CROATICA CHEMICA ACTA CCACAA **62** (4) 763—773 (1989)

YU ISSN 0011-1643
CCA-1905 UDC 541
Conference Paper

Electronic Structure of Superheavy Elements and Their Compounds

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Received February 6, 1989

To determine if element 104 in its compounds has d-or *p*-character the electronic structure of $KuCl_4$ has been calculated using a self-consistent relativistic multiple scattering model with $X\alpha$-exchange. By comparing the data obtained for $KuCl_4$ with those for $HfCl_4$ and $PbCl_4$ it has been established that $KuCl_4$ is not a full analog of $HfCl_4$.

1. INTRODUCTION

Long before the discovery of trans-actinides, questions were asked about the characted of the elements begining with N 103. After the discovery of Lr, the first experiment showed[1] that in water solution this element formed a stable trivalent state. By analogy with Lu its ground state configuration was supposed to be $(Rn)f^{14}ds^2$. In accordance with the fact the elements 103 to 112 were believed to form 6d-series, elements 113 to 118 were taken to form 7p-series. It meant that Lr had to be an analog of the elements of Ga-subgroup, and E104-Ti subgroup.

The following elements, 119 to 120, were considered to be analogs of alkaline and alkaline earth elements with ground state electronic configurations/No/$6d^{10}7p^68s^1$ and /No/$6d^{10}7p^68s^2$. By tradition (La and Ac) element 121 was considered to have the electronic configuration/No/$6d^{10}7p^68s^27d$, and then 32 electrons are to fill $6f^{14}$ and $5g^{18}$-shells up to element 153. Further, there must be a 7d- and 8p-electron shell filling for elements 154 to 162 and 163 to 168. This filled-shell concept doesn't assume any deviations from the periodicity and from what would be expected from a straightforward extrapolation of the Periodic Table.

A number of atomic calculations that appeared in recent years have enabled an insight into the physical and chemical properties of the still unknown superheavy elements. Some results have been reviewed by Hermann[3] and Fricke[4]. Many authors (3—5) have also emphasized that further development in this field must be based on calculations (in this case relativistic adequately describing the electronic structure of molecules, containing superheavy elements. A better knowledge of their chemical and physical properties is the prerequirement for a successful extraction and identification of the possible artificially generated superheavy elements.

It is known that close to the end of the Periodic Table relativistic effects begin to play a more important role influencing the electronic structure of heavy atoms and molecules, and as a result the chemistry of their compounds. Nevertheless, up to now no element is known whose ground state is different compared to the normal continuation of the Periodic Table, due to the direct relativistic influence. The first candidate for such a deviation turned out to be element 103 (Lr). It was Mann[6] who first pointed out that single configuration Dirac-Fock calculations give $5f^{14}7s^27p^1$ as the ground state. Independently Brewer[7] came to the same conclusion using a semi-empirical extrapolation and later he reaffirmed the result taking into account relativistic and correlation effects. Multiconfigurational relativistic Dirac-Fock calculations[9] predict the same ($5f^{14}$ $7s^27p_{1/2}$) electronic ground state configuration which arises from a strong relativistic stabilization of the $7p_{1/2}$ orbital. Furthermore, it has been suggested that the $7s^2$ closed shell might be sufficiently stabilized by relativistic effects to make it an »inert core« so that only $7p_{1/2}$ (or 6d) electron may be removed under reducing conditions, thus producing monovalent Lr. However, the experiments carried out in Darmstadt[11] have not confirmed the existence of monovalent Lr (it turned out to be impossible to reduce Lr^{3+} to the monovalent state in aqueous solution).

Experimental attempts to search for Lr as a volatile p-element[12] using on-line gas chromatography have not given any results so far. These experiments, however, do not allow the authors to exclude the existence of Lr(p). They believe that maybe in the presence of the chromatography column surface, due to the higher adsorption enthalpy of Lr(d) (750 kJ/mol) with respect to Lr(p)(—187kJ/mol), the $/Rn/5f^{14}7s^27p_{1/2}$ configuration promotes to $/Rn/5f^{14}6d7s^2$, which is predicted to be only about 93 kJ/mol higher in energy.

