Angewandte Chemie
Eine Zeitschrift der Gesellschaft Deutscher Chemiker

Supporting Information

Stable Salts of Heteroleptic Iron Carbonyl/Nitrosyl Cations

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1. Supplementary Methods

General Conditions. All manipulations on substrates and products were undertaken in a MBraun glovebox filled with Ar or N_2 (O_2, H_2O < 1 ppm). All experiments were carried out in special double-Schlenk tubes[1] (Supplementary Figure 19) separated by a G3 or G4 frit with grease-free PTFE or glass valves in an inert atmosphere using vacuum and standard Schlenk techniques. Solvents were dried by standard methods using CaH_2 or P_4O_{10}, distilled prior to use and stored over activated molecular sieves. 1,2,3,4-tetrafluorobenzene (TFB) was additionally stirred over Ag[Al(OR^F)$_4$] to remove less fluorinated arene-impurities. NO[F-{Al(OR^F)$_3$}$_2$] {R^F = C(CF$_3$)$_3$} was prepared from NO[PF$_6$] (Acros) and Me$_3$Si-F-Al(OR^F)$_3$[2] according to literature.[3]

NMR Spectroscopy. NMR samples were prepared in 5 mm thick walled NMR tubes with J. Young valves. The ^{1}H, ^{13}C{^{1}H}, ^{19}F and ^{27}Al spectra were recorded either on a Bruker Avance II+ 400 MHz, on a Bruker Avance III HD 300 MHz or on a Bruker Avance 200 MHz spectrometer either in 1,2-$F_2C_6H_4$ (*ortho*-difluorobenzene, *o*DFB) at r.t. Measurements conducted in 1,2-$F_2C_6H_4$ were calibrated by using the ^{19}F signal of the solvent 1,2-$F_2C_6H_4$ (δ = –139.0 ppm[4], rel. to CCl_3F). The field corrections of other nuclei were adjusted accordingly.

The Bruker Topspin software package (version 3.2) was used for measuring and processing of the spectra. Typically, very tiny impurities were detected in the ^{19}F NMR at –74.8 ($HOC(CF_3)_3$) and –75.5 ppm. All graphical representations were done with Topspin (version 4.0.6).

Vibrational Spectroscopy. FTIR measurements were performed on a FTIR Bruker ALPHA with a QuickSnap Platinum ATR sampling module inside the glovebox. The data were processed with the Bruker OPUS 7.5 software package. Unless otherwise stated, the spectra were recorded in the range of 4000-550 cm^{-1} with a resolution of 2 cm^{-1} at r.t. and a base line correction with 3 iterations was applied. FT Raman spectra were recorded on a Bruker VERTEX 70 spectrometer equipped with a RAM II module (1064 nm exciting line of a NdYAG laser) by using a highly sensitive liquid N_2 cooled Ge detector. The samples were measured in flame sealed soda-lime glass Pasteur pipettes in the range of 4000-50 cm^{-1} with a resolution of 4 cm^{-1} at r.t. The data were processed with the Bruker OPUS 7.5 software package. Unless otherwise noted, the Raman spectra were cut off below 75 cm^{-1} and a baseline correction with 5 iterations was applied. All IR and Raman spectra were normalized to 1 and intensities are given as follows: vvw = very very weak (< 0.1), vw = very weak (< 0.2), w = weak (< 0.3), mw = medium weak (< 0.4), m = medium (< 0.5), ms = medium strong (< 0.6), s = strong (< 0.7), vs = very strong (< 0.8), vvs = very very strong (≥ 0.9). Extremely weak bands (< 0.025) are not reported. Typical artefacts in the Raman spectra appear at about 2939 and 2757 cm^{-1}, especially for weakly scattering samples. Graphical representations were done with OPUS 7.5 or with OriginPro (version 9.2).

UV/Vis spectroscopy. Solution UV/VIS spectra were recorded on a Varian Cary® 50 UV-Vis spectrophotometer in quartz cuvettes (thickness 1 mm) in *o*DFB solution and a concentration of about 1 mM.

Single-Crystal X-ray Diffraction. Single crystals were selected at r.t. under perfluoropolyalkylether oil (AB128330, ABCR GmbH & Co. KG) on 0.1, 0.2 or 0.3 mm micromounts (M1-L19-100/200/300). Structural data were collected from shock-cooled crystals on a Bruker SMART APEX II Quazar CCD area detector diffractometer using a D8 goniometer with an Incoatec Mo-Microfocus Source IμS with mirror-monochromated Mo-K_α radiation (λ = 0.71073 Å) at 100(2) K. The diffractometer was equipped with an Oxford Cryosystem 800 low temperature device. The data were processed with APEX v2013.6-2, integrated with SAINT[5] (V8.37A) and an empirical absorption correction using SADABS 2014/5[6] or SADABS 2016/2[6] was applied. The structures were solved by direct methods using SHELXT[7,8]. Unless otherwise stated, all non-hydrogen atoms were refined anisotropically by full matrix least squares methods against weighted F^2 values based on all independent reflections by using SHELXL-2014/7[8,9] with ShelXle as GUI software[10]. Disordered fragments were modelled with the help of the DSR software[11]. The graphical presentation of crystal structures was prepared either with Mercury (version 3.9)[12] or with OLEX2 (version 1.2)[13]. CCDC codes 1962273, 1962274 and 1967545 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via: https://summary.ccdc.cam.ac.uk /structure-summary-form. Note that the nitrogen atom(s) is crystallographically indistinguishable from the carbon atom(s) and was/were only refined for visual clarity.

Powder Diffraction. The powder diffractograms were recorded with the sample in a 0.5 mm thick capillary (Hilgenberg GmbH, wall thickness 0.01 mm) sealed with perfluoropolyalkylether oil (AB128330, ABCR GmbH & Co. KG), at RT and about 100(10) K in the 2-Θ range 2–44° with a STOE STADI P powder diffractometer with Mo-$K_{\alpha 1}$ radiation (λ = 0.709300 Å) equipped with a Ge-(111) monochromator and a silicon microstripe detector (Mythen 1K). Data acquiring, processing and the calculation of powder diffractograms from single-crystal data were performed using STOE WinXPOW® package. Graphical representations were done with OriginPro (version 9.2).

Computational Details. Quantum chemical calculations were performed with the TURBOMOLE[14] program package (version 7.0). All investigated molecular structures were optimized at the density functional theory (DFT) and were run in redundant internal coordinates using the BP86[15] or B3LYP[16] functional with the resolution-of-identity (RI) approximation[17] together with the basis set def2-TZVPP[18] and with dispersion correction (DFT-D3BJ)[19]. A fine integration grid (m4; 5 for NMR calculations) and the default SCF convergence criteria (10^{-6} a.u.) were used. All optimized structures were checked for minima (no imaginary frequencies) with the implemented module AOFORCE[20] and for proper spin occupancies using the implemented module EIGER. Entropic contributions to enthalpy and Gibbs free energy with inclusion of zero point energies (ZPE) were calculated at the BP86-D3BJ/def2-TZVPP level for standard conditions with the FREEH module. For the calculation of the reaction energies in solution, FREEH enthalpy/entropy of the gas phase calculation were used for the COSMO calculations. UV/VIS spectra were calculated based on 50 excited states per orbital symmetry.

2. Detailed Synthesis, Characterization and Spectra of Compounds 1 and 2

Synthesis of $[Fe(CO)_4(NO)][F\text{-}\{Al(OR^F)_3\}_2]$ (1)

To a double-Schlenk tube equipped with about 1200 mg of impure $NO[F\text{-}\{Al(OR^F)_3\}_2]$, first CH_2Cl_2 (4 mL) then $Fe(CO)_5$ (0.35 mL) were added at 0 °C. A beige-grey suspension was formed and gas evolution was visible. After thawing to room temperature (r.t.) and stirring for two hours, some *o*DFB (about 3 mL) was added to dissolve the forming precipitate and accelerate the reaction. Then, the reaction was stirred at RT for another hour and *n*-pentane was added to the brown solution to precipitate the crude product. After subsequent washings, a beige-brown solid was obtained, which was dissolved in *o*DFB (resulting in a brown solution) and crystallized at r.t. by slow vapour diffusion of *n*-pentane, yielding brown crystals of pure **1** (see Supplementary Figure 20). Yield: 650 mg, 49% (referenced to the impure NO^+-salt).

Note: This route displays the robustness of the synthesis against impurities of the starting materials, their stoichiometry and the solvent. The reaction also works similarly without the excess of $Fe(CO)_5$, the homologues $Fe_2(CO)_9$ and $Fe_3(CO)_{12}$ can also be used.

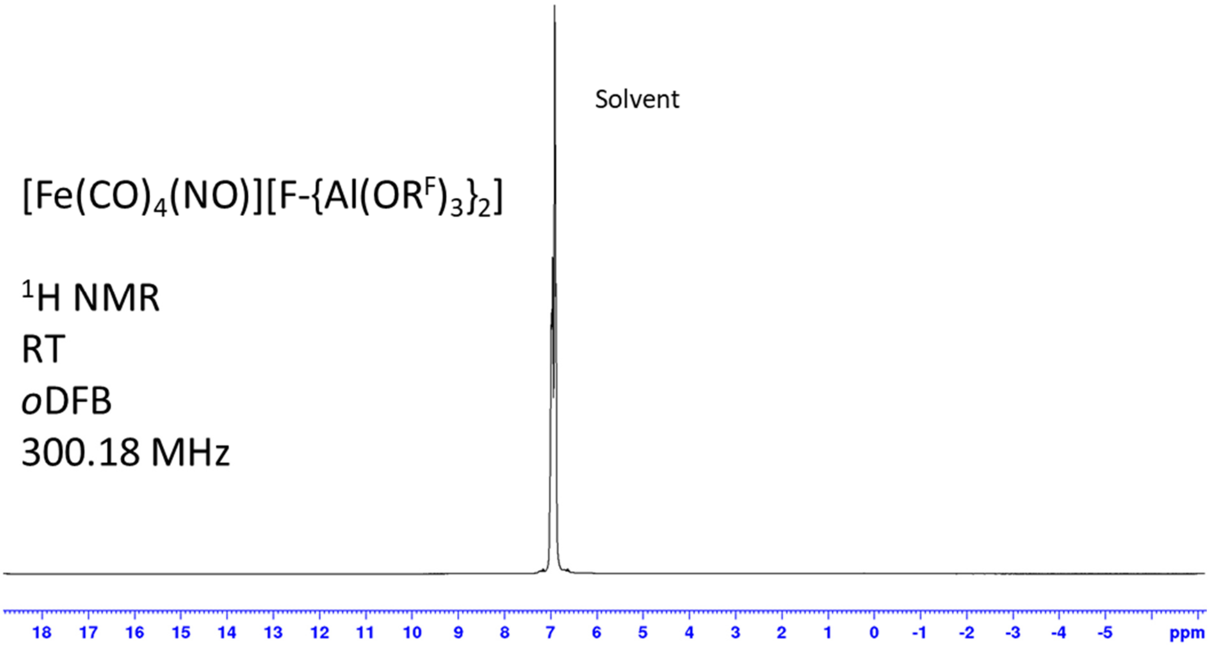
Note: **1** crystallizes in $P2_1/c$ from CH_2Cl_2 and in P–1 from *o*DFB (see "Single-Crystal XRD Data of Compounds **1** and **2**").

