

Protonated decafluorobenzophenone and the decafluorobenzophenone–arsenic pentafluoride adduct

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The reaction of decafluorobenzophenone [perfluorobenzophenone, (C₆F₅)₂CO] with AsF₅ in anhydrous HF yields the protonated salt [bis(2,3,4,5,6-pentafluorophenyl)methylidene]oxidanium hexafluoroarsenate, (C₆F₅)₂COH⁺[AsF₆][−], whereas its reaction with AsF₅ in SO₂ affords the Lewis acid–base adduct decafluorobenzophenone–arsenic pentafluoride, (C₆F₅)₂CO·AsF₅. In both compounds, the decafluorobenzophenone moiety exhibits an elongated C=O bond [1.274 (2) and 1.2526 (15) Å in the salt and adduct, respectively]. The crystal structure of (C₆F₅)₂COH⁺[AsF₆][−] features a short O—H...F hydrogen bond between the cation and the anion, and the crystal structure of (C₆F₅)₂CO·AsF₅ represents a rare example of a ketone coordinated to the strong Lewis acid AsF₅.

1. Introduction

Protonation of small molecules plays an important role in investigating and elucidating the reaction mechanisms of acid-catalysed organic reactions. These reactive cations are typically generated in superacidic media (Olah *et al.*, 2009) and a wide range of compounds has been shown to undergo protonation under such conditions. Examples include nitriles (Haiges *et al.*, 2016; Goetz *et al.*, 2016), organic azides (Saal *et al.*, 2020), carboxylic acids (Saal *et al.*, 2023; Hollenwäger *et al.*, 2024), acyl halides (Steiner *et al.*, 2024a), amides (Axhausen *et al.*, 2013; Saal *et al.*, 2023), esters (Hollenwäger *et al.*, 2025) and amino sulfonic acids (Bockmair *et al.*, 2024).

The protonation of aldehydes and ketones in solution has been studied in detail by low-temperature NMR spectroscopy. For example, the protonation of aliphatic aldehydes (Olah *et al.*, 1967b) and aliphatic ketones (Olah *et al.*, 1967a) was studied in the superacidic media HSO₃F–SbF₅–SO₂, protonated alicyclic ketones in HSO₃F–SbF₅–SO₂ and HSO₃F–SO₂ (Olah & Calin, 1968), protonated acetophenones in HSO₃F (Birchall & Gillespie, 1965) and benzophenones in HSO₃F–SbF₅ (Sekuor & Kranenburg, 1966; van der Linde *et al.*, 1968). The reaction of hexafluoroacetone in an HF–SbF₅ mixture, however, results in HF addition to the ketone, followed by protonation, yielding a rare example of a protonated alcohol (Minkwitz & Reinemann, 1999).

Several crystallographically characterized examples of protonated ketones (Childs *et al.*, 1982, 1990; Chadda *et al.*, 1986; Stuart *et al.*, 2017; Schickinger *et al.*, 2018) and protonated aldehydes (Hwang *et al.*, 2010; Heo *et al.*, 2011; Hayatifar *et al.*, 2014; Stuart *et al.*, 2017) have been reported. The crystal structure of protonated benzophenone has been reported in

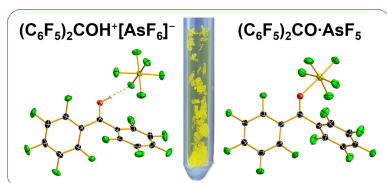


Table 1
Experimental details.

Experiments were carried out at 100 K using a Rigaku OD XtaLAB Synergy-S Dualflex diffractometer with an Eiger2 R CdTe 1M detector. The absorption correction was Gaussian (*CrysAlis PRO*; Rigaku OD, 2025).

	(C ₆ F ₅) ₂ CO	(C ₆ F ₅) ₂ COH ⁺ [AsF ₆] [−]	(C ₆ F ₅) ₂ CO·AsF ₅
Crystal data			
Chemical formula	C ₁₃ F ₁₀ O	C ₁₃ HF ₁₀ O ⁺ AsF ₆ [−]	C ₁₃ AsF ₁₅ O
<i>M</i> _r	362.13	552.06	532.05
Crystal system, space group	Monoclinic, <i>C2</i>	Monoclinic, <i>P2₁/n</i>	Orthorhombic, <i>Pbca</i>
<i>a</i> , <i>b</i> , <i>c</i> (Å)	20.1460 (4), 5.39987 (10), 5.47058 (14)	8.19207 (7), 21.17409 (18), 9.28475 (9)	12.39109 (18), 12.04038 (17), 20.8754 (3)
α , β , γ (°)	90, 95.912 (2), 90	90, 98.2086 (8), 90	90, 90, 90
<i>V</i> (Å ³)	591.96 (2)	1594.03 (2)	3114.47 (8)
<i>Z</i>	2	4	8
Radiation type	Cu <i>K</i> α	Cu <i>K</i> α	Ag <i>K</i> α, λ = 0.56087 Å
μ (mm ^{−1})	2.18	4.70	1.25
Crystal size (mm)	0.43 × 0.1 × 0.07	0.09 × 0.05 × 0.03	0.58 × 0.29 × 0.22
Data collection			
<i>T</i> _{min} , <i>T</i> _{max}	0.491, 1.000	0.842, 1.000	0.290, 1.000
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	10783, 1212, 1193	26147, 3336, 3134	97292, 8537, 7132
<i>R</i> _{int}	0.056	0.032	0.033
(sin θ /λ) _{max} (Å ^{−1})	0.629	0.630	0.914
Refinement			
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.034, 0.095, 1.11	0.025, 0.066, 1.05	0.031, 0.081, 1.09
No. of reflections	1212	3336	8537
No. of parameters	110	285	271
No. of restraints	1	0	0
H-atom treatment	—	All H-atom parameters refined	—
Δρ _{max} , Δρ _{min} (e Å ^{−3})	0.28, −0.24	0.30, −0.49	0.53, −0.64
Absolute structure	Flack <i>x</i> determined using 514 quotients [(<i>I</i> ⁺) − (<i>I</i> [−])]/[(<i>I</i> ⁺) + (<i>I</i> [−])] (Parsons <i>et al.</i> , 2013)	—	—
Absolute structure parameter	0.05 (10)	—	—

Computer programs: *CrysAlis PRO* (Rigaku OD, 2025), *olex2.solve* (Bourhis *et al.*, 2015), *SHELXL* (Sheldrick, 2015), *DIAMOND* (Brandenburg, 2022) and *OLEX2* (Dolomanov *et al.*, 2009).

the form of [HCB₁₁H₅Cl₆][−] carborane (Stasko *et al.*, 2002) and [TaF₆][−] salts (Marchetti *et al.*, 2007), both featuring a hydrogen-bonded dimer, [(C₆H₅)₂C=O—H···O=C(C₆H₅)₂]⁺.

The protonation of decafluorobenzophenone, (C₆F₅)₂CO, in solution was previously studied in H₂SO₄ and HSO₃F (Chambers & Spring, 1969), and in HF–SbF₅–SO₂ClF mixtures (Olah & Mo, 1973) by NMR spectroscopy. Research on Lewis acid–base adducts of AsF₅ with ketones remains scarce (Stuart *et al.*, 2019) and no crystal structures containing a C₂CO–AsF₅ fragment have been reported in the Cambridge Structural Database (CSD, Version 6.00, April 2025; Groom *et al.*, 2016).

In this work, the synthesis and structural characterization of the protonated decafluorobenzophenone (perfluorobenzophenone) salt (C₆F₅)₂COH⁺[AsF₆][−] and a Lewis acid–base adduct of arsenic pentafluoride and decafluorobenzophenone, *i.e.* (C₆F₅)₂CO·AsF₅, are reported.

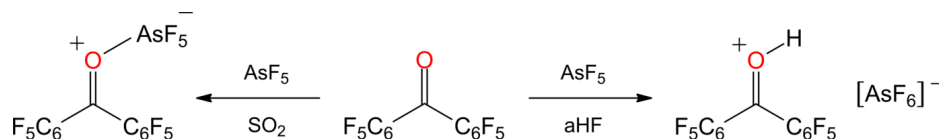
2. Experimental

2.1. Synthesis and crystallization

A fluorinated ethylene propylene (FEP) vessel (outer diameter: 6 mm; inner diameter: 4.6 mm), equipped with an aluminium-encased polychlorotrifluoroethylene (PCTFE)

valve, was passivated with fluorine overnight prior to use. In a nitrogen-filled glovebox (Vigor SG1200/750E–SG1500/750E; H₂O < 0.02 ppm, O₂ < 2 ppm), the vessel was loaded with (C₆F₅)₂CO (23 mg, 0.064 mmol; Thermo Scientific, 97%). Anhydrous HF (0.2 ml; Linde, 99.995%; stored over K₂NiF₆) was then condensed into it using a vacuum line designed for handling elemental fluorine, resulting in a suspension of (C₆F₅)₂CO at room temperature. Upon addition of AsF₅ (0.137 mmol), synthesized as described previously (Mazej & Žemva, 2005), a yellow precipitate formed that dissolved completely upon warming to room temperature. Slow cooling to −30 °C yielded canary-yellow crystals of (C₆F₅)₂COH⁺[AsF₆][−]. The solvent aHF was removed under dynamic vacuum at −78 °C, leaving a yellow crystalline solid. Another synthesis was performed on a slightly larger scale [113 mg, 0.312 mmol (C₆F₅)₂CO; 0.4 ml aHF; 0.936 mmol AsF₅] (Figs. 1–3).

For the synthesis of (C₆F₅)₂CO·AsF₅, (C₆F₅)₂CO (14 mg, 0.039 mmol) was dissolved in dry SO₂ (0.3 ml; Ruše, stored over CaH₂ in a glass bulb) at room temperature. AsF₅ (0.168 mmol) was added at −196 °C. Upon thawing of the SO₂–AsF₅ mixture, a yellow coloration appeared immediately. The vessel was then stored at −78 °C under a nitrogen overpressure (~1000 Torr). Large yellow crystals of (C₆F₅)₂CO·AsF₅ formed over a period of ten days. Volatiles, SO₂ and

**Figure 1**

Synthesis of the $(\text{C}_6\text{F}_5)_2\text{COH}^+[\text{AsF}_6]^-$ salt and the $(\text{C}_6\text{F}_5)_2\text{CO}\cdot\text{AsF}_5$ adduct.

excess AsF_5 were removed under dynamic vacuum between -78 and -50 °C, yielding a yellow solid (Figs. 1 and 2).

A crystalline sample was quickly deposited from the FEP reaction vessel into an aluminium trough of the low-temperature crystal-mounting apparatus, designed and employed for mounting highly reactive moisture-sensitive noble-gas compounds (Lozinšek *et al.*, 2021; Motaln *et al.*, 2024), which was cooled using a stream of cold nitrogen to temperatures ranging from -80 to -100 °C. Suitable crystals were selected under a stereomicroscope and mounted on the tip of a MiTeGen loop using Fomblin oil (Z25, SynQuest) (Motaln *et al.*, 2025). The loop assembly was picked up with cryo-pin tongs cooled to -196 °C and quickly transferred to the magnetic holder on the goniometer head, where the crystal was protected by a cold nitrogen stream at 100 K.

