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A structure calculation for hydrogen like nobelium

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ABSTRACT

Hidrojen benzeri iyonlar bir atomun en basit yapılı halidir, bu konuda çalışmak atomik yapıları tanımlamada kullanılan yöntemlerin test edilmesini sağlar. Hidrojen benzeri iyonlar hakkında çalışmalar yapmak atomik yapıyı anlamak için de bir fırsattır. Bu sebeple hidrojen benzeri nobelyum (No^{101+}, Z=102) için bir çalışma gerçekleştirildi. No^{101+} seviye yapısı hesaplamalarında çok konfigürasyonlu Hartree-Fock ve çok konfigürasyonlu Dirac Fock yöntemlerinin her ikisi de kullanıldı. Hesaplamalar bazı relativisitik düzeltmeleri ve kuantum elektrodinamik etkileri içerir. Ulaşılabilir kaynaklarda No^{101+} için oldukça az sayıda teorik çalışma vardır, deneysel çalışma ise yoktur. Hesaplama sonuçları diğer teorik çalışma sonuçlarıyla karşılaştırılarak yorumlandı.

Anahtar Kelimeler: MCHF method, MCDF method, energy levels, relativistic correction, QED effects

Hidrojen benzeri nobelyumun yapı hesaplaması

ÖZ

The hydrogen like ion is the simplest structure of an atom, so the studying on it gives a change to test of methods using for determinating of atomic structures. It is also an occasion the studying on hydrogen like ions to understand atomic structure. For this reason, it is performed a study for hydrogen like nobelium (No^{101+}, Z=102). It has been used both multiconfiguration Hartree-Fock, MCHF, and multiconfiguration Dirac-Fock method, MCDF, as calculating level structure of No^{101+}. The calculations have contained some relativistic corrections and quantum electrodynamic effects. There are very few theoretical works in available literature and no experimental one for No^{101+}. The calculated results have been interpreted in comparison with other theoretical results.

Keywords: MCHF yöntemi, MCDF yöntemi, enerji seviyeleri, relativistik düzeltmeler, QED etkileri

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1. INTRODUCTION

The developments in the science and technology such as interpretation of astrophysical spectra, atomic collision studies, the improvement of the x-ray lasers and the diagnostics of fusion plasmas, have increased the need of precise spectroscopic data [1]. The origin of the exact spectral characteristic calculations is critically defining the level structure. A few works have been performed levels structure of hydrogen like nobelium (No^{101+}, Z=102). Some of have been listed NIST atomic data base [2]. The energies of $1s_{1/2}$, $2s_{1/2}$ and $2p_{3/2}$ levels for hydrogenic ions have been given in Johnson and Soff's [3] and Yerokhin and Shabaev's [4] lamb shift studies. Jitrik and Bunge [5, 6] have performed more extensive work for hydrogen like ions. The *nl* (up to *n*=26, *l*=25, Z=1-118) levels have been calculated using point-nucleus Dirac eigenfunctions and the data are available on a web site [7] as two sets. But the extensive work is not sufficiently sensitive as it will be explained in the results and discussion section.

Unfortunately, there is no experimental data for No^{101+} levels structure. Their short lifetimes and radioactivity make almost impossible experimentally work with high Z structures.

It has been calculated for *nl* (*n*=1-9 and *l*=0-4) levels for No^{101+} using MCHF atomic structure package [8] and GRASP (MCDF method) code [9]. The present calculations have been performed as a part of large scale study about lithium, helium and hydrogen like actinides, Z=89-103 [10, 11].

2. METHOD OF CALCULATIONS

In this section, it has been given a brief about MCHF and MCDF methods used in the calculations. Both methods have been detailly described in [8, 14] for MCHF and [9, 15] for MCDF.