Simple mixing of the two starting materials, adding a solvent of choice (bearing in mind that NO[WCA] salts are incompatible with *n*-pentane), stirring overnight to ensure a complete transformation, washing of the crude product with CH_2Cl_2 or *n*-pentane (to remove possible neutral iron carbonyl impurities) and subsequent crystallization by slow vapour diffusion of *n*-pentane into an *o*DFB or TFB solution led to crystalline **1** in yields around 80%.

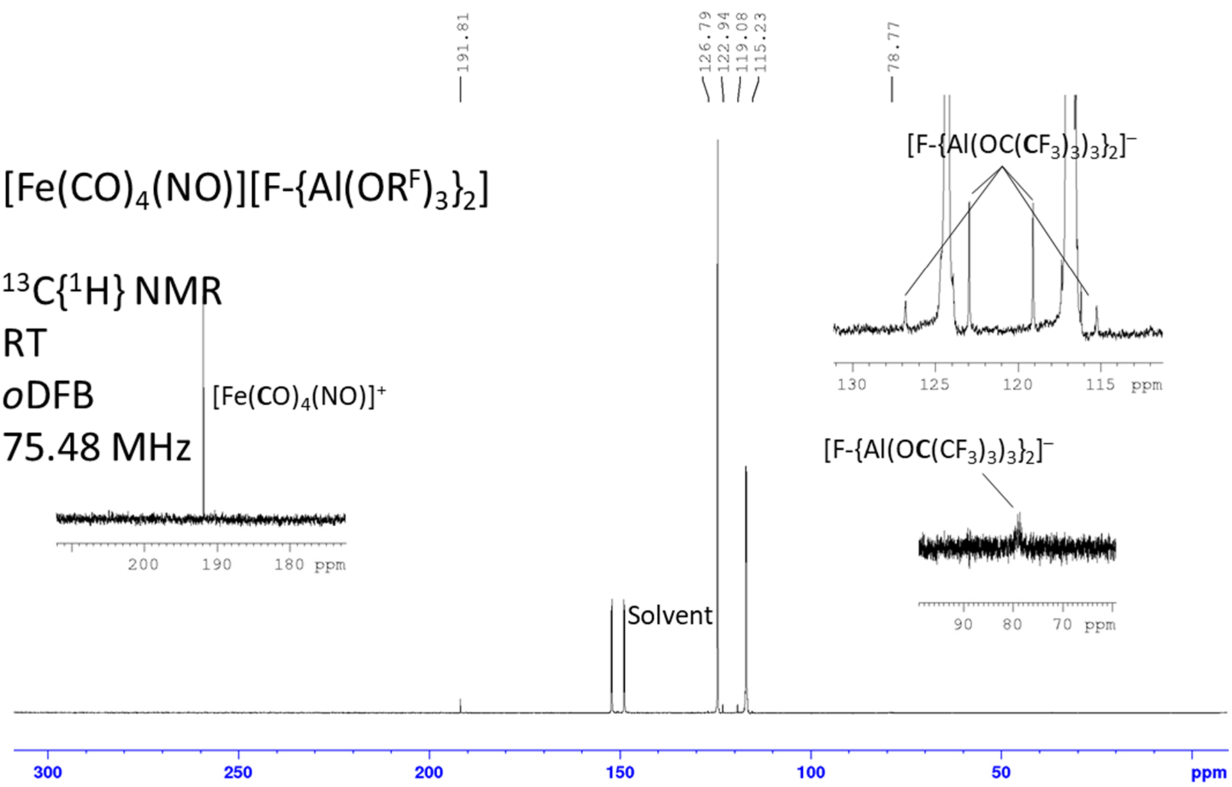
FTIR (ZnSe, ATR): $\tilde{\nu}/cm^{-1}$ (intensity) = 2183 (vvw), 2144 (vw), 2137 (mw), 2119 (m), 2083 (vvw), 1904 (m), 1353 (vw), 1301 (mw), 1277 (ms), 1268 (ms), 1243 (vvs), 1209 (vvs), 972 (vvs), 860 (vw), 760 (vvw), 751 (vvw), 726 (vvs), 634 (vw), 605 (m), 592 (w), 568 (w).

FT Raman (100 scans, 250 mW, 4 cm^{-1}): $\tilde{\nu}/cm^{-1}$ (intensity) = 2183 (vvs), 2145 (vvs), 2121 (vvs), 1905 (w), 1269 (vw), 814 (w), 754 (ms), 606 (vw), 572 (vw), 539 (vw), 499 (vvw), 365 (mw), 325 (mw), 292 (vw), 233 (vvw), 117 (vvs).

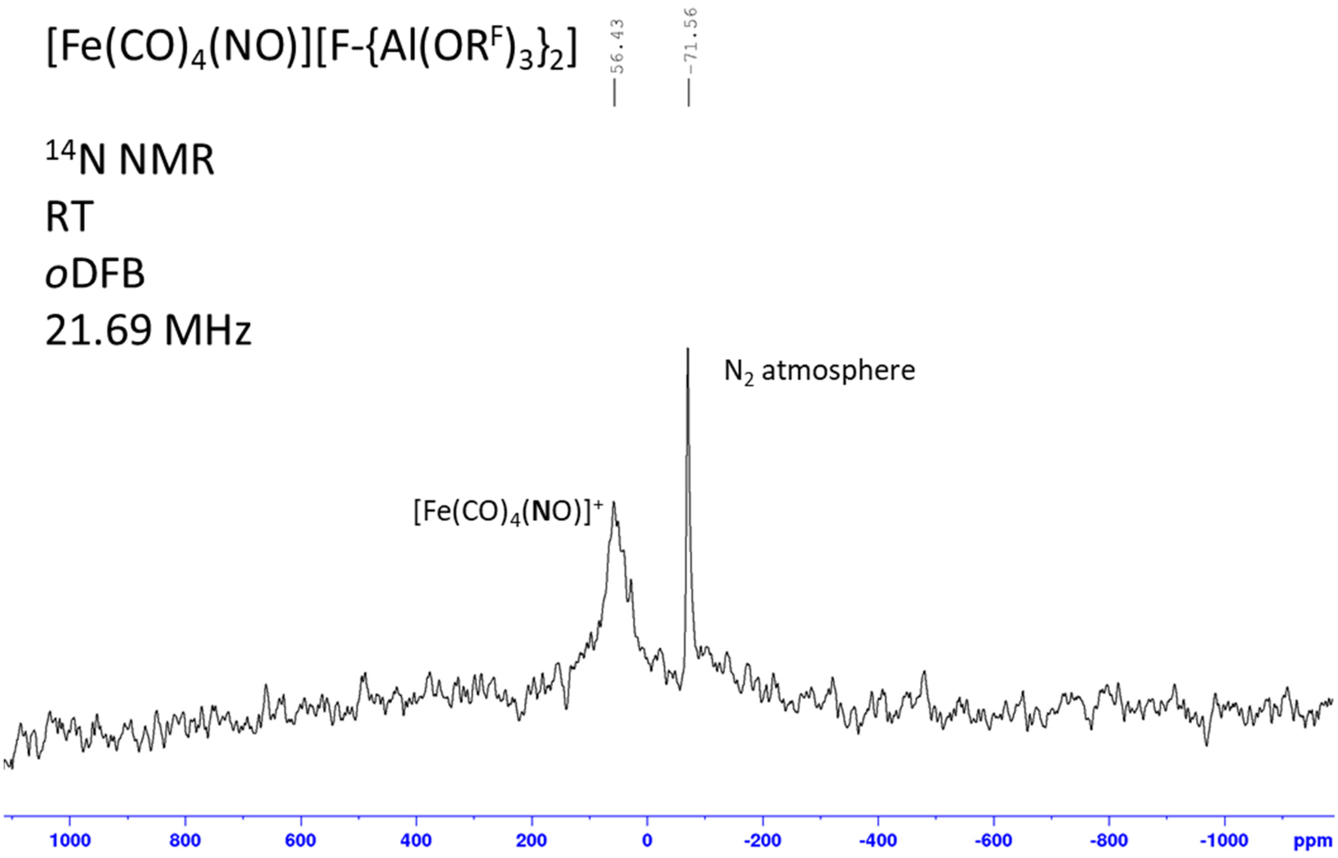
^{1}H NMR (300.18 MHz, *o*DFB, 298 K): *only solvent signals*; **^{13}C{^{1}H} NMR** (75.48 MHz, *o*DFB, 298 K): δ /ppm = 191.8 (s, 4C $[Fe(\mathbf{C}O)_4(NO)]^+$), 121.0 (q, ^1J(C,F) = 291 Hz, 12C, $[F\text{-}\{Al(OC(\mathbf{C}F_3)_3)_3\}_2]^-$), 78.8 (m, 4C, $[F\text{-}\{Al(O\mathbf{C}(CF_3)_3)_3\}_2]^-$); **^{14}N NMR** (21.69 MHz, *o*DFB, 298 K): δ/ppm = 56 (br. s, 1N, $[Fe(CO)_4(\mathbf{N}O)]^+$), –71 (s, N_2 from glovebox atmosphere); **^{19}F NMR** (282.45 MHz, *o*DFB, 298 K): δ/ppm = –76.0 (s, 54F, 6 × $C(C\mathbf{F}_3)_3$), –185.0 (br. s, 1F, $[\mathbf{F}\text{-}\{Al(OC(CF_3)_3)_3\}_2]^-$); **^{27}Al NMR** (78.22 MHz, *o*DFB, 298 K): δ/ppm = 35 (br. s, 1Al, $[F\text{-}\{\mathbf{Al}(OC(CF_3)_3)_3\}_2]^-$).



