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Potential energy curves and dipole transition moments for electronic states of ArHe and HeNe

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Relativistic core-potential calculations have been carried out on the ground and excited Ω states of ArHe and HeNe correlating with the atomic limits Ar*$(3p^5 4s,\ ^3P, ^1P)$ and Ne*$(2p^5 3s,\ ^3P, ^1P)$, respectively, and with ground-state He atoms. The potential energy curves of the excited states of ArHe are repulsive. The potential energy curves of the 0^-(I), 1(I) and 0^+(II)$2p\sigma \rightarrow 3s$ states of HeNe show a local Rydberg minimum at 2.8 bohr and a barrier at 4.0 bohr, while the other excited state potentials of HeNe are repulsive. For both ArHe and HeNe, large dipole transition moments are calculated connecting the ground state with states dissociating to atomic limits from which radiative transitions to the atomic ground state are allowed. Small but nonzero dipole transition moments are obtained for short internuclear distances for the transitions from the 1(I) state, which correlates with the metastable $^3P_2$ state of Ar (in ArHe) or Ne (in HeNe). The radiative lifetime of the 1(I) state of HeNe (estimated from the vertical transition at 2.8 bohr) is 18 μs. *© 2001 American Institute of Physics.* [DOI: 10.1063/1.1398100]

I. INTRODUCTION

The determination of interaction potentials for rare gas dimers in excited states is important for the elucidation of the processes involved in collisions of ground state and excited state rare gas atoms.[1–3] Because they are used as sources in UV lasers, rare gas excimers and exciplexes have attracted a lot of research interest over the past decades. Despite the conceptual simplicity of their electronic structure, however, accurate determinations of the interaction potentials, especially for the heteronuclear dimers, are rare due to the computational difficulties involved. The precise determination of the shallow minima generally found in these systems require large CI expansions, and it is essential to include spin-orbit coupling in order to calculate the atomic limits correctly. Semiempirical[4–6] and model potential calculations[7] have been employed with good success for the determination of the Rg*Rg′ potentials for internuclear distances larger than 5 bohr, covering the region where any shallow minima are to be found in these systems. It is expected that the possible Rydberg minima in the excited states will be at internuclear distances shorter than 5 bohr, however. The potential energy curve of a Rydberg state usually resembles that of the ground state of the core cation, following the simple description of a molecular cation core plus a Rydberg electron. In the case of the rare gas dimers, however, Rydberg minima are not typical for the excited states and instead, generally shallower minima are found at larger *R* than in the cation, as for example has been found in the *6p* states of the RgXe* systems.[8] Furthermore, additional features may be present in a given system, such as for the $\Omega = 0^+$ state of Xe $5p^5 6s[3/2] + \mathrm{Kr}$, for which a double-well potential, including a typical Rydberg minimum at short *R*, and a shallow minimum at large *R*, has been proposed by Pibel *et al.*[9] in a laser-induced fluorescence spectroscopic study of this system. Thus, the elucidation of the electronic structure of the excited states of rare-gas dimers is a very interesting and challenging problem. The most appropriate *ab initio* methods to calculate interaction potentials for the excited states of rare gas dimers, especially for the heavier pairs, make use of relativistic effective core potentials (RECP) and have been applied to states of ArNe[10] and ArKr.[11] Similar work on XeHe and XeAr[12] employed an RECP treatment combined with a model Hamiltonian calculation of the radial coupling matrix elements.

Beyond the determination of the potential energy curves, the interactions and transition moments of the excited states are also of interest. For example, the dipole transition moments are required for the study of radiative processes accompanying collisions between rare gas atoms,[1–3] such as the radiative quenching of the $^3P_2$ metastable states of rare gas atoms by collisions with Ne and He atoms.[13]

In the present work, multireference configuration interaction calculations (MRDCI) employing relativistic effective core potentials (RECP) have been carried out on the electronic states of ArHe and HeNe, analogous to our previous work on ArNe.[10] Potential energy curves and dipole transition moments have been calculated and radiative lifetimes of the excited states have been determined. The present work is part of an effort which started with our previous calculations on ArNe[10] towards a systematic theoretical description of the excited states of heteronuclear rare gas dimers Rg*Rg′ for different combinations of rare gas atoms, which show many

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TABLE I. Transition energies (cm^{-1}) of ArHe and HeNe at internuclear distance of 100.0 bohr compared to experimental atomic Ar and Ne levels, respectively.

