

**Predicted spectrum of atomic nobelium**Anastasia Borschevsky and Ephraim Eliav  
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The electronic spectrum of atomic nobelium (element 102) is calculated in preparation for a planned experiment. The intermediate-Hamiltonian (IH) coupled-cluster method is applied to the ionization potential and excitation energies of the atom, using a large basis set ( $37s\ 31p\ 26d\ 21f\ 16g\ 11h\ 6i$ ) and correlating the outer 42 electrons. All the levels studied are obtained simultaneously by diagonalizing the IH matrix. The rows and columns of this matrix correspond to all excitations from correlated occupied orbitals to virtual orbitals in a large  $P$  space ( $8s\ 6p\ 6d\ 4f\ 2g\ 1h$ ), and the matrix elements are “dressed” by including excitations to the higher virtual orbitals ( $Q$  space) at the coupled cluster singles-and-doubles level. Lamb shift corrections are included. The accuracy is assessed by applying the same method to ytterbium, the lighter homologue of No. The calculated ionization potential of Yb is within 3 meV of experiment, and the average error in the lowest 20 excitation energies of the atom is  $300\text{ cm}^{-1}$ . Nobelium is the heaviest element for which a reliable semiempirical estimate of the ionization potential exists, 6.65(7) eV; the calculated value of 6.632 eV is in excellent agreement. Transition amplitudes are obtained from an extensive relativistic configuration interaction calculation. The outstanding feature of the predicted nobelium spectrum is a very strong line at  $30\ 060\text{ cm}^{-1}$ , with an amplitude  $A=5.0\times 10^8\text{ s}^{-1}$ , corresponding to the  $7s7p\ ^1P_1\rightarrow 7s^2\ ^1S_0$  transition. Putting the error limit conservatively at 0.1 eV, we predict a strong feature in the No spectrum at  $30\ 100\pm 800\text{ cm}^{-1}$ .

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**I. INTRODUCTION**

Spectroscopic studies of superheavy atoms ( $Z\geq 100$ ) present a severe challenge to the experimentalist. The first such study, involving fermium ( $Z=100$ ), was published recently [1]; measurements are now planned [2] for nobelium and lawrencium ( $Z=102$  and  $103$ , respectively), which present even larger difficulties. Their low production rates in nuclear fusion reactions, below ten atoms per second, and short lifetimes, on the order of seconds, make a reliable prediction of transition energies mandatory, since broad spectroscopic scans must be avoided. In addition, theoretical studies are crucial for identifying the lines. Indeed, the Fm measurements [1] were accompanied and guided by multiconfiguration Dirac-Fock (MCDF) calculations. We recently predicted the spectrum of lawrencium [3], and the purpose of the present work is to provide reasonably accurate transition energies and amplitudes for nobelium. The quality of the calculated spectrum is estimated by applying the same method to ytterbium, the lighter homologue of nobelium.

The Fock-space coupled-cluster (FSCC) scheme, a multi-reference variant of the coupled-cluster method, is used here in the framework of the four-component Dirac-Coulomb-Breit Hamiltonian. This method has provided the most accurate transition energies for many atomic and molecular systems [4]. It takes account of nondynamic electron correlation

by the multiconfigurational approach, including the important electron configurations in the model ( $P$ ) space, and at the same time provides a good description of dynamic correlation by incorporating many millions of excitations to  $Q$  space determinants. The FSCC approach has been augmented and improved by the development of intermediate Hamiltonian Fock-space coupled-cluster (IHFSCC) methods [5–8]. These make possible the use of much larger and more flexible  $P$  spaces without running into intruder states and divergence, thereby increasing the accuracy obtained [9–13]. Pilot applications with the extrapolated intermediate-Hamiltonian approach [14,15] reproduced the known ionization potentials and electron affinities of the alkali-metal atoms within 1 meV. The IHFSCC calculation [3] of the excitation energies of Lu, the lighter homologue of Lr, gave an average error of  $400\text{ cm}^{-1}$ , and the application to Lr pinpointed two strong transitions of Lr in the experimentally relevant range of  $20\ 000\text{--}30\ 000\text{ cm}^{-1}$  with comparable accuracy.