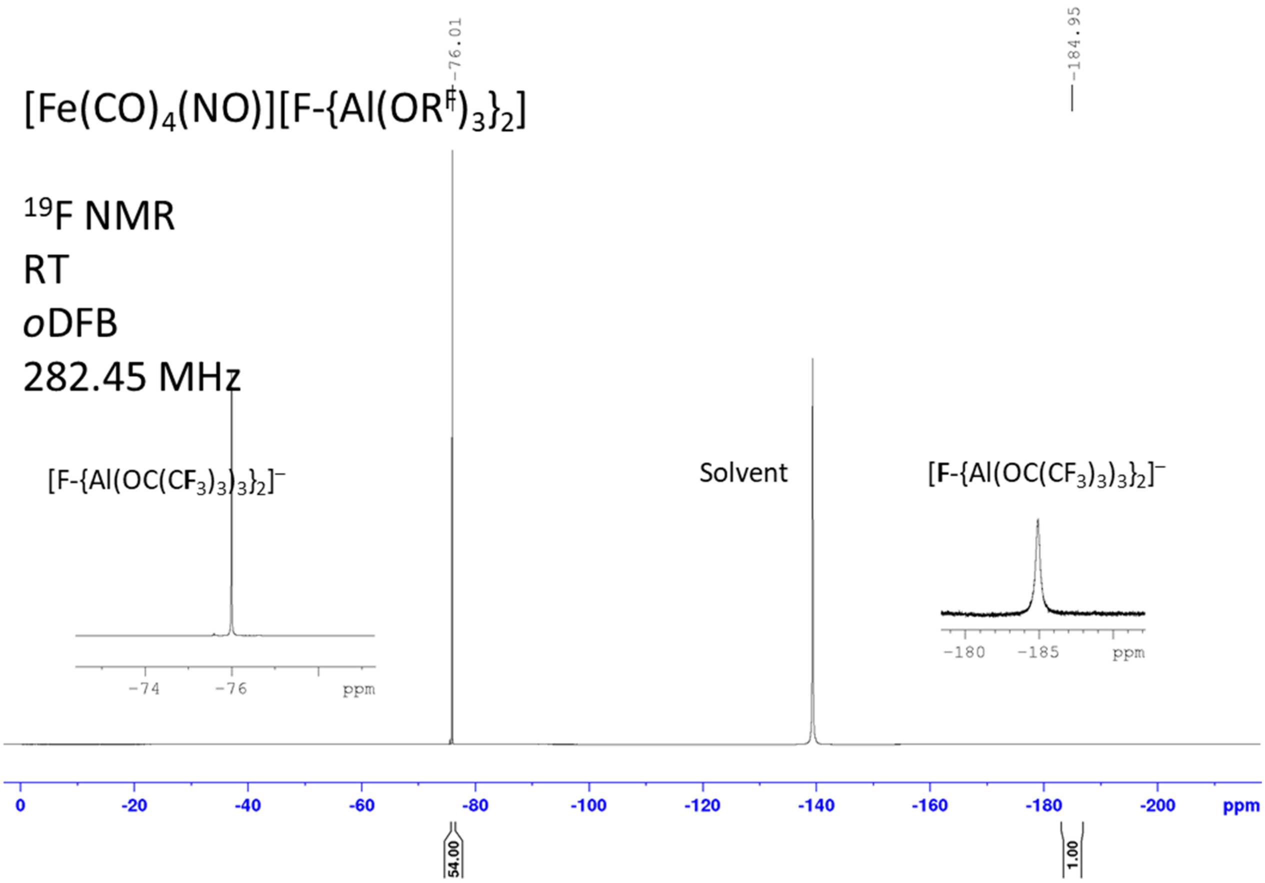
Supplementary Figure 1. ^{1}H NMR (300.18 MHz, *o*DFB, RT) of **1**.



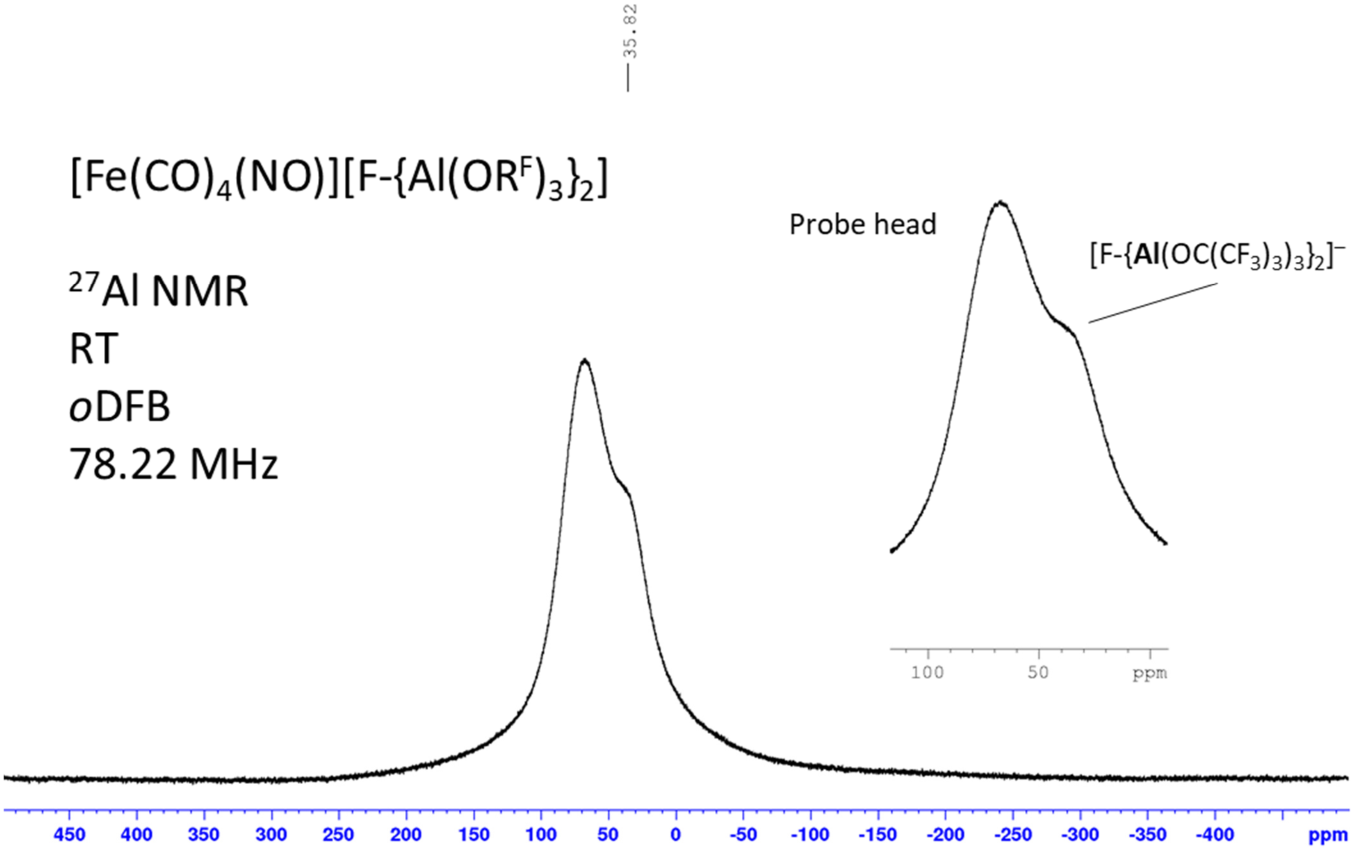
Supplementary Figure 2. ^{13}C{^{1}H} NMR (75.78 MHz, *o*DFB, RT) of **1**.



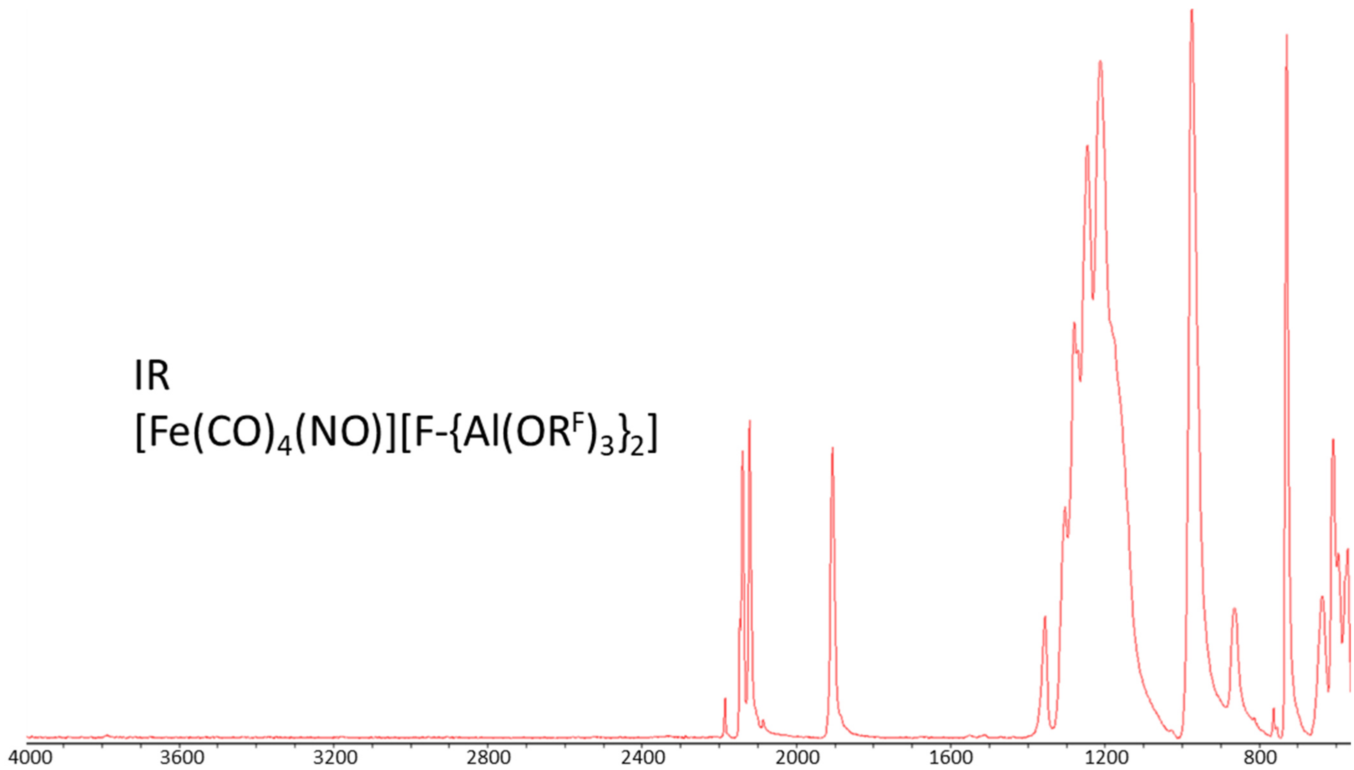
Supplementary Figure 3. ^{14}N NMR (21.69 MHz, *o*DFB, RT) of **1**.