2.2. Refinement

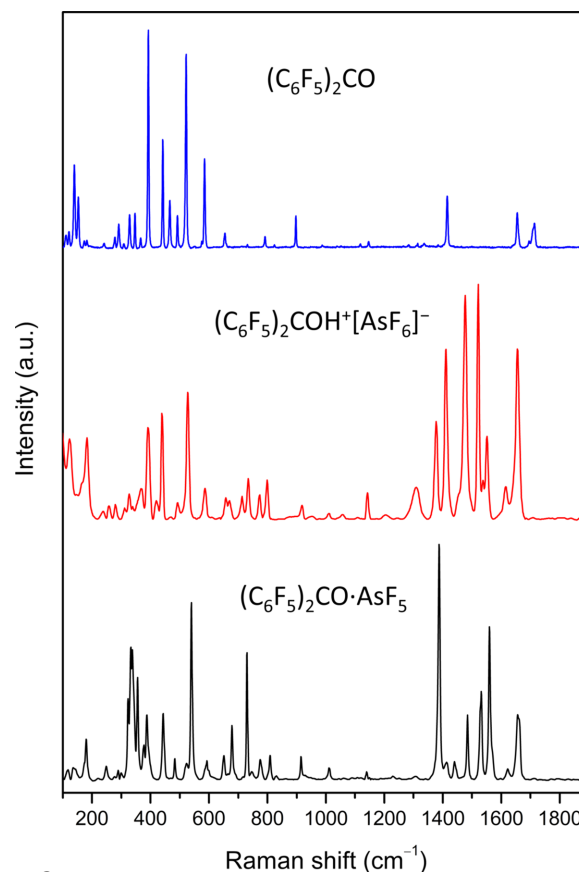
Crystal data, data collection and structure refinement details are summarized in Table 1. The position of the H atom in the crystal structure of $(\text{C}_6\text{F}_5)_2\text{COH}^+[\text{AsF}_6]^-$ was located in a difference electron-density map and refined freely, including its isotropic displacement parameter (Cooper *et al.*, 2010).

2.3. Raman spectroscopy

Raman spectroscopy was performed using either a Horiba Jobin Yvon LabRAM HR spectrometer coupled with an Olympus BXFM-ILHS microscope or a Bruker Senterra II confocal Raman microscope equipped with a Linkam LTS420 low-temperature stage. Red (633 and 785 nm) and green (532 nm) lasers were tested, with the laser power adjusted to the sample. The Raman spectra of $(\text{C}_6\text{F}_5)_2\text{COH}^+[\text{AsF}_6]^-$ and $(\text{C}_6\text{F}_5)_2\text{CO}\cdot\text{AsF}_5$ exhibited fluorescence regardless of the excitation wavelength used. The low-temperature (-90 °C) spectrum of solid $(\text{C}_6\text{F}_5)_2\text{CO}$ (Fig. 2), which is in good agreement with the previously published Raman spectrum (Anandhi & Umapathy, 2000), was recorded using the Bruker spectrometer with a 785 nm red laser at 1.5 cm^{-1} resolution. Low-temperature Raman spectra of the $(\text{C}_6\text{F}_5)_2\text{COH}^+[\text{AsF}_6]^-$ salt and the $(\text{C}_6\text{F}_5)_2\text{CO}\cdot\text{AsF}_5$ adduct (Fig. 2) were acquired on the Horiba system using a 633 nm red laser at 4 cm^{-1} resolution from crystalline material protected by a cold nitrogen stream of the crystal-mounting apparatus. Background subtraction from the spectra was performed using the Bruker *OPUS8.7* software suite, with 15 iterations of concave rubber-band correction and 50 baseline points.

3. Results and discussion

To facilitate a comparison of structural changes in the decafluorobenzophenone moiety upon protonation and coordination to AsF_5 , the crystal structure of $(\text{C}_6\text{F}_5)_2\text{CO}$ was redetermined at 100 K (Table 1; Figs. S1 and S2 in the supporting information). The current structural parameters [$\text{C}=\text{O} = 1.197$ (4) Å; $\text{C}-\text{CO} = 1.498$ (3) Å; $\text{C}-\text{C} = 1.373$ (3)– 1.392 (3) Å; $\text{C}-\text{F} = 1.331$ (3)– 1.341 (3) Å] are in excellent agreement with the previously reported crystal structure measured at 153 K [$\text{C}=\text{O} = 1.201$ (8) Å; $\text{C}-\text{CO} = 1.489$ (6) Å; $\text{C}-\text{C} = 1.361$ (6)– 1.403 (5) Å; $\text{C}-\text{F} = 1.329$ (5)– 1.351 (4) Å; Schwarzer *et al.*, 2004]. Decafluorobenzophenone crystallizes in the Sohncke space group *C2* and the molecule exhibits axial chirality owing to sterically hindered rotation of the C_6F_5 rings about the $\text{C}_{\text{aryl}}-\text{C}(\text{O})-\text{C}_{\text{aryl}}$ bonds (Farmer & Walker, 1967). Similarly,

**Figure 2**

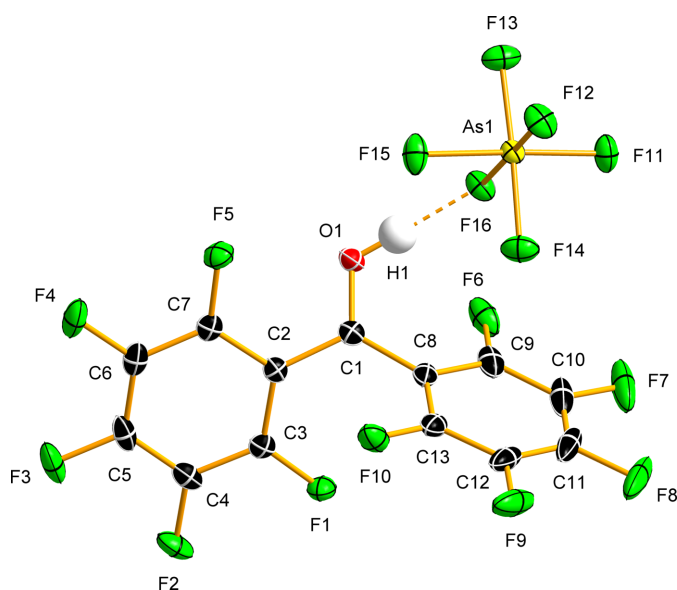
The low-temperature Raman spectra of $(\text{C}_6\text{F}_5)_2\text{CO}$ (top), $(\text{C}_6\text{F}_5)_2\text{COH}^+[\text{AsF}_6]^-$ (middle) and $(\text{C}_6\text{F}_5)_2\text{CO}\cdot\text{AsF}_5$ (bottom) measured at -90 , -90 and -93 °C, respectively.

**Figure 3**

Canary-yellow crystals of $(\text{C}_6\text{F}_5)_2\text{COH}^+[\text{AsF}_6]^-$ that formed upon cooling a solution of $(\text{C}_6\text{F}_5)_2\text{CO}$ and AsF_5 in anhydrous HF to about -10°C using an ethanol bath. The outer diameter of the FEP tube is 6 mm.

chiral crystallization has also been reported for achiral benzophenone (Matsumoto *et al.*, 2016).

The synthetic procedure for the preparation of $(\text{C}_6\text{F}_5)_2\text{COH}^+[\text{AsF}_6]^-$ and $(\text{C}_6\text{F}_5)_2\text{CO}\cdot\text{AsF}_5$ involved the reaction of $(\text{C}_6\text{F}_5)_2\text{CO}$ with AsF_5 in anhydrous HF (aHF) and in liquid SO_2 solvent, respectively (Fig. 1). Although decafluorobenzophenone was poorly soluble in aHF, the addition of AsF_5 resulted in its dissolution at room temperature, accompanied by the development of a yellow coloration. Upon cooling the reaction mixture, canary-yellow plank-shaped crystals began to form

**Figure 4**

The asymmetric unit with the atom-labelling scheme in the crystal structure of $(\text{C}_6\text{F}_5)_2\text{COH}^+[\text{AsF}_6]^-$. The $\text{O}-\text{H}\cdots\text{F}$ hydrogen bond is shown as an orange dashed line. Displacement ellipsoids are depicted at the 50% probability level.

Table 2

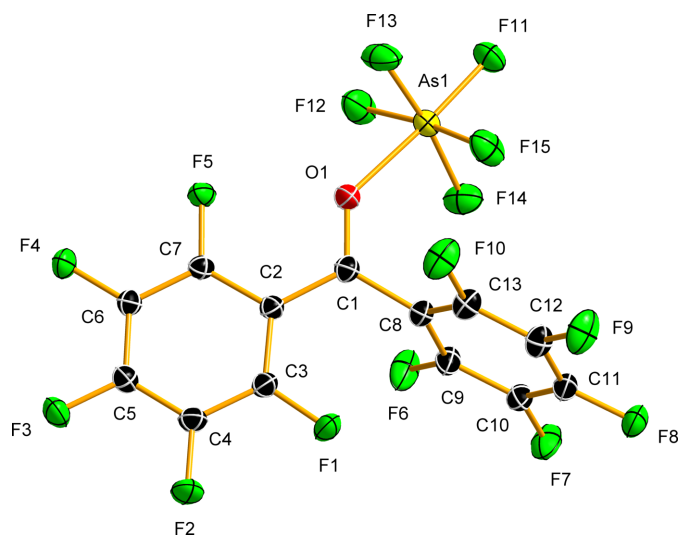
Hydrogen-bond geometry ($\text{\AA}$, $^\circ$) for $(\text{C}_6\text{F}_5)_2\text{COH}^+[\text{AsF}_6]^-$.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O1}-\text{H1}\cdots\text{F16}$	0.90 (3)	1.63 (3)	2.5279 (16)	178 (3)

(Fig. 3). Slow removal of the aHF solvent yielded a crystalline canary-yellow solid, identified as $(\text{C}_6\text{F}_5)_2\text{COH}^+[\text{AsF}_6]^-$.

The protonated salt $(\text{C}_6\text{F}_5)_2\text{COH}^+[\text{AsF}_6]^-$ crystallizes in the monoclinic space group $P2_1/n$ and contains one $(\text{C}_6\text{F}_5)_2\text{COH}^+$ cation and one $[\text{AsF}_6]^-$ anion in the asymmetric unit (Table 1 and Figs. 4 and S3).

In $(\text{C}_6\text{F}_5)_2\text{COH}^+[\text{AsF}_6]^-$ (Fig. 4), the $\text{C}=\text{O}$ bond length [1.274 (2) $\text{\AA}$] is elongated compared to that in $(\text{C}_6\text{F}_5)_2\text{CO}$ [1.197 (4) $\text{\AA}$], and is comparable to values observed in the protonated ketones: acetone, $\text{C}_3\text{H}_6\text{OH}^+$ [1.271 (3) and 1.273 (3) $\text{\AA}$]; adamantan-2-one, $\text{C}_{10}\text{H}_{14}\text{OH}^+$ [1.274 (2) $\text{\AA}$]; and cyclopentanone, $\text{C}_5\text{H}_8\text{OH}^+$ [1.266 (3) and 1.267 (2) $\text{\AA}$] (Stuart *et al.*, 2017). Similar $\text{C}=\text{O}$ bond lengths have been reported for the crystal structures of the hemiprotonated benzophenone salts $[(\text{C}_6\text{H}_5)_2\text{CO}]_2\text{H}^+[\text{CHB}_{11}\text{H}_5\text{Cl}_6]^-$ [1.274 (4) $\text{\AA}$; Stasko *et al.*, 2002] and $[(\text{C}_6\text{H}_5)_2\text{CO}]_2\text{H}^+[\text{TaF}_6]^-$ [1.259 (3) $\text{\AA}$; Marchetti *et al.*, 2007]. The $\text{C}-\text{C}(\text{=O})$ bonds in $(\text{C}_6\text{F}_5)_2\text{COH}^+$ [1.443 (2) and 1.455 (2) $\text{\AA}$] are shorter than the corresponding bonds in $(\text{C}_6\text{F}_5)_2\text{CO}$ [1.498 (3) $\text{\AA}$]. The remaining $\text{C}-\text{F}$ and $\text{C}-\text{C}$ bonds in the $(\text{C}_6\text{F}_5)_2\text{COH}^+$ cation [$\text{C}-\text{C} = 1.370$ (2)–1.406 (2) $\text{\AA}$; $\text{C}-\text{F} = 1.322$ (2)–1.334 (2) $\text{\AA}$] remain within the range of those observed in the crystal structure of $(\text{C}_6\text{F}_5)_2\text{CO}$. The angle between the plane normals of the two arene rings [76.58 (6) $^\circ$] is very similar to that in $(\text{C}_6\text{F}_5)_2\text{CO}$ [77.22 (9) $^\circ$]. The angles between the arene-ring-plane normals and the plane normal of the carbonyl-bond-containing $\text{C}_2\text{C}=\text{O}$ fragment [36.93 (7) and 44.90 (7) $^\circ$] are smaller than the corresponding value observed in the crystal structure of $(\text{C}_6\text{F}_5)_2\text{CO}$ [47.97 (7) $^\circ$].