The available experimental information on the levels of Yb appears in the compendium of Martin *et al.* [16]. Several theoretical treatments used the MCDF approach. Yb transition energies were studied by Migdalek and Baylis [17] and by Kotochigova and Tupizin [18], and the low- $^{1,3}P_1$  states of Yb and No were treated recently with a relatively small basis [19]. Other methods used include density functional theory (DFT) calculations by Vosko *et al.* [20] and pseudopotential and DFT studies of No by Liu *et al.* [21]. The FSCC method was used to obtain excitation energies a decade ago [22]. A similar application reported recently [23] used basis sets with

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TABLE I. Transition energies of Yb ( $\text{cm}^{-1}$ ).

Method Ref.		Expt. [16]	IHFSCC Present	+QED	FSCC [23]	FSCC [22]	MCDF [18]	+CP [17]
Ionization potential								
$6s^2$	$^1S_0$	50 443	50 463		50 552	51 109		48 074
Excitation energies								
$6s6p$	$^3P_0$	17 288	17 011	16 969	17 576	17 359	15 826	
	$^3P_1$	17 992	17 719	17 674	18 424	18 089	16 563	
	$^3P_2$	19 710	19 442	19 399	20 218	19 836	18 167	
$5d6s$	$^3D_1$	24 489	24 770	24 723	25 865	24 936		
	$^3D_2$	24 752	24 981	24 935	25 966	25 180		
	$^3D_3$	25 271	25 422	25 379	26 125	25 676		
$6s6p$	$^1P_1$	25 068	25 777	25 724		27 271	27 838	23 120
$5d6s$	$^1D_2$	27 678	27 512	27 456		28 587		
$6s7s$	$^3S_1$	32 695	32 543	32 495	32 967			
$6s7s$	$^1S_0$	34 351	33 900	33 851	34 932			
$6s7p$	$^3P_0$	38 091	38 293	38 238				
	$^3P_1$	38 174	38 373	38 318				
	$^3P_2$	38 552	38 707	38 648				
$6s7p$	$^1P_1$	40 563	39 214	39 154				
$6s6d$	$^3D_1$	39 809	40 158	40 103				
	$^3D_2$	39 838	40 187	40 131				
	$^3D_3$	39 966	40 280	40 224				
$6s6d$	$^1D_2$	40 062	40 399	40 340				
$6s8s$	$^3S_1$	41 615	41 697	41 582				
$6s8s$	$^1S_0$	41 939	42 049	41 934				
Average absolute errors of excitation energies								
Six lowest levels			246	245	779	262	1 800	
Levels calc. in [23]			260	272	691			
All 20 levels			320	300				
Fine-structure splittings								
$6s6p$	$^3P_1 - ^3P_0$	704	708	705	848	730	737	
	$^3P_2 - ^3P_1$	1 718	1 723	1 725	1 794	1 747	1 604	
$5d6s$	$^3D_2 - ^3D_1$	263	211	212	101	244		
	$^3D_3 - ^3D_2$	519	441	444	159	496		
$6s7p$	$^3P_1 - ^3P_0$	84	80	80				
	$^3P_2 - ^3P_1$	337	334	330				
$6d6s$	$^3D_2 - ^3D_1$	30	29	28				
	$^3D_3 - ^3D_2$	93	93	93				
Average absolute error								
Four splittings			35	34	185	24		
All splittings			18	18				

more  $s$ ,  $p$ , and  $d$  functions than the earlier work [22], but had fewer  $f$  and  $g$  functions and no  $h$  orbitals, resulting in a larger average error in the excitation energies listed there. Most singlet excitation energies were not given, but large errors in them were reported [23].

Here we apply the intermediate-Hamiltonian coupled-cluster approach, an extension of the FSCC method, to the electronic spectra of the Yb and No atoms, comparing the

results to experimental values for Yb and predicting the spectrum of the actinide nobelium.

