67**, 1877 (1977); Chem. Phys. Lett. **51**, 468 (1977); **56**, 484 (1978); E. A. McCullough, Jr., J. Chem. Phys. **75**, 1579 (1981); L. Adamowicz and E. A. McCullough, Jr., *ibid.* **75**, 2475 (1981); E. A. McCullough, Jr., Mol. Phys. **42**, 943 (1981); J. Phys. Chem. **86**, 2178 (1982); L. Adamowicz and E. A. McCullough, Jr., Int. J. Quantum Chem. **24**, 19 (1983); Chem. Phys. Lett. **107**, 72 (1984); J. Phys. Chem. **88**, 2045 (1984); E. A. McCullough, Jr., Comput. Phys. Rep. **4**, 267 (1986).
[24] D. Heinemann, B. Fricke, and D. Kolb, Phys. Rev. A **38**, 4998 (1988); D. Heinemann, A. Rosen, and B. Fricke, Phys. Scr. **42**, 692 (1990).
[25] L. Yang, D. Heinemann, and D. Kolb, Chem. Phys. Lett. **178**, 213 (1991).