Ω states	ArHe, ΔE theor.[a]	Ar* levels Expt.[c]	HeNe, ΔE theor.[b]	Ne* levels Expt.[c]
0^+(I)	0.0	0.0 ($J=0$)	0.0	0.0 ($J=0$)
0^-(I)	93 104		134 037	
1(I)	93 113		134 038	
2(I)	93 144	93 143.8($J=2$)	134 044	134 043.79($J=2$)
0^+(II)	93 738		134 461	
1(II)	93 759	93 750.6($J=1$)	134 470	134 461.24($J=1$)
0^-(II)	94 545	94 553.7($J=0$)	134 804	134 820.59($J=0$)
0^+(III)	95 345		135 957	
1(III)	95 342	95 399.9($J=1$)	135 984	135 890.67($J=1$)

[a] Energies shifted by 3808 cm^{-1}.
[b] Energies shifted by 2602 cm^{-1}.
[c] Reference 24.

common features in their potential energy curves, but also important differences, depending on the interplay of the factors determining them.

II. CALCULATIONS

The present calculations on ArHe include the ground and excited electronic states correlating with the limits Ar $(3p^5 4s,\ ^3P,^1P)$ plus ground state He, and similarly those on HeNe include the ground and excited states correlating with Ne $(2p^5 3s,\ ^3P,^1P)$ plus ground state He. In C_{2V} symmetry, the resulting states in each case comprise two $^1A_1$ states and one of $^3A_1$, $^1B_1$, and $^1B_2$, $^3B_1$ and $^3B_2$ symmetry, which correspond to the lowest two $^1\Sigma^+$, and the lowest $^3\Sigma^+$, $^1\Pi$ and $^3\Pi$ states, respectively. These states give rise to Ω states of $0^+(3)$, $0^-(2)$, 2(1), 1(3), and of total symmetry A_1, A_2, B_1 and B_2.[10,11]

The calculations have been carried out with the aid of a relativistic effective core potentials (RECP) version of the MRDCI programs, using the contracted CI implementation.[14–18] This involves a two-step procedure. In the first step Λ-S electronic states are determined in conventional CI calculations in which all the electronic integrals are calculated with the aid of RECPs and the SCF treatment includes only the scalar relativistic terms in addition to the conventional nonrelativistic Hamiltonian. The resulting Λ-S states are employed in the second step to form the full Hamiltonian matrix, including the spin-orbit interaction. Diagonalization is then carried out for each total symmetry to determine eigenvalues and eigenfunctions. In the present work, the latter are in turn employed for the computation of dipole transition moments between electronic states. These calculations are carried out for different values of the internuclear distance *R*, varying from 2.0 to 30.0 bohr for HeNe and from 2.4 to 20.0 bohr for ArHe and also for $R=100$ bohr.

Relativistic core potentials are employed for Ar (*K* and *L* shells) and Ne (*K* shell).[19] The one-electron basis set employed for Ar is the $(12s\ \ 9p/6s\ \ 5p)$ basis of McLean and Chandler[20] augmented with one set of *d* functions for polarization (exponent 0.736) and three *s* and one *p* diffuse functions with exponents 0.08, 0.04, and 0.015 and 0.0472, respectively. It was found necessary to employ such a triple-zeta basis for the 4*s* function of Ar in order to obtain convergence in the resulting potentials. For He, a $(10s\ \ 3p/6s\ \ 3p)^{21}$ basis has been employed, augmented with one *d* polarization function (exponent 1.965), one diffuse *s*, and one set of diffuse *p* functions with exponents

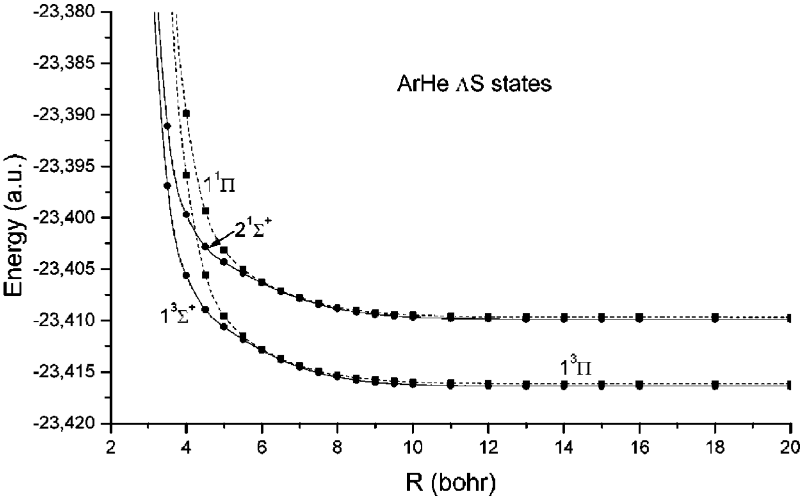

FIG. 1. Potential energy curves of the Λ-S excited states of ArHe.

