

Predicted Properties of the Superheavy Elements. III. Element 115, Eka-Bismuth^{1a}

O. L. Keller, Jr.,*^{1b} C. W. Nestor, Jr.,

Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830

and Burkhard Fricke

Gesellschaft für Schwerionenforschung, Darmstadt, BRD, Germany (Received April 29, 1974)

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Element 115 is expected to be in group V-a of the periodic table and have most stable oxidation states of I and III. The oxidation state of I, which plays a minor role in bismuth chemistry, should be a major factor in 115 chemistry. This change will arise because of the large relativistic splitting of the spherically symmetric $7p_{1/2}$ shell from the $7p_{3/2}$ shell. Element 115 will therefore have a single $7p_{3/2}$ electron outside a $7p_{1/2}^2$ closed shell. The magnitude of the first ionization energy and ionic radius suggest a chemistry similar to Tl^+ . Similar considerations suggest that 115^{3+} will have a chemistry similar to Bi^{3+} . Hydrolysis will therefore be easy and relatively strongly complexing anions of strong acids will be needed in general to effect studies of complexation chemistry. Some other properties of 115 predicted are as follows: ionization potentials I 5.2 eV, II 18.1 eV, III 27.4 eV, IV 48.5 eV, $0 \rightarrow 5^+$ 159 eV; heat of sublimation, 34 kcal (g-atom)⁻¹; atomic radius, 2.0 Å; ionic radius, 115^+ 1.5 Å, 115^{3+} 1.0 Å; entropy, 16 cal deg⁻¹ (g-atom)⁻¹ (25°); standard electrode potential $115^+|115$, -1.5 V; melting and boiling points are similar to element 113.

Introduction

Interest in superheavy elements remains high as new heavy-ion beams are being developed at the Super HILAC accelerator at Berkeley and construction proceeds on the UNILAC in Darmstadt. For over 1 year the Dubna heavy-ion accelerator group has been carrying out reactions that might produce superheavy elements. The recent Russian attempt to use the reaction of ^{76}Ge with ^{232}Th to reach elements in the island of stability was unfortunately unsuccessful.² This suggests that the discovery of superheavy elements will probably be difficult, since the germanium plus thorium reaction was expected to be one of the more favorable cases.³ Chemical separations methods may now take on added importance in the search since they might offer much higher reliability and sensitivity than physical and nuclear methods. This was the case in the discovery of fission, for example.⁴

Element 115, eka-bismuth, is a particularly interesting case scientifically since its chemistry will be strongly altered by relativistic effects.⁵ There is, in fact, no element like 115 available to us in the present periodic system. An approach involving careful comparisons with the periodic table and analogies based on relativistic Hartree-Fock (rel HF) and relativistic Hartree-Fock-Slater (rel HFS) calculations appears to be best under these circumstances. Our predictions therefore involve first calculating electronic energy levels, ionization potentials, promotion energies to excited states, and atomic and ionic radii. The rel HFS programs were those of Oak Ridge and Fricke that we have used previously.^{6,7} The relativistic Hartree-Fock program was very kindly made available to us by Desclaux.⁸

All three atomic calculational methods gave results which were close to each other. Further properties were estimated by combining the calculated quantities with valence bond theory or other general theories and by extrapolations in the periodic system. We first of all present in the following paragraphs our calculational results. These will

then be combined in the following sections to arrive at specific predictions on the chemical properties of element 115.

Ionization Energies

Calculated and experimental ionization energies of the Group V-a elements are given in Table I. The difference, Δ , between the experimental and rel HFS results were used to estimate an "experimental" value for the ionization potentials of 115 and its ions. For comparison we give in Table II the rel HFS and experimental values for the ionization energies of the group III-a elements, Pb, and Po.

Atomic and Ionic Radii

In our considerations of chemical and physical properties the atomic and ionic radii are of considerable importance. Stabilization of an ion in a solution or crystal is dependent on the magnitude of decrease in the ionic radius with increase in its ionization (charge) since the radius strongly influences solvation and lattice energies. The atomic radii, on the other hand, are important for considerations involving valence bond theory. As pointed out by Pauling⁹ and by Drago,¹⁰ metallic atoms with a large volume have weaker covalent bonding because the valence electrons are spread over a larger space so that less overlap with the orbitals of anions results. Calculated atomic radii of the group V-a elements along with their empirical values as given by Slater¹¹ are given in Table III. Values for Tl, Pb, and Po are also given for comparison. The average radius of the outermost electronic shell, $\langle r \rangle$, was calculated both by the rel HF and rel HFS methods for As, Sb, Bi, and 115. The results of the two methods are very similar. Also the radius of maximum radial charge density for the outermost shell, r_{max} , is given. The latter is preferred by Slater¹¹ for comparison with his empirical atomic radii. In Figure 1 we plot Slater's atomic radii and the calculated r_{max} for the group V-a elements *vs.* row of the periodic table. The reproduction of the trend of the empirical radii by the calculations is obviously excel-

