Atomic Properties of Element 113 and Its Adsorption on Inert Surfaces from *ab Initio* Dirac−Coulomb Calculations

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Fully relativistic *ab initio* Dirac-Coulomb Fock-space coupled cluster calculations were performed on Tl and element 113. The calculated polarizabilty of element 113, 29.85 au, is the smallest in group 13, except for B. The estimated atomic and van der Waals radii of element 113 are also the smallest among these elements. Using the calculated atomic properties and an adsorption model, adsorption enthalpies of elements Al through 113 on inert surfaces, such as Teflon and polyethylene, are predicted. The trends in the atomic properties and ΔH_{ads} in group 13 were found to reverse from In to element 113, reflecting the strong relativistic contraction and stabilization of the outer $n\mathrm{p}_{1/2}$ orbital, which are largest for element 113. The small values of ΔH_{ads} for element 113 on Teflon (14 kJ/mol) and polyethylene (16 kJ/mol) guarantee its transport from the target chamber to the chemistry set up, and the 6 kJ/mol difference relative to Tl values makes possible the separation and identification of the superheavy element on the inert surfaces.

I. Introduction

Chemical studies of the heaviest elements are the most fundamental type of studies.[1] They seek to probe the bottom of the periodic table, where nuclei become unstable and relativistic effects on the electronic shells are extremely strong.

The heaviest element whose chemical properties have been experimentally studied is $^{283}112$, with $t_{1/2}$ of 3.8 s.[2] Its adsorption behavior on a gold surface was investigated and compared with that of the nearest homologue, Hg, using gas phase chromatography.[3] Element 112 was found to be rather reactive under the experimental conditions, and predictions of its likeness to rare gases were not supported. It exhibited similar behavior (though somewhat less reactive) to that of Hg, confirming its position in group 12 of the periodic table. Similar experiments are under way to study the chemical behavior of element 114, whose isotopes $^{287}114$ and $^{288}114$ have $t_{1/2} = 0.5$ and 0.8 s, respectively.[4]

The odd element 113 has an isotope ($A = 284$) with $t_{1/2} = 0.48^{+0.58}_{-0.17}$ s, which makes it suitable for chemical studies. This isotope is obtained[5] by α-decay of the $^{288}115$ isotope, produced in the nuclear reaction of a ^{48}Ca beam with a ^{243}Am target. Its adsorption behavior may be investigated by gas chromatography, as was done in the element 112 studies: the 113 isotope will be adsorbed on silicon detectors of the chromatography column covered with a gold layer. Feasibility experiments are underway, studying the adsorption behavior of the nearest homologue, Tl.[6]

Prediction of the adsorption enthalpy, ΔH_{ads}, and temperature, T_{ads}, of element 113 on a gold surface is very important for the planned experiments. Information about adsorption on inert surfaces such as Teflon and polyethylene is also valuable, as these materials are used as transport capillaries from the target chamber to the detection system in the experimental setup.

The fundamental chemical properties of element 113 were predicted as early as 1970 by Keller et al.,[7] using Dirac−Fock atomic calculations and extrapolations in group 13. Some recent studies[8−10] include relativistic calculations for the simple molecules (113)H, (113)F, and $(113)\mathrm{X}_3$ (X = H, F, and Cl). The stability of $113\mathrm{F}_5$ has also been considered.[8]

In earlier works we predicted ΔH_{ads} and T_{ads} of elements 112 and 114 on various surfaces - on metals using results of the fully relativistic density functional theory calculations,[11] and on inert surfaces using results of atomic *ab initio* Dirac−Coulomb (DC) calculations and adsorption models.[12] Here we present atomic property calculations of Tl and element 113, using advanced relativistic *ab initio* methods. On the basis of these calculations we predict adsorption enthalpies of these and other group 13 elements on Teflon and polyethylene. An analysis of trends in the properties for the entire group 13 elements, including element 113, is also presented.

The methodology and details of the calculations are described in the next section. Section III presents the results of the calculations and discusses atomic properties. Adsorption is considered in section IV, and conclusions are given in section V.

II. Methodology and Calculation Details

A. Energy Calculations. Calculations of heavy element properties must take into account relativistic effects and explicit electron correlation. The core electrons, which experience the largest effects of relativity, contribute little to the electronic response properties of the atom. However, these properties experience indirect relativistic effects through the contraction of the valence orbitals, which might be significant.

