

Is E112 a relatively inert element? Benchmark relativistic correlation study of spectroscopic constants in E112H and its cation

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(Received 29 December 2005; accepted 25 April 2006; published online 8 June 2006)

We report the first results of relativistic correlation calculation of the spectroscopic properties for the ground state of E112H and its cation in which spin-orbit interaction is taken into account non-perturbatively. Studying the properties of E112 (eka-Hg) is required for chemical identification of its long-lived isotope, $^{283}\text{112}$. It is shown that appropriate accounting for spin-orbit effects leads to dramatic impact on the properties of E112H whereas they are not so important for E112H⁺. The calculated equilibrium distance, $R_e^{\text{calc}}=1.662 \text{ \AA}$, in E112H is notably smaller than $R_e^{\text{expt}}=(1.738\pm 0.003) \text{ \AA}$ and $R_e^{\text{calc}}=1.738 \text{ \AA}$ in HgH, whereas the dissociation energy, $D_e^{\text{calc}}=0.42 \text{ eV}$, in E112H is close to $D_e^{\text{expt}}=0.46 \text{ eV}$ and $D_e^{\text{calc}}=0.41 \text{ eV}$ in HgH. These data are quite different from $R_e^{\text{NH}}=1.829 \text{ \AA}$ and $D_e^{\text{NH}}=0.06 \text{ eV}$ obtained for E112H within the scalar-relativistic Douglas-Kroll approximation [Nakajima and Hirao, *Chem. Phys. Lett.* **329**, 511 (2000)]. Our results indicate that E112 should not be expected to behave like a noble gas in contrast to the results by other authors.

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INTRODUCTION

The superheavy element 112 (eka-Hg) was discovered at GSI (Darmstadt) in 1996 within the “cold” fusion reaction.¹ The recent observation at FLNR (Dubna) of the “ α -SF” chain, attributed to 4 sec α -decay branch of $^{283}\text{112}$ followed by a 0.2 sec spontaneous fission of $^{279}\text{110}$ (Ds),² raised the question as to what species was observed in the previous “hot” fusion FLNR experiment.³ Moreover, the production of $^{283}\text{112}$ in the reaction of ^{48}Ca and ^{238}U was not confirmed at LBNL (Berkeley).^{4,5} However, a very specific decay mode of the short “ α -SF” chain offered a unique chance to unambiguously identify $^{283}\text{112}$ in a chemical experiment.

To our knowledge, starting from the papers of Pitzer⁶ and Fricke⁷ in 1975 it was mainly suggested by other authors that E112 behaves rather like a rare gas than Hg. In Ref. 8, the confusing conclusions about both the relative inertness of E112 compared to Hg and the similarity of E112 to Hg were made in the abstract and conclusion, respectively. The first attempt to identify E112 chemically was made at FLNR^{9,10} but no spontaneous fissions were detected. It was interpreted as indication of the Rn-like behavior of E112 as well.

Chemical experiments on studying properties of E112 are currently under way at FLNR¹⁰ and similar work is in progress at GSI and PSI (Villigen)¹¹ that involves an attempt to clarify the recent observation of the decay chains and fission products associated with the production of E114 and E116;² being their decay product, E112 should be detectable in gas-phase chromatographic experiments. The experimental study of superheavy element (SHE) properties (see Refs. 12 and 13, and references therein) is very difficult because of their short half-lives and extremely small quantities, with

only single atoms being available for research. In this connection, reliable theoretical prediction of their properties based on *ab initio* benchmark calculations is highly desirable. As a first step in the extensive study of chemistry of E112, bonding in simple diatomic molecules such as E112H should be studied. The earlier studies of eka-mercury fluorides¹⁴ are not so sensitive because both mercury and xenon are known to react in a fluorine atmosphere. On the other hand, the Hg₂, Xe₂, and E112₂ dimers^{8,15} are Van der Waals systems with small dissociation energies. By contrast, the ground state RnH and XeH molecules are not observed in the gas phase, whereas HgH can be obtained by radiofrequency discharge in hydrogen and metal vapor (see, e.g., Ref. 16).