TABLE I: Ionization Energies of Group V-a Elements

Z	Ion	Ionization energies, eV			$\Delta(\text{exptl} - \text{rel HFS})$
		rel HF	rel HFS	Exptl	
15	P		8.6	10.484	1.9
	P ⁺		18.0	19.72	1.7
	P ²⁺		28.5	30.156	1.6
	0 → 5 ⁺		169.8	176.72	6.9
33	As	8.44	8.00	9.81	1.8
	As ⁺	17.0	17.1	18.63	1.6
	As ²⁺	27.6	27.0	28.34	1.4
	As ³⁺	-	49.6	50.1	0.5
51	Sb	162.5	164.2	169.5	5.3
	Sb ⁺	7.49	7.05	8.639	1.6
	Sb ²⁺	15.4	15.5	16.5	1.0
	Sb ³⁺	24.6	24.1	25.3	1.2
83	Bi	142.4	144.6	150.5	5.9
	Bi ⁺	6.58	6.09	7.287	1.2
	Bi ²⁺	15.5	15.7	16.68	0.94
	Bi ³⁺	24.8	24.5	25.56	1.1
115	115	143.7	146.3	150.8	4.5
	115 ⁺	4.79	4.70	(5.2)	(0.5)
	115 ²⁺	17.70	17.4	(18.1)	(0.7)
	115 ³⁺	27.3	26.5	(27.4)	(0.9)
115	115 ³⁺	48.0	48.0	(48.5)	(0.5)
	0 → 5 ⁺	155	155	(159)	(4)

TABLE II: Ionization Potentials of Group III-a, Pb, and Po (eV)

	rel HFS	Exptl	Δ
Ga	5.02	6.00	0.98
	20.21	20.51	0.30
	30.50	30.70	0.20
0 → 3 ⁺	55.73	57.21	1.48
In	4.88	5.785	0.90
	18.41	18.86	0.45
	27.56	28.03	0.47
0 → 3 ⁺	50.85	52.67	1.82
Tl	5.24	6.106	0.87
	19.90	20.42	0.52
	29.30	29.8	0.5
0 → 3 ⁺	54.4	56.3	1.90
113	6.51	(7.4)	(0.9)
	22.78	(23.3)	(0.5)
	32.47	(33.0)	(0.5)
0 → 3 ⁺	61.76	(63.7)	(1.9)
Pb	6.4	7.415	1.0
	14.0	15.028	1.0
	31.6	31.93	0.3
Po	7.2	8.43	1.2
	14.8		
	26.8		

TABLE III: Slater Atomic Radius

Z	Element	rel HF, $\langle r \rangle$	Atomic radius		Slater atomic radius
			rel HFS, $\langle r \rangle$	rel HFS, r_{max}	
15	P		1.21	0.98	1.00
33	As	1.35	1.31	1.07	1.15
51	Sb	1.57	1.52	1.27	1.45
83	Bi	1.72	1.67	1.41	1.60
115	eka-Bi	2.07	2.00	1.77	(2.0)
81	Tl		1.80	1.42	1.90
82	Pb		1.58	1.22	1.80
84	Po		1.52	1.21	1.90

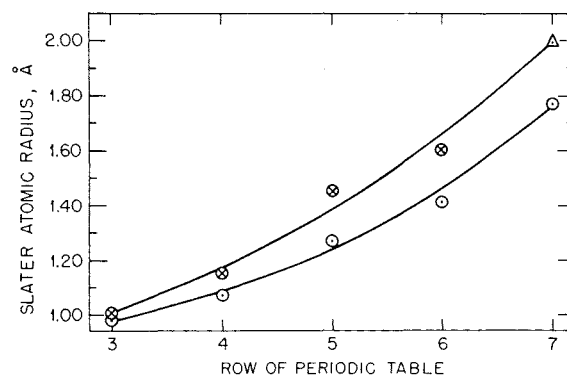


Figure 1. Slater atomic radii of group V-a elements (⊙), extrapolated atomic radius of element 115 (Δ) and maximum radial charge density in the outermost shell computed by rel HFS.