Taking into account the difficulties encountered by experimentators, the theoretical predictions in this area remain urgent.

Analogy on the Basis of Atomic Properties

Considering Lr as a p-element one can hardly relate it to the elements of the Ga-subgroup, whose peculiarity is a high promotion energy to d-state. Thus, Tl which is very often compared with Lr has the first excited state $6s^27s^2$ at 26478 cm^{-1} above the ground state $6s^26p_{1/2}$ ($^2P_{1/2}$) and excitation energy to the d-state is even higher — 36118 cm^{-1}. Lr differs from the typical p-elements both in character of excitation and in its energy. The ground state configuration of Lr ($7f^{14}7s^27p$), as it has been shown[9], has an admixture (24%) of $7s^26d$ and 6d7s7p-electronic states.

But Lr also differs from typical d-elements, *e. g.* the lowest excited levels (states) of Sc arise from the excitation of 4s-electron to 3d-level ($3d^24s$) with energies of the transition being equal to 11500 and 15000 cm^{-1} for ^4F and ^2F-states, respectively.

Earlier in the work[13] it was emphasized that promotion energies $5f^q7s^2 \rightarrow 5f^q7s7p$ for the elements at the end of the actinide series are lower than those for $5f^q7s^2 \rightarrow 5f^q7s6d$ excitation (Table I).

TABLE I

Excitation energy $f^qs^2 \rightarrow f^qsp$ and $f^qs^2 \rightarrow f^qds$, in kcal/mol

	Bk	Cf	Es	Fm	Md	No
$s^2 \rightarrow sp$	49	51	54	55	57	59
$s^2 \rightarrow sd$	54	60	65	74	80	90

It is seen (Table I) that there is a following tendency to the end of actinide series: stabilization of 7p and destabilization of 6d-atomic orbitals (AO). This qualitative effect transforms into a quantitative one that takes place in the case of Lr.

Summing up all the experimental and theoretical data obtained, one can conclude that Lr might be an element with a new quality, and all experimental attempts to obtain it in a pure d or p-state hardly seem to be successful.

As far as E104 is concerned, it is supposed to begin a new series of elements in the Periodic Table, where 6d-shell is to fill with electrons. Data obtained by Zvara[16] about the properties of gaseous Ku halogenides and those obtained by Silva on the basis of the ion exchange behaviour of Ku are used as an evidence of the d-character of Ku. But the increasing role of relativistic effects must probably influence the electronic structure of Ku and its compounds. Keller[14] supposed that under the influence of relativistic stabilization of $7p_{1/2}$—AO the ground state configuration might be $7s^27p_{1/2}^2$ and by its properties Ku might be an analog of Pb($6s^26p^2$) and metallic Ku might be a volatile substance. But the lowest limit for the sublimation enthalpy for Ku $\Delta H_s = 370$ kJ/mol and for Pb $\Delta H_s = 190$ kJ/mol and in contrast to atomic Pb, Ku does not pass through the chromatography column in the hydrogen current[15]. But no final decision about the p-character of Ku could be reached in terms of the used experimental technique because it was impossible to determine the difference between ΔH_s(Ku) and ΔH_s(Hf).

Again, if one considers Ku as an analog of Pb, the latter has the first excited $6s^26p7s$-state at 35500 cm^{-1} above the ground state, and the lowest d-state ($6s^26p6d$) at 38800 cm^{-1}. Nevertheless, the first excited state $6s5d^3$ of d-elements (Hf) is 14500 cm^{-1} above the ground state $6s^25d^2$. Relativistic Hartree-Fock-Slater and Dirac-Fock calculations[4,13,18] have given a number of close-spaced electronic configurations ($7s^26d^2$, $7s^26d7p$, $7s^27p^2$). Recent multiconfigurational Dirac-Fock calculations[19] predict that the ground state of Ku is the $J = 2$ state with the main contribution from $7s^26d7p^2$ single configuration:

$$80\% 7s^26d7p + 18\% 7s7p6d^2 + 2\% \text{ others.}$$

The first excited state $6d^27s^2(95\%)$ at about 0.5 eV is the $J = 2$ state. The ground state of Ku^+ is $7s^26d$ by analogy to Hf, and the $7s^27p$ configuration is 2.4 eV higher.