It was shown in Ref. 17 for the examples of E112 and other SHE's that the errors in calculations due to employing the point nucleus (instead of the realistic Fermi nuclear model) reach 0.4 eV for transition energies between low-lying states, whereas neglecting the Breit effects leads to the errors up to 0.1 eV. Generalized relativistic effective core potentials (GRECP's)¹⁸ were generated for E112 and other SHE's¹⁷ which allow one to simulate the Breit interaction and the Fermi nuclear model in an economic way with very high precision.¹⁹ The accuracy of these GRECP's and of the RECP's of other groups was estimated in atomic finite-difference SCF calculations with Coulomb two-electron interaction and point nucleus as compared to the corresponding all-electron Dirac-Fock-Breit calculations with the Fermi nuclear model. It was justified and checked in Refs. 17 and 19 that the GRECP method allows one to carry out reliable calculations of SHE's and their compounds within the level of “chemical accuracy” (1 kcal/mol, 0.043 eV, or 350 cm⁻¹ for valence transition energies) when the valence and outer core shells are appropriately treated. Hence, the overall accuracy of calculations in heavy-atom molecules is limited, in

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practice, by the current capabilities of correlation methods and codes and not by the GRECP approximation.

In this paper, we present GRECP calculations of spectroscopic constants for the ground states of the E112H molecule and its cation exploiting the MOLGEP code.²⁰ To our knowledge, only three calculations on E112H and E112H⁺ were published.^{8,14,21} In Ref. 21, the third order Douglas-Kroll (DK3) method was applied to calculation of E112H and its ions. The correlations were taken into account by second-order Møller-Plesset perturbation theory (MP2) and by the coupled cluster method with single, double (and triple) cluster amplitudes, CCSD(T), for the 19 outer electrons (in the shells originating from the 6*p*, 6*d*, 7*s*, 7*p* shells of E112 and the 1*s* shell of H) of the E112H molecule. It is not clear from Ref. 21 why the correlations with the 6*p* shell of E112 are considered but correlations with the 6*s* and 5*f* shells are not whereas the small value of calculated dissociation energy, $D_e^{\text{NH}}=0.06$ eV, could be strongly influenced by the latter. The 6*s* and 6*p* shells are closely localized in space, whereas the 5*f* and 6*p* shells have close orbital energies. The effect of the finite nuclear size was taken into account but the Breit effects and even the spin-orbit (SO) interaction were neglected (i.e., only scalar-relativistic calculations were made). It is clear that both effects increase with the nuclear charge *Z*, so these approximations can be inappropriate for SHE compounds even if they are justified for their lighter analogues.

In Refs. 8 and 14, the RECP calculations of E112H⁺ (but not E112H) were carried out by the MP2 and CCSD(T) methods. In Ref. 14, complete active space SCF and multi-reference configuration interaction (MRCI) calculations of E112H⁺ were also performed.⁴² The SO, finite nuclear size and Breit effects were taken into account at the generation stage of the pseudopotential (PP) of Seth *et al.*¹⁴ It should be noted that the parameters of the spin-averaged part of this PP were adjusted with the help of atomic PP calculations in the LS-coupling scheme. However, the SO splittings for SHE's are comparable with energies of splittings between the spinors with different orbital quantum numbers (see, e.g., Ref. 17) and such an approximate PP generation scheme may lead to serious errors (see <http://www.qchem.pnpi.spb.ru/Basis/Bonn03.pdf>). The SO interaction was taken into account in the calculations from Ref. 8. However, the author applied the 20-electron RECP of Nash *et al.*²² The Breit effects were not considered at the generation stage of this RECP. It is not stated in Refs. 8 and 22 which nuclear model was used there. In our test calculations,¹⁷ the errors of this RECP in reproducing the results of the all-electron Dirac-Fock-Breit calculations with the Fermi nuclear model were up to 1 eV for transition energies between low-lying states. Moreover, the basis set superposition errors (BSSE's)^{23,24} were not estimated in the calculations from Ref. 8.

