**Abstract:** \([\text{SnI}_8\{\text{Fe(CO)}_4\}_4]\)[\text{Al}_2\text{Cl}_7]_2\) contains the \([\text{SnI}_8\{\text{Fe(CO)}_4\}_4]\) cation with an unprecedented highly coordinated, bicapped \(\text{SnI}_8\) prism. Given the eightfold coordination with the most voluminous stable halide, it is all the more surprising that this \(\text{SnI}_8\) arrangement is surrounded only by fragile \(\text{Fe(CO)}_4\) groups in a clip-like fashion. Inspite of a predominantly ionic bonding situation in \([\text{SnI}_8\{\text{Fe(CO)}_4\}_4]\), the \(\text{I}^-\cdot\text{I}^-\) distances are considerably shortened (down to 371 pm) and significantly less than the van der Waals distance (420 pm). The title compound is characterized by single-crystal structure analysis, spectroscopic methods (EDXS, FTIR, Raman, UV/Vis, Mössbauer), thermogravimetry, and density functional theory methods.

High coordination numbers (CNs) are preferably realized at high pressure and with small ligands.\(^\text{[1]}\) In the solid state, moreover, high CNs are preferred in densely packed structures (e.g. perovskites) and supported by high lattice energies. For cationic tin (Sn\(^{2+}\), Sn\(^{4+}\)), flexible coordination is possible and most often refers to tetrahedral and octahedral arrangements.\(^\text{[2]}\) To date, higher CNs are known only for chelating ligands (e.g. crown ethers)\(^\text{[3]}\) or chelating oxoanions at high pressure (e.g. CN 10 in \(\text{SnB}_4\text{O}_7\) made at 7.5 GPa/1100°C).\(^\text{[4]}\) In all these cases, multidentate ligands and/or high pressure are a prerequisite. For monodentate ligands, the CN of Sn\(^{2+/4+}\) is typically limited to six. The binary \(\text{SnI}_2\) shows (5+2) coordination with five shorter (303–326 pm) and two significantly longer Sn–I distances (373 pm).\(^\text{[5]}\) Even for fluorine, the smallest halide, only sixfold coordination was reported (e.g. \([\text{NH}_4]_3[\text{SnF}_6]\)\(^\text{[6]}\). Eightfold coordination with iodine, to the best of our knowledge, is also unknown for the significantly larger Pb\(^{2+}\) ion. With this background, \([\text{SnI}_8\{\text{Fe(CO)}_4\}_4]\)-\([\text{Al}_2\text{Cl}_7]\)_2 is surprising for several reasons: 1) eightfold halide coordination of Sn\(^{2+}\) is observed for the first time; 2) despite its size and repulsive \(\text{I}^-\cdot\text{I}^-\) interaction, eightfold coordination occurs with the most voluminous stable halide; 3) the \(\text{SnI}_8\) building unit is surrounded only by fragile \(\text{Fe(CO)}_4\) groups in a clip-like fashion.

\([\text{SnI}_8\{\text{Fe(CO)}_4\}_4]\)[\text{Al}_2\text{Cl}_7]_2\) was prepared by heating \(\text{SnI}_4\) and \(\text{Fe}_2(\text{CO})_9\) in the ionic liquid [BMIm][AlCl\(_3\)] (ratio 1:3; [BMIm]: 1-butyl-3-methylimidazolium) to 130°C in argon-filled, sealed glass ampoules. This temperature was required to dissolve all starting materials. When the reaction mixture was slowly cooled to room temperature (1 K h\(^{-1}\)), numerous large black crystals (up to 0.5 mm\(^3\)) with a slight violet shimmer were obtained starting at about 50°C (Figure 1; Supporting Information: Figures S1–S5). The reaction can be rationalized by reduction of Sn\(^{IV}\) to Sn\(^{III}\) and oxidation of Fe\(^{II}\) to Fe\(^{III}\) (Eq. (1));

\[
4\text{Sn}_4 + 4\text{Fe}_2(\text{CO})_9 + 4\text{AlCl}_3 + 2\text{Cl}^- 
\rightarrow [\text{SnI}_8\{\text{Fe(CO)}_4\}_4][\text{Al}_2\text{Cl}_7]_2 + 2\text{I}^- + 3\text{SnI}_2 + 2\text{CO}
\]

