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Karl Christe (Raytheon) "Hepta-Coordination. Synthesis and Characterization of the IOF_5^{2-} Dianion, an XOF_5 Compound"

(Statement A)

Hepta-Coordination. Synthesis and Characterization of the IOF_5^{2-} Dianion, an XOF_5E Compound

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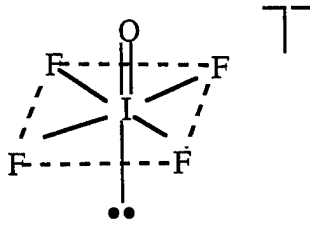
Contribution from the Air Force Research Laboratory, Edwards Air Force Base, California 93524, the Loker Hydrocarbon Research Institute, University of Southern California, Los Angeles, California 90089, and the Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, Washington 99352

Abstract: The new IOF_5^{2-} dianion was prepared in the form of its cesium salt by heating stoichiometric amounts of CsF, I_2O_5 and IF_5 to 162 °C for 14 days. The white stable solid was characterized by vibrational spectroscopy. A normal coordinate analysis was carried out with the help of *ab initio* calculations at the HF/ECP/DZP level of theory and resulted in an excellent agreement between observed and calculated frequencies. The structure of IOF_5^{2-} is that of a pentagonal bipyramid with five equatorial fluorine ligands, and an oxygen atom and one sterically active free valence electron pair occupying the two axial positions. The structure is very similar to that, previously established by vibrational spectroscopy and X-ray diffraction for isoelectronic $XeOF_5^-$, and represents only the second example of a heptacoordinated XOF_5E (E = free valence electron pair) main group species. The possible existence of the IOF_6^{3-} trianion is briefly discussed.

Introduction

The existence of the IOF_4^- anion has been known for many years,[1-4] and its pseudo-octahedral structure (I) has been well established by x-ray diffraction[1] and vibrational spectroscopy.[3,4] Furthermore, the isoelectronic species, $XeOF_4$, is well known.[5-9] The recent discoveries that $TeOF_5^-$,[10] $IO_2F_4^-$,[11] IF_6^-,[12] IF_4^-,[13] and even SbF_6^- and BiF_6^-[14] can all add a second F^-



(I)

ion to form the corresponding dianions and the existence of the isoelectronic $XeOF_5^-$ anion[15] prompted us to explore whether the IOF_5^{2-} anion might also be accessible and stable, and then to establish its structure. The structure of isoelectronic $XeOF_5^-$ had been controversial and was only recently settled by a combined *ab initio*-vibrational spectroscopy[16] and an x-ray diffraction[17] study.

Experimental

Materials and Methods. The I_2O_5 was obtained by heating a commercially available sample of "I_2O_5" from Mallinckrodt, which based on its Raman spectrum was actually HI_3O_8,[18] in a dynamic vacuum at 210 °C for 12 hr. The CsF (KBI) was fused in a platinum crucible, transferred while hot to the drybox, and finely powdered. The IF_5 (Matheson Co.) was treated with ClF_3 (Matheson Co.) at 25 °C until the liquid was colorless, followed by fractional condensation in a dynamic vacuum, using the –64 °C fraction.

Volatile materials were handled in a stainless steel vacuum line equipped with Teflon-FEP U-traps, 316 stainless steel bellows seal valves, and a Heise pressure gauge.[19] Solids were handled in the dry nitrogen atmosphere of a glovebox.

Infrared spectra were recorded on a Mattson Galaxy spectrometer using AgBr disks, which were prepared by pressing the finely powdered samples between two thin AgBr plates in a Barnes Engineering minipress inside the glovebox. Raman spectra were recorded at room

temperature on a Cary Model 83 GT spectrometer using the 488-nm exciting line of an Ar ion laser.

Preparation of Cs_2IOF_5. On the stainless steel vacuum line, IF_5 (9.255 mmol) was condensed at –196 °C into a prepassivated (with ClF_3) 75 mL Monel cylinder which was closed by a Monel valve. The cylinder was taken to the drybox, cooled to –196 °C, opened, and preweighed stoichiometric amounts of finely powdered dry CsF (30.92 mmol) and I_2O_5 (3.086 mmol) were added. The cylinder was closed, evacuated at –196 °C and then heated in an electric oven to 162 °C for 65 hr. Inspection of the white loose product by Raman spectroscopy showed only partial conversion to IOF_5^{2-} with large amounts of I_2O_5,[18] $CsIOF_4$[3,4] and Cs_2IF_7[12] being present. The product was finely powdered, returned to the cylinder and heated to 162 °C for an additional 95 hr. Examination of the solid product indicated a conversion to Cs_2IOF_5 of about 90% and a strong decrease in the amounts of I_2O_5, $CsIOF_4$ and Cs_2IF_7. The product was powdered again and heated to 162 °C for an additional 188 hr. At this point, the resulting white loose powder showed essentially complete conversion to Cs_2IOF_5, with a trace of $CsIOF_4$ being the only impurity detectable by Raman spectroscopy.