TABLE II. Calculated energies (cm^{-1})[a] of the Ω states of ArHe.

R (a.u)	0^+(I)	0^+(II)	0^+(III)	2(I)	0^-(I)	0^-(II)	1(I)	1(II)	1(III)
3.00	2338	100 914	115 372	114 407	99 623	115 370	99 625	114 748	116 307
3.50	8887	95 272	100 518	99 493	94 013	100 503	94 022	99 845	101 420
3.75	5325	94 015	97 078	95 983	92 778	97 033	92 794	96 348	97 947
4.00	3154	93 190	95 063	93 841	92 011	94 946	92 039	94 226	95 850
4.25	1846	92 560	93 960	92 528	91 504	93 701	91 544	92 945	94 586
4.50	1063	92 050	93 388	91 712	91 146	92 955	91 192	92 171	93 815
4.75	599	91 661	93 071	91 188	90 879	92 492	90 920	91 697	93 329
5.00	328	91 373	92 864	90 837	90 670	92 186	90 699	91 392	93 007
5.25	175	91 156	92 708	90 586	90 497	91 966	90 516	91 177	92 779
5.50	87	90 986	92 578	90 398	90 351	91 796	90 362	91 011	92 606
5.75	38	90 845	92 461	90 247	90 221	91 655	90 228	90 874	92 465
6.00	13	90 723	92 355	90 119	90 104	91 532	90 108	90 753	92 344
6.25	2.4	90 617	92 257	90 011	89 999	91 425	90 002	90 647	92 239
6.50	0.0	90 526	92 169	89 918	89 907	91 333	89 909	90 556	92 149
6.75	2	90 445	92 088	89 837	89 823	91 251	89 826	90 473	92 068
7.00	6	90 375	92 017	89 767	89 749	91 179	89 754	90 401	91 997
7.25	12	90 314	91 952	89 707	89 685	91 117	89 690	90 338	91 934
7.50	15	90 261	91 896	89 655	89 631	91 064	89 636	90 284	91 881
7.75	20	90 215	91 847	89 611	89 583	91 018	89 589	90 237	91 834
8.00	23	90 175	91 804	89 572	89 542	90 978	89 549	90 197	91 793
8.50	31	90 113	91 736	89 513	89 479	90 917	89 487	90 135	91 728
9.00	36	90 071	91 689	89 472	89 434	90 875	89 443	90 091	91 682
9.50	40	90 040	91 655	89 443	89 404	90 845	89 413	90 060	91 650
10.00	43	90 019	91 632	89 422	89 383	90 824	89 392	90 039	91 627
11.00	47	89 996	91 606	89 401	89 362	90 803	89 371	90 017	91 603
12.00	48	89 987	91 596	89 392	89 352	90 794	89 361	90 007	91 592
13.00	50	89 983	91 590	89 388	89 348	90 789	89 357	90 003	91 588
14.00	50	89 982	91 589	89 387	89 348	90 789	89 357	90 003	91 587
15.00	51	89 981	91 588	89 386	89 346	90 788	89 356	90 001	91 585
16.00	51	89 982	91 589	89 387	89 347	90 789	89 356	90 002	91 586
18.00	51	89 981	91 589	89 386	89 346	90 788	89 356	90 001	91 585
20.00	51	89 981	91 588	89 387	89 347	90 788	89 356	90 002	91 585

[a] With respect to the lowest energy of the ground state.

0.0256 and 0.052 47, respectively. For Ne the ($10s\,5p\,2d\,1f/4s\,3p\,2d\,1f$) basis of Dunning[22] was modified by omitting the five s functions with the largest s exponents (contributing mostly to the $1s$ orbital for which RECPs are used) and uncontracting the remaining five s functions to obtain a ($5s\,5p\,2d\,1f/5s\,3s\,2d\,1f$) basis set. In addition, three diffuse s functions with exponents 0.04, 0.02, 0.01, and one set of diffuse p functions, with exponent 0.02, were included in the Ne basis. All the above basis functions are Cartesian Gaussian-type functions.