## II. METHOD

The same method is used as in the earlier work on Lu and Lr [3]. The  $P$  space is partitioned into two parts [24], the main  $P_m$  and intermediate  $P_i$ , and an intermediate Hamil-

tonian  $H_I$  in  $P$  is derived, the eigenvalues of which give good approximation to the eigenvalues of  $H$  dominated by the main model-space components. Three projection operators are defined, satisfying

$$P_m + P_i = P, \quad P + Q = 1. \quad (1)$$

Two sets of wavelike operators [24] are expanded in coupled-cluster normal-ordered exponential expressions.  $\Omega = 1 + \chi$  is a standard wave operator in  $P_m$ ,

$$\Omega P_m |\Psi_m\rangle = (\exp S) P_m |\Psi_m\rangle = |\Psi_m\rangle, \quad (2)$$

where  $|\Psi_m\rangle$  denotes an eigenstate of the Hamiltonian  $H$  with the largest components in  $P_m$ , and  $R = 1 + \Delta$  is an operator in  $P$ , satisfying

$$R P |\Psi_m\rangle = (\exp T) P |\Psi_m\rangle = |\Psi_m\rangle. \quad (3)$$

The last equation, and therefore all equations derived from it, applies when operating on  $|\Psi_m\rangle$ , but not necessarily on  $|\Psi_i\rangle$ . This feature distinguishes  $R$  from a bona fide wave operator. The cluster equation for  $S$  in the  $(n)$  sector of the Fock space is [9]

$$Q[S^{(n)}, H_0]P_m = Q(\overline{VQ_i\Omega} - \overline{\chi P_m VQ_i\Omega})^{(n)}P_m, \quad (4)$$

where  $Q_i = 1 - P_i = Q + P_m$ . No  $P_i S P_m$  elements appear in the equation, so that  $P_i$  acts as a buffer between  $P_m$  and  $Q$ , facilitating convergence and avoiding intruder states. Equation (4) is valid provided  $Q S P_m \approx Q T P_m$ , which is rather easy to achieve with a properly defined  $P_i$ ; this condition is monitored in the calculation. After Eq. (4) is solved for  $Q S P_m$ ,  $Q T P_m$  may be obtained by

$$(E - H_0) Q T^{(n)} P = Q[S(E - H_0)P_m + (\overline{VR}) - (\overline{\chi P_m VR})]^{(n)}P. \quad (5)$$

$E$  is an arbitrary constant, chosen to facilitate convergence. Tests have shown that  $E$  may be changed within broad bounds (hundreds of hartrees) with minute effect (a few wave numbers) on calculated transition energies. The final step is the construction of the intermediate Hamiltonian

$$H_I = P H R P, \quad (6)$$

which gives upon diagonalization the correlated energies of  $|\Psi_m\rangle$ ,

$$H_I P |\Psi_m\rangle = E_m P |\Psi_m\rangle. \quad (7)$$

The dimension of the  $H_I$  matrix is that of  $P$ ; however, only the eigenvalues corresponding to  $|\Psi_m\rangle$  are required to satisfy Eq. (7). The other eigenvalues, which correspond to states  $|\Psi_i\rangle$  with the largest components in  $P_i$ , may include larger errors.

The Lamb shifts were estimated for each state by evaluating the electron self-energy and vacuum polarization using the approximation scheme of Indelicato *et al.* [25]. The code described in Refs. [25,26] was adapted to our basis-set expansion procedure by Vilkas and Ishikawa [27]. All the necessary radial integrals were evaluated analytically. In this scheme [26], the screening of the self-energy is estimated by integrating the charge density of a spinor to a short distance

TABLE II. IHFSCC excitation energies of No ( $\text{cm}^{-1}$ ). The ground state is  $7s^2 1S_0$ .

Upper state			+QED
7s7p	$^3P_0$	19 028	18 879
	$^3P_1$	20 605	20 454
	$^3P_2$	25 527	25 374
6d7s	$^3D_1$	28 496	28 338
	$^3D_2$	28 935	28 778
	$^3D_3$	30 040	29 897
7s7p	$^1P_1$	30 224	30 056
6d7s	$^1D_2$	33 071	32 892
7s8s	$^3S_1$	35 263	35 092
7s8s	$^1S_0$	36 701	36 538
7s8p	$^3P_0$	40 742	40 576
	$^3P_1$	40 860	40 692
	$^3P_2$	42 003	41 837
7s8p	$^1P_1$	42 458	42 285
7s7d	$^3D_1$	42 881	42 726
	$^3D_2$	42 934	42 758
	$^3D_3$	43 203	43 033
7s7d	$^1D_2$	43 423	43 079
7s9s	$^3S_1$	44 598	44 247
7s9s	$^1S_0$	45 001	44 828