Figure 1. Decomposition of \([\text{SnI}_8\{\text{Fe(CO)}_4\}_4]\)[\text{Al}_2\text{Cl}_7]_2\) single crystals after separation from the mother liquor (in perfluorinated polyalkylether under argon at 25°C): a) Photos of a crystal taken over a period of 5 minutes (light microscopy); b) scheme of the decomposition with reaction products.
was previously reported only for chlorine-bridged compounds (e.g., [Cp(CO)2FeClSnCl4]).[7]

X-ray structure analysis based on single crystals revealed the title compound to crystallize in the monoclinic space group C2/c (Table S1, Figures S2 and S3) and to contain [SnI4(Fe(CO)4)4]2+ cations and [Al2Cl7]+ anions.[8] Beside crystal structure analysis, the chemical composition was validated by energy-dispersive X-ray spectroscopy (EDXS) with a Sn/I ratio of 1.3:8:4.3 (scaled on iodine as the heaviest element) which fits well with the expectation (1:8:4).

\[\text{[SnI}_4\text{Fe(CO)}_4\text{]}_2^+|\text{Al}_2\text{Cl}_7^+] \rightarrow \text{SnI}_3 + 3 \text{FeI}_2 + \text{FeCl}_3 + 4 \text{AlCl}_3 + 16 \text{CO} \tag{2}\]

The formation of AlCl3 and SnI3 is indicated by characteristic colorless needles (AlCl3) and orange crystals (SnI3). The lack of any \(\text{C}=\text{O}\) vibrations in the FTIR spectra points to the absence of metal carbonyls (e.g., Fe(CO)5, Fe2(CO)9, [cis-Fe(CO)4Cl2] as decomposition products (Figure S1). In contrast to room-temperature decomposition, the heating of the title compound leads to a three-step decomposition between 40–50°C (in the ionic liquid) and the rapid decomposition under inert conditions at 25°C (and below) illustrate the metastability and fragile nature of the title compound.

The unusual [SnI4(Fe(CO)4)4]2+ cation is centered by Sn4+ which in turn is eightfold coordinated by iodide (Figure 2a). The resulting Sn4+ polyhedron can be described as a bicapped triangular prism (Figure 2b,d). The Sn–I distances of 317.3 (2)–330.6 (3) pm in the prism (Figure 2c) are comparable to those of SnI3[9] but significantly longer than in SnI4 (Table 1),[10] which points to Sn4+ and I–Sn4+ bonding. The Sn–I distances of the two capping iodine atoms of the central SnI4 subunit (332.0 (1), 341.2 (3) pm) are slightly longer than the Sn–I distances within the prism (Figure 2c). Even these longer Sn–I distances are nevertheless significantly shorter than the extended distances in SnI3 (373.4 pm)[10] and the sum of the Sn–I van der Waals radii (411 pm).[11] Taking the large volume and the repulsion of the negatively charged neighbors into account, such short Sn–I distances in combination with eightfold coordination in the [SnI4(Fe(CO)4)4]2+ cation are unprecedented.

![Figure 2.](https://www.angewandte.org/doi/10.1002/ange.201910810)

**Figure 2.** [SnI4(Fe(CO)4)4]2+ cation: a) Overview with crystallographic numbering of the atoms; b) side view of the bicapped triangular SnI4 prism; c) Sn–I distances (in pm); d) top view of the bicapped triangular SnI4 prism.

| Compound | d(Sn–I) [pm] | d(Fe–I) [pm] |
|----------|-------------|-------------|
| [SnI4(Fe(CO)4)4]2+ | 317.3(2)–341.2(3) | 262.6(2)–264.9(2) |
| SnI3[9] | 302.7–325.7 | 373.4 |
| [Fe(I2)2]2+ | 269.7 | / |
| FeI2 (solid)[11] | / | 288.5 |
| Fe2I4 (dimer, gas phase)[12a] | / | 248.0, 268.3 |
| [Fe(CO)3(L)I2] [12b]/C0 | / | 265.5, 266.7 |
| [Fe(CO)3(L)I2] [12c]/C13 | / | 265.3 |

The I–I distances in the central SnI4 subunit cover a wide range and can be assigned to two groups. Pairs of iodine atoms are bridged by Fe(CO)5 groups in a clip-like fashion and exhibit distances of 376.3–384.4 pm (Figure 3a). The respective Fe–I distances (262.6(2)–264.9(2) pm) are shorter than in solid FeI2 (288.5 pm)[11] and compare to those of bridging Fe–I pairs of iodide with I–Fe–I angles (in °) including schematic illustration, b) non-Fe(CO)5-clipped pairs of iodide (for longer I–I distances see: Figure S4).