Energy calculations were performed using the DIRAC04 package.[13] The Dirac−Coulomb Hamiltonian is employed, with an external electric field added. The DC Hamiltonian is

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

with

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$$h_D = c\alpha \cdot \mathbf{p} + \beta c^2 + V_{\text{nuc}} \qquad (2)$$

α and β are the four-dimensional Dirac matrices, and V_{nuc} is the nuclear attraction operator, with the nucleus modeled as a finite-size charge. Only the one-electron terms in the DC Hamiltonian are relativistic, while the two-electron repulsion terms remain in the nonrelativistic form.

The ground states of Tl and element 113 have one electron in the $n\text{p}_{1/2}$ shell. The Fock space coupled cluster (FSCC) method with sectors (0,0) and (0,1) was used. The closed-shell cation served as reference, and the (0,1) sector was constructed with the $n\text{p}_{1/2}$ valence orbitals ($n = 6$ for Tl and $n = 7$ for element 113). The Faegri basis set[14] with 26s24p18d13f5g2h uncontracted Gaussian-type orbitals was taken for both atoms. For Tl, 44 electrons were correlated and virtual orbitals above 30 au were omitted. For element 113, 46 electrons were correlated, and virtual orbitals above 100 au were omitted.

B. Atomic Polarizabilities. Atomic polarizabilities were calculated in the same way as in ref 12. In brief, for a uniform electric field F acting in the z direction only ($F_x = F_y = 0$ and $F_z = F$), the polarizability becomes

$$\alpha = -\frac{\partial^2 E(F)}{\partial^2 F}_{F=0} \qquad (3)$$

To obtain α of the elements under study, we calculated the energy $E(F)$ of the atomic ground states for different values of external electric field, $F = 0$, 0.0005 and 0.001 au. For atoms the dipole moment is zero because of parity, and the energy may be expressed as

$$E(F) = E(0) + \frac{1}{2}F^2 \cdot \frac{\partial^2 E(F)}{\partial F^2}_{F=0} + \cdots \qquad (4)$$

The energies $E(F)$ are plotted as a function of F^2, and the derivative is obtained by numerical differentiation. As eq 3 shows, the negative value of the derivative, multiplied by two, gives the static dipole polarizability α.

C. Ionization Potentials and Electron Affinities. Ionization potentials (IP) and energy levels of the neutral through the 5+ ionized states, as well as electron affinities (EA) of Tl and element 113, were calculated previously using the Dirac−Coulomb−Breit (DCB) Hamiltonian and relativistic coupled cluster single double excitations method for correlation.[15] Very large basis sets were used, with l up to 6 (See ref 15 for details). Here we calculate the IPs using the DIRAC04 program[13] and the same basis set[14] as for the polarizabilities (section II.A).

D. Atomic and van der Waals Radii. The atomic (AR) and van der Waals (R_{vdW}) radii of element 113 are obtained from the radius, $R_{\max}$, of the outer $n\text{p}_{1/2}$ maximum charge density,[16] using correlations with the known in group 13 values. See below for details.