METHODS AND CALCULATIONS

The GRECP,^{17–19,25} Fock-space relativistic CC-SD (RCC-SD)^{26,27} and spin-orbit direct configuration interaction (SODCI)^{28,29} methods were used for the present calculations. The gaussian expansions of our GRECP and (16, 21, 16, 12, 14)/[4, 6, 4, 2, 1] basis set for E112 are avail-

able at our website <http://www.qchem.pnpi.spb.ru/Basis/>. In the SODCI calculation, the relativistic scheme of configuration selection was applied.³⁰

Two series of Fock-space RCC-SD calculations were performed for E112H using GRECP. The ground state of the cation E112H⁺ served as the reference in the first series (denoted by RCC-SD-1), and the Fock-space scheme was



with an electron added in the lowest unoccupied σ orbital of E112H⁺. The second series (RCC-SD-2) started from the ground state of the anion E112H⁻ as the reference using the Fock-space scheme



with electrons removed from the highest occupied σ orbital of E112H⁻. Moreover, the RCC-SD calculations of E112 (to calculate counterpoise corrections and D_e) were carried out where the 6*d*¹⁰7*s*² ground state of the E112 atom was used as the reference and the Fock-space scheme was



with an electron removed from the 6*d* or 7*s* shell.

Our test atomic RCC calculations on E112 showed that at least 34 outer electrons of the atom (occupying the 5*f*, 6*s*, 6*p*, 6*d*, 7*s*, and 7*p* shells) should be correlated and the basis set should include up to *i*-type functions (*l*=6) in order to calculate the excitation and ionization energies with “chemical accuracy”. Nevertheless, we expect that the contributions of the core correlations will be less important for the molecule than for the atom as was found in our similar calculations^{25,31,32} on Hg and HgH. This is, in particular, supported by a large orbital energy separation between 5*p* and 5*d* shells in Hg ($\epsilon[5p_{3/2}; 5d_{3/2}] \approx -2.8; -0.65$ a.u.) and by a comparable separation between 6*p* and 6*d* shells in E112 ($\epsilon[6p_{3/2}; 6d_{3/2}] \approx -2.4; -0.56$ a.u.) Therefore, only 13 outer electrons for the E112H molecule (12 electrons for E112H⁺ in the shells originating from the 6*d*, 7*s*, 7*p* shells of E112 and the 1*s* shell of H) were correlated in the present calculations. Precise calculations with the larger number of correlated electrons when the SO interaction is explicitly treated are rather time-consuming and not yet practical.

In scalar-relativistic CC-SD calculations, we have also estimated (see Table I) that correlations with the 6*p* shell of E112 give relatively small contributions to the spectroscopic constants in E112H and E112H⁺ except for D_e in E112H⁺. This cation dissociates to E112⁺(6*d*_{3/2}⁴6*d*_{5/2}⁵7*s*_{1/2}²)+H(1*s*)³³ in contrast to HgH⁺, which dissociates to Hg⁺(5*d*_{3/2}⁴5*d*_{5/2}⁶6*s*_{1/2}¹)+H(1*s*). The 6*p* shell has almost the same spatial extent as the 6*d* shell, so correlations between these shells are important for transitions with an essential change in the occupation number for the 6*d* shell. In principle, the D_e value for E112H⁺ can be easily corrected using our atomic RCC results for the ionization potential of the 6*d*_{5/2} subshell of E112. However, we observed large compensations between contributions accounting for correlations

TABLE I. Spectroscopic constants of the ground states of the E112H molecule and the E112H⁺ ion from two-component RCC-SD and scalar-relativistic CC-SD calculations with GRECP in the H (8, 4, 3)/[4, 2, 1] ANO and E112 (16, 21, 16, 12, 14)/[4, 6, 4, 2, 1] basis set. Our corresponding results for HgH and HgH⁺ and the results of other groups for E112H and E112H⁺ are also presented for comparison. R_e is in Å, D_e in eV, Y_{02} in 10^{-6} cm⁻¹, other values in cm⁻¹.