However, the question arises whether the fact that the ground state of Ku is $7s^26d7p$ instead of $7s6d^2$ is a good reason for believing that its properties would move to the p-elements. In accordance with the Huckel approach the strength of the chemical bonding formed by the atom in compound is determined by the energies of valent orbitals and their space expansion and therefore the authors[19] consider Ku to be a typical d-element (AO energies of Ku are similar to Hf as well as values $< r >$).

The properties (p-or d-) that Ku will have in its compounds can be determined only on the basis of molecular calculations. In a sense, $KuCl_4$ is the most proper species for both d- and p-elements form rather stable tetrachlorides.

Method of Calculations and Parameters

The self-onsistent (SCF) calculations were performed using a version of the multiple scattering Xα-method, a detailed description of which can be found elsewhere, *e. g.* in ref. 20.

In the radial Schrödinger-like equation the »large« radial function G_{nl} has the solution:

$$[H_{NR} + H_m + BH_D] \, G_{nl} = EG_{nl}$$

Here H_{NR} is the usual nonrelativistic operator for the central field problem, H_m and H_D are the standard massvelocity and Darwin operators and B is given by

$$B = \{ 1 + \frac{1}{4} \alpha^2 \, [E - V(r)] \}^{-1}$$

where $\alpha = 1/137$. The spin-orbital interaction is taken into account by using the perturbation theory: $H'_{SO} = BH_{SO}$, where H_{SO} is the standard spin-orbit operator of the Pauli theory. The collection of one-electron energies, obtained by adding the first-order perturbation theory shifts induced by the spin-orbit operator, will be labeled RX_α—SO while the (more accurate) collection obtained by diagonalizing this operator among a group of adjacent levels will be labeled RX_α—SO′. The latter procedure takes into account the effect of mixing several close-spaced electronic states for valent orbitals, which becomes more prominent for the heavy elements.

The band length Ku—Cl was chosen as a sum of ionic radii (4.9905 a. u.) and we employed a Hf—Cl internuclear distance in $HfCl_4$ of 4.8393 a. u. and 4.4045 a. u., and a Pb—Cl distance in $PhCl_4$ of 4.5936 a. u.

We used the model of overlapping atomic spheres with their ratio being determined by the Norman procedure. The value of overlapping changed from 10 to 25%, the virial ratio being the best for 25% (in case $KuCl_4$). SCF molecular calculations were carried out starting with atomic ground state configurations $7s6d^2$, $7s^27p^2$ and $7s^27p6d$.

Results of Molecular Calculations and Discussion

It is well-known that the molecular field splitting of d- and p-orbitals is different. In the T_d field d-orbitals are split into e_g- and t_{2g} components and such a scheme is valid for all d-element compounds. But observing the molecular orbital (MO) scheme of any p-element compounds one can notice a peculiarity: a position of the first antibonding level of a_1-symmetry below t_2-level of pure p-character (Figure 1).

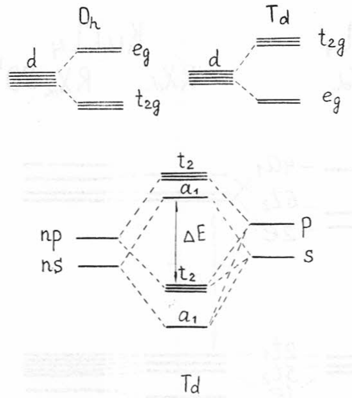

Figure 1. Principal scheme of d- and p-orbital splitting in the T_d molecular field.