In MRDCI, as in all multireference methods, the choice of reference space is very important because it determines the zeroth order description of the states, and the CI spaces are generated by allowing single and double excitations with

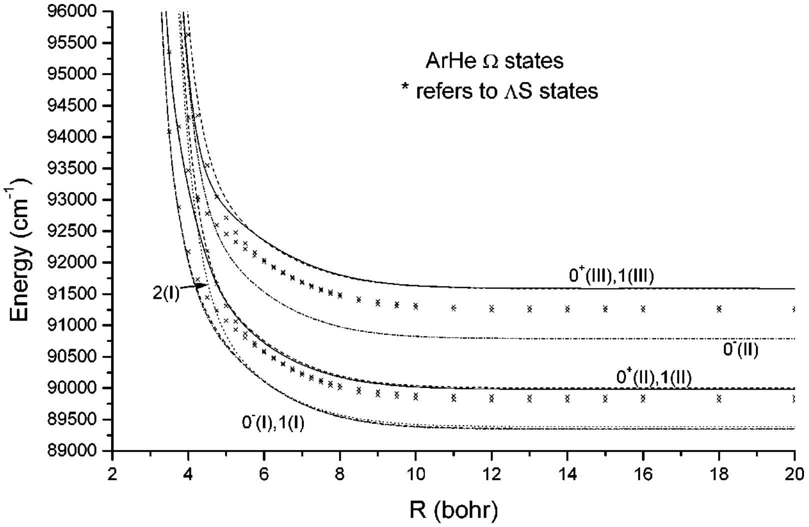

FIG. 2. Potential energy curves of the Ω states of ArHe.

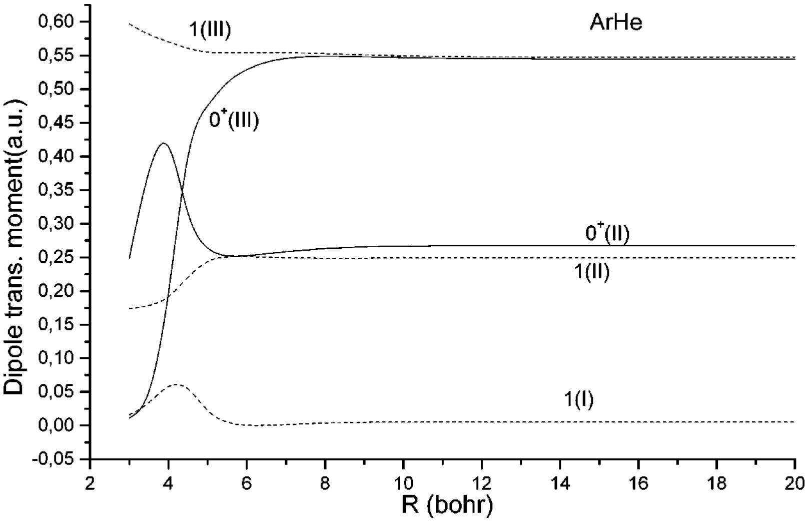

FIG. 3. Dipole transition moments for the allowed transitions from the excited states to the ground state of ArHe.

respect to all the reference configurations. The reference configurations employed in the present work have been determined by test calculations at different values of the internuclear distance in each case and they characterize the calculated wave functions throughout with a contribution of over 90%. For the calculations on ArHe the reference spaces consist of ten configurations for the ${}^1A_1$, nine configurations for the ${}^3A_1$, and six configurations for each of the ${}^1B_1$, ${}^3B_1$, ${}^1B_2$, and ${}^3B_2$ calculations. The CI spaces include each of the configuration functions resulting from all single and double excitations (i.e., selection threshold $T=0$) with respect to the reference configurations. The resulting CI spaces contain 132 979 configuration functions for the ${}^1A_1$, 212 011 for the ${}^3A_1$, 98 904 for the ${}^1B_1$ and the ${}^1B_2$, and 164 748 configuration functions for the ${}^3B_1$ and the ${}^3B_2$ calculations. Exploratory calculations determined that it is desirable to have $T=0$ calculations for the potentials of these systems where small energy differences need to be determined. For the CI calculations on HeNe the reference spaces consist of twelve configurations for the ${}^1A_1$, eleven for the ${}^3A_1$, and nine for each of the ${}^1B_1$, ${}^3B_1$, ${}^1B_2$, and ${}^3B_2$ spaces. The resulting MRDCI spaces consist of 221 198 configuration functions for the ${}^1A_1$, 386 501 for the ${}^3A_1$, 212 592 for the ${}^1B_1$ and the ${}^1B_2$, and 377 869 for the ${}^3B_1$ and the ${}^3B_2$ calculations. A full-CI correction[23] was applied to the eigenvalues in both systems.