Molecule	Method	R_e	w_e	D_e	B_e	$w_e x_e$	α_e	$-Y_{02}$
Our calculations:								
HgH ⁺	GRECP/12e-RCC-SD-1	1.596	2037	2.67	6.60	39	0.200	279
HgH ⁺	GRECP/12e-RCC-SD(T)-1	1.599	2013	2.68	6.58	41	0.208	282
HgH ⁺	Experiment ^{35,37}	1.594±0.000	2031±3	(2.75±0.36) ^a	6.61±0.00	44±3	0.206±0.000	285±0
Our calculations:								
E112H ⁺	GRECP/20e-CC-SD-1	1.537	2587	4.60	7.10	46	0.198	215
E112H ⁺	GRECP/20e-CC-SD-2	1.531	2681	4.46	7.15	35	0.168	205
E112H ⁺	GRECP/18e-CC-SD-1	1.537	2588	4.61	7.10	47	0.198	215
E112H ⁺	GRECP/18e-CC-SD-2	1.531	2680	4.46	7.16	35	0.169	205
E112H ⁺	GRECP/12e-CC-SD-1	1.535	2590	4.96	7.12	47	0.200	216
E112H ⁺	GRECP/12e-CC-SD-2	1.527	2679	4.75	7.19	37	0.175	208
E112H ⁺	GRECP/12e-RCC-SD-1	1.537	2569	3.96	7.11	47	0.201	218
E112H ⁺	GRECP/12e-RCC-SD-2	1.519	2752	3.80	7.28	45	0.187	204
E112H ⁺	GRECP/12e-RCC-SD-1+HOCA	1.540	2547	4.35	7.08	45	0.195	220
Other groups' calculations:								
E112H ⁺	DK3/18e-CCSD ²¹	1.528	2621		7.18			
E112H ⁺	DK3/18e-CCSD(T) ²¹	1.532	2595		7.15			
E112H ⁺	PP/CCSD(T) ^{14b}	1.515	2640	5.15		51		
E112H ⁺	PP/MRCI+SO ^{14b}	1.503	2620	3.86				
E112H ⁺	PP/CCSD(T)+SO ^{14b}	1.517	2673	4.09		52		
E112H ⁺	RECP/RCCSD(T) ^{8b}	1.583		3.50				
Our calculations:								
HgH	GRECP/13e-RCC-SD-1	1.709	1575	0.35	5.76	56	0.262	312
HgH	GRECP/13e-RCC-SD(T)-1	1.738	1395	0.41	5.56	83	0.348	363
HgH	Experiment ^{16,35,36}	1.738±0.003	1403±18	0.46±0.00	5.57±0.02	98±23	0.337±0.067	345±1
HgH	Experiment ³⁷	[1.766] ^c	[1203] ^c	0.46	[5.39] ^c			[395] ^c
Our calculations:								
E112H	GRECP/21e-CC-SD-1	1.742	1438	-0.03	5.53	113	0.409	340
E112H	GRECP/21e-CC-SD-2	1.801	1104	-0.02	5.15			
E112H	GRECP/19e-CC-SD-1	1.741	1439	-0.03	5.53	113	0.409	340
E112H	GRECP/19e-CC-SD-2	1.801	1102	-0.02	5.15			
E112H	GRECP/13e-CC-SD-1	1.746	1402	-0.03	5.50	119	0.429	354
E112H	GRECP/13e-CC-SD-2	1.808	1038	-0.05	5.10			
E112H	GRECP/13e-RCC-SD-1	1.638	1859	0.36	6.25	95	0.338	288
E112H	GRECP/13e-RCC-SD-2	1.663	1649	0.32	6.06	123	0.425	340
E112H	GRECP/13e-RCC-SD-1+HOCA	1.662	1800	0.42	6.07	152	0.385	287
Other groups' calculations:								
E112H	DK3/19e-CCSD ²¹	1.823	991	0.04	5.05			
E112H	DK3/19e-CCSD(T) ²¹	1.829	1007	0.06	5.02			

^aCited in Refs. 35 and 37 as uncertain.

^bNote that the RCCSD(T), RMRCI+SO, RCCSD(T)+SO values from Ref. 14 and the CCSD(T) values from Ref. 8 are listed. The acronyms for these calculations (the last one is in the *jj*-coupling scheme, the other ones are scalar-relativistic where the second and third ones are corrected for the SO effects) are redefined in accordance with the other notations in this paper.

^cCited in Ref. 37 as corresponding to the zero vibrational level.

with core shells and for basis functions with high angular momenta. Thus, the above ionization potential from the calculation with 12 correlated electrons in the basis including up to *g* functions (*l*=4) differs from that with 52 electrons and *l* up to 8 only by +773 cm⁻¹ (0.10 eV).

The calculations were carried out for 15 internuclear distances from 2.3 to 3.7 a.u. at an interval of 0.1 a.u. The spec-

troscopic constants were calculated by the Dunham method in the Born-Oppenheimer approximation. All our RCC and SODCI results reported in Table I, were improved using counterpoise corrections (CPC's)^{23,24} calculated for the E112 $6d^{10}7s^2$ state with a ghost H atom. CPC's calculated for the ground state of the H atom are about 1 cm⁻¹, and are therefore ignored.

