Theoretical Predictions of Properties of Element 120 and its Adsorption on Noble Metal Surfaces

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In the present work, we predict chemical properties and adsorption behaviour of element 120 whose production was attempted recently at the GSI, Darmstadt [1]. The most promising nuclear reaction appears to be ^{50}Ti + ^{249}Cf giving the ^{295}120 and ^{296}120 isotopes in the 4*n* and 3*n* evaporation channel, respectively [2]. Expected lifetime, of the order of μs, is too short for study of chemical properties of this element using current gas-phase chromatography techniques. However, development of vacuum chromatography could open new prospects in this field.

An analysis of atomic properties, calculated within the Dirac-Coulomb-Breit approach [3], shows that the relativistic stabilization and contraction of the valence ns AO in group 2 results in the inversion of trends beyond Ba, so that element 120 will be more electronegative than Ca. In this work, chemical reactivity of element 120 in comparison with its lighter homologs Ca through Ra was studied on the example of the M_2 and MAu dimers. Knowledge of properties of these compounds is indispensable for estimating quantities measured in the chromatography studies, i.e., sublimation, ΔH_{sub}, and adsorption enthalpies, ΔH_{ads}, on gold.

Molecular calculations were performed with the use of our fully relativistic, 4-component, Density Functional Theory method in the non-collinear spin-polarized approximation [4]. Results for M_2 and MAu are given in Tables 1 and 2, respectively.

Table 1. Spectroscopic properties of M_2 (M = K through element 120): bond lengths, R_e (in Å), dissociation energies, D_e (in eV) and vibrational frequencies, ω_e (in cm^{-1})[a]

Mol.	R_e	D_e	ω_e
Ca_2	4.236	0.141	66
	4.277	*0.137*	*65*
Sr_2	4.493	0.133	44
	4.498	*0.137*	*40*
Ba_2	4.831	0.226	43
Ra_2	5.193	0.106	25
$(120)_2$	5.646	0.018	9

[a] Values in italics are experimental.

The data of Table 1 show that $D_e(M_2)$ have a reversal of the trend beyond Ba. Thus, $(120)_2$ should be most weakly bound in the row of homologs, due to the 8s(120) AO contraction and van der Waals nature of bonding in M_2.

D_e(MAu) (Table 2) have also a reversal of the trend beyond Ba, so that 120Au should be the most weakly bound in the row of homologs due to the 8s(120) AO stabilization. ΔH_{sub} of the 120 metal and ΔH_{ads}(120) on gold were obtained via a correlation with the binding energies of the corresponding dimes in the group. According to the results, ΔH_{sub}(120) and -ΔH_{ads}(120) on Au (also on Pt and Ag) should be the smallest among the homologs.

Table 2. Properties of MAu (M = Ca through element 120): bond lengths, R_e (in Å), dissociation energies, D_e (in eV) and vibrational frequencies, ω_e (in cm^{-1})[a]

Mol.	R_e	D_e	ω_e
CaAu	2.627	2.706	221
	2.67	*2.545*	*221*
SrAu	2.808	2.629	159
BaAu	2.869	3.006	145
RaAu	2.995	2.564	105
120Au	3.050	1.902	97

[a] Values in italics are experimental.

Predicted trends in the adsorption of group-2 elements on noble metals are shown in Fig 1. The moderate values of ΔH_{ads}(120) are indicative of the feasibility of the chromatography chemical studies on this element.

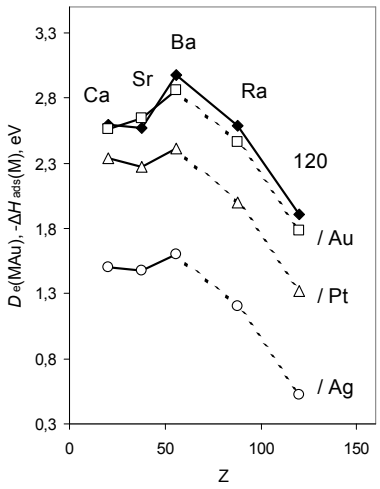

Fig. 1. Calculated D_e(MAu) (filled symbols) and -ΔH_{ads}(M) (open symbols), where M = Ca through element 120, on Au, Pt and Ag.

References

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