The wave function, $\Psi(\gamma LS)$, is a linear combination of configuration state functions, $\Phi(\gamma_i LS)$,

$$\Psi(\gamma LS)=\sum_{i=1}^{M} c_i \Phi(\gamma_i LS), \qquad \sum_{i=1}^{M} c_i^2 = 1 . \qquad (1)$$

$$H_{NR}=\sum_{j=1}^{N}\left(\frac{1}{2}\nabla_j^2-\frac{Z}{r_j}\right)+\sum_{j<k}\frac{1}{r_{jk}} \qquad (2)$$

The non-relativistic hamiltonian of an atom or ion is given in formula (2) and the energy functional is based on this hamiltonian. In the fully relativistic MCDF method, wavefunction and hamiltonian are like the following equations.

$$\Psi_\alpha(PJM)=\sum_{r}^{n_c} c_r(\alpha)\left|\gamma_r PJM\right\rangle \qquad (3)$$

$$H_{DC}=\sum_{j=1}^{N}\left(c\vec{\alpha}_j.\vec{p}_j+(\beta_j-1)c^2+V(r_j)\right)+\sum_{j<k}^{N}\frac{1}{r_{jk}} \qquad (4)$$

The two-component Fermi function is used modelling the nuclear charge distribution for both method. Moreover, the first order corrections to the MCHF approximation is evaluated via Breit-Pauli (mass and Darwin corrections, spin-orbit, spin-other orbit, orbit-orbit and spin-spin contact) operators using in configuration interaction, CI, procedure. The transverse (photon) Breit interactions and quantum electrodynamics (self-energy and vacuum polarization) corrections are considered in MCDF method. In addition, MCHF and MCDF methods include both the correlation effect.

3. RESULTS AND DISCUSSION

Hydrogenic nobelium has just one electron around Z=102 nucleus which creates strong coulomb filed. No^{101+} has a simple structure, but it is difficult to calculate a situation contains highly excited levels. In the calculations, *nl* (*n*=1-9 and *l*=0-4) levels have been considered for both methods. Furthermore, the Breit-Pauli relativistic corrections for MCHF calculation, the transverse photon interaction and QED effects consist of self energy (SE) plus vacuum polarization (VP) contributions for MCDF have been taken into account.

The excitation energies have been given in Table 1. In Table 1, the vacuum polarization (VP) and self energy (SE) contributions to MCDF, MCDF+QED (QED=SE+VP) energies, MCHF energies and other work energies have been presented in the columns respectively. The Breit-Pauli and the transverse photon effects are almost zero because there is just one electron in the ion structure. But the magnitude of VP and SE corrections could not be neglected. For this reason, SE and VP have been given in sperate columns of

Table 1. The multipers of value have been shown in the column headings.

The ground state $1s_{1/2}$ energy has been computed as -1313574147.31 cm^{-1} by MCHF and -1358557647.77 cm^{-1} (SE= 1486470 cm^{-1}, VP=-4552460 cm^{-1}) by MCDF method. This level had been calculated as -1394776000 cm^{-1} in ref [3] and -1360764272 cm^{-1} in ref [4]. The percentage errors between MCHF and other works are 5.82% [3] and 3.46% [4] and between MCDF and other works are 2.59% [3] and 0.16% [4]. It has been good agreement especially with MCDF for the ground state of No^{101+}. Reference [3] and [4] have also presented the energy levels of $2s_{1/2}$ and $2p_{1/3, 3/2}$. The same agreements have been seen for these levels. A graph has been drawn between this work results and other work [7] to make a comparison for excited levels in Figure 1 and 2.

As Figure 1 and 2 has examined, it has revealed the results of MCHF and MCDF have been compatible with both set 1 and set 2 of reference 7. The MCDF results have been more fit than the MCHF results to other work because MCHF method contains just the Breit-Pauli corrections but MCDF involves QED effects besides the transverse photon interactions. The linear correlation coefficients, R^2, of the comparison with set 1 [7] have been obtained as 0.8130 for MCHF and 0.8140 for MCDF. R^2 of comparison set 2 has been 0.9985 for MCHF and 1.0000 for MCDF calculation. The present excitation energies results have been in an excellent agreement with set 2 calculation.

The crosscheck of this work methods has been represented in the Figure 3. The coefficient of determination for MCHF-MCDF calculation is 0.9987. The agreement between different methods in present paper has supported the reliability of this work calculations. On the other hand, nl_j energy values are same $n(l+1)_j$ of reference [7] (except $d_{5/2}$-$4f_{5/2}$, $f_{7/2}$-$g_{7/2}$ states in set 1). For example, $E(2s_{1/2})=E(2p_{1/2})=1.0112968730$ cm^{-1} in both sets, $E(3p_{3/2})=E(3d_{3/2})= 1.2174868013$ cm^{-1} in both sets and $E(4d_{5/2})=E(4f_{5/2})=1.2962577170$ cm^{-1} in set 2 etc. It has been pointed out that this work especially MCDF results are more sensible and reliable than reference [7].