RESULTS AND DISCUSSION

Our results for the ground states of E112H and E112H⁺ are collected in Table I. The corresponding results^{25,32} for HgH and HgH⁺ and the results of other groups^{8,14,21} for E112H and E112H⁺ are also presented for comparison. In the GRECP/RCC-SD-1 calculations one can observe the bond length contractions for E112H and E112H⁺ of 0.07 and 0.06 Å with respect to HgH and HgH⁺. Detailed comparison of our results for HgH and HgH⁺ with the results of other groups and the experimental data can be found in Ref. 32.

Our RCC-SD values for spectroscopic constants show considerable differences between two Fock-space schemes, GRECP/RCC-SD-1 and GRECP/RCC-SD-2. Such differences are caused by the truncation of the CC operator and indicate significant contributions from the omitted higher-order (triple, etc.) cluster amplitudes (HOCA). The HOCA influence on the total energies at each point of the potential curves was estimated with the help of the configuration interaction corrections on HOCA³⁴ calculated as differences in the total energies of the SODCI and RCC-SD-1 values. In these calculations, the same numbers of electrons were correlated as in the above RCC-SD case, but a reduced basis set, [4, 4, 3, 1] on E112 and [3, 2] on H, was used because approaching the full configuration interaction limit in SODCI calculations becomes too time-consuming for larger basis sets.

Except for the dissociation limit, HOCA have a small effect on E112H⁺ since the cation is a closed shell system. It is well known that the CC approach works particularly well for closed-shell states, which is confirmed by the comparison of the GRECP/12e-RCC-SD-1 results with and without HOCA correction for E112H⁺. The change in D_e is mainly due to different ionization potentials for the $6d_{5/2}$ electron of the E112 atom in the RCC-SD-1 and SODCI calculations. The GRECP/12e-RCC-SD-2 results show considerable distinctions from the results corrected by HOCA because E112H⁺ is calculated in the high Fock-space sector, (2,0), in which some loss of accuracy takes place. The HOCA contribution for E112H is important. Similar trend was observed in our GRECP/RCC calculations³² on HgH when the effect of the triple cluster amplitudes was taken into account for 13 electrons that essentially improved the agreement with the experimental data.

The differences between DK3/CCSD(T)²¹ and our GRECP/RCC-SD-1+HOCA results are small for E112H⁺, but are importantly larger for E112H. In particular, unlike our GRECP/13e-RCC-SD-1+HOCA bond length, the DK3/19e-CCSD(T) value²¹ for E112H is larger than the experimental data^{16,35-37} for HgH. It is worthwhile to note that the DK3/CCSD(T) calculations²¹ are scalar-relativistic whereas our RCC and SODCI calculations are performed with the spin-dependent GRECP. To check the effect of the SO interaction, we have also carried out scalar-relativistic CC calculations with the spin-averaged GRECP part. The same basis, number of correlated electrons, Fock-space schemes, etc. were taken as in the RCC calculations. One can see from

comparing our CC-SD and RCC-SD results that the SO effect is small for E112H⁺ (except for D_e) but is essential for E112H.

The R_e and w_e values for E112H⁺ by the PP/CCSD(T) method from Ref. 14 (see the footnote in Table I) differ from the DK3/18e-CCSD(T) results²¹ by -0.017 Å and $+45\text{cm}^{-1}$. The corresponding PP/CCSD(T)+SO values differ from our GRECP/12e-RCC-SD-1+HOCA results by -0.023 Å and $+126\text{cm}^{-1}$. The RECP/RCCSD(T) equilibrium distance for E112H⁺ from Ref. 8 differs from our GRECP/RCC-SD-1+HOCA result by $+0.04$ Å and even more from the results of other groups.^{14,21} The difference between the RECP/RCCSD(T) equilibrium distance calculated in Ref. 8 for HgH⁺ and the experimental datum is -0.04 Å. Thus, in contrast to our results, the RECP/RCCSD(T) calculations⁸ give a larger bond length for E112H⁺ than for HgH⁺ by 0.03 Å.

One can, however, expect some increase in R_e for E112H⁺ and decrease for E112H when accounting for correlations with the inner shells. In our scalar-relativistic calculations, a small increase in D_e was observed with a larger basis set.