III. Atomic Properties

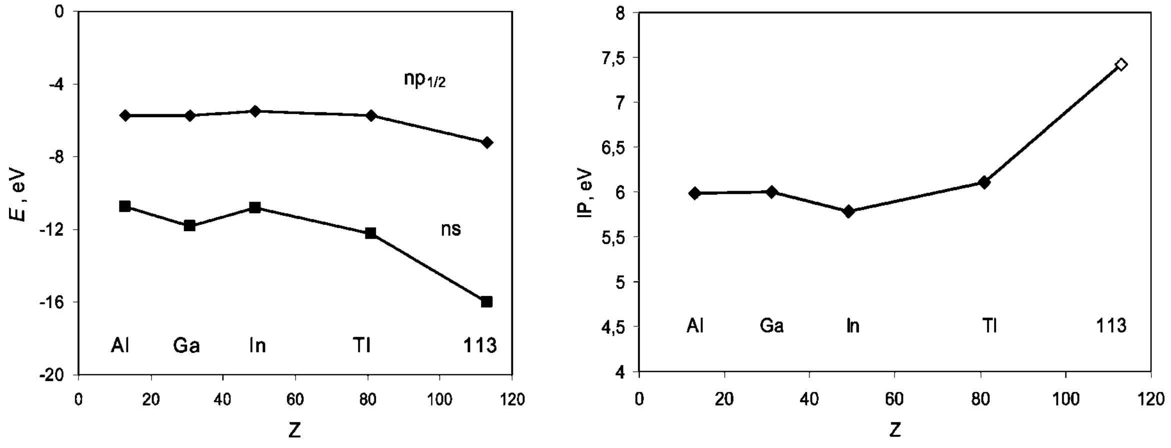
A. Electronic Configurations and Stability of Oxidation States. The chemistry of element 113 will be defined by the valence $7\text{p}_{1/2}$ orbital, which is relativistically stabilized and contracted. The 7s electrons, with even stronger stabilization, are less accessible for bonding, as indicated by their energies, E, and $R_{\max}$ (see Table 1 and Figures 1a and 2a). The principal oxidation state of this element will therefore be 1+, as indicated by consecutive IPs.[15] Molecular calculations[8−10] have also shown that the stability of the 1+ oxidation state with respect to the 3+ state increases with Z in group 13. The stability of the 1+ oxidation state with respect to the neutral atom, however, decreases from Tl to element 113, so that the latter will be less reactive than Tl. Thus, the standard redox potential $E°(113^{1+}/113)$ is 0.6 V, compared to −0.34 V[8] for $E°(\text{Tl}^{1+}/\text{Tl})$. The possibility of a 5+ oxidation state and formation of 113F_6^- was discussed in ref. 8, due to the involvement of the relativistically destabilized 6d AOs in bonding.

B. Ionization Potentials and Electron Affinities. The results of DCB RCC[15] and present DC FSCC calculations of the first IPs are presented and compared with experiment[17] in Table 1. The DC values reported here are very close to the earlier DCB results,[15] obtained with a better Hamiltonian and larger basis, confirming the good accuracy of the present calculations. The DCB RCC EAs[15] of Tl and element 113 are also shown; note the close agreement with the experimental[18] EA of Tl, measured several years after the calculations. The $l > 4$ basis functions have been shown[15] to change the EA by 0.01 eV or less, and the Breit term has similar effect on transitions not involving f electrons.

The first three IPs[15] of element 113 are higher than those of Tl, reflecting the relativistic stabilization of the $7\text{p}_{1/2}$ and 7s AOs, and predicting a reduced reactivity of the heavier element. The larger EA of element 113 is also indicative of the relativistically stabilized $7\text{p}_{1/2}$ AO. Figure 1 shows the $n\text{p}_{1/2}$ orbital energies and first IPs of Al through element 113. The decrease observed from Al to In is reversed to Tl and element 113, reflecting their

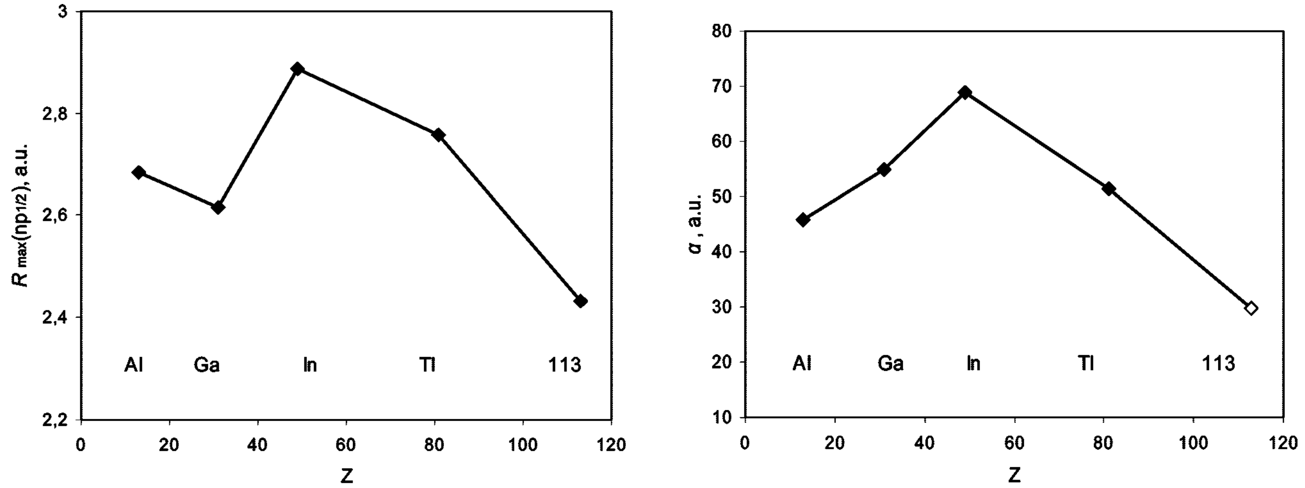
TABLE 1: Atomic Properties: Maxima of the Radial Charge Density $R_{\max}$ (in Å) and Energies E (in eV) of the Outer ns and $n\text{p}_{1/2}$ AOs, Ionization Potentials IP (in eV), Electron Affinities (EA) (in eV), Polarizabilities α (in au), van der Waals R_{vdW} (in Å) and Atomic Radii AR (in Å) of Tl and Element 113