Table II contains eigenvalues (MO energies) for $HfCl_4$, $KuCl_4$ and $PbCl_4$. Figure 2 combines this tabular information with the arrow indicating the intervening energy gap. It is obvious that the energy level oderings for $HfCl_4$ and $KuCl_4$ are similar except for the almost degenerate lower $2a_1$—$1t_1$ MOs. Eigenvalues for $HfCl_4$ and $KuCl_4$ practically do not differ either. A more prominent distinction is in the antibonding MO ordering. Thus, in $HfCl_4$ the classical scheme of d-orbitals splitting in T_d-crystal field is preserved, whereas in $KuCl_4$ $4a_1$-antibonding level dramatically decreases being the lowest unoccupied (LU) MO in the case of 25% ovelapping (Figure 3). Figure 2 and Table II show that such a situation takes place in the MO scheme for $PbCl_4$ where $3a_1$ level is the LUMO. Thus, the electron structure of $KuCl_4$ has an element peculiar for the p-element compounds.

TABLE II

Eigenvalues (RXα), eV

MO	$HfCl_4$ 25%	$KuCl_4$		MO	$PbCl_4$ 25%
		20%	25%		
$1t_2$	39.05	35.87	35.51		
$1a_1$	20.98	20.90	20.99		
$2t_2$	20.86	20.72	20.80	$1t_2$	21.86
$2a_1$	18.91	19.19	18.97	1e	20.61
$3t_2$	18.90	19.21	18.98	$1a_1$	21.47
$1t_1$	18.90	19.22	18.98	$2t_2$	19.82
$3a_1$	10.64	10.62	10.82	$2a_1$	13.58
$4t_2$	9.90	9.61	9.83	$3t_2$	9.80
1e	8.99	8.86	8.84	2e	8.58
$5t_2$	8.78	8.70	8.63	$4t_2$	8.54
$2t_1$	8.52	8.50	8.48	$1t_1$	8.46
2e	3.92	3.06	2.70	$3a_1$	4.82
$6t_2$	3.07	2.30	2.00	$5t_2$	0.93
$4a_1$	1.97	2.94	2.80	$4a_1$	0.32

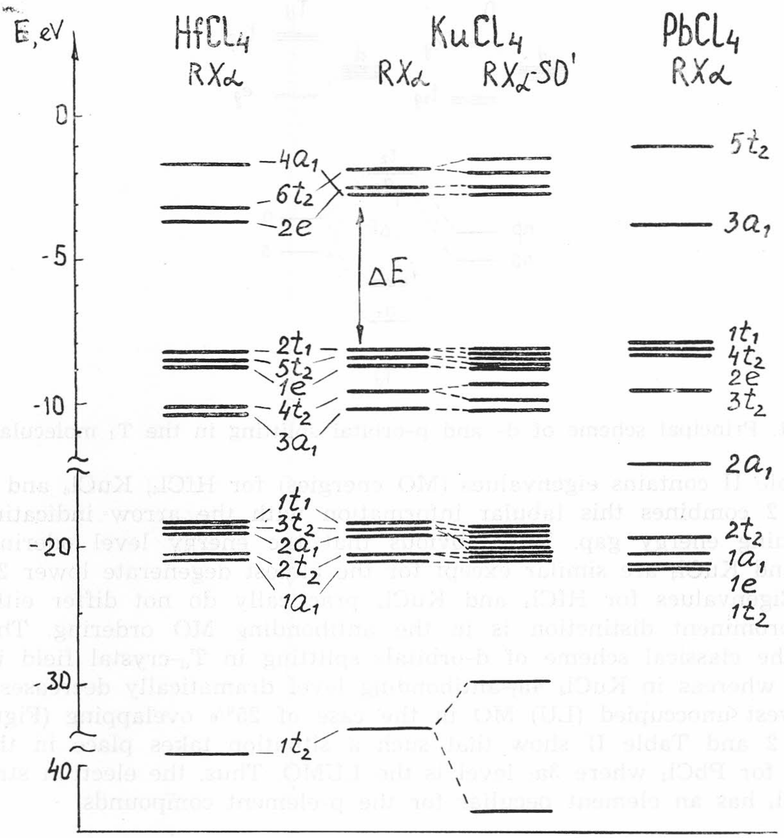

Figure 2. Energy level scheme (eigenvalues) for $HlCl_4$, $KuCl_4$ and $PbCl_4$.