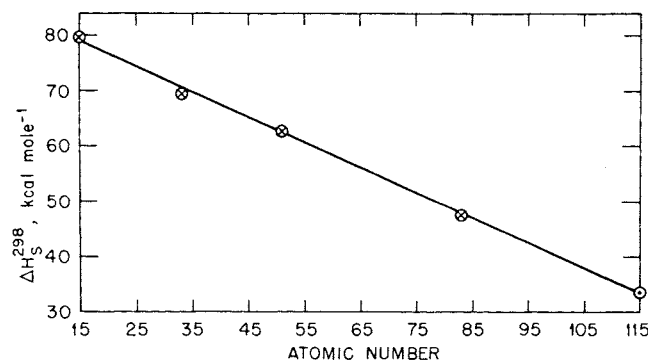


Figure 2. Heat sublimation of element 115.

lent, so we can use the plot of r_{max} with confidence as a guide in extrapolating to the value of 2.0 Å for the atomic radius of 115. This value is the same as our calculated values of $\langle r \rangle$.

In Table IV the computed values of $\langle r \rangle$ and r_{max} are given for the +1 and +2 or +3 ions of thallium, lead, bismuth, polonium, 113, and 115. Empirical ionic radii from Shannon and Prewitt¹² are given in the last column for the known ions. By comparison of the calculated radii with the elements whose radii are known, we estimate the radii of Bi⁺, Po²⁺, 113⁺, 113³⁺, 115⁺, and 115³⁺. The ionic radius of 115⁺ as derived in this way (1.5 Å) is found to be close to that of Tl⁺ and Bi⁺. The ionic radius of 115³⁺ (1.0 Å) is found to be close to that of Bi³⁺, but somewhat larger than Tl³⁺.

Heat of Sublimation

The heat of sublimation, ΔH_s^{298} , was obtained by extrapolation of the values¹³ for P, As, Sb, and Bi *vs.* atomic number, Z . As shown in Figure 2, ΔH_s^{298} for 115 is 34 kcal (g-atom)⁻¹. David¹⁴ extrapolated $\log \Delta H_s^{298}$ *vs.* $\log Z$ to obtain 35 kcal (g-atom)⁻¹. These simple extrapolations^{6,14} also yield 34 kcal (g-atom)⁻¹ for the ΔH_s^{298} of element 113. Since 115 and 113 are close together in the periodic system and both have a single 7p electron outside of closed shells, it is not surprising that their heats of sublimation would be similar. The higher first ionization potential of element 113 (Tables I and II) and its possibly smaller atomic radius might indicate that it would have a higher heat of sublimation than 115. The results obtained by extrapolation indicate a higher polarizability of 115 than 113 to counteract

TABLE IV: Radii of Ions of Tl, Pb, Bi, Po, 113, and 115 (Å)

Z	Ion	rel HFS (calcd)		Ionic radius ^a
		(r)	r _{max}	
81	Tl ⁺	1.23	1.11	1.50
	Tl ³⁺	0.69	0.60	0.88
82	Pb ⁺	1.43	1.18	
	Pb ²⁺	1.12	0.99	1.18
83	Bi ⁺	1.33	1.19	(1.5)
	Bi ³⁺	1.04	0.97	1.02
84	Po ⁺	1.41	1.18	
	Po ²⁺	1.18	1.03	(1.2)
113	113 ⁺	1.16	1.05	(1.4)
	113 ³⁺	0.82	0.72	(1.0)
115	115 ⁺	1.25	1.12	(1.5)
	115 ³⁺	1.01	0.95	(1.0)

^a Estimated values in parentheses. Empirical values from ref 12.

the ionization energy and possible radius differences. The rather high promotion energy of 7.4 eV from the 7s²7p ground state of element 113 to the 7s7p² trigonally hybridized valence state is an indication of a low polarizability compared to element 115 whose promotion energy from the 7p²_{1/2}7p^{3/2} state to the 7p²_{1/2}7p²_{3/2 state is calculated to be 4.8 eV (Table V where 115 is included under group III-a for tabular convenience).}

The melting point and boiling point of 115 can be expected to be close to the values for 113 given in paper I of this series.⁶

Excited State Energies

For 115(V) the promotion energy to the trigonal-bipyramidal sp³d valence state is needed. The promotion energies for the group V-a elements from the s²p³ ground state to the sp³d valence state are therefore also given in Table V. The rather high promotion energy for 115(V) of 18.4 eV compared to the value for Bi(V) of 15.5 eV indicates that the group valence will be even less important for eka-bismuth than for bismuth.