from the origin, typically 0.3 Compton wavelengths. The ratio of the integral computed with a spinor and that obtained from the corresponding hydrogenic spinor is used to scale the self-energy correction for a bare nuclear charge that has been computed by Mohr [28]. Extensive relativistic configuration interaction (RCI) wave functions are used. While the IHFSCC excitation energies are expected to be more accurate, the RCI functions reproduced them in most cases within a few percent, so that the QED corrections should be quite accurate. The RCI functions are also used to obtain the No transition amplitudes.

### III. APPLICATION

Within the framework of the Dirac-Coulomb-Breit Hamiltonian, the Dirac-Fock-Breit orbitals are first calculated and correlation is included at the coupled-cluster singles-and-doubles (CCSD) level. The closed-shell reference states for the Yb and No atoms are the dications  $(\text{Xe})4f^{14}$  and  $(\text{Rn})5f^{14}$ , respectively. The states of the neutral atoms are reached by adding two electrons to the reference determinants in a designated set of valence orbitals. The  $P_m$  and total  $P$  spaces were augmented to convergence of the excitation energies. The final  $P_m$  for Yb included two  $s$  orbitals and one  $p$ ,  $d$ , and  $f$  orbitals beyond those occupied in the reference determinant, and the total  $P$  comprised  $7s 5p 3f 2g 1h$  orbitals, including those in  $P_m$ . Somewhat larger spaces were taken for No,  $2s 2p 2d 1f$  in  $P_m$  and  $8s 6p 6d 4f 2g 1h$  in  $P$ .

The universal basis set [29] was used, consisting of even-tempered Gaussian-type orbitals with exponents given by

TABLE III. RCI electric dipole transition amplitudes of the strongest transitions of nobelium.  $\tau$  is the lifetime of the upper level.

$\lambda$ (Å)	Upper state		$\tau$ (s)	Lower state		$A$ (s <sup>-1</sup> )
2 365	<i>7s8p</i>	<sup>1</sup> <i>P</i> <sub>1</sub>	$2.9 \times 10^{-8}$	<i>7s</i> <sup>2</sup>	<sup>1</sup> <i>S</i> <sub>0</sub>	$3.2 \times 10^7$
2 457	<i>7s8p</i>	<sup>3</sup> <i>P</i> <sub>1</sub>	$2.9 \times 10^{-8}$	<i>7s</i> <sup>2</sup>	<sup>1</sup> <i>S</i> <sub>0</sub>	$1.0 \times 10^7$
3 327	<i>7s7p</i>	<sup>1</sup> <i>P</i> <sub>1</sub>	$2.0 \times 10^{-9}$	<i>7s</i> <sup>2</sup>	<sup>1</sup> <i>S</i> <sub>0</sub>	$5.0 \times 10^8$
4 103	<i>7s9s</i>	<sup>3</sup> <i>S</i> <sub>1</sub>	$1.2 \times 10^{-8}$	<i>7s7p</i>	<sup>3</sup> <i>P</i> <sub>1</sub>	$1.8 \times 10^7$
4 484	<i>7s7d</i>	<sup>3</sup> <i>D</i> <sub>2</sub>	$4.5 \times 10^{-8}$	<i>7s7p</i>	<sup>3</sup> <i>P</i> <sub>1</sub>	$1.4 \times 10^7$
5 140	<i>7s9s</i>	<sup>3</sup> <i>S</i> <sub>1</sub>	$1.2 \times 10^{-8}$	<i>7s7p</i>	<sup>3</sup> <i>P</i> <sub>2</sub>	$4.2 \times 10^7$
5 663	<i>7s7d</i>	<sup>3</sup> <i>D</i> <sub>3</sub>	$6.1 \times 10^{-8}$	<i>7s7p</i>	<sup>3</sup> <i>P</i> <sub>2</sub>	$1.7 \times 10^7$
6 168	<i>7s8s</i>	<sup>3</sup> <i>S</i> <sub>1</sub>	$1.4 \times 10^{-8}$	<i>7s7p</i>	<sup>3</sup> <i>P</i> <sub>0</sub>	$1.1 \times 10^7$
6 832	<i>7s8s</i>	<sup>3</sup> <i>S</i> <sub>1</sub>	$1.4 \times 10^{-8}$	<i>7s7p</i>	<sup>3</sup> <i>P</i> <sub>1</sub>	$3.3 \times 10^7$
7 679	<i>7s7d</i>	<sup>1</sup> <i>D</i> <sub>2</sub>	$8.0 \times 10^{-8}$	<i>7s7p</i>	<sup>3</sup> <i>P</i> <sub>1</sub>	$1.2 \times 10^7$
8 171	<i>7s8p</i>	<sup>3</sup> <i>P</i> <sub>0</sub>	$3.7 \times 10^{-8}$	<i>7s6d</i>	<sup>3</sup> <i>D</i> <sub>1</sub>	$1.6 \times 10^7$
10 290	<i>7s8s</i>	<sup>3</sup> <i>S</i> <sub>1</sub>	$1.4 \times 10^{-8}$	<i>7s7p</i>	<sup>3</sup> <i>P</i> <sub>2</sub>	$2.8 \times 10^7$
15 427	<i>7s8s</i>	<sup>1</sup> <i>S</i> <sub>0</sub>	$8.9 \times 10^{-8}$	<i>7s7p</i>	<sup>1</sup> <i>P</i> <sub>1</sub>	$1.1 \times 10^7$
18 235	<i>7s8p</i>	<sup>3</sup> <i>P</i> <sub>0</sub>	$3.7 \times 10^{-8}$	<i>7s8s</i>	<sup>3</sup> <i>S</i> <sub>1</sub>	$1.1 \times 10^7$