The upper valence level ordering for $PbCl_4$ is like that for $KuCl_4$ ($2a_1$ — — $1t_1$) with similar eigenvalues. The lower valence levels for $PbCl_4$ ($1t_2$ — — $2t_2$) differ from $KuCl_4$ by either their ordering or eigenvalues. Besides, there is a MO of 1e-symmetry (100% d) in $PbCl_4$. Looking for some analogy one can believe that $4f^{14}$ and $5f^{14}$ — inner shells in $HfCl_4$ and $KuCl_4$ (lower valence levels $2a_1$ — $1t_1$) influence to the same extent the electronic structure of upper valence levels whereas the $5d^{10}$-shell in $PbCl_4$ influences the upper valence levels to a different extent ($1t_2$ and 1e levels of 5d (100%)-character lie by 2 and 3 eV lower $2a_1$ — $1t_1$-levels of f(100%) character in $KuCl_4$ and $HfCl_4$).

Before analyzing the MO composition let us consider the influence of relativistic effects on the electronic structure of the species under consideration. For $HfCl_4$ such effects as mass-velocity dependence and Darwin interaction do not change the energy level ordering in going from X_α to RX_α calculation. There is only a slight upward shift of unoccupied levels of d-character owing to an indirect relativistic effect leading to the destabilization of d-orbitals. As a result, the energy gap increases from 3.67 to 4.6 eV.

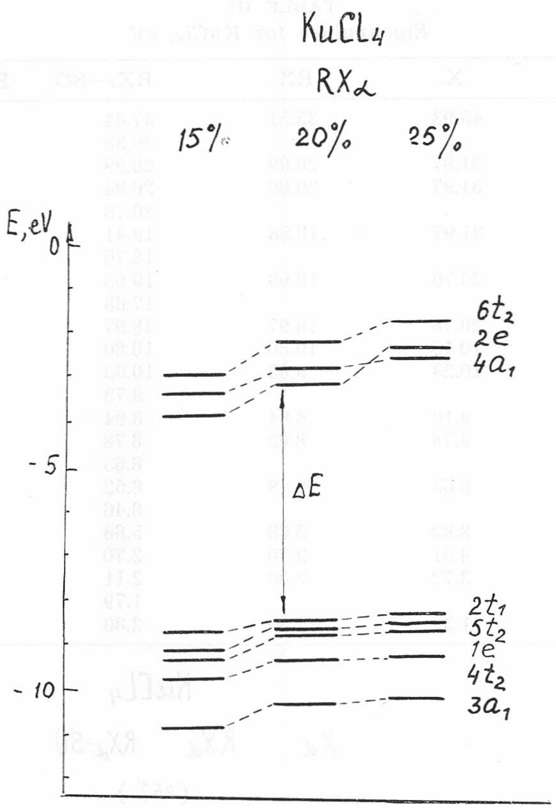

Figure 3. Upper bonding and low antibonding molecular orbitals for $KuCl_4$ as a function of overlapping of atomic spheres.

In the case of $PbCl_4$ there is also a slight shifth of unoccupied levels in going from X_α to RX_α calculation, resulting, however, in a lowering of the LU $3a_1$—MO of s-character as a consequence of relativistic stabilization of 6s-orbitals. In this case the energy gap decreases from 4.58 to 3.64 eV. Spin-orbit interaction only slightly splits t_1 and t_2-MO.

Table III (Figure 4) contains the results of all stages of calculations for $KuCl_4$. Relativistic effects (RX_α-calculation) result in destabilization of d-orbitals (2e and $6t_2$) and stabilization of $4a_1$-MO of 7s-character so that $4a_1$-MO becomes LUMO. Spin-orbit interaction (RX_α-SO) does not influence the energy level ordering. The more accurate RX_α-SO′ procedure results in the LUMO being t_2-MO of mixed d-p-character. Thus, both RX_α-SO and RX_α-SO′ calculations show that in $KuCl_4$ the classical scheme of d-orbital splitting in the T_d-molecular field is not observed.