The present study has provided data for $8g_{7/2}$, $8g_{9/2}$, $9g_{7/2}$ and $9g_{9/2}$ for the first time as well as more accurate estimation of energy levels.

4. CONCLISION

It has been presented the excited energy levels of hydrogen like nobelium as a part of three, two and one electron actinide ions. The applying MCHF and MCDF methods to bring out the structure of hydrogenic nobelium (No^{101+}, Z=102) in high accuracy. The relativistic and radiative effects underlying of atomic theory have been taken consideration in both method calculations. Thus, energy levels have been precisely determinated.

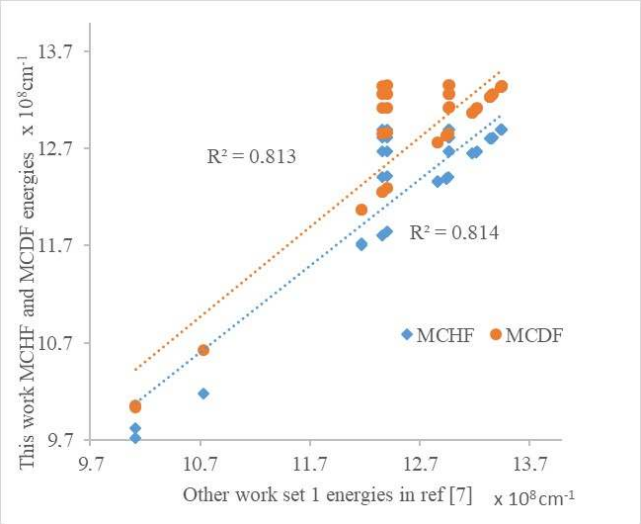

Figure 1. The comparison for excited levels of No^{101+} between set 1 calculation of other work [7] and this work MCHF and MCDF calculations

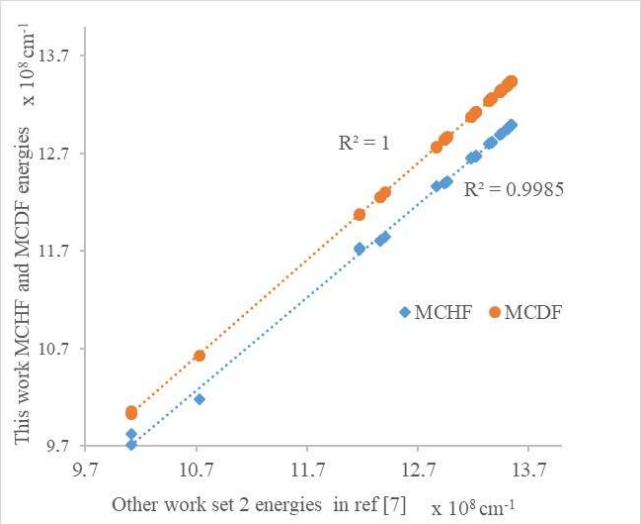

Figure 2. The comparison for excited levels of No^{101+} between set 2 calculation of other work [7] and this work MCHF and MCDF calculations

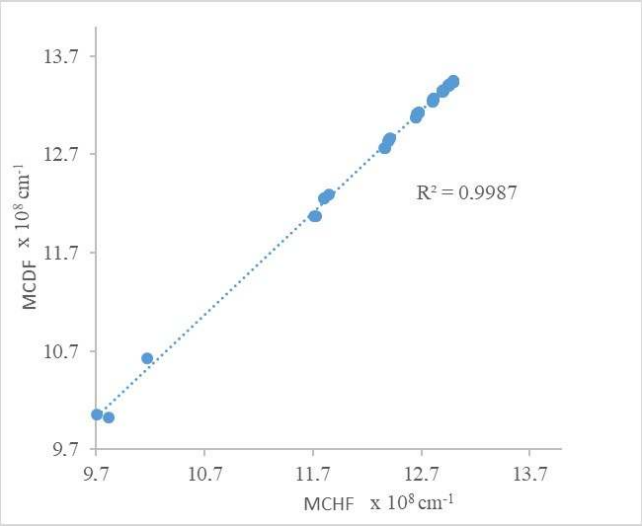

Figure 3. The crosscheck of this work MCHF and MCDF results

Table 1. Energy levels (cm^{-1}) of hydrogen like nobelium, No^{101+}. The values indicated with * and ** are taken from reference [3] and [4], respectively.