The Nature of the 115⁺ Ion

We expect that the chemistry of 115⁺ will be found more analogous to Tl⁺ than any other ion in the periodic system. This prediction is based on the values we have obtained for its ionization energy, ionic radius, and polarizability. The background for these conclusions follows.

The ground-state electronic configuration of element 115 is 7s²_{1/2}7p²_{1/2}7p^{3/2}. The presence of the 7p²_{1/2}7p^{3/2} ground-state configuration of 115 invites comparison to the s²p ground state of the group III-a elements. This is true because the 7p_{1/2} orbital is spherically symmetric (Figure 3) in the relativistic limit and is therefore rather like an s orbital. Most particularly, the 7p²_{1/2} shell is closed analogous to an s² closed shell. Thus the 7p^{3/2} electron is the first electron added outside closed shells and as a result its ionization energy is rather low (5.2 eV). The situation with respect to ionization energy is found to be similar to Tl which has a 6p_{1/2} electron outside of closed shells and has a first ionization energy of 6.1 eV.

A second important determining factor in the chemistry of 115⁺ will be its ionic radius compared to its atomic radius. A large decrease in radius indicates stabilization for the oxidation state involved. This stabilization is due to the accompanying increase in solvation or lattice energy. The decrease in radius on ionizing the 7p^{3/2} electron to form 115⁺

TABLE V: Promotion Energies^a

	ΔE, eV
I Group III-a (s ² p → sp ²)	
Ga	6.4
In	5.5
Tl	6.3
113	7.4
115 (7p ² _{1/2} 7p ^{3/2} → 7p ² _{1/2} 7p ² _{3/2})	4.8
II Group V-a (s ² p ³ → sp ³ d)	
P	15.8
As	16.4
Sb	14.2
Bi	15.5
115	18.4
III Tl ⁺ (6s ² _{1/2} → 6s _{1/2} 6p _{1/2})	7.0
Bi ⁺ (6s ² _{1/2} 6p ² _{1/2} → 6s ² _{1/2} 6p _{1/2} 6p ² _{3/2})	2.2
Po ²⁺ (6s ² _{1/2} 6p ² _{1/2} → 6s ² _{1/2} 6p _{1/2} 6p ² _{3/2})	3.1
113 ⁺ (7s ² _{1/2} → 7s _{1/2} 7p _{1/2})	6.9
115 ⁺ (7s ² _{1/2} 7p ² _{1/2} → 7s ² _{1/2} 7p _{1/2} 7p ² _{3/2})	5.6

^a Differences of total energies by rel HFS.

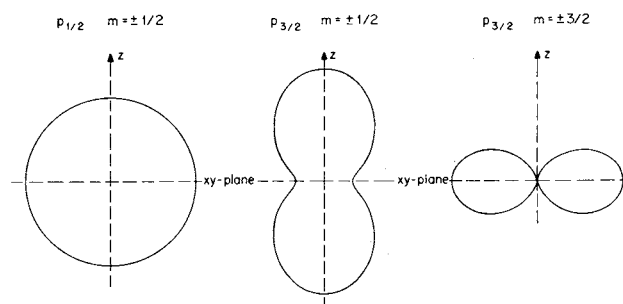


Figure 3. Angular distributions of relativistic p orbitals.

with a 7p²_{1/2} outer shell is 0.5 Å, quite comparable to the change of 0.4 Å in going from Tl to Tl⁺. In the case of Bi⁺ the decrease is only about 0.1 Å. This small decrease in radius coupled with the higher first ionization energy of 7.3 eV explains why Bi⁺ is not found in aqueous solutions (although it is found in molten salt media¹⁶). Tl⁺ is, of course, stable in aqueous solutions. At bismuth the relativistic effects have not become large enough to allow the two electrons in the 6p_{1/2} orbital to form a strongly closed shell. For this reason, 115⁺ is found to be more analogous to Tl⁺ than to Bi⁺ in its ionization potential and ionic radius.