property	Tl	method	ref	113	method	ref
$R_{\max}(n\text{p}_{1/2})$	1.459	DF	16	1.287	DF	16
$R_{\max}(n\text{s})$	1.133	DF	16	1.091	DF	16
$E(n\text{p}_{1/2})$	5.751	DF	16	7.223	DF	16
$E(n\text{s})$	12.22	DF	16	16.00	DF	16
IP	6.108	DCB RCC	15	7.306	DCB RCC	15
	6.096	DC FSCC	this work	7.420	DC FSCC	this work
	6.110	exp	17	7.4	DF	7
EA	0.40(5)	DCB RCC	15	0.68(5)	DCB RCC	15
	0.377(13)	exp	18			
α	51.3	DC FSCC	this work	29.9	DC FSCC	this work
	51(7)	exp	17			
R_{vdW}	1.90	correlation	this work	1.84(1)	correlation	this work
	1.96	exp	19			
AR	1.38	correlation	this work	1.22	correlation	this work
	1.90	exp	20			



(a) (b)

Figure 1. (a) Energies (E) of the ns and $np_{1/2}$ AOs[16] and (b) the first ionization potentials (IP) of group 13 elements. The IP for Al through Tl are experimental values (filled symbols),[17] for element 113 (open symbol)—our calculations.



(a) (b)

Figure 2. (a) Radii of the maximum charge density of the $np_{1/2}$ AOs[16] and (b) polarizabilities of group 13 elements. The α for Al through Tl are experimental, except for Ga, which is calculated;[17] the element 113 value is from present calculations.

TABLE 2: Selected Values of the Group 13 Element Properties: Ionization Potentials IP (in eV), Electron Affinities EA (in eV), Polarizabilities α (in au), Atomic (AR) and van der Waals Radii R_{vdW} (in Å)

element	IP[a]	EA[b]	α[a]	AR[c]	R_{vdW}[d]
Al	5.98577	0.43283(5)	45.889	1.25	1.89
Ga	5.999301	0.43(3)	54.796	1.30	1.87
In	5.78636	0.404(9)	68.833	1.55	1.93
Tl	6.108194	0.377(13)	51.287	1.38[e]	1.90[e] (1.91[c])
113	7.306[f]	0.68(5)[f]	29.85[e]	1.22[e]	1.84 ± 0.01[e]

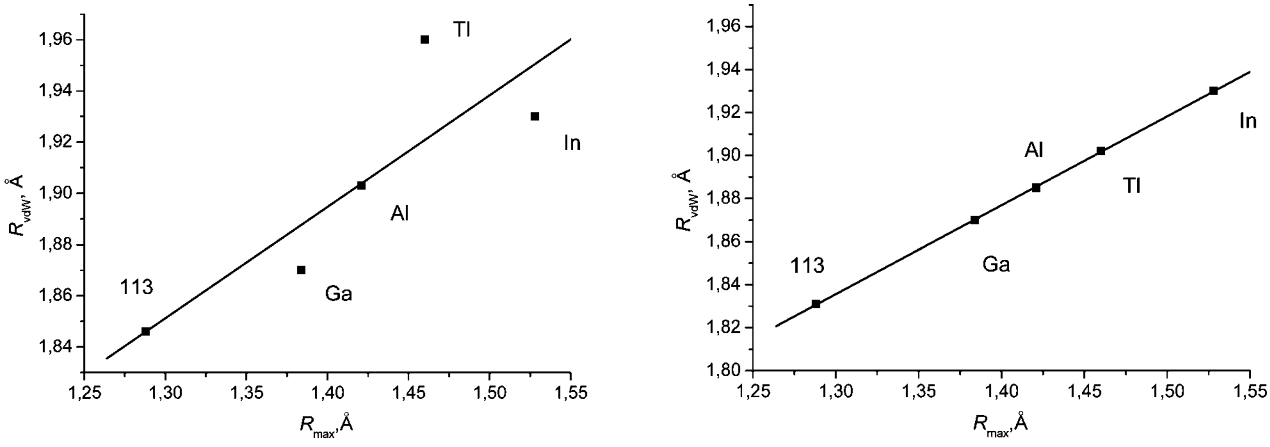
[a] Reference 17. [b] Reference 18. [c] Reference 21. [d] Reference 19. [e] This work. [f] Reference 15.