![Figure 3.](https://www.angewandte.org/doi/10.1002/ange.201910810)

**Figure 3.** I–I distances (in pm) in the [SnI4(Fe(CO)4)4]2+ cation: a) Fe(CO)5-clipped pairs of iodide with I–Fe–I angles (in °) including schematic illustration, b) non-Fe(CO)5-clipped pairs of iodide (for longer I–I distances see: Figure S4).
in the Fe–I dimer and other carboxylidoiron compounds (Table 1).[12] A second group of I–I distances relates to non-
Fe(CO)₅-clipped pairs of iodine with shorter (370.6–423.8 pm, Figure 3b) and longer distances (412.6–453.7 pm, Figure S4).
Several I–I distances are significantly less than the twofold
distance of iodine (420 pm).[13] Such close
contacts typically indicate attractive bonding as they are
known from iodine–iodide interactions (I⁻⁻⁻⁻I⁻) in poly-
iodides.[13] In [SnI₈(Fe(CO)₄)₄]⁺⁺, however, the close contacts
occur between negatively charged iodide atoms (I⁻⁻⁻⁻I⁻). This
finding can be attributed predominantly to the Fe(CO)₄ clips
since increasing the I–I distance would cause a widening of
the I-Fe-I angle, which, however, is more or less constrained
without the Fe(CO)₄ ligands.

The [SnI₈(Fe(CO)₄)₄]⁺⁺ cation could also be formally
described as a Sn²⁺-centered coordination complex with four
uncharged [cis-Fe(CO)₄]⁺⁺ ligands. However, it should be
noted that no equilibrium of Sn²⁺ and [cis-Fe(CO)₄]⁺⁺ was
observed—neither for the presence of Sn²⁺ (Table S2 and Figure S7).
Unfortunately, ⁵⁷Fe Mössbauer spectra could not be recorded
due to the strong absorption of iodine (see the Supporting
Information). With regards to iron, however, FTIR spectra
are indicative and show two strong (2156, 2100 cm⁻¹) and two
weak (2115, 2135 cm⁻¹) CO vibrations (Figure 4a; Table S3
and Figure S8), which are well in agreement with references
such as [cis-Fe(CO)₄]⁺⁺ (2129, 2084, 2060 cm⁻¹).[14] In
contrast, the CO vibrations of zero-valent iron carbonyls
like Fe(CO)₅ (2000, 2025 cm⁻¹)[15] and Fe₄(CO)₁₆ (2084,
2034 cm⁻¹)[16] occur at lower wavenumbers. This observation
can be ascribed to stronger σ-bonding and weaker π-back-
bonding, which confirms the lower electron density and the
positive valence state of iron in [SnI₈(Fe(CO)₄)₄]⁺⁺. These
findings are confirmed by Raman spectroscopy (Figure 4b;
Figure S9). With the help of theoretical calculations, Raman
bands close to 590, 390, 200, and 185 cm⁻¹ can be attributed to
ν(Fe-C) and δ(Fe-C-O) as well as to νₓₓₓₓₓ(FeI₂) and νₓₓₓₓₓₓₓₓ(FeI₂). Calculated Raman spectra of the [SnI₈(Fe(CO)₄)₄]⁺⁺
cation are also in good agreement with the experimental data
(Table S4 and Figure S10).