There is, however, a further question about 115⁺, and this concerns how strong a "b" metal character it will have.¹⁵ Tl⁺ is intermediate in its behavior between Cu⁺, Ag⁺, and Au⁺ and the alkali metals.¹⁷ In analogy to the "b" cations, Tl⁺ forms an insoluble chloride, bromide, iodide, sulfate, and sulfide. On the other hand, Tl⁺ resembles the alkali metals in forming a soluble cyanide, hydroxide, carbonate, and oxalate. In contrast to Cu⁺, Ag⁺, and Au⁺, Tl⁺ forms only weak complexes with anions such as Cl⁻, Br⁻, and I⁻. It is for this reason, for example, that TlCl is not made more soluble¹⁸ by excess HCl whereas AgCl dissolves.

Dunitz and Orgel¹⁹ found a rough correlation between d-s separation energies and the tendency of d¹⁰ ions to distort or to show covalency effects in their bonding. The d-s separation energies for the "b" type ions Cu⁺, Ag⁺, and Au⁺ are 2.7, 4.8, and 1.9 eV, respectively.⁷ Of course, their radii would be expected to have an importance as well. The Slater atomic radii¹¹ are Cu (1.35 Å), Ag (1.60 Å), and Au (1.35 Å). The energies of separation in Tl⁺, Bi⁺, and 115⁺ between the ground and first excited states are given in

TABLE VI: Standard Electrode Potential for the 115⁺|115 Couple^{a,b}

ΔH_s^{298}	Ionization energy	$\Delta H_{\text{hyd}}(115^+(\text{aq}))$	$\bar{S}_{115^+(\text{aq})}^\circ$	$\bar{S}_{115(\text{s})}^\circ$	$-T\Delta S$	E°
1.5	5.2	-3.22	13.4×10^{-4}	6.9×10^{-4}	+0.4	-1.5

^a All quantities in appropriate units with energies in eV. ^b $0.5S^\circ_{\text{H}_2(\text{g})} = 6.8 \times 10^{-4} \text{ deg}^{-1}$. ΔH for reaction $0.5\text{H}_2(\text{g}) \rightarrow \text{H}^+(\text{aq}) + \text{e}^-$ is taken as 4.6 eV.

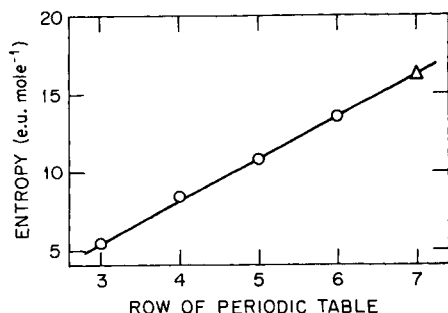


Figure 4. Entropy of elemental 115 (298°K).

Table V (where the values of Po^{2+} and 113^+ are also given for comparison). The calculated energies are Tl^+ (7.0 eV), Bi^+ (2.2 eV), and 115^+ (5.6 eV). 115^+ is thus seen to be intermediate between Tl^+ and Ag^+ in its promotion energy, but the much larger atomic radius of 115 (2.0 Å) will weaken covalent bonding effects in 115^+ as it does in Tl^+ (atomic radius = 1.90 Å).

Also the large ionic radius of 115^+ of 1.5 Å (Table IV) is similar to that of Tl^+ (1.5 Å), so the polarizing power of 115^+ on anions is expected to be weak as well.

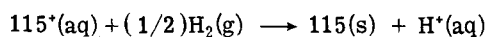
The conclusion we reach then is that the ionic picture of bonding is applicable to 115^+ to a degree that is similar to that found for Tl^+ .

Smith and Davis²⁰ have already pointed out expected relationships between Bi^+ and 115^+ with emphasis on spectroscopic and polycationic features.

Standard Electrode Potential of the 115⁺|115 Couple

For the cations of an ionic nature it is found that a calculation based on the Born-Haber cycle yields a reasonably quantitative value for the standard electrode potential.¹⁷ In paper I of this series,⁶ it was found that the Born-Haber cycle approach plus the inclusion of the entropy term gave quantitative agreement for the $\text{Tl}^+|\text{Tl}$ couple. We therefore expect a similar calculation to be helpful in interpreting the chemistry of 115^+ .