relativistic stabilization. The same trend is observed in the subsequent IPs[15] due to the relativistic stabilization of the ns AOs.

C. Polarizabilities. Table 1 shows the polarizabilities of Tl and element 113, derived from the DC-FSCC energy calculations as described in section II.B. The calculated α(Tl) agrees very well with experiment[17] (Tables 1 and 2), and similar accuracy is expected for element 113. Data for all group 13 elements are shown in Table 2 and Figure 2b. Experimental values are given when available;[17] the number for Ga is calculated,[17] with an expected accuracy of 2%, and our DC FSCC result is listed for element 113. A reversal of the trend is observed beyond In, similar to that of $R_{\max}(np_{1/2})$. Element 113 shows the lowest α in the group (except B), a result of the large relativistic contraction and stabilization of the $7p_{1/2}$ orbital.

D. Atomic and van der Waals Radii. Empirical van der Waals[19] and atomic radii[20] are available for some of the group 13 atoms (see Table 2). The unknown or uncertain values may be estimated using a correlation between the known values and $R_{\max}$ of the $np_{1/2}$ AOs.[16] The correlation between $R_{\max}(np_{1/2})$ and R_{vdW}, using the experimental radii[19] for In, Ga and Tl, is shown in Figure 3(a). It gives $R_{\mathrm{vdW}}(\mathrm{Al}) = 1.90$ Å and $R_{\mathrm{vdW}}(113) = 1.85$ Å. Tl lies rather far from the correlation line, and another correlation, using only the Ga and In points, is shown in Figure 3(b). The estimated values of R_{vdW} are now 1.89 Å for Al, 1.90 Å for Tl, and 1.83 Å for element 113. R_{vdW} of element 113 is therefore taken as 1.84(1) Å. Calculations of adsorption enthalpies below show that $R_{\mathrm{vdW}}(\mathrm{Tl}) = 1.90$ Å is a better value than the 1.96 Å (ref 19) and is, therefore, recommended. The R_{vdW} values used in the calculations of adsorption enthalpies are summarized in Table 2.

The AR[20] of B through In are very close to the corresponding $R_{\max}(np_{1/2})$, while AR(Tl) = 1.90 Å (ref 20) is much too large. Using a linear correlation between AR and $R_{\max}(np_{1/2})$ (Figure 4), the AR values were obtained for Tl and element 113 (Table



(a) (b)

Figure 3. Correlation between $R_{max}(np_{1/2})$ and R_{vdW}: (a) values for Ga, In and Tl are experimental,[19] those for Al (1.90 Å) and element 113 (1.85 Å) are present calculations; (b) values for In and Ga are experimental,[19] those for Al (1.89 Å), Tl (1.90 Å) and element 113 (1.83 Å) are present calculations.

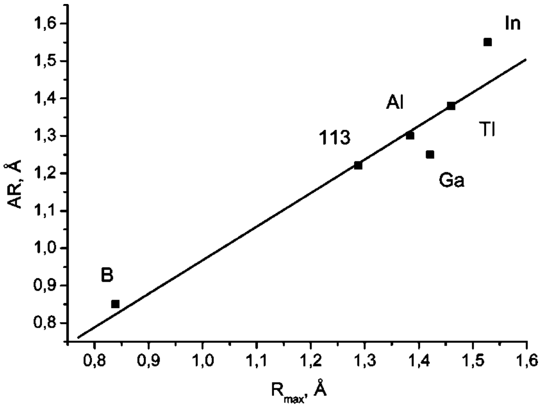


Figure 4. Correlation between $R_{max}(np_{1/2})$ and AR: The values for B, Al, Ga, and In are experimental,[20] and those for Tl (1.38 Å) and element 113 (1.22 Å) are from present work.