**Figure 5**

The asymmetric unit with the atom-labelling scheme in the crystal structure of adduct $(\text{C}_6\text{F}_5)_2\text{CO}\cdot\text{AsF}_5$. Displacement ellipsoids are depicted at the 50% probability level.

Table 3

Selected geometric parameters ($\text{\AA}$, $^\circ$) for crystallographically characterized compounds featuring AsF_5 coordinated to a carbonyl group.

$\text{S}_2\text{N}_2\text{CO} = 5\text{-oxo-1,3}\lambda^4,2,4\text{-dithiadiazole}$, $\text{C}_4\text{H}_2\text{F}_2\text{O}_2 = \text{fumaryl fluoride}$, $\text{CH}_2\text{ClCFO} = \text{chloroacetyl fluoride}$ and $\text{CH}_2\text{FCFO} = \text{fluoroacetyl fluoride}$.

Compound (moiety)	C=O	O—As	As—F _{ax}	C—O—As	Reference
$(\text{C}_6\text{F}_5)_2\text{CO}\cdot\text{AsF}_5$	1.2526 (15)	1.9897 (10)	1.6890 (8)	133.83 (8)	This work
$\text{S}_2\text{N}_2\text{CO}\cdot\text{AsF}_5$	1.279 (4)	1.879 (7)	1.695 (6)	127.3 (1)	Gieren <i>et al.</i> (1980)
$\text{C}_4\text{H}_2\text{F}_2\text{O}_2\cdot 4(\text{C}_4\text{H}_2\text{F}_2\text{O}_2\cdot\text{AsF}_5)\cdot(\text{C}_4\text{H}_2\text{F}_2\text{O}_2\cdot 2\text{AsF}_5)$					Bayer <i>et al.</i> (2021)
$(\text{C}_4\text{H}_2\text{F}_2\text{O}_2\cdot\text{AsF}_5)$	1.221 (2)	2.0367 (15)	1.6840 (14)	132.33 (15)	
$(\text{C}_4\text{H}_2\text{F}_2\text{O}_2\cdot 2\text{AsF}_5)$	1.220 (2)	2.0472 (14)	1.6835 (13)	130.67 (14)	
$(\text{C}_4\text{H}_2\text{F}_2\text{O}_2\cdot 2\text{AsF}_5)$	1.215 (3)	2.0444 (14)	1.6926 (13)	130.83 (14)	
$\text{CH}_2\text{ClCFO}\cdot\text{AsF}_5$	1.213 (3)	2.0418 (16)	1.6854 (14)	128.96 (17)	Steiner <i>et al.</i> (2024b)
$\text{CH}_2\text{FCFO}\cdot\text{AsF}_5$	1.210 (3)	2.0306 (15)	1.6835 (13)	130.49 (15)	Steiner <i>et al.</i> (2024b)

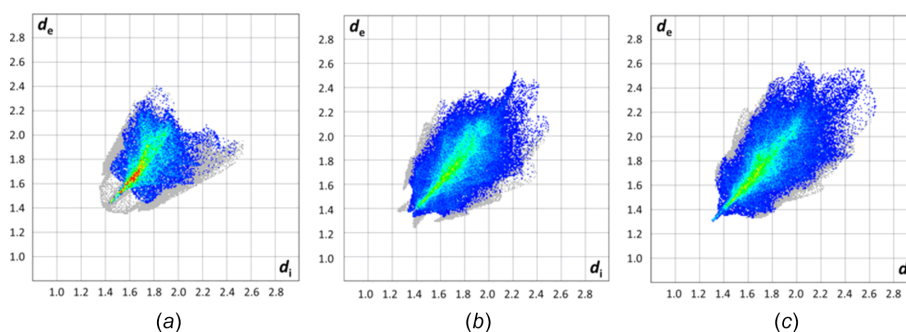
The crystal structure exhibits a short hydrogen bond between the $(\text{C}_6\text{F}_5)_2\text{COH}^+$ cation and the $[\text{AsF}_6]^-$ anion (Table 2). The H atom lies only slightly out of the $\text{C}_2\text{C}=\text{O}$ plane [0.14 (3) $\text{\AA}$]. The $\text{O}\cdots\text{F}$ hydrogen-bond distance [2.5279 (16) $\text{\AA}$] is shorter than those observed in the crystal structures of $[\text{PnF}_6]^-$ (Pn = As or Sb) salts of protonated ketones – acetone, cyclopentanone and adamantane-2-one [2.560 (3)–2.6233 (16) $\text{\AA}$; Stuart *et al.*, 2017] – due to the greater Brønsted acidity of the perfluorinated conjugate acid $(\text{C}_6\text{F}_5)_2\text{COH}^+$. The hydrogen-bonded As—F bond is elongated [As—F(H) = 1.7853 (10) $\text{\AA}$; As—F = 1.6943 (10)–1.7237 (11) $\text{\AA}$], resulting in a distortion of the $[\text{AsF}_6]^-$ anion from idealized octahedral geometry. Interestingly, similar As—F_{bridging} bond lengths have been observed in metal complexes where the $[\text{AsF}_6]^-$ anion is coordinated to a metal centre, for example, in $[\text{Mg}(\text{KrF}_2)_4(\text{AsF}_6)_2]$ [1.7856 (14) and 1.7965 (13) $\text{\AA}$] (Lozinšek *et al.*, 2017).

The supporting information includes an additional crystal structure determination of $(\text{C}_6\text{F}_5)_2\text{COH}^+[\text{AsF}_6]^-$ employing Ag $K\alpha$ radiation, providing results essentially similar to those presented in the text.

The reaction of decafluorobenzophenone with an excess of AsF_5 in SO_2 at low temperature (Fig. 1) resulted in the formation of a yellow solution, from which large yellow plate-like crystals of the Lewis acid–base adduct $(\text{C}_6\text{F}_5)_2\text{CO}\cdot\text{AsF}_5$ crystallized at -78°C over a period of ten days. The compound crystallizes in the orthorhombic space group $Pbca$ (Table 1) and represents a rare crystallographically characterized example of a ketone coordinated to AsF_5 (Figs. 5 and S4).

The C=O bond length [1.2526 (15) $\text{\AA}$] in the crystal structure of the adduct is elongated compared to that in $(\text{C}_6\text{F}_5)_2\text{CO}$ [1.197 (4) $\text{\AA}$], although to a lesser extent than in the protonated salt [1.274 (2) $\text{\AA}$]. A similar C=O bond length was observed in the benzophenone adduct with TaCl_5 [1.265 (3) $\text{\AA}$; Marchetti *et al.*, 2007], in the adducts of BF_3 with ethylene carbonate [1.2486 (14) $\text{\AA}$], dimethyl carbonate [1.2559 (14) $\text{\AA}$], diethyl carbonate [1.2562 (18) $\text{\AA}$] and γ -butyrolactone [1.2541 (16) $\text{\AA}$] (Bodin *et al.*, 2023), and in the amide moiety of capsaicin [1.2459 (19) $\text{\AA}$; Lozinšek, 2025]. The elongation of the C=O bond is accompanied by a significant shortening of the *anti*-C—C(=O) bond [1.4549 (16) $\text{\AA}$], whereas the *syn*-C—C(=O) bond length remains virtually unchanged [1.4879 (16) $\text{\AA}$] compared to the corresponding distance observed in $(\text{C}_6\text{F}_5)_2\text{CO}$ [1.498 (3) $\text{\AA}$]. All other bond lengths in the $(\text{C}_6\text{F}_5)_2\text{CO}$ moiety within $(\text{C}_6\text{F}_5)_2\text{CO}\cdot\text{AsF}_5$ [C—C = 1.3788 (17)–1.4133 (15) $\text{\AA}$; C—F = 1.3162 (13)–1.3359 (15) $\text{\AA}$] are similar to those observed in $(\text{C}_6\text{F}_5)_2\text{COH}^+[\text{AsF}_6]^-$ and $(\text{C}_6\text{F}_5)_2\text{CO}$. The angle between the plane normals of the two arene rings [81.57 (4) $^\circ$] differs from those in the crystal structures of $(\text{C}_6\text{F}_5)_2\text{CO}$ and $(\text{C}_6\text{F}_5)_2\text{COH}^+[\text{AsF}_6]^-$. Of the two rings, one is almost coplanar with the plane formed by the $\text{C}_2\text{C}=\text{O}$ moiety [9.44 (5) $^\circ$], while the other is nearly perpendicular [75.63 (5) $^\circ$].

The O—As bond [1.9897 (10) $\text{\AA}$] in the crystal structure of $(\text{C}_6\text{F}_5)_2\text{CO}\cdot\text{AsF}_5$ is substantially longer than that reported for the adduct of Roesky's ketone, $\text{S}_2\text{N}_2\text{CO}\cdot\text{AsF}_5$ [1.879 (7) $\text{\AA}$; Gieren *et al.*, 1980], and shorter than the O—As bond lengths (Table 3) observed in the limited number of crystal structures of compounds featuring a C=O—AsF₅ linkage, involving acyl

**Figure 6**

Hirshfeld fingerprint plots of (a) $(\text{C}_6\text{F}_5)_2\text{CO}$ (56.8%), (b) $(\text{C}_6\text{F}_5)_2\text{COH}^+[\text{AsF}_6]^-$ (69.6%) and (c) $(\text{C}_6\text{F}_5)_2\text{CO}\cdot\text{AsF}_5$ (72.8%), showing the prevalent F $\cdots$ F intermolecular contacts.

fluorides (Bayer *et al.*, 2021; Steiner *et al.*, 2024b). The As atom resides slightly out of the C₂C=O plane [0.417 (2) Å]. The C=O—As bond angle [133.83 (8)°] is comparable to those in other compounds where a C=O group acts as a ligand to AsF₅ (Table 3). The As—F_{ax} (ax is axial) bond *trans* to As—O is somewhat shorter [1.6890 (8) Å] than the As—F_{eq} (eq is equatorial) bonds in the AsF₅ moiety [1.6960 (10)–1.7018 (9) Å]. The O—As—F_{ax} angle [176.30 (5)°] is close to linear. The acute O—As—F_{eq} angles [83.84 (5)–89.06 (5)°], the obtuse F_{ax}—As—F_{eq} angles [92.94 (5)–94.16 (5)°] and the *trans*-F_{eq}—As—F_{eq} angles deviating from linearity [171.85 (5) and 172.89 (5)°] reflect the smaller bond domain (Gillespie, 2008) and lower bond order (Stuart *et al.*, 2019) of the As—O bond compared to the As—F bonds.