Computational Methods. Quantum chemical calculations employing the Hartree-Fock (HF) self-consistent-field method and the program Gaussian 94[20] were performed for the free, C_{5v} symmetry IOF_5^{2-} dianion. A double-ζ plus polarizatrion (DZP) basis on the oxygen and fluorine atoms[21] and a DZP basis set for the valence shell and an effective core potential (ECP)[22] for the inner shells of iodine were used. This level of calculation has been shown to provide excellent structures and frequencies for hyper-valent main group compounds.[10-14] The geometry and vibrational freguencies were calculated using analytic derivative methods.[23] The calculated Hessian matrixes (second derivatives of the energy with respect to Cartesian coordinates) were

converted to symmetry-adapted internal coordinates for further analysis using the program Bmtrx.[24]

Results and Discussion

Synthesis and Properties of Cs_2IOF_5. The synthesis of Cs_2IOF_5 was achieved by heating stoichiometric mixtures of I_2O_5, CsF and IF_5 to 162 °C for extended time periods (eq 1).

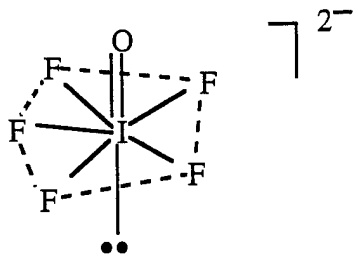
$$10CsF + I_2O_5 + 3IF_5 \xrightarrow[14\ d]{162\ ^oC} 5Cs_2IOF_5 \qquad (1)$$

The initial reaction products were mainly $CsIOF_4$[3,4] and Cs_2IF_7,[12] in addition to some Cs_2IOF_5. It was found important to stop periodically the reaction and intimately grind the sample. Two regrinds and a total heating time of 14 days were found sufficient to achieve essentially complete conversion to Cs_2IOF_5, with a trace of $CsIOF_4$ being the only impurity detectable by Raman spectroscopy. When only half the amount of CsF was used in this reaction, the principal product was $CsIOF_4$.

The Cs_2IOF_5 salt is a white stable solid which was characterized by its vibrational spectra (see below). The growing of single crystals for x-ray diffraction or NMR studies was ~~were~~ preempted by its poor solubility and ready loss of F^- ions in the usual solvents. The loss of F^- from multi-fluorine substituted mononuclear dianions in solution is a typical reaction induced by the more favorable solvation energies.

Vibrational Spectra and Computational Results. The Raman and infrared spectra of solid Cs_2IOF_5 are shown in Figure 1, and the observed frequencies and their assignment in point group C_{5v} are summarized in Table 1. As can be seen, the observed spectra are in excellent agreement with the scaled HF/ECP/DZP frequencies and those of the closely related IF_5^{2-} [16] and isoelectronic $XeOF_5^-$ [13] anions. The excellent correspondence between the vibrational spectra of $XeOF_5^-$ and IOF_5^{2-} leaves no doubt that IOF_5^{2-} also possesses the pseudo-pentagonal bipyramidal

C_{5v} structure found for $XeOF_5^-$ in $NO^+XeOF_5^-$ by x-ray diffraction.[7] This C_{5v} structure for IOF_5^{2-} was also confirmed by the results of our *ab initio* calculations which showed it to be the minimum energy structure with the oxygen atom and a sterically active free valence electron pair of iodine occupying the two axial positions of a pentagonal bipyramid.



The geometry, predicted for IOF_5^{2-} on the basis of the *ab initio* calculations, is given in Table 2.

Since our evidence for the structure of IOF_5^{2-} rests mainly on the vibrational spectra, a normal coordinate analysis was carried out for this anion. Its symmetry force constants and potential energy distribution (PED) are listed in Table 3, and in Table 4 its internal stretching force constants are compared to those of the closely related IOF_4^-,[3] IF_5^{2-},[16] and IF_4^-[25] anions and their isoelectronic xenon counterparts.[13,16,25,26]

The PED of Table 3 shows that the vibrations in the A_1 block are highly characteristic, but that the similarities of the frequencies of the antisymmetric IF_5 stretching modes with those of the closest deformation modes result in strong mixing in the E blocks. This similarity is caused by the high ionicity and weakness of the equatorial IF_5 bonds which cause, for example, the antisymmetric IF_5 stretching frequency, ν_8 (E_2), to have a lower frequency than the in plane IF_5 scissoring mode, ν_7 (E_2).