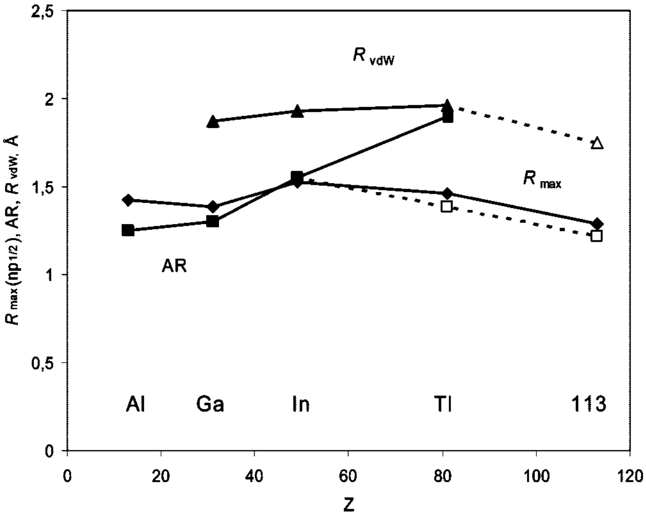


Figure 5. Maximum of the radial charge density (R_{max}, diamonds) of the $np_{1/2}$ orbitals,[16] atomic radii (AR, squares) and van der Waals radii (R_{vdW}, triangles) of group 13 elements. The filled symbols are experimental data,[19,20] open symbols are present estimates.

1, Figures 4 and 5). The AR and R_{vdW} of Al through element 113 are given in Table 2 and shown in Figure 5 along with $R_{max}(np_{1/2})$. The R_{vdW} values for In and Tl are in excellent agreement with those of 1.98 Å and 1.91 Å, respectively, obtained from the *ab initio* calculations[21] for the model $[M(Cp)]_2$ systems. Both types of the radii exhibit a trend reversal beyond In, due to the relativistic contraction of the outer $np_{1/2}$ AOs. R_{vdW} and AR of element 113 are, therefore, the smallest in the series.

A summary of the atomic properties used in the calculations of the adsorption enthalpies is presented in Table 2.

IV. Adsorption on Inert Surfaces

It was shown[12,22] that the dispersion interaction energy of an atom with a solid surface can be rather accurately calculated via the following equation, derived from a model of an atom−slab interaction[23]

$$E(x) = -\frac{3}{16}\left(\frac{\varepsilon - 1}{\varepsilon + 2}\right)\frac{\alpha_{at}}{\left(\frac{1}{IP_{slab}} + \frac{1}{IP_{at}}\right)x^3} = -\frac{C_3}{x^3} \qquad (5)$$

Here IP_{slab} and IP_{at} are the ionization potentials of the surface material and adsorbed atom, respectively, α_{at} is the polarizability of the adsorbed atom, ε is the dielectric constant of the surface material and x is the adatom-surface distance. It was also shown[12,24] that x can be well approximated by R_{vdW} of the adsorbed species.

The properties of the inert materials of interest are the following: for Teflon $\varepsilon = 2.04$ and IP = 10.12 eV;[12] for polyethylene (PE) $\varepsilon = 2.26$ and IP is in the range 9.6−9.8 eV.[25] Using these values and the atomic IP, α and R_{vdW} of Table 2, the C_3 coefficients and adsorption enthalpies $\Delta H_{ads} = -E(x)$ were calculated by eq 5. The resulting values are shown in Table 3 and in Figure 6.

The calculated ΔH_{ads} of group 13 elements on Teflon are somewhat smaller than those on PE. An inversion of trend beyond In is observed for both surfaces (Figure 6). The inversion is caused by the drastically decreasing atomic polarizabilities, as seen by comparing the polarizability graph, Figure 2b, with that of ΔH_{ads}, Figure 6. The smaller α is not compensated by a decrease of x or R_{vdW} in eq 5; the latter is nearly the same for all these elements (Figure 5). $E(x)$ of element 113, which has the smallest α, is therefore the lowest, making this element the most volatile in group 13, and there should be no problem with its transport from the target chamber to the chromatography setup.