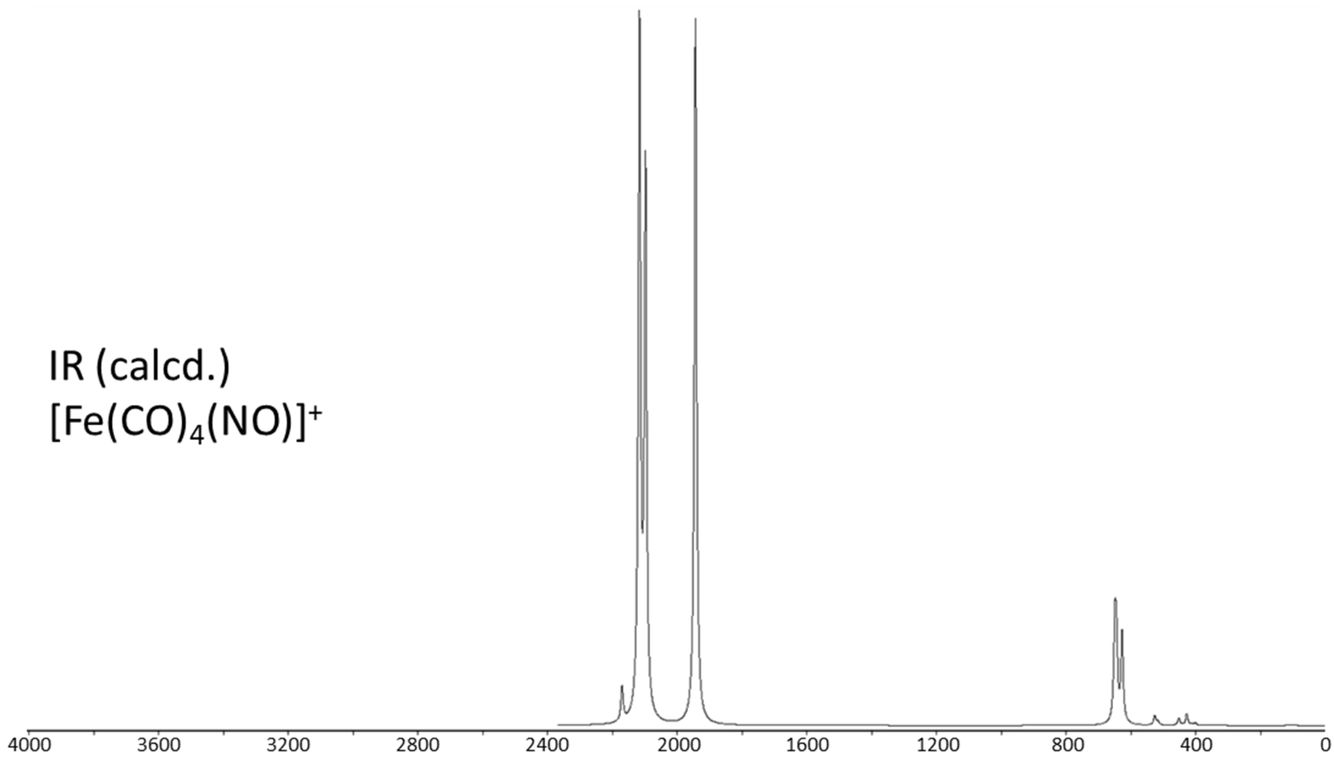
Supplementary Figure 4. ^{19}F NMR (282.45 MHz, *o*DFB, RT) of **1**.



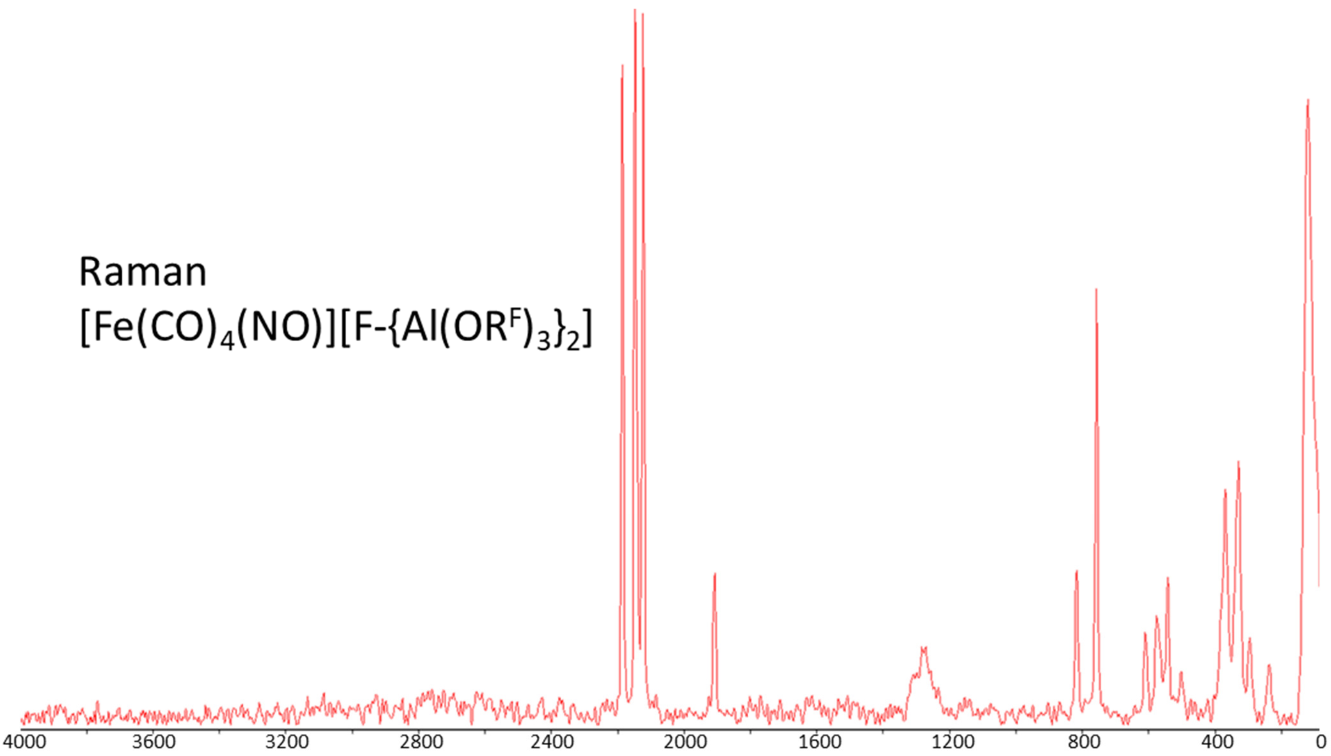
Supplementary Figure 5. ^{27}Al NMR (78.22 MHz, *o*DFB, RT) of **1**.



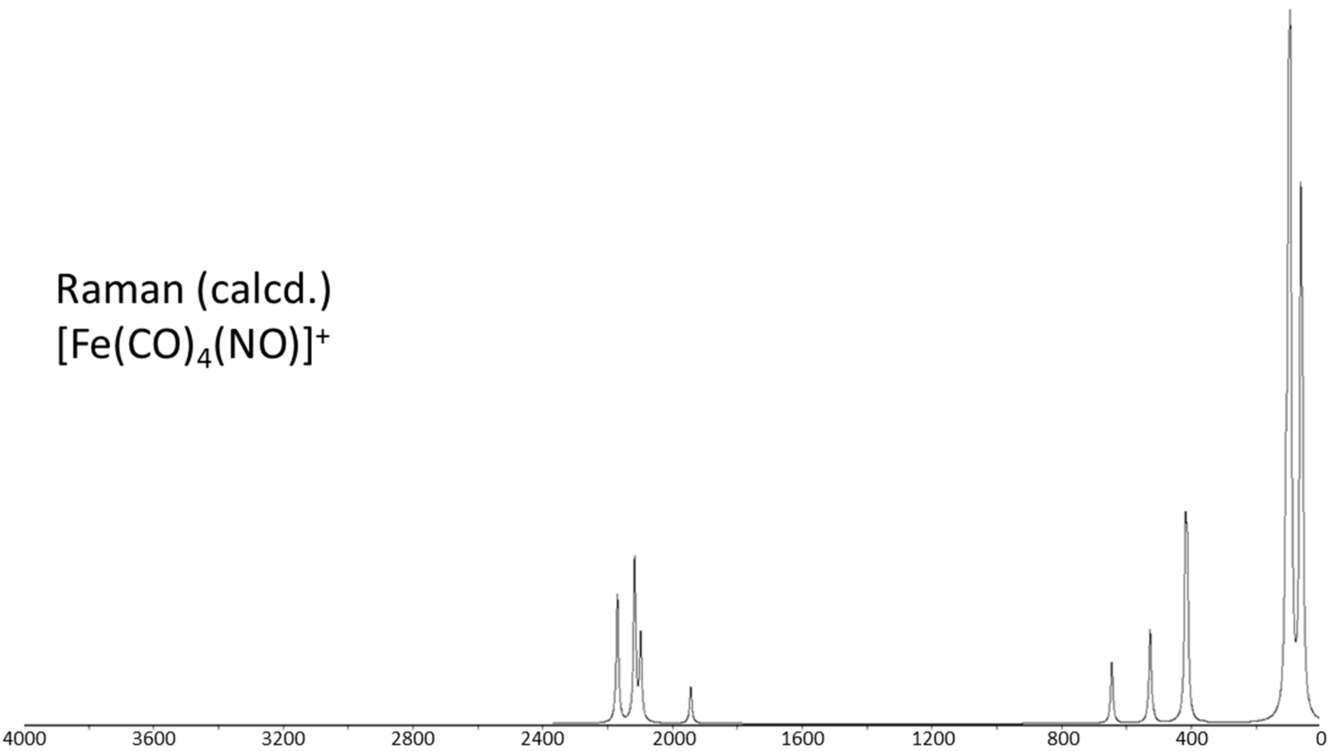
Supplementary Figure 6. Experimental ATR-IR (ZnSe) spectrum of **1**.



Supplementary Figure 7. Calculated (BP86-D3BJ/def2-TZVPP) IR spectrum of $[Fe(CO)_4(NO)]^+$.



Supplementary Figure 8. Experimental Raman spectrum (100 scans, 250 mW) of **1**.



Supplementary Figure 9. Calculated (BP86-D3BJ/def2-TZVPP) Raman spectrum of $[Fe(CO)_4(NO)]^+$.