Inspection of Table 4 shows the expected trends. The stretching force constants of the IF_5 part of IOF_5^{2-} are very similar to those of IF_5^{2-}, except for the increase in fr on going from IF_5^{2-} to IOF_5^{2-}, caused by the change in the iodine oxidation state from +III to +V and the concommitant

increase in the covalency of the I-F bonds. On going from IOF_4^- to IOF_5^{2-}, both the I-O and I-F stretching force constants decrease, as expected for an increased polarity of these bonds due to the additional negative charge in the dianion. The same trends hold for the isoelectronic xenon species of Table 4.

The I-F stretching force constants in IOF_5^{2-} and IF_5^{2-} exhibit very low values of 1.84 and 1.53 mdyn/Å, when compared to the values of 5.60 and 4.68 mdyn/Å for the highly covalent I-F bonds in IF_6^+ and F_{ax}-IF_4, respectively.[28] These low fr values for IOF_5^{2-} lend strong support to the highly ionic, 6-center 10-electron bond model for the five equatorial fluorine ligands, which was previously proposed and discussed in detail for XeF_5^- [16] and IF_7.[27] The value of 6.01 mdyn/Å for the I-O bond in IOF_5^{2-}, although on the low side of the usual range for mainly covalent I=O double bonds, confirms that the negative charges in IOF_5^{2-} are concentrated on the fluorine ligands.[28]

Possible Existence of Cs_3IOF_6. The use of a $CsF:I_2O_5:IF_5$ stoichiometry of 15:1:3, which corresponds to a final product having a composition of Cs_3IOF_6, resulted in a white solid, the Raman spectrum of which was distinct from that of Cs_2IOF_5. After 83 days of heating to 162°C and periodic grinding of the sample, a new composition was obtained which gave the following Raman spectrum (cm^{-1}, rel int): 865(100), 468(100), 372(2), 327(24), 265(1), 246(7), 177(7). The IOF_4^- and IOF_5^{2-} anions, observable in the early stages of its synthesis had vanished, and the only impurities detectable by Raman spectroscopy were traces of I_2O_5 and IF_7^{2-}.

In order to judge if this composition could represent the novel IOF_6^{3-} anion, *ab initio* calculations, similar to those previously used for evaluating the feasibility of IF_6^{3-},[16] were carried out. The most likely structure for IOF_6^{3-}, possessing either a sterically active or a sterically inactive free valence electron pair on iodine, are shown in Figure 2 and were tested for their

tendencies to spontaneously lose fluoride ions. In all four calculations, spontaneous fluoride ion loss and no energy minima for the different IOF_6^{3-} structures were found. The C_{5v} IOF_6^{3-} structure lost one F^-, the C_{2v} structure two F^-, and the C_{3v} structures three F^- to give the stable IOF_5^{2-} and IOF_4^- ions and IOF_3 molecule, respectively. In view of these calculations, no reliable interpretation can be offered at this time for the Raman spectrum of the "Cs_3IOF_6" composition. The fact that the I=O stretching vibration of "Cs_3IOF_6" is actually 11 cm^{-1} higher than that in IOF_5^{2-} might be interpreted as evidence against the presence of discrete IOF_6^{3-} ions.

Conclusions

This study conclusively demonstrates the existence of the IOF_5^{2-} dianion as its stable cesium salt. This dianion is only the second known example of a pseudo-pentagonal bipyramidal main group species possessing, in addition to the five equatorial fluorine ligands, one doubly bonded oxygen ligand and one sterically active free valence electron pair in the axial positions. The results from a normal coordinate analysis of the vibrational spectra show that the five equatorial ligands are relatively weakly bound through highly ionic 6-center 10-electron bonds, similar to those found for the pentagonal planar XeF_5^- [16] and IF_5^{2-} [13] anions. The possible existence of the IOF_6^{3-} trianion was also studied, and the presence of a new composition was indicated by the Raman spectra but *ab initio* calculations and a slight shift of the I=O stretching mode to higher frequency augur against the presence of IOF_6^{3-}.

Acknowledgment. This paper is dedicated to Professor Wolfgang Sawodny on the occasion of his retirement. The authors thank Dr. S. Rodgers and Prof. G. Olah for their active support. The work at the Air Force Research Laboratory was supported by the Propulsion Directorate and Office of Scientific Research of the U. S. Air Force, while that at USC was sponsored by the

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(28) The Mulliken charges for IOF_5^{2-} are 2.35 e for I, -0.86 e for O, and –0.70 e for F. Thus, most of the negative charge is found in the ring of the five equatorial fluorines. Even though the oxygen has a slightly larger negative Mulliken charge than fluorine, it is partially compensated by the high positive charge on I.