TABLE 3: Calculated C_3 Coefficients and Adsorption Enthalpies ΔH_{ads} of Group 13 Atoms on Teflon and Polyethylene (PE), Where the ΔH_{ads} for Tl Is Calculated with R_{vdW} = 1.90 Å

	Teflon			PE		
	C_3	ΔH_{ads}		C_3	ΔH_{ads}	
element	eV·au^3	eV	kJ/mol	eV·au^3	eV	kJ/mol
Al	8.325	0.170	17.28	9.420	0.203	19.54
Ga	9.959	0.226	21.78	11.264	0.255	24.63
In	12.226	0.252	24.32	13.835	0.285	27.51
Tl	9.429	0.203[a]	19.65[a]	10.660	0.230[b]	22.22[b]
113	6.100	0.145	14.00	6.899	0.164	15.83

[a] ΔH_{ads} = 0.18 eV or 17.90 kJ/mol for R_{vdW} = 1.96Å; [b] ΔH_{ads} = 0.21 eV or 20.24 kJ/mol for R_{vdW} = 1.96Å.

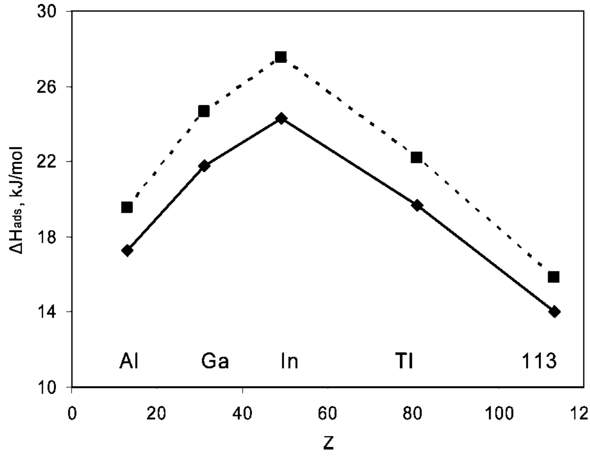


Figure 6. Calculated adsorption enthalpies, ΔH_{ads}, of group 13 elements on Teflon (solid line) and polyethylene (dashed line). R_{vdW} = 1.90 Å was taken for Tl.

V. Conclusion

The static dipole polarizabilities and ionization potentials for Tl and element 113 were calculated using the DC FSCC method. The calculated α(Tl) agrees very well with experiment. The DC FSCC IP for Tl is also very close to experiment, and the IP of element 113 agrees with the most accurate DCB RCC calculations. Atomic and van der Waals radii of Tl and element 113 were estimated from the radius R_{max} of the outer valence electron distribution. The atomic properties served to calculate the adsorption enthalpies of elements Al through 113 on the inert surfaces Teflon and polyethylene.

The atomic properties and adsorption enthalpies for Al through element 113 exhibit trend reversal beyond In. This is caused by the strong contraction and stabilization of the outer $np_{1/2}$ orbitals of Tl and element 113. The effect is strongest for element 113, resulting in the smallest polarizability and atomic and van der Waals radii in group 13 (except B), while the ionization potential and electron affinity are the largest. The extremely small α of element 113 is the main reason for its low adsorption enthalpy on inert surfaces. The calculated ΔH_{ads} of 14 kJ/mol on Teflon and 16 kJ/mol on polyethylene will allow easy transport of element 113 from the target chamber to the chemistry set up. These adsorption enthalpies are about 6 kJ/mol weaker below corresponding Tl values, making possible the separation and identification of the heavier element by the use of inert surfaces.

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References and Notes

(1) *The Chemistry of the Superheavy Elements*; Schädel, M., Ed.; Kluwer: Dordrecht, The Netherlands, 2003.

(2) Oganessian, Yu. Ts.; Utyonkov, V. K.; Lobanov, Yu. V.; Abdulin, F. Sh.; Polyakov, A. N.; Sagaidak, R. N.; Shirokovsky, I. V.; Tsyganov, Yu. Ts.; Voinov, A. A.; Gulbekian, G. G.; Bogomolov, S. L.; Gikal, B. N.; Mezentsev, A. N.; Iliev, S.; Subbotin, V. G.; Sukhov, A. M.; Subotnic, K.; Zagrebaev, V. I.; Vostokin, G. K.; Itkis, M. G. *Phys. Rev. C* **2006**, *74*, 044602.

(3) Eichler, R.; Aksenov, N. V.; Belozerov, A. V.; Bozhikov, G. A.; Vhepigin, V. I.; Dmitriev, S. N.; Dressler, R.; Gäggeler, H. W.; Gorshkov, V. A.; Haenssler, F.; Itkis, M. G.; Laube, A.; Lebedev, V. Ya.; Malyshev, O. N.; Oganessian, Yu. Ts.; Petrushkin, O. V.; Piguet, D.; Rasmussen, P.; Shishkin, S. V.; Shutov, S. V.; Svirikhin, A. I.; Tereshatov, E. E.; Vostokin, G. K.; Wegrzecki, M.; Yeremin, A. V. *Nat. Lett.* **2007**, *447*, 72.

