

# Empirical Relation between the Adsorption Properties on Gold Surfaces and Volatility of the Elements 112 and 114

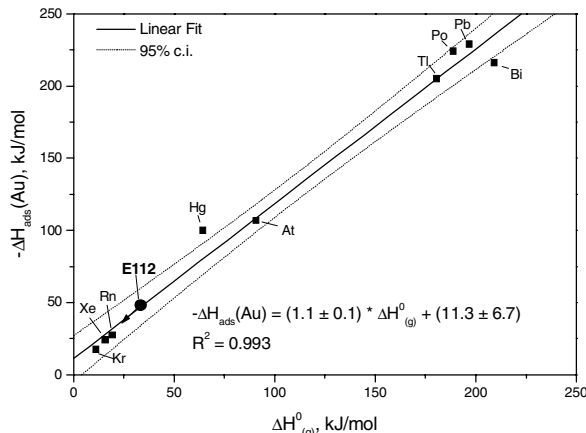
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The typical result of gas phase chemical investigations on a one-atom-at-a-time level are standard adsorption enthalpies ( $\Delta H_{\text{ads}}$ ) of chemical species on stationary chromatographic surfaces. The standard adsorption enthalpies are deduced from experimental results using either the model of linear gas chromatography assuming mobile adsorption [1] or Monte-Carlo based models [2]. The obtained enthalpy values are independent on experimental conditions. The absolute amounts of these enthalpies represent the strength of interaction of the species with the surface. For example the deposition temperatures represent a comparable measure for this interaction strength only in the case of comparable experimental conditions. Thermochemical data describe collective properties of macroscopic amounts of the chemical species. Hence, links are needed for the derivation of thermochemical data from the experiments with single atoms. Nowadays, the only links are empirical correlations between  $\Delta H_{\text{ads}}$  and collective data related to evaporation or sublimation as boiling points (b.p.) or standard sublimation enthalpies ( $\Delta H_{\text{subl}}$ ) of the type (eqn. 1):

$$-\Delta H_{\text{ads}} = A \cdot \Delta H_{\text{subl}} + B \quad (1)$$

The other way around, these correlations are used to predict the behavior of new chemical species in gas phase chemical adsorption studies using predicted thermochemical properties of these elements or compounds (see [3] for review). Empirical correlations as (eqn. 1) are established for chlorides and oxychlorides, oxides, and hydroxides, and for elements on quartz surfaces [3]. These correlations presuppose small or comparable netto adsorption enthalpies for all species on the respective stationary phase. Recently, the gas phase chemical investigation of the new transactinide p-elements are focused on the determination of the adsorption properties of their elemental state on noble metal surfaces. Especially, the elements 112 and 114 are expected to be very inert. Their metallic character is assessable only in the interaction with strongly oxidizing agents or in contact with noble metal surfaces. Hence, for the design of gas phase chemical experiments with these elements and for the data analysis of experimental results empirical correlations similar to that described above are indispensable. Here we present a correlation between the standard adsorption enthalpy of various elements on gold surfaces ( $-\Delta H_{\text{ads}}(\text{Au})$ ) and their standard sublimation enthalpy at 0 K ( $\Delta H^0(\text{g})$ ) (see Fig. 1). Other models can be used to describe directly the adsorption interaction of these elements on metal surfaces or to predict standard sublimation enthalpies. We use this correlation in order to predict the adsorption properties of the elements 112 and 114 in the experiments and to derive thermochemical data from first experimental results for element 112 [3][4] (see Table 1). Either  $-\Delta H_{\text{ads}}(\text{Au})$  is given for the element due to various predictions or  $\Delta H^0(\text{g})$ . The given correlation is used to derive the corresponding value.



**Fig. 1:** Correlation between  $-\Delta H_{\text{ads}}(\text{Au})$  and  $\Delta H^0(\text{g})$  (black squares). The upper limit experimental result for element 112 [3] is shown (black dot).

**Table 1:** Summary of predicted data (bold) together with the corresponding calculated data (eqn. in Fig. 1).

Element	$-\Delta H_{\text{ads}}(\text{Au})$ , kJ/mol	$\Delta H^0_{\text{subl}}$ , kJ/mol	Lit
112	35	<b>22</b>	[5]
112	<b>38-60</b>	25-44	[6]
112	53	<b>38</b>	[6]
112	<b>80</b>	63	[7]
112	-82	<b>-85</b>	[8]
112	<b>30</b>	<b>17</b>	[9]
112	34.4	<b>21</b>	[10]
112exp	<b>≤60</b>	<b>≤44</b>	[11]
112exp	<b>&lt;48</b>	<b>&lt;33</b>	[4]
114	90	<b>71.5</b>	[5]
114	<b>143</b>	120	[6]
114	220	<b>190</b>	[6]
114	<b>60</b>	44	[9]
114	35.5	<b>22</b>	[10]

## References

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