The computed excitation energies at the internuclear distance of 100.0 bohr for both ArHe and HeNe are listed in Table I, along with the experimental values[24] for the levels of Ar* and Ne*, respectively. The theoretical levels have been shifted upward by 3766 cm^{-1} for ArHe and by 2602 cm^{-1} for HeNe, as the calculations tend to favor the Rydberg states over the ground state for which there is more correlation energy to be accounted for. This is a typical practice in such calculations as, for example, was the case for the calculations on ArKr.[11] As shown in Table I, the calculated splittings of the Ar*$(3p^5 4s, {}^3P, {}^1P)$ and the Ne*$(2p^5 3s, {}^3P, {}^1P)$ levels are in excellent agreement with the corresponding experimental values.

III. RESULTS AND DISCUSSION

A. ArHe

The potential energy curves of the excited Λ-S states of ArHe are plotted in Fig. 1, where it may be seen that they are totally repulsive. The spin-orbit coupling matrix elements be-

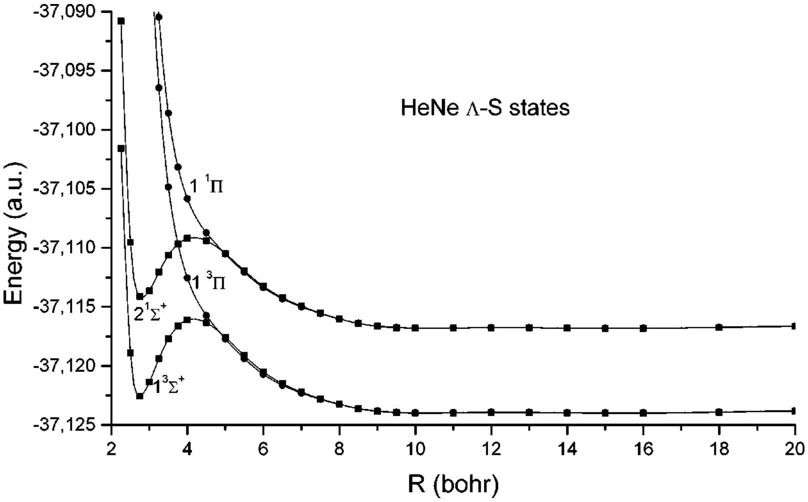

FIG. 4. Potential energy curves of the Λ-S excited states of HeNe.

TABLE III. Calculated energies[a] of the Ω states of HeNe.

R (bohr)	0^+(I)	0^+(II)	0^+(III)	2(I)	0^-(I)	0^-(II)	1(I)	1(II)	1 (III)
2.25	37 842	139 027	175 219	174 715	136 665	175 219	136 665	174 920	176 095
2.50	21 467	134 914	157 096	156 589	132 865	157 096	132 865	156 797	158 022
2.75	12 136	133 905	146 970	146 458	132 054	146 969	132 054	146 669	147 945
3.00	6804	134 002	141 285	140 764	132 308	141 283	132 309	140 980	142 318
3.25	3759	134 335	138 075	137 537	132 735	138 066	132 738	137 758	139 156
3.50	2037	134 602	136 278	135 695	133 085	136 241	133 092	135 925	137 378
3.75	1082	134 639	135 390	134 635	133 295	135 210	133 311	134 880	136 376
4.0	561	134 323	135 181	134 004	133 368	134 623	133 393	134 276	135 797
4.25	280	133 982	135 130	133 599	133 326	134 270	133 355	133 915	135 434
4.50	134	133 711	135 052	133 306	133 211	134 026	133 228	133 679	135 175
4.75	60	133 486	134 938	133 072	133 059	133 826	133 062	133 492	134 966
5.00	25	133 288	134 799	132 870	132 892	133 642	132 886	133 316	134 782
5.50	2	132 926	134 482	132 506	132 541	133 286	132 531	132 965	134 441
6.00	0	132 634	134 193	132 213	132 242	132 990	132 234	132 667	134 154
6.50	9	132 429	133 978	132 008	132 029	132 781	132 023	132 455	133 947
7.00	21	132 284	133 821	131 864	131 877	132 633	131 874	132 305	133 797
7.50	28	132 168	133 694	131 749	131 755	132 515	131 754	132 185	133 675
8.00	35	132 072	133 589	131 653	131 655	132 417	131 655	132 086	133 573
8.50	40	131 995	133 504	131 577	131 575	132 339	131 576	132 007	133 491
9.00	42	131 948	133 451	131 530	131 525	132 291	131 526	131 958	133 441
9.50	43	131 926	133 427	131 509	131 502	132 269	131 504	131 935	133 417
10.00	43	131 919	133 417	131 501	131 494	132 261	131 496	131 928	133 408
11.00	43	131 922	133 418	131 505	131 497	132 264	131 499	131 931	133 410
12.00	44	131 927	133 423	131 510	131 503	132 270	131 505	131 936	133 414
13.00	46	131 926	133 422	131 509	131 502	132 269	131 504	131 935	133 412
14.00	48	131 922	133 417	131 504	131 498	132 265	131 500	131 931	133 408
15.00	49	131 917	133 412	131 499	131 493	132 260	131 494	131 926	133 403
16.00	50	131 916	133 412	131 499	131 492	132 259	131 494	131 925	133 403
18.00	52	131 932	133 429	131 514	131 508	132 275	131 510	131 941	133 420
20.00	53	131 952	133 450	131 535	131 528	132 295	131 530	131 961	133 440