Table IV gives the charge composition (%) of the MOs. For bonding levels ($3a_1$ — $2t_1$) d-orbitals of Ku participate to a greater extent in the chemical bond formation than p-orbitals ($4t_2$-MO), whereas in $PbCl_4$ this orbital ($3t_2$) is characterized by strong participation of p-AO and in the region of bonding orbitals ($2a_1$ — $1t_1$) the s- and p-orbitals are predominant.

TABLE III

Eigenvalues for *$KuCl_4$, eV*

MO	X_α	RX_α	RX_α—SO	RX_α—SO′
$1t_2$	45.93	35.51	47.84	
			29.33	
$1a_1$	31.97	20.99	20.99	21.99
$2t_2$	31.97	20.80	20.84	20.97
			20.78	20.86
$1t_1$	31.97	18.98	19.41	20.53
			18.76	17.67
$3t_2$	20.70	18.98	19.63	20.53
			17.68	17.66
$2a_1$	20.78	18.97	18.97	17.65
$3a_1$	10.10	10.80	10.80	10.80
$4t_2$	10.23	9.83	10.03	10.04
			9.73	9.80
1e	9.10	8.84	8.84	8.85
$5t_2$	8.78	8.63	8.78	8.77
			8.63	8.63
$2t_1$	8.63	8.48	8.52	8.52
			8.46	8.45
ΔE	3.82	5.68	5.66	5.42
2e	4.81	2.70	2.70	3.03
$6t_2$	3.72	2.00	2.11	1.81
			1.79	1.77
$4a_1$	1.32	2.80	2.80	2.80

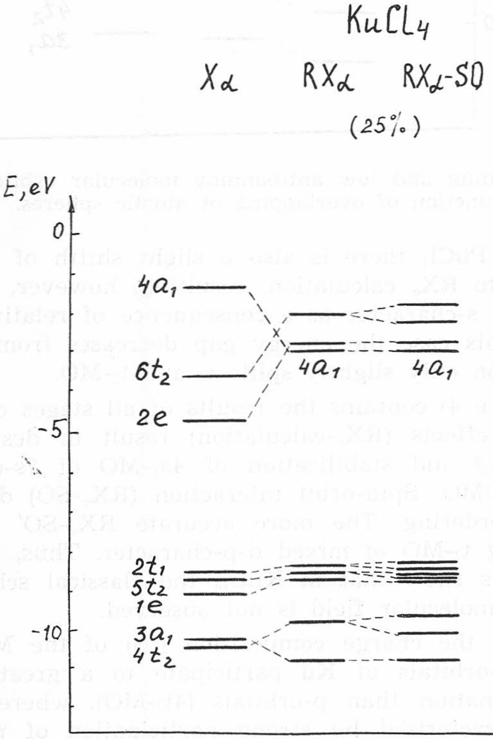

Figure 4. MO scheme for $KuCl_4$ displaying the strong influence of relativistic effects on the unoccupied ($2e$—$4a_1$) levels.

TABLE IV

MO composition (%). Only the predominant orbital contributions are given

MO	AO	$HfCl_4$	$KuCl_4$	MO	AO	$PbCl_4$
$1a_1$	f	10.59	12.96	1e	d	99.98
	s (Cl)	85.99	83.48	$1a_1$	s	7.96
$2t_2$	f	3.30	4.32		f	1.10
	s (Cl)	93.21	92.50		s (Cl)	89.60
$2a_1$	f	99.70	99.94	$2t_2$	p	2.56
$3t_2$	f	99.90	99.98		d	2.64
$1t_1$	f	99.99	100.00		s Cl)	94.36
$3a_1$	s	21.53	26.64	$2a_1$	s	43.54
	f	1.70	2.02		f	0.58
	p (Cl)	74.80	69.07		p (Cl)	48.23
$4t_2$	p	4.76	5.26	$3t_2$	p	17.10
	d	16.41	13.51		d	1.72
	p (Cl)	77.94	79.80		p (Cl)	79.85
1e	d	9.69	7.24	2e	d	2.02
	p (Cl)	90.31	92.76		p (Cl)	97.98
$5t_2$	p	2.86	2.61	$4t_2$	p	0.02
	d	1.24	0.94		d	2.59
	p (Cl)	95.78	96.30		p (Cl)	96.53
$2t_1$	p (Cl)	98.80	98.55	$1t_1$	p (Cl)	98.57
2e	d	90.89	92.39			
	p (Cl)	9.11	7.69			
$6t_2$	p	7.93	10.28	$5t_2$	p	39.21
	d	75.13	74.71		d	8.19
	p (Cl)	12.61	10.85		p (Cl)	12.53
$4a_1$	s	35.22	43.02	$3a_1$	s	32.59
	s (Cl)	40.43	24.42		s (Cl)	70.64
	p (Cl)	14.54	22.99		p (Cl)	47.39