Index	Levels	VP $\times 10^6$	SE $\times 10^6$	MCDF+QED $\times 10^9$	MCHF $\times 10^9$	Set 1 of Ref [7] $\times 10^9$	Set 2 of Ref [7] $\times 10^9$
1	$1s_{1/2}$	-	-	0.00	0.00	0.00	0.00
2	$2s_{1/2}$	1.199403	-3.653314	1.00295171537	0.98170785980	1.0112968730 1.027979000*	1.0112968730 1.004712978**
3	$2p_{1/2}$	1.420165	0.4266115	1.00591039533	0.97145482573	1.0112968730 1.005272000*	1.0112968730 1.003420974**
4	$2p_{3/2}$	1.484548	-4.435453	1.06261310485	1.01758437757	1.0730450211 1.066867000*	1.0730450211 1.064980029**
5	$3s_{1/2}$	1.402018	-4.286438	1.20759934475	1.17298231838	1.2174868013	1.2174868013
6	$3p_{1/2}$	1.463886	-4.498713	1.20705754637	1.17080276176	1.2174868013	1.2174868013
7	$3p_{3/2}$	1.485723	-4.517838	1.22539976005	1.18073671769	1.2359128787	1.2359128787
8	$3d_{3/2}$	1.486442	-4.552460	1.22536585595	1.18040002362	1.2359128787	1.2359128787
9	$3d_{5/2}$	1.486465	-4.552460	1.22968681078	1.18467594967	1.2402338172	1.2402338172
10	$4s_{1/2}$	1.452259	-4.440670	1.27649802170	1.23666708945	1.2867719827	1.2867719827
11	$4p_{1/2}$	1.476917	-4.529927	1.27627503218	1.23595578708	1.2867719827	1.2867719827
12	$4p_{3/2}$	1.486132	-4.537904	1.28388022889	1.23925150592	1.2944129481	1.2944129481
13	$4d_{3/2}$	1.486452	-4.552460	1.28386598753	1.23908721727	1.2944129481	1.2944129481
14	$4d_{5/2}$	1.486467	-4.552460	1.28571075514	1.24073993087	1.2962577170	1.2962577170
15	$4f_{5/2}$	1.486470	-4.552460	1.28571073022	1.24070927528	1.2359128787	1.2962577170
16	$4f_{7/2}$	1.486470	-4.552460	1.28657248864	1.24158077579	1.2402338172	1.2971194802
17	$5s_{1/2}$	1.469779	-4.495653	1.30727319558	1.26519700740	1.3176837517	1.3176837517
18	$5p_{1/2}$	1.481716	-4.541061	1.30716240524	1.26489927488	1.3176837517	1.3176837517
19	$5p_{3/2}$	1.486294	-4.545056	1.31099153137	1.26629926445	1.3215310351	1.3215310351
20	$5d_{3/2}$	1.486460	-4.552460	1.31098426238	1.26621661828	1.3215310351	1.3215310351
21	$5d_{5/2}$	1.486468	-4.552460	1.31193004472	1.26698235196	1.3224768529	1.3224768529
22	$5f_{5/2}$	1.486470	-4.552460	1.31192996799	1.26695912027	1.2359128787	1.3224768529
23	$5f_{7/2}$	1.486470	-4.552460	1.31237414349	1.26738978638	1.2402338172	1.3229210407
24	$5g_{7/2}$	1.486470	-4.552460	1.31237407241	1.26738494782	1.2962577170	-
25	$5g_{9/2}$	1.486470	-4.552460	1.31263364740	1.26764750773	1.2971194802	-
26	$6s_{1/2}$	1.477373	-4.519991	1.32354784701	1.28036965412	1.3340174158	1.3340174158
27	$6p_{1/2}$	1.483847	-4.545993	1.32348608608	1.28022479241	1.3340174158	1.3340174158
28	$6p_{3/2}$	1.486369	-4.548222	1.32567148843	1.28091567910	1.3362135094	1.3362135094
29	$6d_{3/2}$	1.486464	-4.552460	1.32566726056	1.28087078294	1.3362135094	1.3362135094
30	$6d_{5/2}$	1.486469	-4.552460	1.32621367602	1.28127212882	1.3367600323	1.3367600323
31	$6f_{5/2}$	1.486470	-4.552460	1.32621348029	1.28125693553	1.2359128787	1.3367600323
32	$6f_{7/2}$	1.486470	-4.552460	1.32647104448	1.28149331788	1.2402338172	1.3370176301
33	$6g_{7/2}$	1.486470	-4.552460	1.32647086220	1.28148825852	1.2962577170	-
34	$6g_{9/2}$	1.486470	-4.552460	1.32662166687	1.28163732545	1.2971194802	-
35	$7s_{1/2}$	1.481075	-4.532249	1.33316476898	1.28938685310	1.3436626667	1.3436626667