In all three crystal structures, *i.e.* (C₆F₅)₂CO, (C₆F₅)₂COH⁺[AsF₆][−] and (C₆F₅)₂CO·AsF₅, the dominant intermolecular contacts are F⋯F (Figs. 6 and S5), which involve contributions of 56.8, 69.6 and 72.8%, respectively, whereas the C⋯F contacts (Fig. S6) cover 30.7, 23.7 and 25.2% of the surface area, respectively. The similarity in the intermolecular interactions between (C₆F₅)₂COH⁺[AsF₆][−] and (C₆F₅)₂CO·AsF₅ is evident from a comparison of their Hirshfeld fingerprint plots (Figs. 6 and S5–S7) (Spackman & McKinnon, 2002; Spackman *et al.*, 2021). In the crystal structure of (C₆F₅)₂CO, O⋯F contacts (Fig. S7) also contribute to the packing, accounting for 8.5% of the surface area. However, in the crystal structures of (C₆F₅)₂COH⁺[AsF₆][−] and (C₆F₅)₂CO·AsF₅, this contribution is reduced to 4.4 and 1.9%, respectively, as the O atom is bonded to hydrogen and arsenic, respectively. In the protonated salt, F⋯H contacts involve 2.3% of the surface area (Fig. S8).

4. Conclusion

In this work, the syntheses, crystal structure determination and Raman spectra of a protonated decafluorobenzophenone salt, (C₆F₅)₂COH⁺[AsF₆][−], and a Lewis acid–base adduct, (C₆F₅)₂CO·AsF₅, are reported. The crystal structure of (C₆F₅)₂CO was also redetermined at 100 K. These crystal structures represent rare examples of a protonated perfluorinated aromatic ketone and a ketone–arsenic pentafluoride adduct.

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supporting information

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Protonated decafluorobenzophenone and the decafluorobenzophenone–arsenic pentafluoride adduct

Erik Uran and Matic Lozinšek

Computing details

Bis(2,3,4,5,6-pentafluorophenyl)methanone (pfbp_1)

Crystal data

C₁₃F₁₀O

$M_r = 362.13$

Monoclinic, C2

$a = 20.1460(4) \text{ \AA}$

$b = 5.39987(10) \text{ \AA}$

$c = 5.47058(14) \text{ \AA}$

$\beta = 95.912(2)^\circ$

$V = 591.96(2) \text{ \AA}^3$

$Z = 2$

$F(000) = 352$

$D_x = 2.032 \text{ Mg m}^{-3}$

Cu $K\alpha$ radiation, $\lambda = 1.54184 \text{ \AA}$

Cell parameters from 8190 reflections

$\theta = 4.4\text{--}75.7^\circ$

$\mu = 2.18 \text{ mm}^{-1}$

$T = 100 \text{ K}$

Plank, clear colourless

$0.43 \times 0.1 \times 0.07 \text{ mm}$

Data collection

Rigaku OD XtaLAB Synergy-S Dualflex
diffractometer with an Eiger2 R CdTe 1M
detector

Radiation source: micro-focus sealed X-ray
tube, PhotonJet (Cu) X-ray Source

Mirror monochromator

Detector resolution: $13.3333 \text{ pixels mm}^{-1}$

ω scans

Absorption correction: gaussian
(CrysAlis PRO; Rigaku OD, 2025)

$T_{\min} = 0.491$, $T_{\max} = 1.000$

10783 measured reflections

1212 independent reflections

1193 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.056$

$\theta_{\max} = 75.8^\circ$, $\theta_{\min} = 4.4^\circ$

$h = -24 \rightarrow 25$

$k = -6 \rightarrow 6$

$l = -6 \rightarrow 6$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.034$

$wR(F^2) = 0.095$

$S = 1.11$

1212 reflections

110 parameters

1 restraint

Primary atom site location: iterative

$w = 1/[\sigma^2(F_o^2) + (0.0725P)^2 + 0.0709P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.28 \text{ e \AA}^{-3}$

$\Delta\rho_{\min} = -0.24 \text{ e \AA}^{-3}$

Absolute structure: Flack x determined using

514 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)

Absolute structure parameter: 0.05 (10)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.500000	0.5279 (6)	0.000000	0.0254 (6)
F1	0.55011 (6)	0.9228 (3)	0.3092 (2)	0.0297 (3)
O1	0.500000	0.3063 (5)	0.000000	0.0363 (6)
C2	0.56145 (10)	0.6731 (4)	−0.0384 (4)	0.0248 (5)
F2	0.65871 (7)	1.1917 (3)	0.2293 (3)	0.0386 (4)
C3	0.58311 (10)	0.8685 (4)	0.1153 (4)	0.0245 (5)
F3	0.72843 (7)	1.0815 (4)	−0.1543 (3)	0.0393 (4)
C4	0.63891 (11)	1.0062 (4)	0.0784 (4)	0.0287 (5)
F4	0.69032 (7)	0.6982 (3)	−0.4572 (3)	0.0399 (4)
C5	0.67484 (11)	0.9486 (4)	−0.1160 (4)	0.0288 (5)
F5	0.58043 (7)	0.4335 (3)	−0.3865 (3)	0.0379 (4)
C6	0.65533 (11)	0.7512 (5)	−0.2692 (4)	0.0294 (5)
C7	0.59954 (11)	0.6169 (4)	−0.2295 (4)	0.0279 (5)

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0312 (15)	0.0190 (14)	0.0261 (15)	0.000	0.0031 (11)	0.000
F1	0.0328 (6)	0.0324 (7)	0.0249 (6)	0.0001 (6)	0.0080 (5)	−0.0056 (6)
O1	0.0367 (12)	0.0214 (11)	0.0519 (15)	0.000	0.0095 (10)	0.000
C2	0.0275 (10)	0.0215 (10)	0.0252 (10)	0.0037 (8)	0.0017 (8)	0.0011 (8)
F2	0.0376 (7)	0.0349 (8)	0.0433 (9)	−0.0090 (6)	0.0052 (6)	−0.0128 (7)
C3	0.0267 (9)	0.0247 (11)	0.0225 (10)	0.0031 (8)	0.0043 (8)	0.0017 (7)
F3	0.0287 (7)	0.0438 (8)	0.0466 (9)	−0.0078 (6)	0.0097 (6)	0.0009 (7)
C4	0.0305 (11)	0.0263 (11)	0.0288 (12)	0.0003 (9)	0.0005 (9)	−0.0021 (10)
F4	0.0345 (7)	0.0559 (10)	0.0311 (8)	0.0034 (7)	0.0130 (6)	−0.0047 (8)
C5	0.0240 (10)	0.0308 (12)	0.0317 (11)	−0.0003 (9)	0.0035 (8)	0.0043 (10)
F5	0.0401 (7)	0.0378 (8)	0.0368 (8)	−0.0026 (7)	0.0089 (6)	−0.0160 (7)
C6	0.0280 (10)	0.0360 (13)	0.0244 (10)	0.0069 (9)	0.0048 (8)	0.0009 (9)
C7	0.0295 (10)	0.0260 (10)	0.0281 (11)	0.0033 (9)	0.0018 (8)	−0.0037 (9)

Geometric parameters ($\text{\AA}$, $^\circ$)

C1—O1	1.197 (4)	C3—C4	1.380 (3)
C1—C2 ⁱ	1.498 (3)	F3—C5	1.331 (3)
C1—C2	1.498 (3)	C4—C5	1.382 (3)
F1—C3	1.341 (2)	F4—C6	1.336 (3)
C2—C3	1.391 (3)	C5—C6	1.388 (3)
C2—C7	1.392 (3)	F5—C7	1.341 (3)

F2—C4	1.332 (3)	C6—C7	1.373 (3)
O1—C1—C2 ⁱ	121.54 (13)	C3—C4—C5	119.4 (2)
O1—C1—C2	121.54 (13)	F3—C5—C4	119.8 (2)
C2 ⁱ —C1—C2	116.9 (3)	F3—C5—C6	120.2 (2)
C3—C2—C1	121.61 (18)	C4—C5—C6	119.96 (19)
C3—C2—C7	117.1 (2)	F4—C6—C5	119.4 (2)
C7—C2—C1	121.2 (2)	F4—C6—C7	120.9 (2)
F1—C3—C2	119.60 (18)	C7—C6—C5	119.7 (2)
F1—C3—C4	118.4 (2)	F5—C7—C2	119.8 (2)
C4—C3—C2	122.0 (2)	F5—C7—C6	118.3 (2)
F2—C4—C3	120.7 (2)	C6—C7—C2	121.8 (2)
F2—C4—C5	119.9 (2)		
C1—C2—C3—F1	2.9 (3)	C3—C2—C7—F5	−178.74 (19)
C1—C2—C3—C4	−178.70 (18)	C3—C2—C7—C6	−1.4 (3)
C1—C2—C7—F5	1.6 (3)	C3—C4—C5—F3	179.50 (19)
C1—C2—C7—C6	178.88 (19)	C3—C4—C5—C6	−1.1 (3)
F1—C3—C4—F2	−1.2 (3)	F3—C5—C6—F4	−0.9 (3)
F1—C3—C4—C5	178.09 (18)	F3—C5—C6—C7	−179.3 (2)
O1—C1—C2—C3	−131.84 (16)	C4—C5—C6—F4	179.7 (2)
O1—C1—C2—C7	47.8 (2)	C4—C5—C6—C7	1.3 (3)
C2 ⁱ —C1—C2—C3	48.16 (16)	F4—C6—C7—C2	−178.4 (2)
C2 ⁱ —C1—C2—C7	−132.2 (2)	F4—C6—C7—F5	−1.0 (3)
C2—C3—C4—F2	−179.69 (19)	C5—C6—C7—C2	0.0 (3)
C2—C3—C4—C5	−0.4 (3)	C5—C6—C7—F5	177.4 (2)
F2—C4—C5—F3	−1.2 (3)	C7—C2—C3—F1	−176.83 (17)
F2—C4—C5—C6	178.2 (2)	C7—C2—C3—C4	1.6 (3)

Symmetry code: (i) $-x+1, y, -z$.