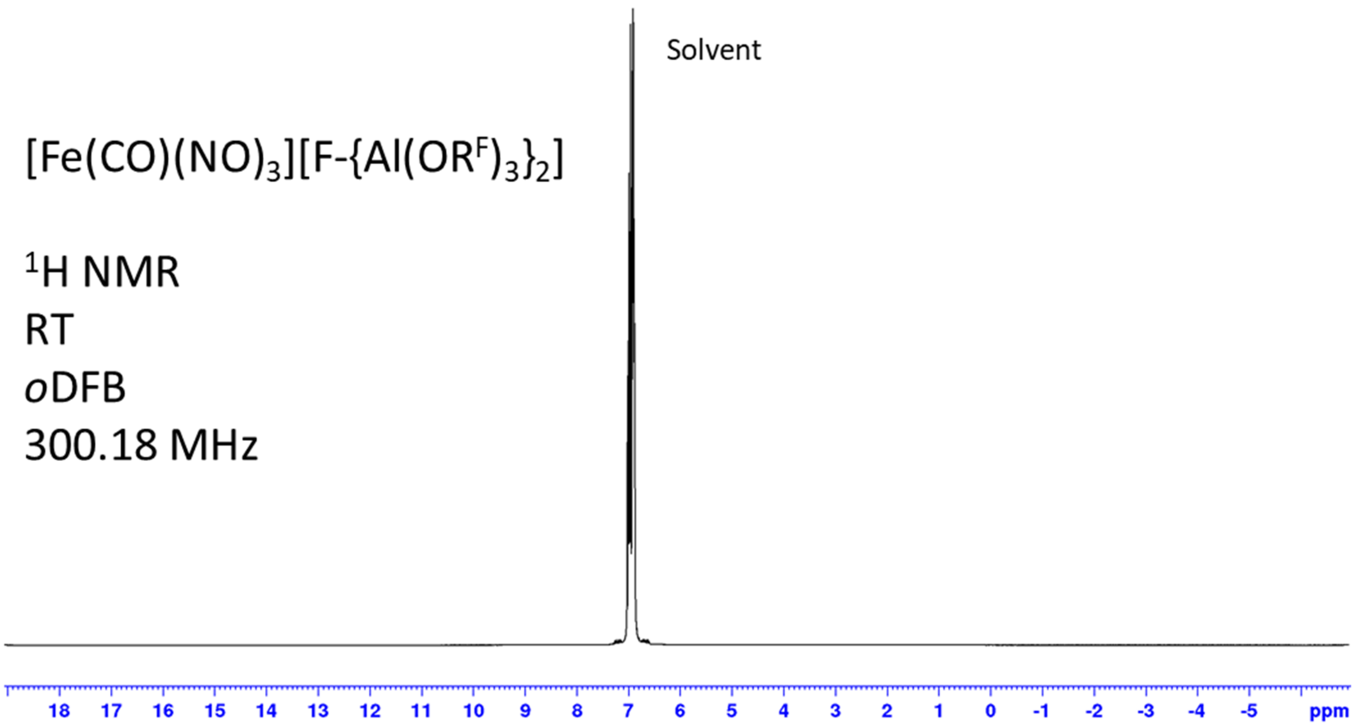
Synthesis of $[Fe(CO)(NO)_3][F\text{-}\{Al(OR^F)_3\}_2]$ (2)

Inside the glovebox, $Fe_3(CO)_{12}$ (44.4 mg, 0.088 mmol) and $NO[F\text{-}\{Al(OR^F)_3\}_2]$ (400 mg, 0.264 mmol) were added to a double-Schlenk tube. Then, TFB (ca. 4 mL) was added and gas evolution and formation of brown **1** were visible upon contact of the solvent and the solids. The brown solution was immediately frozen (*l*N_2*)* and the whole system was evacuated. The flask was filled with $NO_{(g)}$ (ca. 1.3 bar) and was allowed to reach r.t. After 5 min of stirring, the solution turned dark green. Additional stirring for three hours ensured a complete conversion. Then, the atmosphere was exchanged with Ar and the crude dark green reaction solution was crystallized by slow vapour diffusion of *n*-pentane at r.t., resulting in dark green crystals (see Supplementary Figure 20). Yield: 352 mg, 80%.

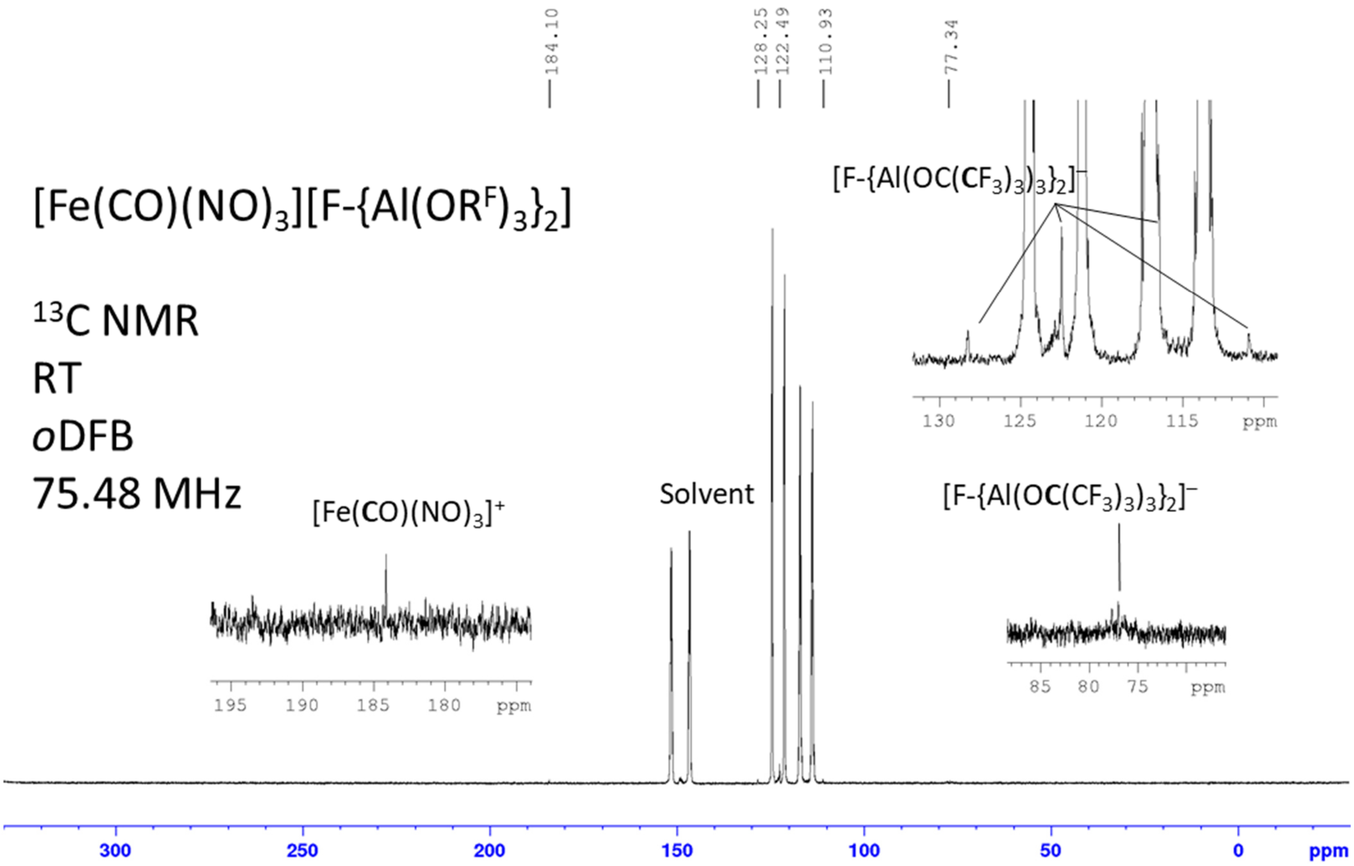
FTIR (ZnSe, ATR): $\tilde{\nu}/cm^{-1}$ (intensity) = 2189 (vw), 1971 (vw), 1876 (s), 1354 (vw), 1301 (vvw), 1266 (vvw), 1244 (w), 1213 (vvs), 1176 (vw), 972 (vvs), 862 (vw), 638 (vw), 810 (vvw), 760 (vvw), 727 (vvs), 628 (w), 567 (w).

FT Raman (1000 scans, 250 mW, 4 cm^{-1}): $\tilde{\nu}/cm^{-1}$ (intensity) = 2190 (s), 1972 (vw), 1881 (vw), 1308 (vvw), 1272 (vvw), 1134 (vvw), 977 (vvw), 817 (vw), 753 (m), 683 (vvw), 629 (vvw), 569 (w), 540 (vw), 490 (w), 367 (vw), 326 (mw), 291 (vw), 233 (vvw), 90 (vvs).

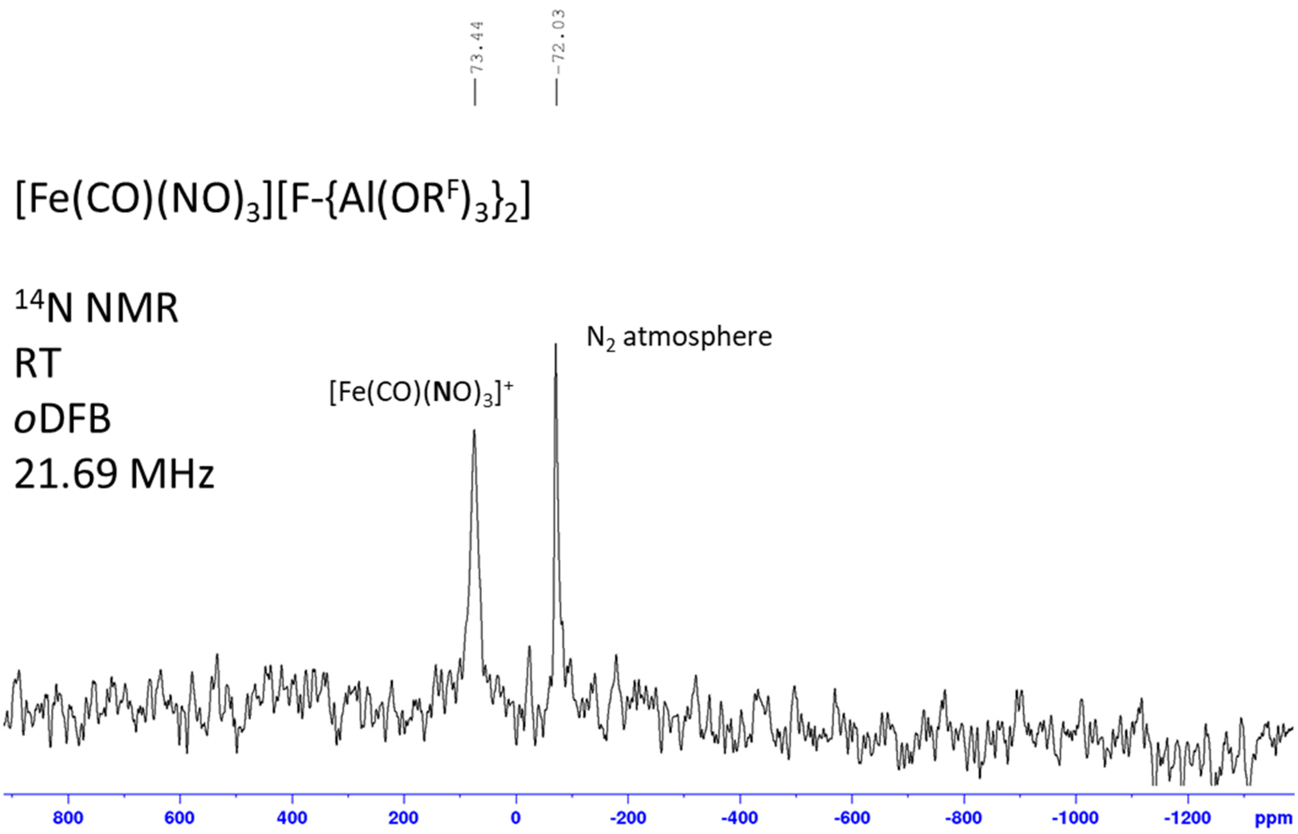
^{1}H NMR (300.18 MHz, *o*DFB, 298 K): *only solvent signals*; **^{13}C NMR** (75.48 MHz, *o*DFB, 298 K): δ /ppm = 184.1 (s, 1C $[Fe(\mathbf{C}O)(NO)_3]^+$), 119.6 (q, ^{1}J(C,F) = 291 Hz, 12C, $[F\text{-}\{Al(OC(\mathbf{C}F_3)_3)_3\}_2]^-$), 77.3 (m, 4C, $[F\text{-}\{Al(O\mathbf{C}(CF_3)_3)_3\}_2]^-$); **^{14}N NMR** (21.69 MHz, *o*DFB, 298 K): δ /ppm = 73 (br. s, 3N, $[Fe(CO)(\mathbf{N}O)_3]^+$), –72 (s, N_2 from glovebox atmosphere); **^{19}F NMR** (282.45 MHz, *o*DFB, 298 K): δ /ppm = –75.5 (s, 54F, 6 × $C(C\mathbf{F}_3)_3$), –184.4 (br. s, 1F, $[\mathbf{F}\text{-}\{Al(OC(CF_3)_3)_3\}_2]^-$); **^{27}Al NMR** (78.22 MHz, *o*DFB, 298 K): δ /ppm = 34 (br. s, 1Al, $[F\text{-}\{\mathbf{Al}(OC(CF_3)_3)_3\}_2]^-$).