CONCLUSIONS

It is well known that properties of SHE's are somewhat different from those of their lighter analogues particularly due to very strong relativistic effects (see Ref. 27 and references therein). Therefore, even those approximations which work well for the lighter analogues (neglecting the SO interaction for Σ states, the suggested effective state of an atom in a molecule, the preferred valency, etc.) should not be used for SHE's without serious checking and analyzing. The calculated equilibrium distance, R_e , in E112H is notably smaller than that in HgH. Therefore, one can also expect smaller bond lengths for the other E112 compounds in comparison with Hg compounds. There is a long-term discussion in scientific community whether E112 will behave like Hg or Rn. Ground-state RnH and XeH molecules are not observed in the gas phase. Our calculations for the E112H molecule do not predict a large dissociation energy, D_e , but it is close to that of HgH. It is sometimes suggested that the interaction between E112 and H can be well described by the dispersion interaction only. However, the latter is correct at large distances, much larger than the sum of atomic radii, whereas at short distances, the dispersion interaction becomes divergent. We have calculated the average radii $\langle r \rangle$ of the outermost shell for some atoms within Hartree-Fock-Dirac-Breit approximation and have also tabulated below the experimental data for polarizability (α) and ionization potential (I) of Hg, Xe, and H. The calculated values from Refs. 14 and 33 are presented for E112. The dispersion interaction energy is defined

$$E_{\text{disp}}(R_{AB}) = \frac{3}{2} \frac{I_A I_B}{I_A + I_B} \frac{\alpha_A \alpha_B}{R_{AB}^6}, \quad (4)$$

where R_{AB} is the internuclear distance between atoms A and B. The Xe atom has the smaller atomic radius than E112 and Hg, therefore, the stronger dispersion interaction energy should be expected for XeH than E112H and HgH (at $R_{AB} = r_A + r_B$),

$$\begin{aligned} r_{\text{Hg}} &= 2.85 \text{ a.u.} \\ r_{\text{E112}} &= 2.50 \text{ a.u.} \\ r_{\text{Xe}} &= 2.35 \text{ a.u.} \\ r_{\text{H}} &= 1.50 \text{ a.u.} \end{aligned}$$

$$\begin{aligned} \alpha_{\text{Hg}} &= 34. \text{ a.u.} \\ \alpha_{\text{E112}} &= 26. \text{ a.u.} \\ \alpha_{\text{Xe}} &= 27. \text{ a.u.} \\ \alpha_{\text{H}} &= 4.5 \text{ a.u.} \end{aligned}$$

$$\begin{aligned} I_{\text{Hg}} &= 0.384 \text{ a.u.} \\ I_{\text{E112}} &= 0.440 \text{ a.u.} \\ I_{\text{Xe}} &= 0.446 \text{ a.u.} \\ I_{\text{H}} &= 0.500 \text{ a.u.} \end{aligned}$$

$$\begin{aligned} E_{\text{disp}}(r_{\text{Hg}}+r_{\text{H}}) &= 0.20 \text{ eV} \\ E_{\text{disp}}(r_{\text{E112}}+r_{\text{H}}) &= 0.27 \text{ eV} \\ E_{\text{disp}}(r_{\text{Xe}}+r_{\text{H}}) &= 0.36 \text{ eV} \end{aligned}$$

Thus, the dispersion interaction do not describe satisfactory the bonding of the atoms of our interest. In turn, our GRECP/RCC-SD-1+HOCA calculations demonstrate the presence of a chemical bond between E112 and H. Therefore, we believe that the chemistry of singly-valent E112 rather resemble Hg than noble gas. That point is also supported by calculations of other E112 compounds^{38–41} though the relativistic DFT results obtained in Refs. 38 and 39 are rather contradictory and cannot be considered as reliable.

ACKNOWLEDGMENTS

The RCC-SD code of U. Kaldor, E. Eliav, and A. Landau together with the SODCI code of R. J. Buenker and his colleagues H. -P. Liebermann and A. B. Alekseyev were used in our calculations. We are grateful to A. Zaitsevskii and Yu. Tchuvil'sky for discussions and corrections in the paper. The present work is supported by the RFBR grant 06-03-33060. T. I. thanks the Russian Science Support Foundation.

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