$$\zeta_n = \gamma \delta^{(n-1)}, \quad \gamma = 106\,111\,395.371\,615,$$

$$\delta = 0.486\,752\,256\,286. \quad (8)$$

Orbitals were added to the basis until the transition energies converged. The orbitals are left uncontracted. Virtual orbitals with energies higher than 200 hartrees are omitted. The outer 42 electrons are correlated in both atoms, leaving 28 inner electrons of Yb and 60 inner electrons of No out at the correlation stage. The basis for both atoms includes 37 *s* functions ( $n=1-37$ ), 31 *p* ( $n=5-35$ ), 26 *d* ( $n=9-34$ ), 21 *f* ( $n=13-33$ ), 16 *g* ( $n=17-32$ ), 11 *h* ( $n=21-31$ ), and 6 *i* ( $n=25-30$ ) orbitals.

#### IV. RESULTS AND DISCUSSION

Since many transition energies of Yb are known with high accuracy [16], their calculation provides a check on the accuracy of the method and the validity of predictions for No. Our results for the lighter element are presented and compared with experiment and previous computations in Table I. The *LS* notation is given, but *J* is the only good quantum number, particularly for nobelium. The transition energies of Yb show very good agreement with experiment, with the ionization potential (IP) within 20 cm<sup>-1</sup> of the measured value and an average error of about 300 cm<sup>-1</sup> or 40 meV for the 20 lowest excitation energies calculated. Fine-structure splittings are also very good, with an average absolute error of 23 cm<sup>-1</sup> (3 meV) and maximum error of 80 cm<sup>-1</sup>. The QED effects are rather small and do not change the picture. The present results have on average half the error of our previous FSCC values [22], due to the use of larger basis sets and *P* spaces. The recent FSCC results of Nayak and Chaudhuri [23] are rather disappointing, giving a good IP, but relatively poor excitation energies, worse even than the 1995 calculations [22]. The probable cause is the basis used. The *spd* basis is good, but the *f* and *g* functions are few and

seem to be concentrated in the low-exponent region, neglecting the regions important for correlating the lower-*l* orbitals. The early MCDF calculations [17,18], with or without inclusion of core polarization, have much larger errors. The relatively small basis sets and short correlation expansions used in the recent MCDF work [19] lead to considerable errors of about 1200 cm<sup>-1</sup> in the excitation energies, indicating the need for extensive inclusion of correlation to obtain reliable results.