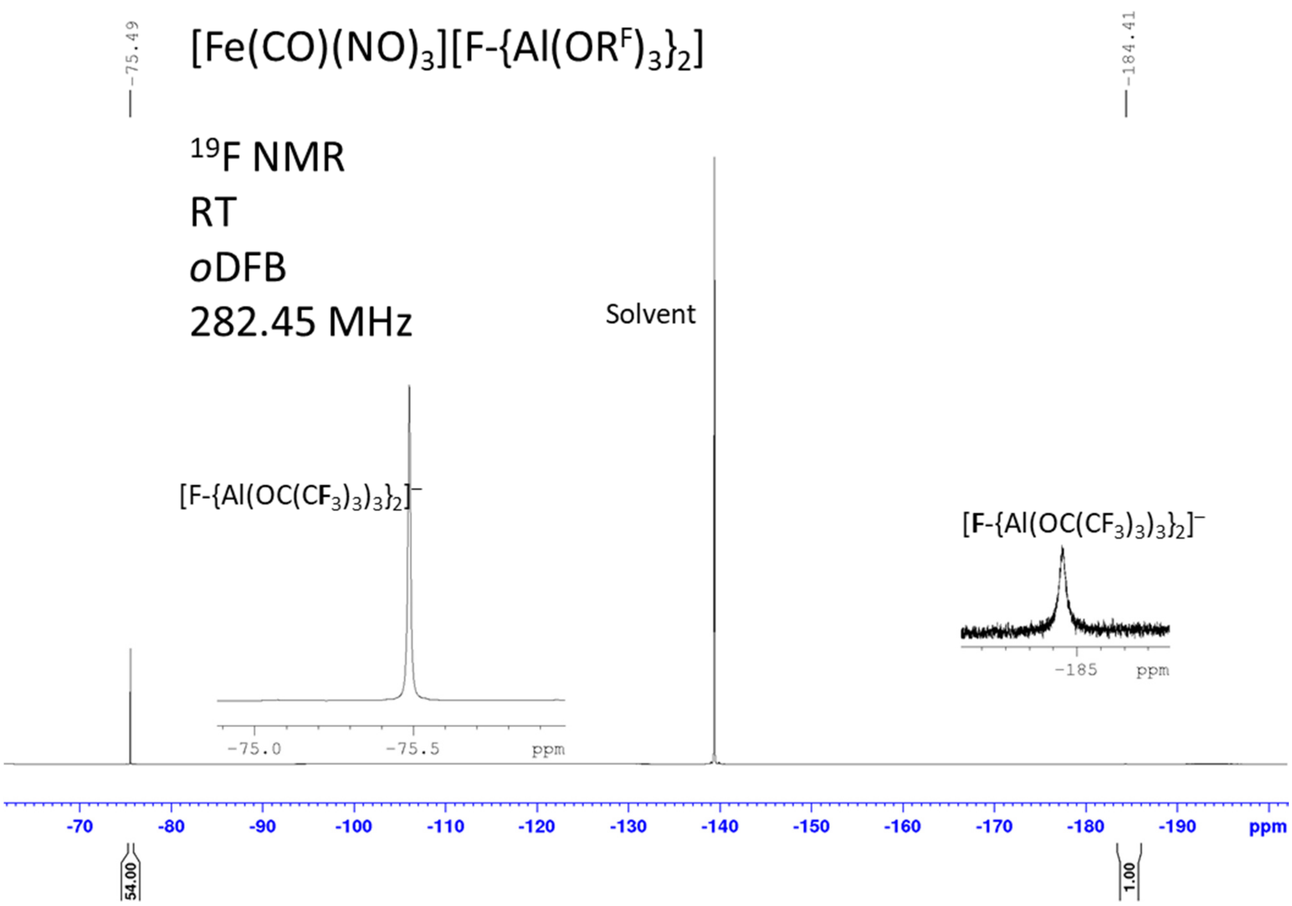
Supplementary Figure 10. ^{1}H NMR (300.18 MHz, *o*DFB, RT) of **2**.



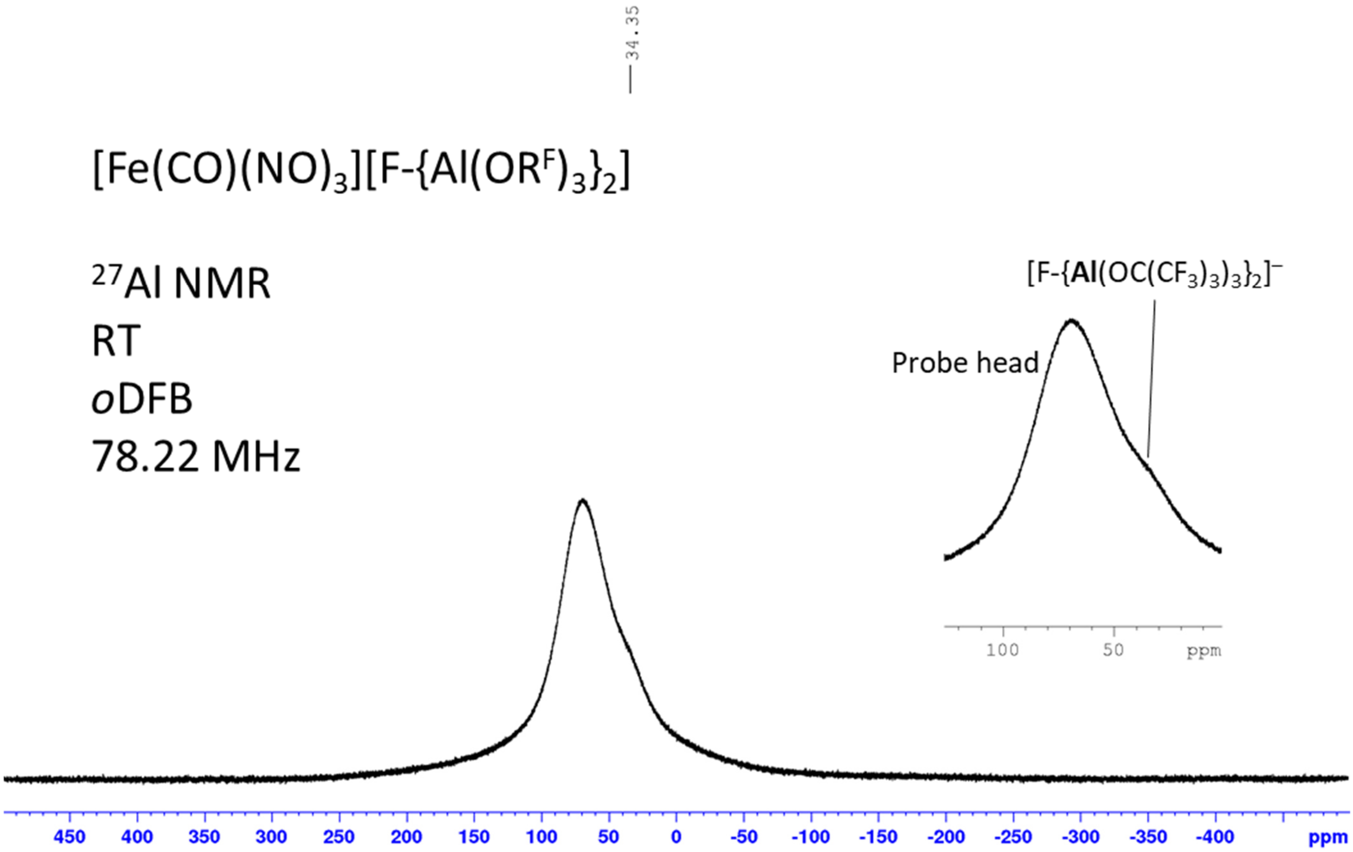
Supplementary Figure 11. ^{13}C NMR (75.48 MHz, *o*DFB, RT) of **2**.



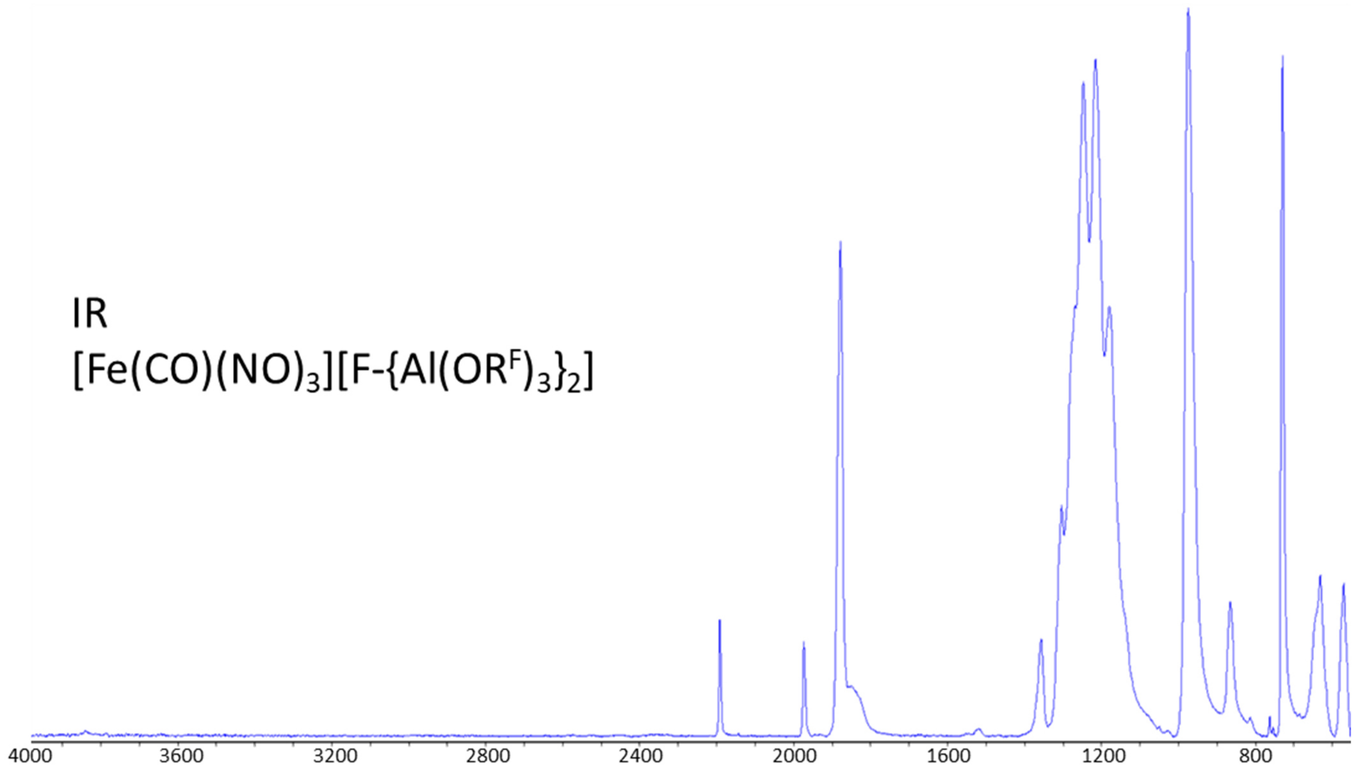
Supplementary Figure 12. ^{14}N NMR (21.69 MHz, *o*DFB, RT) of **2**.