[a] With respect to the minimum of the ground state.

tween the Λ-S excited states of ArHe vary between 440 and 475 cm^{-1}. The energies obtained after the final diagonalization including the spin-orbit coupling are listed in Table II, in which the unshifted values (see above) are listed, and the potential energy curves of the excited Ω states of ArHe are plotted in Fig. 2, with the Λ-S states also indicated for comparison. As shown in Figs. 1 and 2 the excited electronic states of this system, which correlate with the first two excited atomic limits, are repulsive, both the Λ-S and the Ω states. In agreement with the present results, repulsive potentials for the excited states of ArHe, have been obtained at large internuclear distances ($R > 6.0$ bohr) in model potential calculations.[25] Similarly, a repulsive potential was obtained for the 1(I) state by semiempirical calculations[26] and also derived from experimental data for internuclear distances larger than 4.0 bohr.[27] The absence of any typical Rydberg minima at short R in the calculated potentials is consistent with the fact that the ground state potential of the cation, ArHe^+, has a very shallow minimum of only 262 cm^{-1} at 4.89 bohr[28] and Rydberg minima usually have smaller well depths than the corresponding cation potentials. The ground state potential of ArHe is also included in Table II for refer-

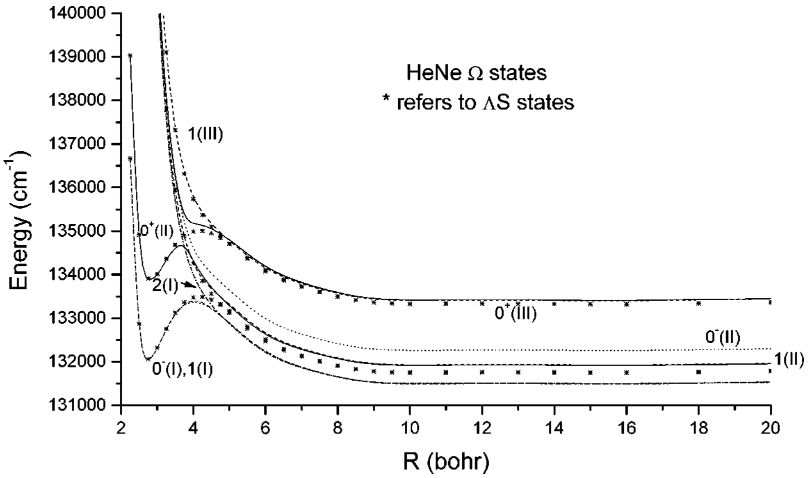

FIG. 5. Potential energy curves of the Ω states of HeNe.