The structure and bonding of the [SnI₈(Fe(CO)₄)₄]⁺⁺
cation were finally verified by quantum chemical calculations
based on density functional theory (DFT). Accordingly,
a square antiprism of SnI₈ with D₄h symmetry turned out to
be a local minimum on the potential energy surface (Table S5
and Figure S11). Distortion of the D₄h-symmetric structure,
however, resulted in D₃d symmetry being 32.5 kJ mol⁻¹ more
stable than D₄h symmetry. Due to two imaginary vibrational
frequencies, however, this D₃d structure represents only
a saddle point on the potential energy surface, which
relaxes to a subgroup with D₃h symmetry (torsion angle 11-Sn1-18-12:
15.1°) and a "real" local energy minimum being 1.9 kJ mol⁻¹
even more stable (HOMO–LUMO gap: 1.66 eV). Although
the potential energy surface is rather flat with regards to the
torsion angle, DFT methods indicate that a bicoordinated trigonal
SnI₈ prism is more stable (~34.5 kJ mol⁻¹) than square
antiprismatic coordination, which excellently reflects the
experimental observation (Table 2, Figure 5; Figure S11). In
comparison to a calculated [cis-Fe(CO)₄]⁺⁺ molecule, the

**Table 2**: Selected distances (d) and angles (χ) in the [SnI₈(Fe(CO)₄)₄]⁺⁺ cation according to DFT calculations and experimental data (calculated [cis-Fe(CO)₄]⁺⁺ molecule as a reference).

| Species                  | d(Sn–I) [pm] | d(Fe–I) [pm] | d(I–I) [pm] | χ(I–Fe–I) [°] |
|--------------------------|-------------|--------------|-------------|---------------|
| Calculated (DFT)         |             |              |             |               |
| [SnI₈(Fe(CO)₄)₄]⁺⁺       | 333.9       | 267.9        | 367.6       | 91.3          |
| [cis-Fe(CO)₄]⁺⁺          | /           | 267.4        | 397.1       | 95.9          |
| Experimental data (single-crystal structure analysis) | | | | |
| [SnI₈(Fe(CO)₄)₄]⁺⁺       | 317.3(2)–341.2(3) | 262.6(2)–370.6(2) | 384.4(2) | 93.4(1) |
| [cis-Fe(CO)₄]⁺⁺          | /           | 387.6        |             |               |

Figure 4. Vibrational spectroscopy of [SnI₈(Fe(CO)₄)₄]⁺⁺[AlCl₄]⁻; a) FTIR spectrum (detailed view of CO vibrations as inset, crystals of the title compound embedded in ionic liquid for stabilization (Figure S8); b) FT-Raman spectrum (Figure S9).

Figure 5. Bonding in [SnI₈(Fe(CO)₄)₄]⁺⁺ with regard to the shortest I–I contacts: a) Calculated bonding MO (DFT) indicating a slight electron transfer from nonbonding iodide electron pairs into the formally
vacant valence p atomic orbital of Sn⁺ (isosurface values at ± 0.04; calculated 12-18/13-16 are symmetry equivalent due to S₈ symmetry); b) Experimental data (single-crystal structure analysis).
larger I–I distance and I-Fe-I angle in [cis-Fe(CO)₄]⁺ are noticeable and point to the strong influence of tin in [SnI₄{Fe(CO)₄}₄]²⁺.

With regard to the I–I distances, DFT calculations confirm the variability of distances and the presence of short I–I contacts in the S₄-symmetric [SnI₄{Fe(CO)₄}₄]²⁺ cation for the Fe(CO)₄-clipped and non-Fe(CO)₄-clipped pairs of iodide (Table 2). To verify whether the shortest I–I distances result from attractive interactions, Bader AIM analysis was performed (AIM: atoms in molecules; see the Supporting Information). Here, bond-critical points (electron density \( \rho_{BCP} \)) were observed only for the I₃–I₂/I₂–I₈ couple (367.6 pm) (Figure 5a, Figure S12). The electron density at this bond-critical point, however, is five to six times lower than for the polyiodide I₉ (\( \rho_{BCP} : 0.052, 0.038 \)), which was calculated as a reference system (Figure S13). Moreover, this weak interaction does not result from direct I–I bonding but from slight electron transfer of nonbonding electron pairs on iodide to the formally vacant valence p atomic orbital of Sn⁺ (Figure 5a; Figure S14). All additional I–I contacts in the central SnI₄ subunit did not result in bond-critical points. In comparison to the calculated distances, finally, the respective I···I distances in the experimentally observed non-S₄-symmetric [SnI₄{Fe(CO)₄}₄]²⁺ cation (I₃–I₁: 370.6, I₂–I₈: 379.4 pm) are in part significantly longer (Table 2, Figure 5b). Taken together, the influence of attractive I–I interactions can be considered to be negligible.