[Bis(2,3,4,5,6-pentafluorophenyl)methylidene]oxidanium hexafluoroarsenate (pfbphas_1)

Crystal data

$C_{13}HF_{10}O^+ \cdot AsF_6^-$
 $M_r = 552.06$
 Monoclinic, $P2_1/n$
 $a = 8.19207$ (7) Å
 $b = 21.17409$ (18) Å
 $c = 9.28475$ (9) Å
 $\beta = 98.2086$ (8)°
 $V = 1594.03$ (2) Å³
 $Z = 4$

$F(000) = 1056$
 $D_x = 2.300$ Mg m^{−3}
 Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
 Cell parameters from 17949 reflections
 $\theta = 4.2\text{--}75.8^\circ$
 $\mu = 4.70$ mm^{−1}
 $T = 100$ K
 Irregular, clear yellow
 $0.09 \times 0.05 \times 0.03$ mm

Data collection

Rigaku OD XtaLAB Synergy-S Dualflex
 diffractometer with an Eiger2 R CdTe 1M
 detector
 Radiation source: micro-focus sealed X-ray
 tube, PhotonJet (Cu) X-ray Source
 Mirror monochromator

Detector resolution: 13.3333 pixels mm^{−1}
 ω scans
 Absorption correction: gaussian
 (CrysAlis PRO; Rigaku OD, 2025)
 $T_{\min} = 0.842$, $T_{\max} = 1.000$
 26147 measured reflections

3336 independent reflections
 3134 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.032$
 $\theta_{\text{max}} = 76.2^\circ$, $\theta_{\text{min}} = 4.2^\circ$

$h = -10 \rightarrow 10$
 $k = -26 \rightarrow 26$
 $l = -11 \rightarrow 11$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.025$
 $wR(F^2) = 0.066$
 $S = 1.05$
 3336 reflections
 285 parameters
 0 restraints
 Primary atom site location: iterative
 Hydrogen site location: difference Fourier map

All H-atom parameters refined
 $w = 1/[\sigma^2(F_o^2) + (0.0365P)^2 + 1.1067P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.30 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.49 \text{ e } \text{\AA}^{-3}$
 Extinction correction: SHELXL2019
 (Sheldrick, 2015),
 $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.00062 (9)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
As1	−0.04788 (2)	0.36662 (2)	0.08141 (2)	0.01629 (8)
C1	0.0308 (2)	0.24086 (8)	0.45829 (18)	0.0173 (3)
F1	0.08742 (14)	0.22108 (5)	0.76315 (11)	0.0250 (2)
O1	0.08150 (15)	0.23385 (6)	0.33572 (13)	0.0206 (3)
H1	0.095 (4)	0.2690 (14)	0.285 (3)	0.047 (8)*
C2	−0.0159 (2)	0.18363 (8)	0.52632 (18)	0.0169 (3)
F2	0.04697 (14)	0.10757 (6)	0.88119 (13)	0.0316 (3)
C3	0.0209 (2)	0.17462 (8)	0.67751 (19)	0.0192 (3)
F3	−0.09505 (16)	0.01254 (5)	0.71399 (15)	0.0365 (3)
C4	−0.0006 (2)	0.11675 (9)	0.7396 (2)	0.0226 (4)
F4	−0.18184 (14)	0.02812 (5)	0.42358 (14)	0.0330 (3)
C5	−0.0702 (2)	0.06760 (8)	0.6537 (2)	0.0254 (4)
F5	−0.12336 (14)	0.13815 (5)	0.29942 (12)	0.0257 (2)
C6	−0.1127 (2)	0.07546 (8)	0.5054 (2)	0.0236 (4)
F6	0.28339 (14)	0.33217 (6)	0.46949 (13)	0.0354 (3)
C7	−0.0819 (2)	0.13200 (8)	0.4428 (2)	0.0198 (3)
F7	0.2469 (2)	0.45084 (6)	0.56574 (17)	0.0600 (5)
C8	0.0198 (2)	0.30331 (8)	0.52164 (18)	0.0206 (3)
F8	−0.0351 (3)	0.48440 (6)	0.66527 (16)	0.0652 (6)
C9	0.1433 (3)	0.34851 (10)	0.5171 (2)	0.0285 (4)
F9	−0.2831 (2)	0.39958 (7)	0.67083 (14)	0.0508 (4)
C10	0.1259 (3)	0.40887 (10)	0.5671 (2)	0.0402 (6)
F10	−0.24547 (15)	0.28072 (5)	0.58219 (13)	0.0294 (2)
C11	−0.0181 (4)	0.42584 (9)	0.6190 (2)	0.0435 (6)
F11	0.05490 (13)	0.43629 (5)	0.09411 (13)	0.0284 (2)

C12	−0.1439 (3)	0.38265 (10)	0.6241 (2)	0.0352 (5)
F12	−0.21720 (13)	0.39793 (6)	−0.02074 (12)	0.0289 (2)
C13	−0.1225 (3)	0.32160 (9)	0.57846 (19)	0.0246 (4)
F13	0.03949 (14)	0.34708 (6)	−0.06940 (11)	0.0312 (3)
F14	−0.12650 (14)	0.38246 (6)	0.23962 (12)	0.0298 (2)
F15	−0.13957 (14)	0.29328 (5)	0.07867 (14)	0.0305 (3)
F16	0.12598 (12)	0.33179 (5)	0.19056 (11)	0.0226 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
As1	0.01455 (12)	0.01742 (12)	0.01641 (12)	−0.00053 (6)	0.00052 (7)	0.00166 (6)
C1	0.0135 (7)	0.0208 (8)	0.0168 (7)	0.0006 (6)	−0.0011 (6)	0.0017 (6)
F1	0.0323 (6)	0.0247 (5)	0.0169 (5)	0.0007 (4)	−0.0001 (4)	−0.0010 (4)
O1	0.0224 (6)	0.0214 (6)	0.0187 (6)	0.0009 (5)	0.0055 (5)	0.0037 (5)
C2	0.0141 (7)	0.0175 (7)	0.0191 (8)	0.0020 (6)	0.0024 (6)	0.0016 (6)
F2	0.0332 (6)	0.0380 (6)	0.0248 (5)	0.0101 (5)	0.0084 (4)	0.0153 (5)
C3	0.0170 (8)	0.0204 (8)	0.0205 (8)	0.0029 (6)	0.0040 (6)	0.0003 (6)
F3	0.0364 (6)	0.0202 (5)	0.0567 (8)	0.0023 (5)	0.0192 (6)	0.0163 (5)
C4	0.0188 (8)	0.0267 (9)	0.0236 (9)	0.0070 (7)	0.0074 (7)	0.0088 (7)
F4	0.0297 (6)	0.0196 (5)	0.0513 (7)	−0.0072 (4)	0.0120 (5)	−0.0097 (5)
C5	0.0194 (8)	0.0180 (8)	0.0415 (11)	0.0046 (7)	0.0133 (8)	0.0091 (7)
F5	0.0260 (6)	0.0290 (6)	0.0210 (5)	−0.0039 (4)	−0.0007 (4)	−0.0045 (4)
C6	0.0164 (8)	0.0182 (8)	0.0377 (10)	0.0002 (6)	0.0085 (7)	−0.0034 (7)
F6	0.0287 (6)	0.0374 (7)	0.0366 (6)	−0.0143 (5)	−0.0072 (5)	0.0131 (5)
C7	0.0161 (8)	0.0200 (8)	0.0234 (9)	0.0018 (6)	0.0033 (7)	−0.0011 (6)
F7	0.0829 (11)	0.0277 (7)	0.0563 (9)	−0.0295 (7)	−0.0355 (8)	0.0150 (6)
C8	0.0289 (9)	0.0173 (8)	0.0142 (7)	−0.0010 (7)	−0.0022 (6)	0.0019 (6)
F8	0.1303 (16)	0.0168 (6)	0.0379 (8)	0.0131 (8)	−0.0242 (9)	−0.0088 (5)
C9	0.0358 (11)	0.0243 (9)	0.0211 (9)	−0.0069 (8)	−0.0106 (8)	0.0069 (7)
F9	0.0868 (11)	0.0415 (8)	0.0255 (6)	0.0362 (8)	0.0124 (7)	−0.0008 (5)
C10	0.0623 (15)	0.0200 (9)	0.0293 (10)	−0.0127 (10)	−0.0240 (10)	0.0073 (8)
F10	0.0339 (6)	0.0272 (6)	0.0304 (6)	0.0071 (5)	0.0156 (5)	0.0044 (4)
C11	0.0855 (19)	0.0155 (9)	0.0215 (9)	0.0079 (10)	−0.0190 (11)	−0.0016 (7)
F11	0.0230 (5)	0.0196 (5)	0.0431 (7)	−0.0029 (4)	0.0059 (5)	0.0021 (4)
C12	0.0640 (15)	0.0247 (10)	0.0151 (8)	0.0176 (10)	−0.0009 (9)	−0.0013 (7)
F12	0.0208 (5)	0.0323 (6)	0.0317 (6)	0.0036 (4)	−0.0028 (4)	0.0089 (5)
C13	0.0381 (10)	0.0203 (8)	0.0148 (8)	0.0056 (8)	0.0017 (7)	0.0016 (6)
F13	0.0311 (6)	0.0432 (7)	0.0194 (5)	0.0059 (5)	0.0036 (4)	−0.0032 (5)
F14	0.0222 (5)	0.0440 (7)	0.0240 (5)	−0.0001 (5)	0.0066 (4)	−0.0015 (5)
F15	0.0223 (5)	0.0211 (5)	0.0455 (7)	−0.0043 (4)	−0.0042 (5)	0.0014 (5)
F16	0.0162 (5)	0.0265 (5)	0.0242 (5)	−0.0014 (4)	−0.0003 (4)	0.0074 (4)

Geometric parameters (Å, °)

As1—F11	1.6943 (10)	C4—C5	1.383 (3)
As1—F12	1.6992 (10)	F4—C6	1.334 (2)
As1—F13	1.7118 (11)	C5—C6	1.382 (3)

As1—F14	1.7191 (11)	F5—C7	1.332 (2)
As1—F15	1.7237 (11)	C6—C7	1.370 (2)
As1—F16	1.7853 (10)	F6—C9	1.333 (3)
C1—O1	1.274 (2)	F7—C10	1.333 (3)
C1—C2	1.443 (2)	C8—C9	1.397 (3)
C1—C8	1.455 (2)	C8—C13	1.401 (3)
F1—C3	1.332 (2)	F8—C11	1.326 (2)
O1—H1	0.90 (3)	C9—C10	1.374 (3)
C2—C3	1.406 (2)	F9—C12	1.326 (3)
C2—C7	1.403 (2)	C10—C11	1.385 (4)
F2—C4	1.331 (2)	F10—C13	1.333 (2)
C3—C4	1.376 (2)	C11—C12	1.383 (4)
F3—C5	1.322 (2)	C12—C13	1.379 (3)
F11—As1—F12	93.28 (5)	F3—C5—C4	119.70 (18)
F11—As1—F13	90.33 (6)	F3—C5—C6	119.75 (18)
F11—As1—F14	90.79 (6)	C6—C5—C4	120.54 (16)
F11—As1—F15	175.30 (5)	F4—C6—C5	120.19 (17)
F11—As1—F16	88.39 (5)	F4—C6—C7	120.29 (18)
F12—As1—F13	92.35 (6)	C7—C6—C5	119.52 (17)
F12—As1—F14	91.45 (6)	F5—C7—C2	119.96 (15)
F12—As1—F15	91.38 (5)	F5—C7—C6	118.23 (16)
F12—As1—F16	178.18 (5)	C6—C7—C2	121.73 (17)
F13—As1—F14	175.97 (6)	C9—C8—C1	121.55 (18)
F13—As1—F15	90.14 (6)	C9—C8—C13	117.82 (17)
F13—As1—F16	88.38 (5)	C13—C8—C1	120.42 (16)
F14—As1—F15	88.43 (6)	F6—C9—C8	119.55 (18)
F14—As1—F16	87.79 (5)	F6—C9—C10	119.3 (2)
F15—As1—F16	86.95 (5)	C10—C9—C8	121.1 (2)
O1—C1—C2	115.69 (15)	F7—C10—C9	120.3 (3)
O1—C1—C8	120.91 (15)	F7—C10—C11	120.2 (2)
C2—C1—C8	123.39 (15)	C9—C10—C11	119.6 (2)
C1—O1—H1	117.0 (19)	F8—C11—C10	119.3 (2)
C3—C2—C1	121.21 (15)	F8—C11—C12	119.6 (3)
C7—C2—C1	121.16 (15)	C12—C11—C10	121.07 (19)
C7—C2—C3	117.20 (15)	F9—C12—C11	120.8 (2)
F1—C3—C2	120.48 (15)	F9—C12—C13	120.5 (2)
F1—C3—C4	118.27 (16)	C13—C12—C11	118.8 (2)
C4—C3—C2	121.12 (16)	F10—C13—C8	120.21 (16)
F2—C4—C3	120.45 (18)	F10—C13—C12	118.09 (19)
F2—C4—C5	119.84 (17)	C12—C13—C8	121.6 (2)
C3—C4—C5	119.70 (17)		
C1—C2—C3—F1	5.8 (2)	F4—C6—C7—C2	177.19 (16)
C1—C2—C3—C4	−169.91 (16)	F4—C6—C7—F5	0.3 (3)
C1—C2—C7—F5	−9.2 (2)	C5—C6—C7—C2	−3.5 (3)
C1—C2—C7—C6	173.94 (16)	C5—C6—C7—F5	179.64 (15)
C1—C8—C9—F6	−8.1 (2)	F6—C9—C10—F7	1.1 (3)