36	$7p_{1/2}$	1.484901	-4.548463	1.33312736739	1.28930952102	1.3436626667	1.3436626667
37	$7p_{3/2}$	1.486408	-4.549818	1.33448785164	1.28968379020	1.3450304679	1.3450304679
38	$7d_{3/2}$	1.486466	-4.552460	1.33448511491	1.28965785688	1.3450304679	1.3450304679
39	$7d_{5/2}$	1.486469	-4.552460	1.33482830308	1.28988619015	1.3453738564	1.3453738564
40	$7f_{5/2}$	1.486470	-4.552460	1.33482798363	1.28987636786	1.2359128787	1.3453738564
41	$7f_{7/2}$	1.486470	-4.552460	1.33499019352	1.29001604087	1.2402338172	1.3455361331
42	$7g_{7/2}$	1.486470	-4.552460	1.33498987932	1.29001205305	1.2962577170	-
43	$7g_{9/2}$	1.486470	-4.552460	1.33508498816	1.29010265117	1.2971194802	-
44	$8s_{1/2}$	1.483065	-4.539069	1.33931051329	1.29518106447	-	1.3498225418
45	$8p_{1/2}$	1.485473	-4.549829	1.33928653668	1.29513776539	-	1.3498225418
46	$8p_{3/2}$	1.486429	-4.550708	1.34018888741	1.29535087625	-	1.3507307246
47	$8d_{3/2}$	1.486467	-4.552460	1.34018700953	1.29533536056	-	1.3507307246
48	$8d_{5/2}$	1.486469	-4.552460	1.34041618933	1.29547159580	-	1.3509602301
49	$8f_{5/2}$	1.486470	-4.552460	1.34041577042	1.29546521546	-	1.3509602301
50	$8f_{7/2}$	1.486470	-4.552460	1.34052432524	1.29555163713	-	1.3510689029
51	$8g_{7/2}$	1.486470	-4.552460	1.34052389031	1.29554872445	-	-
52	$8g_{9/2}$	1.486470	-4.552460	1.34058761106	1.29560631980	-	-
53	$9s_{1/2}$	1.484219	-4.543155	1.34347515123	1.29913143014	-	1.3539919993
54	$9p_{1/2}$	1.485807	-4.550644	1.34345940586	1.29910772150	-	1.3539919993
55	$9p_{3/2}$	1.486442	-4.551241	1.34408699418	1.29922718188	-	1.3546251952
56	$9d_{3/2}$	1.486468	-4.552460	1.34408584581	1.29921806919	-	1.3546251952
57	$9d_{5/2}$	1.486469	-4.552460	1.34424612611	1.29929889415	-	1.3547860299
58	$9f_{5/2}$	1.486470	-4.552460	1.34424573268	1.29929485386	-	1.3547860299
59	$9f_{7/2}$	1.486470	-4.552460	1.34432178469	1.29934848979	-	1.3548623039
60	$9g_{7/2}$	1.486470	-4.552460	1.34432136978	1.29934647776	-	-
61	$9g_{9/2}$	1.486470	-4.552460	1.34436605195	1.29938345510	-	-

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