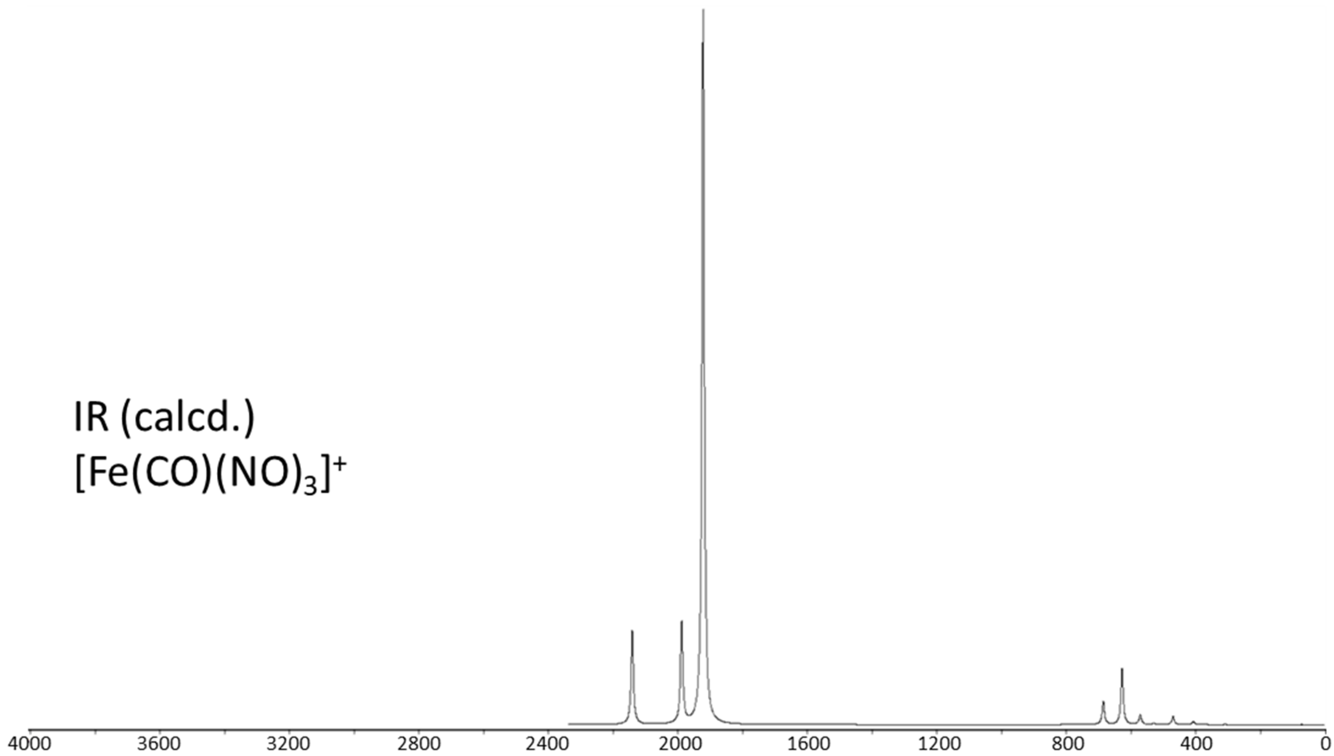
Supplementary Figure 13. ^{19}F NMR (282.45 MHz, *o*DFB, RT) of **2**.



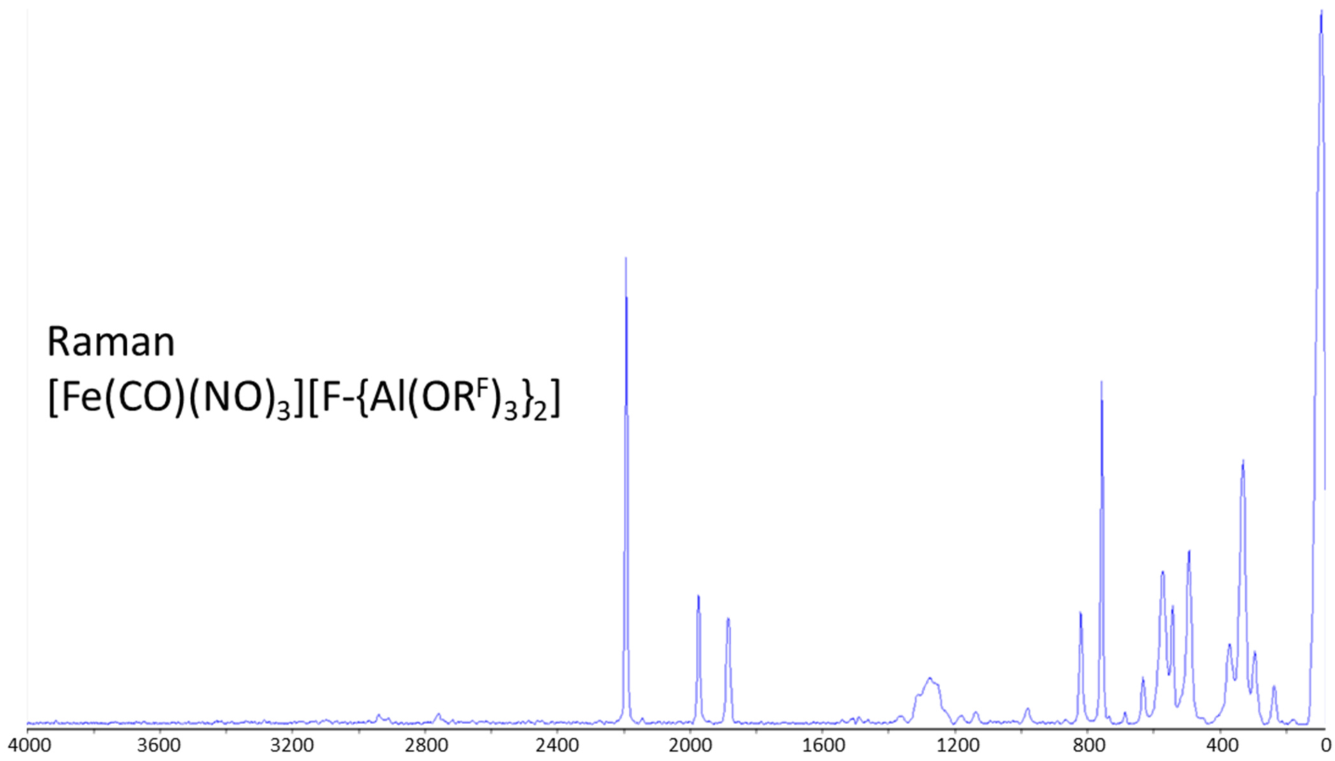
Supplementary Figure 14. ^{27}Al NMR (78.22 MHz, *o*DFB, RT) of **2**.



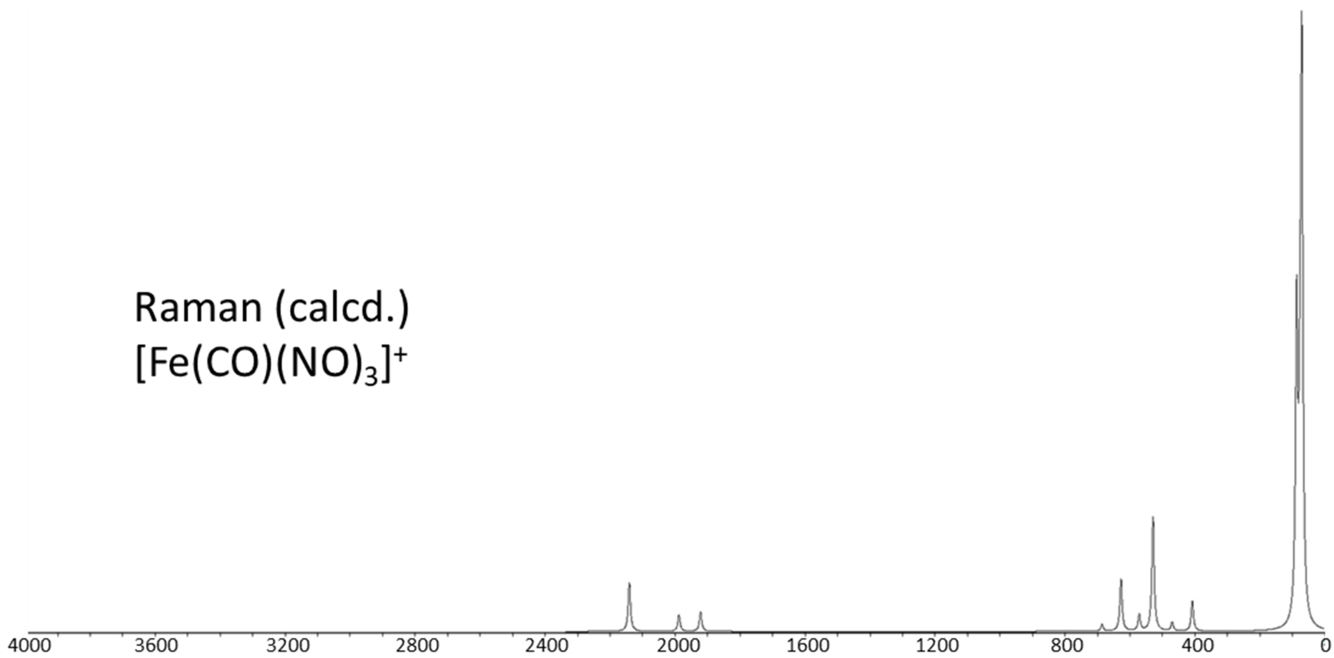
Supplementary Figure 15. Experimental ATR-IR (ZnSe) spectrum of **2**.