C1—C8—C9—C10	174.91 (17)	F6—C9—C10—C11	−178.91 (17)
C1—C8—C13—F10	3.7 (2)	C7—C2—C3—F1	178.40 (15)
C1—C8—C13—C12	−172.58 (16)	C7—C2—C3—C4	2.6 (2)
F1—C3—C4—F2	−1.2 (2)	F7—C10—C11—F8	1.0 (3)
F1—C3—C4—C5	179.64 (15)	F7—C10—C11—C12	−178.71 (17)
O1—C1—C2—C3	141.13 (16)	C8—C1—C2—C3	−39.8 (2)
O1—C1—C2—C7	−31.1 (2)	C8—C1—C2—C7	147.93 (17)
O1—C1—C8—C9	−41.8 (2)	C8—C9—C10—F7	178.10 (16)
O1—C1—C8—C13	132.82 (17)	C8—C9—C10—C11	−1.9 (3)
C2—C1—C8—C9	139.21 (17)	F8—C11—C12—F9	1.9 (3)
C2—C1—C8—C13	−46.2 (2)	F8—C11—C12—C13	−178.59 (17)
C2—C3—C4—F2	174.68 (15)	C9—C8—C13—F10	178.48 (15)
C2—C3—C4—C5	−4.5 (3)	C9—C8—C13—C12	2.2 (3)
F2—C4—C5—F3	2.7 (3)	C9—C10—C11—F8	−179.08 (17)
F2—C4—C5—C6	−176.82 (16)	C9—C10—C11—C12	1.3 (3)
C3—C2—C7—F5	178.22 (15)	F9—C12—C13—C8	176.69 (16)
C3—C2—C7—C6	1.4 (3)	F9—C12—C13—F10	0.4 (3)
C3—C4—C5—F3	−178.10 (16)	C10—C11—C12—F9	−178.45 (18)
C3—C4—C5—C6	2.4 (3)	C10—C11—C12—C13	1.1 (3)
F3—C5—C6—F4	1.4 (3)	C11—C12—C13—C8	−2.8 (3)
F3—C5—C6—C7	−177.95 (16)	C11—C12—C13—F10	−179.17 (17)
C4—C5—C6—F4	−179.09 (16)	C13—C8—C9—F6	177.20 (15)
C4—C5—C6—C7	1.6 (3)	C13—C8—C9—C10	0.2 (3)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
O1—H1···F16	0.90 (3)	1.63 (3)	2.5279 (16)	178 (3)

[Bis(2,3,4,5,6-pentafluorophenyl)methylidene]\ (pentafluoro- λ^6 -arsanyl)oxidanium (pfbpasf5_1_1)

Crystal data

C₁₃AsF₁₅O
M_r = 532.05
 Orthorhombic, *Pbca*
a = 12.39109 (18) Å
b = 12.04038 (17) Å
c = 20.8754 (3) Å
V = 3114.47 (8) Å³
Z = 8
F(000) = 2032

D_x = 2.269 Mg m^{−3}
 Ag *Kα* radiation, λ = 0.56087 Å
 Cell parameters from 47122 reflections
 θ = 2.0–30.5°
 μ = 1.25 mm^{−1}
T = 100 K
 Block, clear yellow
 0.58 × 0.29 × 0.22 mm

Data collection

Rigaku OD XtaLAB Synergy-S Dualflex
 diffractometer with an Eiger2 R CdTe 1M
 detector
 Radiation source: micro-focus sealed X-ray
 tube, PhotonJet (Ag) X-ray Source
 Mirror monochromator
 Detector resolution: 13.3333 pixels mm^{−1}
 ω scans

Absorption correction: gaussian
 (CrysAlis PRO; Rigaku OD, 2025)
T_{min} = 0.290, *T_{max}* = 1.000
 97292 measured reflections
 8537 independent reflections
 7132 reflections with *I* > 2 σ (*I*)
R_{int} = 0.033
 $\theta_{\max}$ = 30.9°, $\theta_{\min}$ = 2.0°

$h = -22 \rightarrow 20$
 $k = -19 \rightarrow 20$

$l = -33 \rightarrow 34$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.031$
 $wR(F^2) = 0.081$
 $S = 1.09$
 8537 reflections
 271 parameters

0 restraints
 Primary atom site location: iterative
 $w = 1/[\sigma^2(F_o^2) + (0.0274P)^2 + 2.135P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.002$
 $\Delta\rho_{\max} = 0.53 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.64 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
As1	0.50792 (2)	0.40911 (2)	0.64848 (2)	0.02257 (3)
C5	0.28261 (10)	0.19309 (10)	0.92493 (6)	0.02246 (19)
C4	0.24222 (10)	0.12768 (11)	0.87612 (6)	0.0234 (2)
C3	0.27171 (10)	0.14865 (10)	0.81359 (6)	0.02212 (19)
C2	0.34450 (9)	0.23460 (9)	0.79776 (5)	0.01867 (17)
C7	0.38522 (9)	0.29831 (9)	0.84923 (5)	0.01876 (17)
C6	0.35415 (9)	0.27853 (10)	0.91164 (5)	0.02070 (18)
C1	0.37817 (9)	0.25751 (10)	0.73232 (5)	0.02101 (18)
C8	0.32579 (9)	0.20170 (10)	0.67684 (5)	0.02081 (18)
C9	0.22534 (10)	0.23470 (12)	0.65449 (6)	0.0252 (2)
C10	0.18101 (10)	0.18654 (12)	0.60053 (6)	0.0253 (2)
C11	0.23673 (11)	0.10312 (11)	0.56902 (6)	0.0242 (2)
C12	0.33583 (12)	0.06706 (10)	0.59150 (6)	0.0256 (2)
C13	0.37967 (11)	0.11747 (10)	0.64512 (6)	0.0240 (2)
F11	0.55613 (8)	0.48758 (8)	0.58783 (4)	0.03464 (19)
F12	0.48259 (10)	0.52132 (9)	0.69524 (5)	0.0447 (3)
F13	0.63035 (8)	0.39401 (10)	0.68384 (5)	0.0445 (3)
F15	0.52715 (9)	0.28689 (8)	0.60916 (5)	0.0378 (2)
F14	0.37842 (8)	0.41244 (8)	0.62149 (5)	0.0356 (2)
F5	0.45393 (7)	0.37995 (6)	0.83950 (4)	0.02408 (14)
F4	0.39370 (7)	0.33967 (7)	0.95905 (4)	0.02815 (16)
F3	0.25376 (8)	0.17360 (7)	0.98480 (4)	0.03145 (17)
F2	0.17660 (8)	0.04381 (8)	0.89019 (4)	0.03378 (19)
F1	0.22986 (8)	0.08292 (8)	0.76879 (4)	0.03288 (19)
F6	0.17231 (7)	0.31596 (10)	0.68461 (5)	0.0414 (2)
F7	0.08585 (7)	0.22050 (10)	0.57809 (5)	0.0386 (2)
F8	0.19484 (8)	0.05827 (8)	0.51654 (4)	0.03254 (18)
F9	0.38834 (9)	−0.01392 (8)	0.56135 (5)	0.0397 (2)
F10	0.47526 (8)	0.08443 (8)	0.66693 (5)	0.0355 (2)

O1	0.45443 (8)	0.32420 (9)	0.72383 (4)	0.0294 (2)
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Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
As1	0.02273 (6)	0.02432 (6)	0.02067 (6)	−0.00182 (4)	0.00199 (4)	0.00121 (4)
C5	0.0242 (5)	0.0227 (5)	0.0205 (5)	−0.0004 (4)	0.0030 (4)	0.0015 (4)
C4	0.0226 (5)	0.0228 (5)	0.0249 (5)	−0.0053 (4)	−0.0008 (4)	0.0033 (4)
C3	0.0223 (5)	0.0223 (5)	0.0218 (5)	−0.0040 (4)	−0.0031 (4)	0.0007 (4)
C2	0.0180 (4)	0.0192 (4)	0.0188 (4)	−0.0007 (3)	−0.0008 (3)	0.0004 (3)
C7	0.0181 (4)	0.0170 (4)	0.0212 (4)	−0.0003 (3)	0.0014 (3)	−0.0007 (3)
C6	0.0218 (4)	0.0200 (4)	0.0202 (4)	−0.0008 (4)	0.0016 (3)	−0.0028 (3)
C1	0.0204 (4)	0.0225 (5)	0.0201 (4)	0.0000 (4)	−0.0017 (3)	0.0011 (3)
C8	0.0209 (4)	0.0228 (5)	0.0187 (4)	−0.0005 (4)	−0.0020 (3)	−0.0003 (3)
C9	0.0192 (4)	0.0353 (6)	0.0211 (5)	0.0026 (4)	−0.0004 (3)	−0.0052 (4)
C10	0.0195 (4)	0.0353 (6)	0.0211 (5)	−0.0010 (4)	−0.0022 (4)	−0.0014 (4)
C11	0.0284 (5)	0.0254 (5)	0.0188 (4)	−0.0050 (4)	−0.0026 (4)	−0.0006 (4)
C12	0.0323 (6)	0.0195 (5)	0.0251 (5)	0.0020 (4)	−0.0029 (4)	−0.0020 (4)
C13	0.0261 (5)	0.0194 (4)	0.0265 (5)	0.0029 (4)	−0.0054 (4)	0.0005 (4)
F11	0.0407 (5)	0.0354 (4)	0.0278 (4)	−0.0089 (4)	0.0053 (3)	0.0073 (3)
F12	0.0583 (7)	0.0336 (5)	0.0421 (5)	−0.0139 (5)	0.0196 (5)	−0.0138 (4)
F13	0.0248 (4)	0.0637 (7)	0.0450 (5)	−0.0123 (4)	−0.0074 (4)	0.0217 (5)
F15	0.0465 (5)	0.0276 (4)	0.0393 (5)	0.0008 (4)	0.0153 (4)	−0.0043 (4)
F14	0.0271 (4)	0.0348 (4)	0.0450 (5)	−0.0006 (3)	−0.0076 (4)	0.0128 (4)
F5	0.0261 (3)	0.0209 (3)	0.0252 (3)	−0.0068 (3)	0.0045 (3)	−0.0034 (3)
F4	0.0343 (4)	0.0287 (4)	0.0215 (3)	−0.0061 (3)	0.0031 (3)	−0.0079 (3)
F3	0.0401 (5)	0.0327 (4)	0.0215 (3)	−0.0072 (3)	0.0075 (3)	0.0021 (3)
F2	0.0369 (4)	0.0331 (4)	0.0313 (4)	−0.0178 (4)	−0.0015 (3)	0.0063 (3)
F1	0.0398 (5)	0.0345 (4)	0.0243 (4)	−0.0176 (4)	−0.0072 (3)	−0.0001 (3)
F6	0.0254 (4)	0.0632 (7)	0.0356 (5)	0.0168 (4)	−0.0046 (3)	−0.0227 (4)
F7	0.0220 (4)	0.0611 (6)	0.0327 (4)	0.0062 (4)	−0.0084 (3)	−0.0100 (4)
F8	0.0385 (5)	0.0358 (4)	0.0234 (4)	−0.0070 (4)	−0.0066 (3)	−0.0059 (3)
F9	0.0515 (6)	0.0266 (4)	0.0410 (5)	0.0127 (4)	−0.0099 (4)	−0.0134 (4)
F10	0.0359 (4)	0.0278 (4)	0.0429 (5)	0.0139 (3)	−0.0153 (4)	−0.0052 (3)
O1	0.0285 (4)	0.0392 (5)	0.0205 (4)	−0.0126 (4)	−0.0014 (3)	0.0035 (3)