(4) Eichler, R. Manuscript in preparation.

(5) Oganessian, Y. *J. Phys. G: Nucl. Part. Phys.* **2007**, *34*, R165.

(6) König, S., Gäggeler, H. W.; Eichler, R.; Haenssler, F.; Soverna, S.; Dressler, R.; Friedrich, S.; Piguet, D.; Tobler, L. *PSI Annual Report* 2005 (http://lch.web.psi.ch/pdf/anrep05/03.pdf).

(7) Keller, O. L., Jr.; Burnett, J. L.; Carlson, T. A.; Nestor, C. W., Jr. *J. Phys. Chem.* **1970**, *74*, 1127.

(8) Seth, M.; Schwerdtfeger, P.; Faegri, K. *J. Chem. Phys.* **1999**, *111*, 6422.

(9) Seth, M. *The Chemistry of the Superheavy Elements*; Thesis, University of Auckland, 1998.

(10) Han, Y. K.; Bae, C.; Lee, Y. S. *J. Chem. Phys.* **1999**, *110*, 8986.

(11) Sarpe-Tudoran, C.; Anton, J.; Fricke, B.; Pershina, V. *J. Chem. Phys.* **2007**, *126*, 174702.

(12) Pershina, V.; Borschevsky, A.; Eliav, E.; Kaldor, U. *J. Chem. Phys.* **2008**, *128*, 024707.

(13) Dirac, a relativistic *ab initio* electronic structure program, Release DIRAC04.0 (2004). Written by: Jensen, H. J. Aa.; Saue, T.; Visscher L. With contributions from: Bakken, V.; Eliav, E.; Enevoldsen, T.; Fleig, T.; Fossgaard, O.; Helgaker, T.; Laerdahl, J.; Larsen, C. V.; Norman, P.; Olsen, J.; Pernpointner, M.; Pedersen, J. K.; Ruud, K.; Salek, P.; van Stralen, J. N. P.; Thyssen, J.; Visser, O.; Winther, T. (http://dirac.chem.sdu.dk).

(14) Faegri, K. *Theor. Chim. Acta* **2001**, *105*, 252.

(15) Eliav, E.; Ishikawa, Y.; Pyykkö, P.; Kaldor, U. *Phys. Rev. A* **1997**, *56*, 4532. Eliav, E.; Kaldor, U.; Ishikawa, Y.; Seth, M.; Pyykkö, P. *Phys. Rev. A* **1996**, *53*, 3926.

(16) Desclaux, J. P. *At. Data Nucl. Data Tables* **1973**, *12*, 311.

(17) *CRC Handbook of Chemistry and Physics*, 86th ed. (2005−2006); Lide, D. R., Ed.; CRC Press: Boca Raton, 2005; (http://hbcpnetbase.com). Miller, T. M.; Bederson, B. *Adv. At. Mol. Phys.* **1988**, *25*, 37.

(18) Carpenter, D. L.; Covington, A. M.; Thompson, J. S. *Phys. Rev. A* **2000**, *61*, 042501, and references therein.

(19) Bondi, A. *J. Phys. Chem.* **1964**, *68*, 441.

(20) Slater, J. C. *J. Chem. Phys.* **1964**, *41*, 3199.

(21) Pyykkö, P.; Straka, M.; Tamm, T. *Phys. Chem. Chem. Phys.* **1999**, *1*, 3441.

(22) Pershina, V.; Anton, J.; Fricke, B. *J. Chem. Phys.* **2007**, *127*, 134310. Pershina, V.; Bastug, T.; Fricke, B.; Varga, S. *J. Chem. Phys.* **2001**, *115*, 792.

(23) Adamson, A. W. *Physical Chemistry of Surfaces*; John Wiley and Sons: New York, 1976; p 317.

(24) Zaremba, E.; Kohn, W. *Phys. Rev. B* **1976**, *13*, 2270.

(25) Seki, K.; Ueno, N.; Karlsson, U. O.; Engelhardt, R.; Koch, E. E. *Chem. Phys.* **1986**, *105*, 247.

JP8061306