Electrode potentials are usually related to the standard $\text{H}^+(\text{aq})|\frac{1}{2}\text{H}_2(\text{g})$ couple whose potential is set equal to zero. We therefore consider the change in state for reduction of the aqueous metallic cation, $115^+(\text{aq})$, to the metal, $115(\text{s})$



The change in Gibbs free energy for this one electron reaction is related to the reduction potential and to the enthalpy and entropy by the equation

$$\Delta G = -E^\circ = \Delta H - T\Delta S \text{ (units in eV)}$$

The enthalpy change can be obtained using the Born-Haber cycle.⁶ The entropy change requires obtaining the elemental entropy of 115 metal by extrapolation as shown in Figure 4. The entropy of the aqueous metal ion can be calculated using the equation of Powell and Latimer.^{6,21} The results are given in Table VI. The $115^+|115$ couple is found to have the standard electrode potential -1.5 V com-

pared to the $\text{Tl}^+|\text{Tl}$ couple of -0.34 V and the $113^+|113$ couple of +0.6 V. (Please note that in paper I the so-called "american convention" on sign was used so that the couple referred to an oxidation potential.)

The Chemistry of the 115⁺ Ion

The 115^+ ion emerges as being more like the Tl^+ ion than any other species. It may even be still more ionic in its nature since the $115^+|115$ couple is calculated to be more negative, although this calculation cannot be taken too literally. Nonetheless, as for Tl^+ , the complexing ability of 115^+ can be expected to be low with such anions as the halides, cyanide, and ammonia. Hydrolysis should not be a problem for 115 in the oxidation state of I, and the hydroxide, carbonate, oxalate, and fluoride should be soluble. The sulfide should be insoluble and the chloride, bromide, iodide, and thiocyanate only slightly soluble. Excess HCl will not affect the solubility of $(115)\text{Cl}$ appreciably, for example. 115^+ should be more similar to Tl^+ in this respect than to Ag^+ .

The Chemistry of 115³⁺

The other possible oxidation state of element 115 is +3. We have not found it possible to predict the relative stabilities of the +1 and +3 states. In fact, their relative stabilities may well depend strongly on the state of complexation or hydrolytic conditions. As one might expect from simple extrapolation in the periodic table, we shall find that 115^{3+} is analogous to Bi^{3+} .

The sum of the first three ionization energies of Bi is 49.53 eV, of Tl^{3+} 56.3 eV, and of 115^{3+} (51 eV) (Table I). The ionization energy of 115^{3+} is therefore close to Bi^{3+} , but quite a bit below Tl^{3+} . Furthermore, the ionic radius of 115^{3+} is found to be close to that of Bi^{3+} (1.0 Å) but somewhat larger than that of Tl^{3+} (0.88 Å) (Table IV). On this basis 115^{3+} would be predicted to be more similar to Bi^{3+} than to Tl^{3+} . However the differences between the chemistry of Bi^{3+} and Tl^{3+} are more of degree than of kind, Bi^{3+} being a relatively weak "b" cation whereas Tl^{3+} is "super b."

In the first aqueous chemical studies of 115^{3+} hydrolysis should be avoided in order to obtain the more regular behavior usually associated with complex ion chemistry. In this connection, it should be remembered that mostly only the anions of strong acids are able to compete with hydrolysis in Bi^{3+} and Tl^{3+} aqueous chemistry. In their studies, Graner and Sillen²² found that 0.05 M Bi^{3+} hydrolyzes below an acidity of 0.5 M in 3 M perchlorate. Ahrlund and Grenthe²³ worked at an acidity of 1 M in their studies of the chloride, bromide, and iodide complexes of bismuth. They still found BiOCl and BiOBr precipitating in the absence of extra halide. Tl^{3+} behaves similarly except that its complexation powers are stronger. Ahrlund and Johansson²⁴ studied the chloride and bromide complexes of Tl^{3+} at an acidity of 3 M. Woods, Gallagher, Hugus and King²⁵ worked at an acidity of 0.5 and 3 M in their determinations of the association of Cl^- with Tl^{3+} . A helpful study has been done on this whole question by Biedermann and

Spiro.²⁶ These various studies suggest that the first ion-exchange or solvent-extraction studies of 115^{3+} should be tried at a concentration of around 3 M of a complexing acid such as HCl and/or a suitably high concentration of a relatively strongly complexing anion such as Cl^- .

In the general chemistry of 115^{3+} we expect a behavior similar to Bi^{3+} . The trichloride, tribromide, and triiodide of 115^{3+} will probably be soluble, and they may show a tendency to hydrolyze to form salts analogous to BiOCl and BiOBr . The trifluoride should be insoluble like BiF_3 . Bismuth shows slight amphoteric character and thallium shows essentially none; so 115^{3+} is not expected to be amphoteric to any degree. Like Tl_2S_3 and Bi_2S_3 , $(115)_2\text{S}_3$ will be insoluble. The sulfate and nitrate will be soluble in the respective acids and the phosphate will be insoluble.

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