Based on the results of DFT calculations, the bonding situation in [SnI₄{Fe(CO)₄}₄]²⁺ is predominantly ionic in nature. This ionic bonding was further confirmed by Ahlrichs–Heinzmann population analysis (Table S6), which results in the “ionic” fragments Sn, Fe, and Fe(CO)₄ with partial charges of +0.27, −0.07, and +0.57, respectively. Thus, the bonding situation in [SnI₄{Fe(CO)₄}₄]²⁺ can be best described by a predominately ionic interaction of tin and iodine and a predominately covalent interaction of iodine and iron, where, of course, contributions of both bonding types are included in all cases. Further stabilization of [SnI₄{Fe(CO)₄}₄][Al₂Cl₇] results from lattice energy and the long-range cation–anion interaction.

In summary, [SnI₄{Fe(CO)₄}₄][Al₂Cl₇] is a novel carbonyl compound that was synthesized in an ionic liquid. The title compound is highly sensitive and decompenses rapidly (<5 min) after removal from the mother liquor under argon even at room temperature. The fact that its temperature of decomposition (<25°C) is below the temperature of synthesis (40–50°C) points to the metastable nature of [SnI₄{Fe(CO)₄}₄][Al₂Cl₇]. Most remarkable is the [SnI₄{Fe(CO)₄}₄]²⁺ cation with a central bicapped SnI₄ prism and an unusually high eighthfold coordination of Sn²⁺. Comparably short I–I contacts (down to 371 pm) are observed despite the negatively charged iodide and negligible attractive I–I interactions. The existence of this predominately ionic, Sn²⁺-centered [SnI₄{Fe(CO)₄}₄]²⁺ cation with fragile Fe(CO)₄ clips, eighthfold coordination of tin, and short iodide–iodide contacts is unprecedented. The synthesis in weakly coordinating ionic liquids near room temperature seems to be essential to obtain such a fragile compound at the border between formation and decomposition.

**Experimental Section**

**Chemicals.** All sample handling was strictly conducted under argon, applying standard Schlenk or glovebox techniques. Reactions were performed in argon-filled and sealed glass ampoules, which were dried under reduced pressure (1 × 10⁻² mbar) at 300°C prior to use. Fe(CO)₄ (99.99 %, ABCR) and AlCl₃ (99.99 %, ABCR) were used as supplied. SnI₄ was synthesized by reacting Sn and I₂ in toluene. [BMMIm][Cl] (99 %, IoLiTec) was dried under vacuum at 130°C for 30 hours prior to use.

[SnI₄{Fe(CO)₄}₄][Al₂Cl₇], SnI₄ (80 mg, 0.13 mmol) and Fe(CO)₄ (45.5 mg, 0.13 mmol) were added to a 1:3 mixture of [BMMIm][Cl] (500 mg, 2.86 mmol) and AlCl₃ (1145 mg, 8.59 mmol) as the ionic liquid. This mixture was heated in sealed glass ampoules at 130°C for 4 days to guarantee the dissolution of all AlCl₃ and all starting materials. When the reaction mixture was cooled to room temperature at a rate of 1 K h⁻¹, the formation of black crystals with a weak violet shimmer was observed at a temperature of ≤50°C along with tiny orange needles of SnI₄. The crystals were separated from the ionic liquid by filtration through a glass frit and washed with the pure ionic liquid to remove unreacted starting materials and SnI₄. Whereas the title compound was stable in the ionic liquid, its removal from the mother liquor even under inert conditions (argon) and even at room temperature results in rapid decomposition (<5 min). The decomposition with release of CO was decelerated at lower temperature and stopped at about ~50°C.

Further details regarding synthesis, crystal structure analysis, spectroscopic characterization, and quantum chemical calculations can be obtained from the Supporting Information.

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**Conflict of interest**

The authors declare no conflict of interest.

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