Nobelium is the heaviest element for which an experimental ionization potential appears in the NIST database [30] and in the *Handbook of Chemistry and Physics* [31]. In reality, no measurements on the atom have been performed and the quoted value originates from semiempirical estimates. Sugar [32] extrapolated the measured term energy intervals  $5f^N 7s^2 - 5f^N 7s8s$  for Ra ( $N=0$ ) and the actinides Pu–Es ( $N=6-11$ ) to other *N* values up to nobelium ( $N=14$ ). The Rydberg-Ritz formula for term energies was then used to derive the IP. Application of the method to lanthanides [33] proved its robustness and accuracy, so that the derived actinide IPs are reliable. The value quoted for nobelium is 6.65(7) eV. The calculated IP is 53 489 cm<sup>-1</sup> or 6.632 eV, in excellent agreement with this value. It is about 3000 cm<sup>-1</sup> higher than for Yb, demonstrating the well-known relativistic stabilization of *s* orbitals. The nobelium excitation energies are shown in Table II. The pattern is similar to that of ytterbium, with energies higher by 0.2–0.5 eV, again due to relativistic stabilization. Lamb shifts are significant, reducing the excitation energies by  $\sim 200$  cm<sup>-1</sup>. Only states with a full  $5f^{14}$  shell are treated by the IHFSCC application. Multireference Møller-Plesset calculations found  $5f^{13} 7s^2 7p$  states in the same energy range, but they will not show in the spectrum, since their transition to the ground state is electric-dipole forbidden.

The RCI electric-dipole transition amplitudes and lifetimes are shown in Table III. The lifetimes of a state are obtained by considering its transition to all lower states and

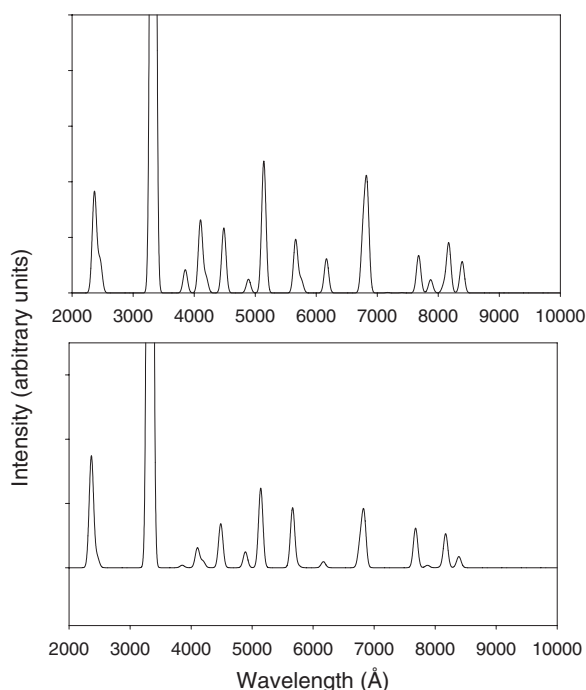


FIG. 1. Simulated  $E1$  spectrum of No, assuming equal population of all excited levels. The lower panel is corrected for the total lifetime of the levels.

include the effect of magnetic dipole and electric quadrupole transitions. The synthesized spectrum of No is shown in Fig. 1. It is obtained by convolution of the lines with a Gaussian function having a 50-Å full width at half maximum, assuming all excited states have equal population. The top panel shows amplitudes of individual transitions, and the lower panel includes the influence of the level lifetime, showing  $A^2\tau$  ( $s^{-1}$ ), with  $A$  the amplitude and  $\tau$  the lifetime. The outstanding feature is the very strong line at  $30\,060\text{ cm}^{-1}$ , corresponding to the  $7s\,7p\,J=1 \rightarrow 7s^2$  transition. As shown in Table III, the amplitude of this transition is higher by an order of magnitude than all others. Assuming error bounds of 0.1 eV, we predict the strongest feature of the No spectrum at  $30\,100 \pm 800\text{ cm}^{-1}$ . Other strong (though