Geometric parameters ($\text{\AA}$, $^\circ$)

As1—F11	1.6890 (8)	C7—F5	1.3162 (13)
As1—F12	1.6960 (10)	C6—F4	1.3271 (14)
As1—F13	1.6967 (10)	C1—C8	1.4879 (16)
As1—F15	1.7018 (9)	C1—O1	1.2526 (15)
As1—F14	1.7012 (9)	C8—C9	1.3874 (17)
As1—O1	1.9897 (10)	C8—C13	1.3830 (17)
C5—C4	1.3817 (18)	C9—C10	1.3808 (17)
C5—C6	1.3861 (17)	C9—F6	1.3359 (15)
C5—F3	1.3209 (14)	C10—C11	1.3850 (19)
C4—C3	1.3788 (17)	C10—F7	1.3331 (15)

C4—F2	1.3293 (14)	C11—C12	1.3844 (19)
C3—C2	1.4120 (16)	C11—F8	1.3270 (14)
C3—F1	1.3303 (14)	C12—C13	1.3844 (18)
C2—C7	1.4133 (15)	C12—F9	1.3304 (15)
C2—C1	1.4549 (16)	C13—F10	1.3300 (15)
C7—C6	1.3792 (16)		
F11—As1—F12	92.94 (5)	F5—C7—C2	121.25 (10)
F11—As1—F13	94.01 (5)	F5—C7—C6	117.09 (10)
F11—As1—F15	94.16 (5)	C7—C6—C5	119.72 (11)
F11—As1—F14	94.14 (5)	F4—C6—C5	119.91 (10)
F11—As1—O1	176.30 (5)	F4—C6—C7	120.37 (10)
F12—As1—F13	90.03 (6)	C2—C1—C8	121.34 (10)
F12—As1—F15	172.89 (5)	O1—C1—C2	118.07 (10)
F12—As1—F14	89.84 (6)	O1—C1—C8	120.57 (11)
F12—As1—O1	83.84 (5)	C9—C8—C1	121.59 (11)
F13—As1—F15	89.54 (6)	C13—C8—C1	119.55 (11)
F13—As1—F14	171.85 (5)	C13—C8—C9	118.82 (11)
F13—As1—O1	84.20 (5)	C10—C9—C8	120.73 (12)
F15—As1—O1	89.06 (5)	F6—C9—C8	119.52 (11)
F14—As1—F15	89.58 (5)	F6—C9—C10	119.73 (11)
F14—As1—O1	87.69 (4)	C9—C10—C11	119.59 (11)
C4—C5—C6	120.47 (11)	F7—C10—C9	120.65 (12)
F3—C5—C4	119.90 (11)	F7—C10—C11	119.76 (11)
F3—C5—C6	119.62 (11)	C12—C11—C10	120.57 (11)
C3—C4—C5	119.86 (11)	F8—C11—C10	119.49 (12)
F2—C4—C5	119.44 (11)	F8—C11—C12	119.94 (12)
F2—C4—C3	120.69 (11)	C13—C12—C11	118.99 (12)
C4—C3—C2	121.67 (11)	F9—C12—C11	120.22 (12)
F1—C3—C4	116.95 (11)	F9—C12—C13	120.79 (12)
F1—C3—C2	121.38 (11)	C8—C13—C12	121.28 (12)
C3—C2—C7	116.61 (10)	F10—C13—C8	119.04 (11)
C3—C2—C1	122.81 (10)	F10—C13—C12	119.68 (12)
C7—C2—C1	120.58 (10)	C1—O1—As1	133.83 (8)
C6—C7—C2	121.66 (10)		
C5—C4—C3—C2	1.28 (19)	C9—C8—C13—F10	−179.02 (12)
C5—C4—C3—F1	−179.82 (12)	C9—C10—C11—C12	0.6 (2)
C4—C5—C6—C7	−0.01 (18)	C9—C10—C11—F8	−178.84 (12)
C4—C5—C6—F4	−178.94 (11)	C10—C11—C12—C13	−1.5 (2)
C4—C3—C2—C7	−0.25 (17)	C10—C11—C12—F9	179.28 (13)
C4—C3—C2—C1	179.10 (12)	C11—C12—C13—C8	0.8 (2)
C3—C2—C7—C6	−0.93 (16)	C11—C12—C13—F10	−179.39 (12)
C3—C2—C7—F5	179.67 (10)	C13—C8—C9—C10	−1.7 (2)
C3—C2—C1—C8	8.79 (17)	C13—C8—C9—F6	−179.98 (13)
C3—C2—C1—O1	−169.78 (12)	F5—C7—C6—C5	−179.50 (11)
C2—C7—C6—C5	1.07 (18)	F5—C7—C6—F4	−0.58 (17)
C2—C7—C6—F4	180.00 (11)	F3—C5—C4—C3	179.49 (12)

C2—C1—C8—C9	77.33 (16)	F3—C5—C4—F2	−1.65 (19)
C2—C1—C8—C13	−105.02 (14)	F3—C5—C6—C7	179.35 (11)
C2—C1—O1—As1	−163.21 (9)	F3—C5—C6—F4	0.42 (18)
C7—C2—C1—C8	−171.88 (11)	F2—C4—C3—C2	−177.56 (12)
C7—C2—C1—O1	9.55 (17)	F2—C4—C3—F1	1.33 (19)
C6—C5—C4—C3	−1.15 (19)	F1—C3—C2—C7	−179.10 (11)
C6—C5—C4—F2	177.71 (12)	F1—C3—C2—C1	0.26 (18)
C1—C2—C7—C6	179.70 (11)	F6—C9—C10—C11	179.32 (13)
C1—C2—C7—F5	0.30 (17)	F6—C9—C10—F7	0.2 (2)
C1—C8—C9—C10	175.95 (12)	F7—C10—C11—C12	179.77 (12)
C1—C8—C9—F6	−2.32 (19)	F7—C10—C11—F8	0.33 (19)
C1—C8—C13—C12	−176.95 (12)	F8—C11—C12—C13	177.92 (12)
C1—C8—C13—F10	3.27 (18)	F8—C11—C12—F9	−1.3 (2)
C8—C1—O1—As1	18.2 (2)	F9—C12—C13—C8	−179.97 (12)
C8—C9—C10—C11	1.0 (2)	F9—C12—C13—F10	−0.2 (2)
C8—C9—C10—F7	−178.12 (12)	O1—C1—C8—C9	−104.14 (15)
C9—C8—C13—C12	0.76 (19)	O1—C1—C8—C13	73.51 (16)

[Bis(2,3,4,5,6-pentafluorophenyl)methylidene]oxidanium hexafluoroarsenate (pfpah_asf6_3_1)

Crystal data

$\text{C}_{13}\text{HF}_{10}\text{O}^+\text{AsF}_6^-$

$M_r = 552.06$

Monoclinic, $P2_1/n$

$a = 8.18723$ (9) Å

$b = 21.1810$ (3) Å

$c = 9.28084$ (11) Å

$\beta = 98.1450$ (11)°

$V = 1593.19$ (3) Å³

$Z = 4$

$F(000) = 1056$

$D_x = 2.302$ Mg m^{−3}

Ag $K\alpha$ radiation, $\lambda = 0.56087$ Å

Cell parameters from 57924 reflections

$\theta = 1.9\text{--}30.9^\circ$

$\mu = 1.23$ mm^{−1}

$T = 100$ K

Plank, clear yellow

$0.79 \times 0.3 \times 0.24$ mm

Data collection

Rigaku OD XtaLAB Synergy-S Dualflex
diffractometer with an Eiger2 R CdTe 1M
detector

Radiation source: micro-focus sealed X-ray
tube, PhotonJet (Ag) X-ray Source

Mirror monochromator

Detector resolution: 13.3333 pixels mm^{−1}

ω scans

Absorption correction: gaussian
(CrysAlis PRO; Rigaku OD, 2025)

$T_{\min} = 0.184$, $T_{\max} = 1.000$

111309 measured reflections

7721 independent reflections

6714 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.061$

$\theta_{\max} = 27.9^\circ$, $\theta_{\min} = 2.3^\circ$

$h = -12 \rightarrow 13$

$k = -35 \rightarrow 35$

$l = -15 \rightarrow 15$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.029$

$wR(F^2) = 0.081$

$S = 1.07$

7721 reflections

284 parameters

0 restraints

Primary atom site location: iterative

Hydrogen site location: difference Fourier map

All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0409P)^2 + 0.4919P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.66$ e Å^{−3}

$\Delta\rho_{\min} = -0.38$ e Å^{−3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
As1	0.54834 (2)	0.13336 (2)	0.41865 (2)	0.01973 (4)
C1	0.46962 (13)	0.25916 (5)	0.04191 (11)	0.02022 (16)
F1	0.41347 (10)	0.27895 (4)	−0.26302 (8)	0.02849 (14)
O1	0.41878 (11)	0.26616 (4)	0.16450 (9)	0.02390 (15)
H1	0.406 (3)	0.2335 (10)	0.208 (2)	0.037 (5)*
C2	0.51636 (13)	0.31646 (5)	−0.02621 (11)	0.02003 (16)
F2	0.45354 (11)	0.39248 (5)	−0.38122 (10)	0.03437 (18)
C3	0.47961 (13)	0.32522 (5)	−0.17732 (12)	0.02224 (18)
F3	0.59551 (12)	0.48756 (4)	−0.21390 (12)	0.0392 (2)
C4	0.50127 (14)	0.38327 (6)	−0.23956 (14)	0.0258 (2)
F4	0.68203 (11)	0.47191 (4)	0.07670 (11)	0.03656 (19)
C5	0.57042 (15)	0.43260 (6)	−0.15354 (16)	0.0283 (2)
F5	0.62363 (11)	0.36183 (4)	0.20083 (9)	0.02891 (15)
C6	0.61357 (14)	0.42482 (5)	−0.00478 (15)	0.0263 (2)
F6	0.21692 (11)	0.16787 (5)	0.03032 (10)	0.0380 (2)
C7	0.58212 (14)	0.36794 (5)	0.05826 (13)	0.02212 (18)
F7	0.25325 (18)	0.04921 (5)	−0.06609 (14)	0.0610 (4)
C8	0.48102 (15)	0.19681 (5)	−0.02156 (12)	0.02330 (18)
F8	0.5357 (2)	0.01558 (5)	−0.16518 (13)	0.0678 (4)
C9	0.35678 (18)	0.15161 (6)	−0.01683 (14)	0.0312 (2)
F9	0.78382 (17)	0.10049 (5)	−0.17057 (10)	0.0528 (3)
C10	0.3746 (2)	0.09099 (7)	−0.06737 (17)	0.0422 (4)
F10	0.74618 (11)	0.21943 (4)	−0.08188 (10)	0.03250 (16)
C11	0.5179 (3)	0.07409 (6)	−0.11909 (16)	0.0460 (4)
F11	0.44533 (10)	0.06363 (4)	0.40625 (10)	0.03148 (16)
C12	0.6446 (2)	0.11726 (7)	−0.12362 (14)	0.0380 (3)
F12	0.71773 (10)	0.10213 (4)	0.52117 (9)	0.03215 (16)
C13	0.62350 (18)	0.17847 (6)	−0.07816 (13)	0.0275 (2)
F13	0.46089 (11)	0.15294 (5)	0.56951 (9)	0.03438 (18)
F14	0.62696 (10)	0.11747 (5)	0.26024 (9)	0.03248 (16)
F15	0.64003 (10)	0.20678 (4)	0.42139 (11)	0.03370 (17)
F16	0.37452 (9)	0.16812 (4)	0.30944 (8)	0.02551 (13)