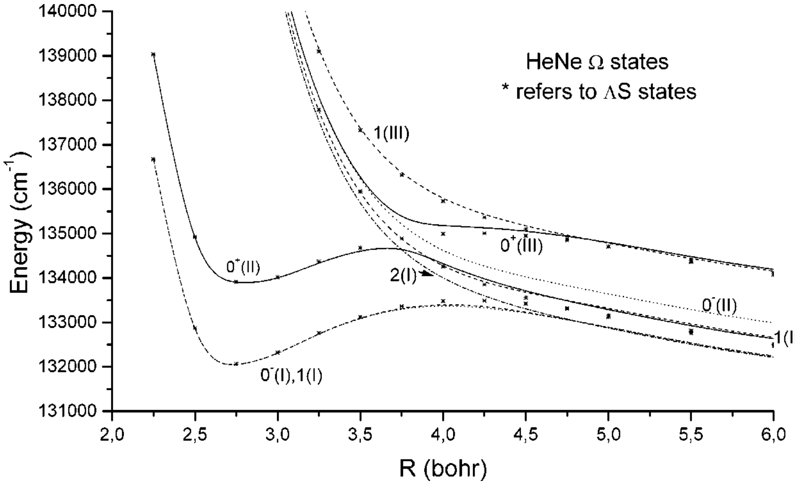

FIG. 6. Potential energy curves of the Ω states of HeNe in the short *R* region.

ence, from which it may be seen that the present calculations obtain a well depth of 51 cm^{-1}, whereas the experimental value is closer to 20.4 cm^{-1}.[29] As the interest of the present work is focused on the excited states, it was not considered necessary to pursue the ground-state potential more accurately, especially since there have been previous accurate determinations of it by various methods.[30,31]

The calculated dipole transition moments between the ground and the excited states are plotted in Fig. 3. As shown, large transition moments are calculated for the states correlating with atomic limits possessing allowed radiative transitions to the ground state. Small but nonzero transition moments are calculated at internuclear distances between 3 and 5 bohr for the radiative transition to the ground state from 1(I), which correlates with the $^3P_2$ metastable state of Ar.

B. HeNe

The results of the calculations on HeNe show some distinctions relative to the results on ArHe, as will be discussed in the following. In Fig. 4, the potential energy curves of the lowest Λ-*S* excited states of HeNe have been plotted. As shown therein, the potential energy curves of the $1\,^3\Sigma^+$ and the $2^1\Sigma^+$ $2p\sigma \rightarrow 3s$ states have Rydberg minima for *R* very close to the R_e of the ground state of the NeHe$^+$ cation,[32] whereas the $1\,^3\Pi$ and the $1\,^1\Pi$ states of HeNe do not show any such minima. It might be noted that all the above excited states are mainly characterized by a single p^5s type of configuration.

The spin orbit coupling matrix elements between the Λ-*S* excited states of HeNe vary between 200 and 250 cm^{-1} at large *R* and are slightly smaller (172–250 cm^{-1}) for shorter *R*. The results of the final diagonalization of the full Hamiltonian, including the spin-orbit coupling, are listed in Table III and plotted in Fig. 5, where again the Λ-*S* states are also indicated. As shown in Fig. 5, the spin-orbit interaction has no effect on the position of the Rydberg minima, which now appear in the potentials of the 0^-(I), 1(I), and 0^+(II) states of HeNe, but an avoided crossing between the 0^+ (II) and the 0^+ (III) states results in a smaller well depth for the 0^+(II) state than the corresponding minimum in the $2\,^1\Sigma^+$ state (see Fig. 6 in which the potentials at short *R* are plotted). Besides the above-mentioned Rydberg minima, there are no other minima in the excited electronic states of HeNe. This is consistent with previously derived potentials of the excited states of HeNe at large internuclear distances.[7,27]

The energies listed in Table III are as calculated, i.e., unshifted. As in Table II for ArHe, the ground state potential is included in Table III for reference. In this case, the calculated well depth of the ground state is 53 cm^{-1}, with the experimental only 14.5 cm^{-1}. Again the accurate determination of the ground state potential has not been pursued. Such small energy differences require a different level of theoretical treatment than employed here, as has been found in previous RECP calculations on KrAr.[11] In any case, this error is small compared to the calculated well depths in the excited states of HeNe (see the following).