weaker) transitions are expected at  $42\,300\text{ cm}^{-1}$  ( $7s\,8p\,J=1 \rightarrow 7s^2$ ),  $18\,900\text{ cm}^{-1}$  ( $7s\,9s\,J=1 \rightarrow 7s\,7p\,J=2$ ),  $14\,600\text{ cm}^{-1}$  ( $7s\,8s\,J=1 \rightarrow 7s\,8p\,J=1$ ), and  $9\,700\text{ cm}^{-1}$  ( $7s\,8s\,J=1 \rightarrow 7s\,7p\,J=2$ ).

## V. SUMMARY AND CONCLUSION

Transition energies and amplitudes of the nobelium atom in the range  $20\,000\text{--}30\,000\text{ cm}^{-1}$  are calculated in preparation for the planned experiment [2]. The intermediate-Hamiltonian Fock-space coupled-cluster formalism at the singles-and-doubles level is used in the framework of the Dirac-Coulomb-Breit Hamiltonian, and Lamb shifts are included. Very large basis sets and model ( $P$ ) spaces are used, and are augmented until convergence of the transition energies is achieved. The main remaining error comes from omitting connected triple and higher excitations in the coupled-cluster expansion to the  $Q$  space (interactions within  $P$  are included to all orders by diagonalization of the intermediate Hamiltonian  $H_I$  matrix).

The accuracy of the method and computational scheme is tested by application to ytterbium, the lower homologue of nobelium. The calculated ionization potential is within  $20\text{ cm}^{-1}$  of experiment, and the average error for the lowest 20 excitation energies (both singlet and triplet) is  $300\text{ cm}^{-1}$ . The IP of nobelium falls within the error bounds of the reliable semiempirical estimate. The outstanding feature of the calculated spectrum of No is a line at  $30\,060\text{ cm}^{-1}$ , corresponding to the  $7s\,7p\,^1P_1 \rightarrow 7s^2\,^1S_0$  transition, with an amplitude  $A=5.0 \times 10^8\text{ s}^{-1}$ . Considering that deviation from experimental energies in Yb is larger for singlets than for triplets, and accounting for possible larger uncertainties in No, we put the error limits for the No transition at a conservative  $0.1\text{ eV}$ . We therefore predict a strong feature in the No spectrum at  $30\,100 \pm 800\text{ cm}^{-1}$ .

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- [1] M. Sewtz, H. Backe, A. Dretzke, G. Kube, W. Lauth, P. Schwamb, K. Eberhardt, C. Grüning, P. Thörle, N. Trautmann, P. Kunz, J. Lassen, G. Passler, C. Z. Dong, S. Fritzsche, and R. G. Haire, *Phys. Rev. Lett.* **90**, 163002 (2003).
- [2] H. Backe, P. Kuns, W. Leuth, A. Dretzke, R. Horn, T. Kolb, M. Laatiaoui, D. Ackermann, M. Block, F. Herfurth, F. P. Hessberger, S. Hofmann, and R. Mann, *Eur. Phys. J. D* (to be published).
- [3] A. Borschevsky, E. Eliav, M. J. Vilkas, Y. Ishikawa, and U. Kaldor, *Eur. Phys. J. D* (to be published).
- [4] For a review of multireference CC methods and particularly the FSCC approach, see D. Mukherjee and S. Pal, *Adv. Quantum Chem.* **20**, 292 (1989). For a review of nonrelativistic FSCC applications see U. Kaldor, *Theor. Chim. Acta* **80**, 427 (1991). For a review of relativistic FSCC applications see U. Kaldor and E. Eliav, *Adv. Quantum Chem.* **31**, 313 (1998).
- [5] A. Landau, E. Eliav, and U. Kaldor, *Chem. Phys. Lett.* **313**, 399 (1999).
- [6] A. Landau, E. Eliav, and U. Kaldor, *Adv. Quantum Chem.* **39**, 171 (2001).
- [7] A. Landau, E. Eliav, Y. Ishikawa, and U. Kaldor, *J. Chem. Phys.* **121**, 6634 (2004).
- [8] U. Kaldor, E. Eliav, and A. Landau, in *Fundamental World of Quantum Chemistry*, edited by E. J. Brandas and E. S. Kryachko (Kluwer, Dordrecht, 2004), Vol. III, pp. 365–406.
- [9] A. Landau, E. Eliav, Y. Ishikawa, and U. Kaldor, *J. Chem. Phys.* **113**, 9905 (2000).
- [10] A. Landau, E. Eliav, Y. Ishikawa, and U. Kaldor, *J. Chem.*