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
As1	0.01778 (5)	0.02108 (6)	0.02005 (5)	−0.00054 (3)	0.00171 (4)	0.00169 (3)
C1	0.0193 (4)	0.0212 (4)	0.0197 (4)	0.0002 (3)	0.0012 (3)	0.0017 (3)
F1	0.0355 (4)	0.0284 (3)	0.0207 (3)	0.0004 (3)	0.0012 (3)	−0.0009 (3)

O1	0.0261 (4)	0.0244 (4)	0.0222 (3)	0.0013 (3)	0.0065 (3)	0.0030 (3)
C2	0.0192 (4)	0.0197 (4)	0.0212 (4)	0.0004 (3)	0.0031 (3)	0.0012 (3)
F2	0.0351 (4)	0.0400 (5)	0.0293 (4)	0.0094 (3)	0.0090 (3)	0.0141 (3)
C3	0.0215 (4)	0.0233 (4)	0.0223 (4)	0.0022 (3)	0.0046 (3)	0.0023 (3)
F3	0.0389 (4)	0.0247 (4)	0.0576 (6)	0.0025 (3)	0.0198 (4)	0.0162 (4)
C4	0.0233 (4)	0.0280 (5)	0.0272 (5)	0.0053 (4)	0.0078 (4)	0.0085 (4)
F4	0.0334 (4)	0.0239 (3)	0.0547 (5)	−0.0075 (3)	0.0141 (4)	−0.0096 (3)
C5	0.0239 (5)	0.0220 (5)	0.0413 (6)	0.0036 (4)	0.0130 (4)	0.0090 (4)
F5	0.0292 (4)	0.0321 (4)	0.0245 (3)	−0.0040 (3)	0.0004 (3)	−0.0045 (3)
C6	0.0219 (4)	0.0201 (4)	0.0384 (6)	−0.0008 (3)	0.0093 (4)	−0.0016 (4)
F6	0.0305 (4)	0.0405 (5)	0.0400 (4)	−0.0137 (3)	−0.0056 (3)	0.0129 (4)
C7	0.0198 (4)	0.0209 (4)	0.0259 (5)	−0.0001 (3)	0.0039 (3)	−0.0012 (3)
F7	0.0822 (8)	0.0301 (5)	0.0585 (7)	−0.0272 (5)	−0.0321 (6)	0.0133 (4)
C8	0.0301 (5)	0.0192 (4)	0.0194 (4)	−0.0013 (4)	−0.0003 (4)	0.0013 (3)
F8	0.1302 (13)	0.0209 (4)	0.0418 (5)	0.0122 (6)	−0.0241 (7)	−0.0088 (4)
C9	0.0378 (6)	0.0255 (5)	0.0264 (5)	−0.0085 (5)	−0.0084 (4)	0.0061 (4)
F9	0.0854 (8)	0.0455 (6)	0.0290 (4)	0.0349 (6)	0.0136 (5)	−0.0016 (4)
C10	0.0640 (10)	0.0219 (5)	0.0328 (6)	−0.0111 (6)	−0.0211 (6)	0.0056 (5)
F10	0.0361 (4)	0.0304 (4)	0.0343 (4)	0.0063 (3)	0.0160 (3)	0.0040 (3)
C11	0.0862 (13)	0.0192 (5)	0.0253 (5)	0.0066 (6)	−0.0176 (7)	−0.0022 (4)
F11	0.0264 (3)	0.0225 (3)	0.0460 (5)	−0.0034 (3)	0.0066 (3)	0.0022 (3)
C12	0.0659 (10)	0.0265 (5)	0.0200 (5)	0.0165 (6)	0.0002 (5)	−0.0016 (4)
F12	0.0243 (3)	0.0358 (4)	0.0345 (4)	0.0039 (3)	−0.0023 (3)	0.0088 (3)
C13	0.0405 (6)	0.0232 (5)	0.0189 (4)	0.0057 (4)	0.0038 (4)	0.0012 (4)
F13	0.0339 (4)	0.0464 (5)	0.0233 (3)	0.0060 (3)	0.0056 (3)	−0.0037 (3)
F14	0.0249 (3)	0.0477 (5)	0.0261 (3)	0.0003 (3)	0.0082 (3)	−0.0018 (3)
F15	0.0251 (3)	0.0240 (3)	0.0497 (5)	−0.0052 (3)	−0.0026 (3)	0.0015 (3)
F16	0.0195 (3)	0.0287 (3)	0.0275 (3)	−0.0008 (2)	0.0008 (2)	0.0076 (3)

Geometric parameters (Å, °)

As1—F11	1.6965 (8)	C4—C5	1.386 (2)
As1—F12	1.7006 (8)	F4—C6	1.3270 (15)
As1—F13	1.7115 (8)	C5—C6	1.386 (2)
As1—F14	1.7196 (8)	F5—C7	1.3250 (14)
As1—F15	1.7254 (8)	C6—C7	1.3793 (16)
As1—F16	1.7849 (7)	F6—C9	1.3279 (19)
C1—O1	1.2743 (13)	F7—C10	1.3316 (19)
C1—C2	1.4448 (15)	C8—C9	1.4021 (17)
C1—C8	1.4545 (16)	C8—C13	1.4004 (18)
F1—C3	1.3282 (14)	F8—C11	1.3258 (17)
O1—H1	0.82 (2)	C9—C10	1.382 (2)
C2—C3	1.4044 (15)	F9—C12	1.325 (2)
C2—C7	1.4049 (15)	C10—C11	1.376 (3)
F2—C4	1.3317 (15)	F10—C13	1.3313 (17)
C3—C4	1.3806 (16)	C11—C12	1.388 (3)
F3—C5	1.3206 (14)	C12—C13	1.3820 (18)

F11—As1—F12	93.29 (4)	F3—C5—C4	119.71 (13)
F11—As1—F13	90.28 (5)	F3—C5—C6	119.64 (13)
F11—As1—F14	90.82 (5)	C6—C5—C4	120.66 (11)
F11—As1—F15	175.32 (4)	F4—C6—C5	120.39 (11)
F11—As1—F16	88.39 (4)	F4—C6—C7	120.26 (12)
F12—As1—F13	92.24 (4)	C7—C6—C5	119.34 (11)
F12—As1—F14	91.60 (4)	F5—C7—C2	120.34 (10)
F12—As1—F15	91.36 (4)	F5—C7—C6	118.16 (10)
F12—As1—F16	178.19 (4)	C6—C7—C2	121.40 (11)
F13—As1—F14	175.95 (4)	C9—C8—C1	121.26 (12)
F13—As1—F15	90.06 (5)	C13—C8—C1	120.55 (11)
F13—As1—F16	88.41 (4)	C13—C8—C9	117.97 (12)
F14—As1—F15	88.52 (5)	F6—C9—C8	119.77 (12)
F14—As1—F16	87.72 (4)	F6—C9—C10	119.36 (14)
F15—As1—F16	86.95 (4)	C10—C9—C8	120.80 (15)
O1—C1—C2	115.67 (10)	F7—C10—C9	119.99 (19)
O1—C1—C8	121.00 (10)	F7—C10—C11	120.26 (15)
C2—C1—C8	123.32 (10)	C11—C10—C9	119.75 (15)
C1—O1—H1	115.1 (15)	F8—C11—C10	119.60 (18)
C3—C2—C1	121.02 (10)	F8—C11—C12	119.3 (2)
C3—C2—C7	117.75 (10)	C10—C11—C12	121.13 (13)
C7—C2—C1	120.81 (10)	F9—C12—C11	120.99 (14)
F1—C3—C2	120.80 (10)	F9—C12—C13	120.17 (17)
F1—C3—C4	118.18 (10)	C13—C12—C11	118.84 (16)
C4—C3—C2	120.89 (11)	F10—C13—C8	120.05 (10)
F2—C4—C3	120.42 (12)	F10—C13—C12	118.42 (13)
F2—C4—C5	119.80 (11)	C12—C13—C8	121.44 (14)
C3—C4—C5	119.77 (11)		
C1—C2—C3—F1	−5.76 (16)	F4—C6—C7—C2	−177.21 (10)
C1—C2—C3—C4	170.02 (10)	F4—C6—C7—F5	−0.68 (17)
C1—C2—C7—F5	9.38 (16)	C5—C6—C7—C2	3.87 (17)
C1—C2—C7—C6	−174.16 (10)	C5—C6—C7—F5	−179.59 (10)
C1—C8—C9—F6	8.22 (17)	F6—C9—C10—F7	−1.18 (19)
C1—C8—C9—C10	−174.99 (11)	F6—C9—C10—C11	178.73 (12)
C1—C8—C13—F10	−3.88 (16)	C7—C2—C3—F1	−178.36 (10)
C1—C8—C13—C12	172.49 (11)	C7—C2—C3—C4	−2.58 (16)
F1—C3—C4—F2	1.38 (16)	F7—C10—C11—F8	−1.2 (2)
F1—C3—C4—C5	−179.79 (10)	F7—C10—C11—C12	178.90 (12)
O1—C1—C2—C3	−141.22 (11)	C8—C1—C2—C3	39.75 (15)
O1—C1—C2—C7	31.15 (15)	C8—C1—C2—C7	−147.89 (11)
O1—C1—C8—C9	41.84 (16)	C8—C9—C10—F7	−177.98 (11)
O1—C1—C8—C13	−132.65 (12)	C8—C9—C10—C11	1.93 (19)
C2—C1—C8—C9	−139.18 (11)	F8—C11—C12—F9	−1.3 (2)
C2—C1—C8—C13	46.33 (15)	F8—C11—C12—C13	178.68 (12)
C2—C3—C4—F2	−174.51 (10)	C9—C8—C13—F10	−178.55 (11)
C2—C3—C4—C5	4.32 (17)	C9—C8—C13—C12	−2.18 (17)
F2—C4—C5—F3	−3.13 (17)	C9—C10—C11—F8	178.84 (12)

F2—C4—C5—C6	176.89 (10)	C9—C10—C11—C12	−1.0 (2)
C3—C2—C7—F5	−178.01 (10)	F9—C12—C13—C8	−176.93 (11)
C3—C2—C7—C6	−1.55 (16)	F9—C12—C13—F10	−0.50 (18)
C3—C4—C5—F3	178.03 (10)	C10—C11—C12—F9	178.55 (13)
C3—C4—C5—C6	−1.95 (17)	C10—C11—C12—C13	−1.5 (2)
F3—C5—C6—F4	−1.01 (17)	C11—C12—C13—C8	3.08 (18)
F3—C5—C6—C7	177.91 (11)	C11—C12—C13—F10	179.51 (12)
C4—C5—C6—F4	178.98 (11)	C13—C8—C9—F6	−177.15 (11)
C4—C5—C6—C7	−2.11 (17)	C13—C8—C9—C10	−0.36 (17)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
O1—H1 $\cdots$ F16	0.82 (2)	1.71 (2)	2.5280 (11)	176 (2)