

Fully Relativistic *ab initio* Dirac-Coulomb Calculations of Atomic Properties of Rn and Element 118

A. Borschevsky¹, E. Eliav¹, U. Kaldor¹, and V. Pershina²

¹Tel Aviv University, Israel; ²GSI, Darmstadt, Germany

Experiments on the production of elements 112-116 in Dubna, Russia, have proven the existence of the enhanced stability of their neutron-rich isotopes. Furthermore, the existence of element 118 has been demonstrated using the ⁴⁸Ca beam and the ²⁴⁹Cf target [1]. The produced ²⁹⁴118 isotope has half-life $T_{\alpha}=0.89^{+1.07}_{-0.31}$ ms in agreement with the theoretical predictions and decays into ²⁸⁶114 or ²⁸²112, which undergo spontaneous fission,.

Chemical identification of element 118 is a matter of the near future. Predictions of its chemical properties, especially those important for gas-phase chromatography experiments [2] are, therefore, needed. Very accurate calculations can nowadays be performed using fully relativistic methods and algorithms. Thus, in this work we predict atomic properties of element 118 and its homolog Rn on the basis of *ab initio* Dirac-Coulomb (DC) calculations using the DIRAC package [3]. In the DC *ab initio* method, the many-electron relativistic Dirac-Coulomb Hamiltonian

$$H_{DC} = \sum_i h_D + \sum_{i<j} 1/r_{ij} \quad (1)$$

is employed, where

$$h_D = c\vec{\alpha} \cdot \vec{p} + \beta c^2 + V_{nuc}. \quad (2)$$

The atomic orbitals are four-component spinors

$$\phi_{nk} = \begin{pmatrix} P_{nk}(r) \\ Q_{nk}(r) \end{pmatrix}, \quad (3)$$

where $P_{nk}(r)$ and $Q_{nk}(r)$ are large and small component, respectively. The Faegri uncontracted 26s24p18d13f5g2h basis set was used for Rn and element 118 [4]. The electron correlation was taken into account at various levels of theory - Moller-Plesset (MP2) and Coupled Cluster Single Double (Triple) excitations [CCSD(T)]. The Hartree-Fock (HF) values were also obtained for comparison in order to elucidate the influence of correlation.

The calculations of polarizability (α) were performed with the use of the finite field method. The strengths of the field were chosen as 0.0001, 0.001 and 0.01 a.u. The results are summarized in Table 1. The obtained DC CCSD(T) values are in very good agreement with experiment for Rn [5] and much better than those calculated in Ref. [6] using the MOLFDIR code. The latter values are not accurate due to the small basis sets used. The $\alpha(118)$ is larger than α of the other gases due to the relativistic expansion of the outer $7p_{3/2}$ atomic orbitals (AOs).

Table I. Polarizabilities α (in a.u.) for Rn and element 118 calculated at different levels of correlation.

Atom	α				Ref.
	HF	MP2	CCSD	CCSD(T)	
Rn	34.99	34.96	34.78	35.04	present
	29.22	28.48	28.61	28.61	calc. [6]
	-	-	-	35.766	exp. [5]
118	50.01	44.45	46.64	46.33	present
	54.46	49.47	52.50	52.43	calc. [6]

We also give here estimates of atomic, or van der Walls radii (R_{vdW}) of element 118. They were determined using a correlation between the maximum of the radial charge density of the outer valence $np_{3/2}$ AOs [7] and known R_{vdW} (Fig. 1). The obtained $R_{vdW}(118)$ is larger than R_{vdW} of the other gases due to the same reason as that for α .

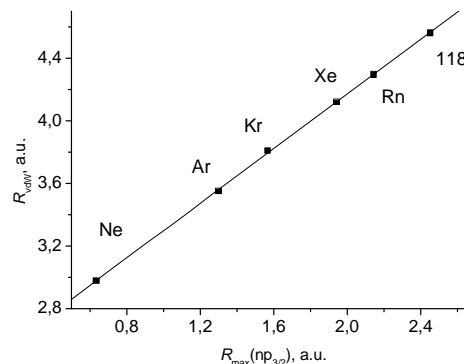


Fig. 1. Correlation between $R_{max}(np_{3/2})$ and R_{vdW} for the rare gases. The obtained value for $R_{vdW}(118) = 4.55$ a.u.

The calculated properties can be used for further predictions of adsorption behaviour of these elements on various surfaces.

References

- [1] Yu. Ts. Oganessia *et al.* Phys. Rev. C 74 (2006) 044602.
- [2] H. W. Gäggeler, A. Türler, In: Chemistry of Superheavy Elements, ed. M. Schädel, Kluwer, 2003.
- [3] DIRAC 04, written by H.J. Ja. Jensen *et al.* (2004).
- [4] K. Faegri, Theor. Chim. Acta 105 (2001) 252.
- [5] CRC Handbook of Chemistry and Physics, 86th edition, ed. D. R. Lide (2005).
- [6] C. Nash, J. Phys. Chem. 109 (2005) 3493.
- [7] J. P. Desclaux, At. Data Nucl Data Tables, 12 (1973) 311.