Table 1. Vibrational Spectra of Cs_2IOF_5 and their Assignments in Point Group C_{4v} Compared to Those Observed for $XeOF_5^-$ and IF_5^{2-}

assignt (activity)	approx mode description	obsd freq, cm^{-1}(intens) Ra	IR	calcd freq,cm^{-1} (IR intens)[a] HF/ECP/DZP	IF_5^{2-}[b]	$XeOF_5^-$[c]
A_1(IR,Ra)	ν_1 νI=O	854(100)	855s	847(71)	-	880
	ν_2 νsym IF5	485(58)	485w	488(0)	474	515
	ν_3 δumbrella IF_5	289(4)	290sh	298(86)	[307][d]	296
E_1(IR,Ra)	ν_4 antisym comb of νas IF_5 and δwag I=O	-	415vs,br	414(1032)	335	495
	ν_5 sym comb of νas IF_5 and δwag I=O	334(5)	330sh	343(230)	-	370
	ν_6 δas in plane IF_5	254(7)		255(0)	245	273
E_2(-,Ra)	ν_7 δsciss in plane IF_5	409(11)		385(0)	396	460
	ν_8 νas IF_5	367(2) 355(15)		363(0)	339 325	397
	ν_9 δpucker IF_5	-		115(0)	[100][d]	[115][d]

[a]Empirical scaling factors of 0.9724 and 0.9244 were used for the stretching and the deformation modes, respectively. [b]Data from ref 16. [c]Data from ref 13. [d]Calculated value.

Table 2. Calculated HF/ECP/DZP Geometry for C_{5v}-IOF_5^{2-}

	unscaled	scaled[a]
r(I=O), Å	1.7220	1.70
r(I-F), Å	2.0409	2.08
<O=I-F, deg	91.476	91.7
<F-I-F, deg	71.972	72.4

[a]Predicted values based on scale factors from $XeOF_4$ in ref 13 and a comparison between predicted HF/ECP/DZP values for isoelectronic $XeOF_5^-$ in ref 13 and the experimental data from ref 17.

Table 3. Symmetry Force Constants[a] and Potential Energy Distribution[b] of C_{5v} IOF_5^{2-} Calculated from the Scaled HF/ECP/DZP Second Derivatives

	freq. cm^{-1} obsd	calcd		sym force consts F_{11}	F_{22}	F_{33}	PED
A_1	854	847	F_{11}	6.006			98.0(1) + 1.6(3) + 0.4(2)
	485	488	F_{22}	0.320	2.655		98.1(2) + 1.0(3) + 0.8(2)
	289	298	F_{33}	0.265	-0.466	2.751	91.7(3) + 8.3(2)
				F_{44}	F_{55}	F_{66}	
E_1	415	414	F_{44}	1.237			47.7(4) + 43.8(5) + 8.5(6)
	334	343	F_{55}	-0.181	2.013		54.4(4) + 45.2(5) + 0.4(6)
	254	255	F_{66}	0.089	-0.262	1.008	63.3(6) + 34.7(5) + 2.0(4)
				F_{77}	F_{88}	F_{99}	
E_2	409	385	F_{77}	1.375			78.9(7) + 21.1(8)
	367 355	363	F_{88}	0.143	2.027		82.6(8) + 17.0(7) + 0.3(9)
	-	115	F_{99}	-0.302	0.031	0.685	94.0(10) + 5.9(8) + 0.1(7)

[a]Stretching Constants in mdyn/Å, deformation constants in mdyn Å/rad^2, and stretch-bend interaction constants in mdyn/rad. [b]PED in percent; symmetry coordinates: S_1=ν I=O; S_2=νsym IF_5; S_3=δumbrella IF_5; S_4=νas IF_5; S_5=δwag I=O; S_6=δas in plane IF_5; S_7=δsciss in plane IF_5; S_8=νas IF_5; S_9=δpucker IF_5.

Table 4. Internal Force Constants (mdyn/Å) of IOF_5^{2-}, IOF_4^-, IF_5^{2-}, and IF_4^- compared to those of the Isoelectronic Xenon Species

	f X=O	fr (XF)	frr (XF)	frr' (XF)
IOF_5^{2-} [a]	6.01	1.84	0.027	0.380
IOF_4^- [b]	6.56	2.46	0.16	0.45
$IF5_2^-$ [c]	—	1.53	0.035	0.423
IF_4^- [d]	—	2.22	0.183	0.466
$XeOF_5^-$ [e]	6.33	2.25	0.15	0.20
$XeOF_4$ [f]	7.08	3.26	0.12	0.10
XeF_5^- [c]	—	2.10	0.14	0.26
XeF_4 [d]	—	3.06	0.12	0.01

[a] Values from this study. [b] Values from ref. 3. [c] Values from ref. 16. [d] Values from ref. 25. [e] Values from ref. 13. [f] Values from ref. 28.