In Table IV, some data relevant to the Rydberg minima and the barriers found in the 0^-(I), 1(I) and 0^+(II) states of HeNe are listed. As shown therein, the well depths of the Rydberg minima with respect to the barrier height, which are in fact local minima lying above the corresponding dissociation limits, are 1344 cm^{-1} at $R_{\min}$, 2.72 bohr for the 0^-(I), and 1(I) states and 744 cm^{-1} at 2.81 bohr for the minimum in the 0^+(II) state of HeNe. These minima lie at vertical energies from the ground state (T_e in Table IV) of 134 651 and 136 500 cm^{-1}, respectively, and the well depths are calculated with respect to the barrier in each case found at 4.00 bohr in the potential energy curves of the 0^-(I) and 1(I) states and at 3.75 for 0^+(II). For comparison, the well depth of the ground state of HeNe$^+$ is 6216 cm^{-1} (Refs. 32 and 33) and the experimental values for R_e vary between 2.46 and 2.82 bohr,[33] whereas the theoretical R_e values lie between 2.67 and 2.745 bohr. Thus the calculated minima in the po-

TABLE IV. Well depths and radiative lifetimes $\tau_{\rm rad}$ for the Rydberg minima of the 0^-(I), 1(I), and 0^+(II) excited states of HeNe.

State	$R_{\min}$, $R_{\rm barrier}$ (bohr)	T_e[a] (cm^{-1})	$E_{\min}$[b] (cm^{-1})	$\tau_{\rm rad}$
0^-(I), 1(I)	2.72, 4.00	134 651	1344	18 μs
0^+(II)	2.81, 3.75	136 500	744	6.9 ns

[a] Vertical energy difference with respect to the ground state. Shifted energy employed.

[b] Well-depth with respect to the barrier.

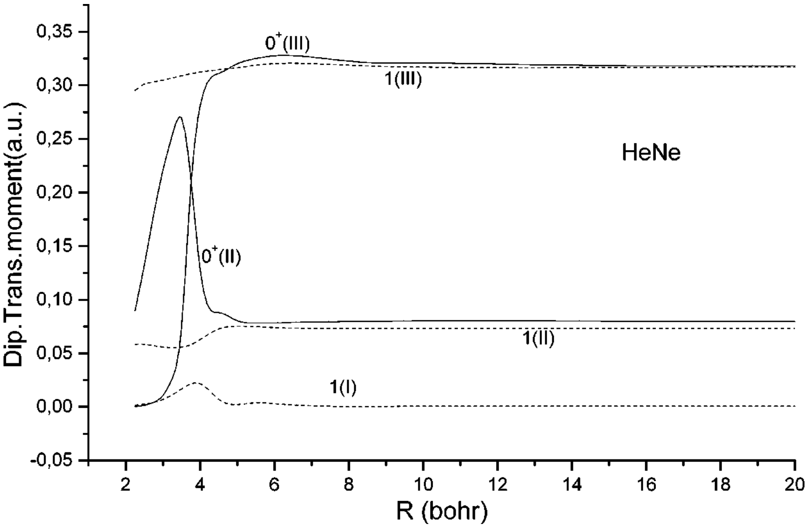

FIG. 7. Dipole transition moments for the allowed transitions from the excited states to the ground state of HeNe.

tential energy curves of the excited states of HeNe are typical Rydberg minima, as they occur at internuclear distance similar to R_e of the cation ground state. It may be noted that the well depth of the Rydberg minima is much smaller than the D_e value of the ground state of the cation.

The calculated transition dipole moments between the excited states and the ground state are plotted in Fig. 7. A comparison of Figs. 3 and 7 shows that the general features of the two plots are similar except that larger transition moments are calculated for the ArHe system than for HeNe. The radiative lifetimes corresponding to the local minima in the excited states of HeNe, have been estimated from the vertical electronic dipole transition moment at $R_{\min}$ in each case and are also given in Table IV. They are 6.9 ns for the minimum of the 0^+(II) state and 18 μs for the minimum of the 1(I) state, which correlates with the metastable $^3P_2$ state of Ne plus ground state He.

IV. CONCLUSIONS

Potential energy curves and dipole transition moments have been calculated for the lower-lying Ω states of ArHe and HeNe by RECP-MRDCI calculations. Repulsive potential energy curves are obtained for all the states of ArHe correlating with Ar* $(3p^5 4s, {}^3P, {}^1P)+$He. Similarly, repulsive potential energy curves are obtained for the Ω states of NeHe except for the 0^-(I), 1(I), and 0^+(II) states, for which typical Rydberg minima are obtained at $R_{\text{He-Ne}}$ 2.72 (for the first two states) and 2.81 bohr, respectively. The calculated dipole transition moments and radiative lifetimes of the excited states show that strong transitions occur for the states correlating with atomic limits from which radiative transitions to the atomic ground state are allowed, while nonzero dipole transition moments are calculated at short R for the transition to the ground state from 1(I), indicating the possibility of radiative quenching of metastable $^3P_2$ rare gas atoms in collisions with other rare gas atoms.

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