- Phys. **115**, 6862 (2001).
- [11] A. Landau, E. Eliav, Y. Ishikawa, and U. Kaldor, *J. Chem. Phys.* **114**, 2977 (2001).
- [12] A. Landau, E. Eliav, Y. Ishikawa, and U. Kaldor, *J. Chem. Phys.* **115**, 2389 (2001).
- [13] E. Eliav, A. Landau, Y. Ishikawa, and U. Kaldor, *J. Phys. B* **35**, 1693 (2002).
- [14] E. Eliav, M. J. Vilkas, Y. Ishikawa, and U. Kaldor, *Chem. Phys.* **311**, 163 (2005).
- [15] E. Eliav, M. J. Vilkas, Y. Ishikawa, and U. Kaldor, *J. Chem. Phys.* **122**, 224113 (2005).
- [16] W. C. Martin, R. Zalubas, and L. Hagan, *Atomic Energy Levels—The Rare-Earth Elements*, U.S. Natl. Bur. Stand. Ref. Data Ser., U.S. Natl. Bur. Stand. Circ. No. NBS 60 (U.S. GPO, Washington, DC, 1978); J. E. Sansonetti, W. C. Martin, and S. L. Young, *Handbook of Basic Atomic Spectroscopic Data* (National Institute of Standards and Technology, Gaithersburg, MD, 2005).
- [17] J. Migdalek and W. E. Baylis, *Phys. Rev. A* **33**, 1417 (1986).
- [18] S. A. Kotochigova and I. I. Tupizin, *J. Phys. B* **20**, 4759 (1987).
- [19] S. Fritzsche, *Eur. Phys. J. D* **33**, 15 (2005).
- [20] S. H. Vosko, J. A. Chevary, and I. L. Mayer, *J. Phys. B* **24**, L225 (1991); S. H. Vosko and J. A. Chevary, *ibid.* **26**, 873 (1993).
- [21] W. Liu, W. Kuchle, and M. Dolg, *Phys. Rev. A* **58**, 1103 (1998).
- [22] E. Eliav, U. Kaldor, and Y. Ishikawa, *Phys. Rev. A* **52**, 291 (1995).
- [23] M. K. Nayak and R. K. Chaudhuri, *Eur. Phys. J. D* **37**, 171 (2006).
- [24] J.-P. Malrieu, Ph. Durand, and J.-P. Daudey, *J. Phys. A* **18**, 809 (1985).
- [25] P. Indelicato, O. Gorcex, and J. P. Desclaux, *J. Phys. B* **20**, 651 (1987).
- [26] Y.-K. Kim, in *Atomic Processes in Plasmas*, edited by Y.-K. Kim and R. C. Elton, AIP Conf. Proc. No. 206 (AIP, New York, 1990), p. 19.
- [27] M. J. Vilkas and Y. Ishikawa, *Phys. Rev. A* **68**, 012503 (2003); *J. Phys. B* **37**, 1803 (2004).
- [28] P. J. Mohr, *Phys. Rev. A* **46**, 4421 (1992).
- [29] G. L. Malli, A. B. F. Da Silva, and Y. Ishikawa, *Phys. Rev. A* **47**, 143 (1993).
- [30] <http://www.physics.nist.gov/PhysRefData/Elements/index.html>
- [31] *Handbook of Chemistry and Physics*, 76th ed., edited by D. R. Lide (CRC Press, Boca Raton, 1996), pp. 10–208.
- [32] J. Sugar, *J. Chem. Phys.* **60**, 4103 (1974).
- [33] J. Reader and J. Sugar, *J. Opt. Soc. Am.* **56**, 1189 (1966); **60**, 1421 (1970).