Comparing $HfCl_4$ and $KuCl_4$ one can notice that in the latter molecule the chemical bond is weaker due to the relativistic destabilization of the 6d-orbital, but at the same time it becomes stronger by the relativistic stabilization of p-orbitals (*e. g.* $4t_2$-MO). The highest ossupied MO in all species is similar in composition (~99% 3s(Cl)).

For antibonding levels the MO composition for $KuCl_4$ is like that for $HfCl_4$ but with a slightly prominent p-character ($6t_2$-MO).

Table V summarizes the results of AO population analysis. One can see that both in $HfCl_4$ and $KuCl_4$ 6p- and 7p-AOs have a similar electronic

TABLE V

AO populations for $HfCl_4$, $KuCl_4$ and $PbCl_4$ (25% overlapping)

AO	$HfCl_4$	AO	$KuCl_4$	AO	$PbCl_4$
6s	0.49	7s	0.59	6s	1.03
5p + 6p	6.49	6p + 7p	6.50	6p	1.18
5d	1.55	6d	1.26	5d + 6d	10.33
4f + 5f	14.54	5f + 6f	14.70	5f	0.21
Charges on metal atom and ligand (Cl)					
q_{Me}	0.93	q_{Me}	0.95	q_{Me}	1.24
q_L	—0.23	q_L	—0.24	q_L	—0.31

charge. This is quite reasonable because from atomic calculations it follows that the 5d-6p (2.95 eV) and 6d—7p (2.57 eV) energy differences in Hf and Ku, respectively, are similar. In $PbCl_4$ the 6d-orbital spatial configuration is such as to lead to the population of this AO equal to 0.33e, the fact being in contradiction with atomic calculations where 6d-state lies much above the ground state. $KuCl_4$ in comparison with $HlCl_4$ has a more prominent 7p-character and a less prominent 6d one.

The highest occupied MO ($2t_1$) in all these systems is responsible for the ionization potential. These values for $KuCl_4$ and $HfCl_4$ will be similar owing to virtually the same value of negative sharge on Cl ions and similar $2t_1$-eigenvalues.

By the character of chemical bond $KuCl_4$ is likely to be close to $HfCl_4$ than to $PbCl_4$, though with a difference in electron density redistribution between d- and p-orbitals. Estimating the chemical bond strength by such an indirect characteristic as crystal field splitting of d-orbitals one can see that the interaction is stronger in $HfCl_4$ than in $KuCl_4$ (energy difference between 2e and $6t_2$-orbitals is larger by 0.15 eV in the first molecule compared to the second one). But notwithstanding the close similarity between $HfCl_4$ and $KuCl_4$ there is no full analogy between them, especially in the region of antibonding MOs where strong relativistic stanbilization of 7s-AO will result in a difference in the spectroscopic properties of $KuCl_4$.

Irrespective of what atomic ground state configuration we started from ($7s^26d^2$, $7s^26d7p$ or $7s^27p^2$), the results were approximately the same as a consequence of the SCF procedure.

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SAŽETAK

Elektronska struktura superteških elemenata i njihovih spojeva

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Samousklađena relativistička X_α metoda višestrukog raspršenja primijenjena je na sustav $KuCl_4$. Ustanovljeno je da $KuCl_4$ nije potpuni analog spoja $HfCl_4$.