Supplementary Figure 16. Calculated (BP86-D3BJ/def2-TZVPP) IR spectrum of $[Fe(CO)(NO)_3]^+$.

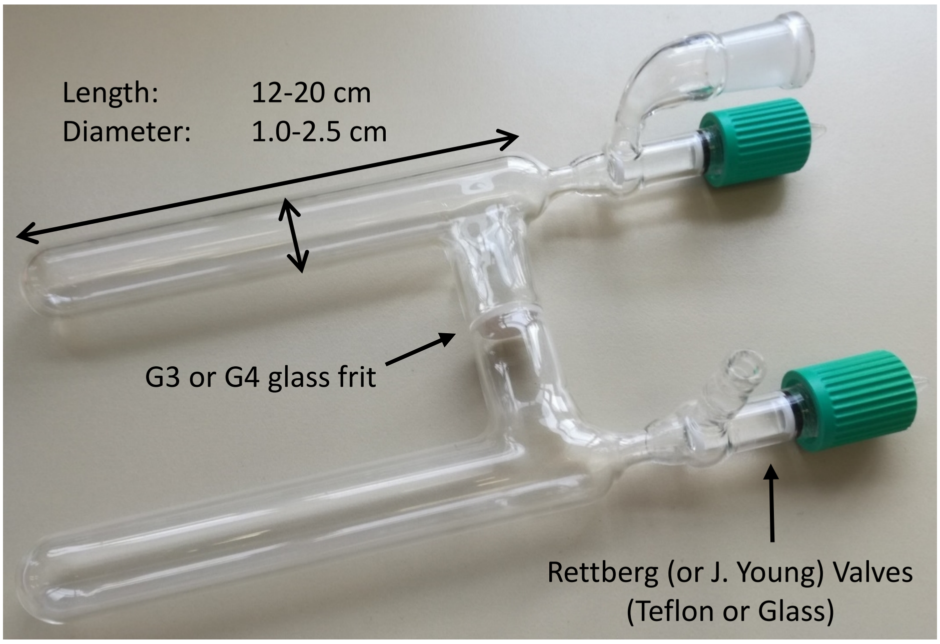


Supplementary Figure 17. Experimental Raman spectrum (1000 scans, 250 mW) of **2**.

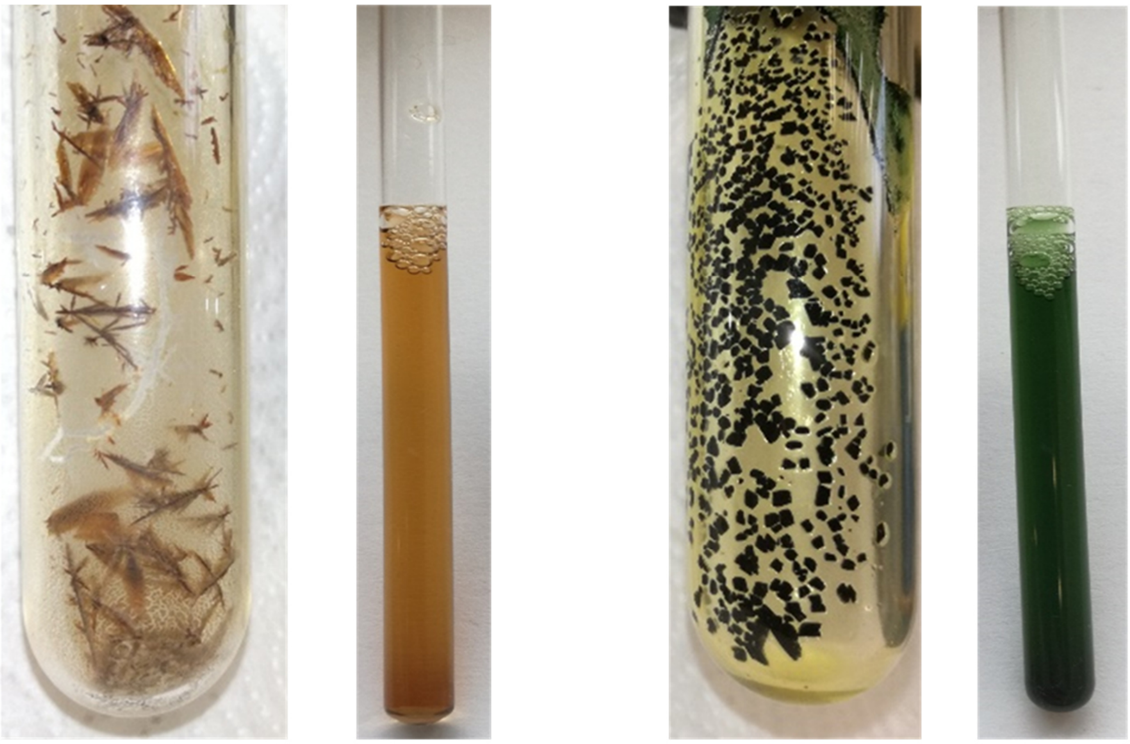


Supplementary Figure 18. Calculated (BP86-D3BJ/def2-TZVPP) Raman spectrum of $[Fe(CO)(NO)_3]^+$.

3. Glassware used and Pictures of compounds 1 and 2



Supplementary Figure 19. Double-Schlenk tube that was typically used for most reactions and crystallizations. Note that different varieties (sizes, Rettberg or J. Young valves) were used. Picture taken by Jan Bohnenberger.



$[Fe(CO)_4(NO)][F\text{-}\{Al(OR^F)_3\}_2]$ $[Fe(CO)(NO)_3][F\text{-}\{Al(OR^F)_3\}_2]$

Supplementary Figure 20. Brown crystals and brown *o*DFB solution of **1** (left) and green crystals and green *o*DFB solution of **2**. Pictures taken by Jan Bohnenberger.

4. Vibrational Analysis

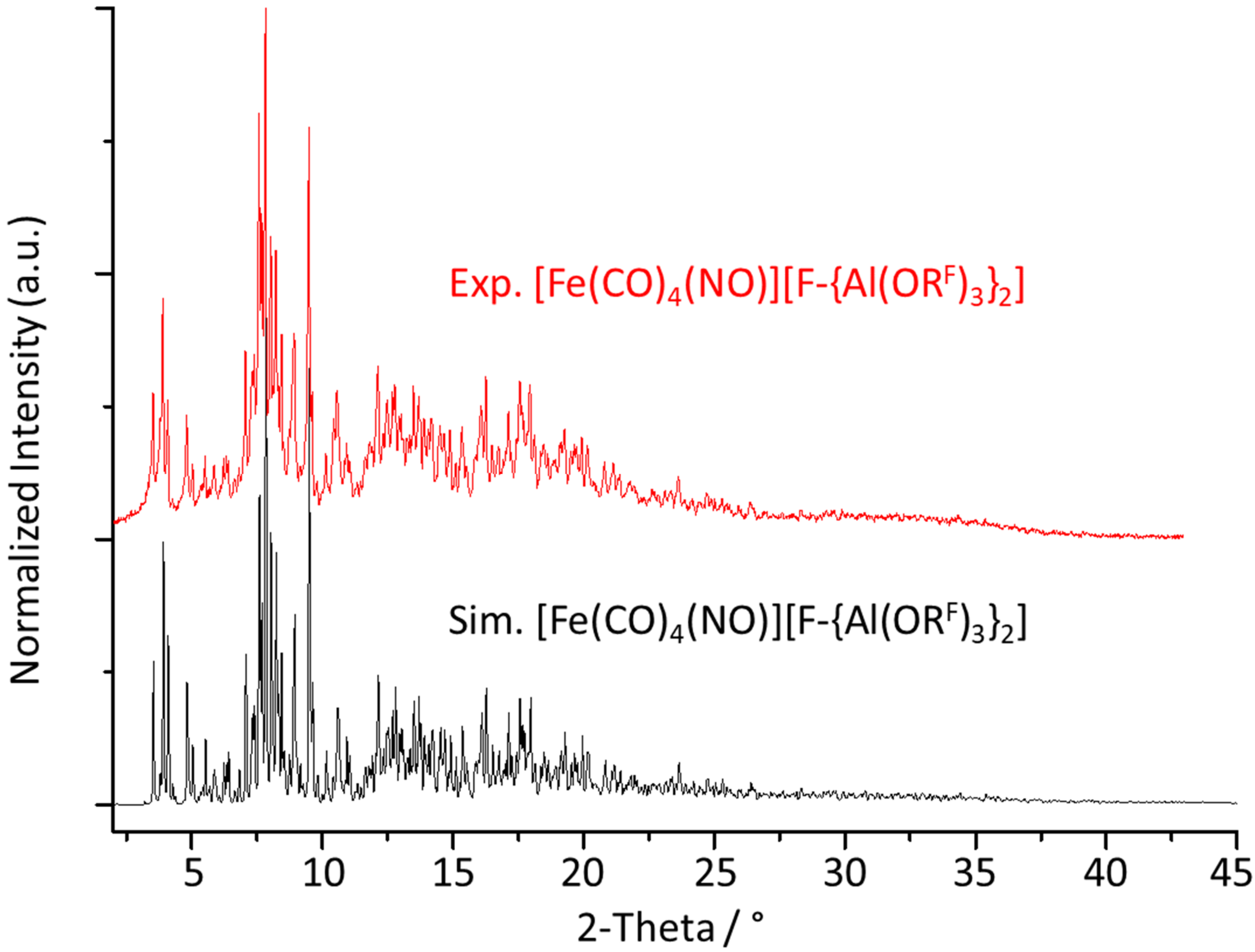
Supplementary Table 1. Full assignment of all IR and Raman vibrations for complexes **1** and **2**.

$[Fe(CO)_4(NO)]$ $[F\text{-}\{Al(OR^F)_3\}_2]$ (1)		**$[Fe(CO)_4(NO)]^+$ calcd.**[a)]		**$[Fe(CO)(NO)_3]$ $[F\text{-}\{Al(OR^F)_3\}_2]$ (2)**		**$[Fe(CO)(NO)_3]^+$ calcd.**[b)]		**$[F\text{-}\{Al(OR^F)_3\}_2]^-$** [21]	**Assignment** [21] c)
IR	Raman	IR	Raman	IR	Raman	IR	Raman	IR	
	117 (vvs)		59 (vvs) 92 (vvs)		90 (vvs)		68 (vvs) 84 (ms)		δ(Fe–N) B_1/E δ(Fe–C) B_2/E
	233 (vvw)				233 (vvw)				C–C
	292 (vw)				291 (vw)				C–C, Al–O
	325 (mw)				326 (mw)				C–C, Al–O
	365 (mw)		410 (w)		367 (vw)		405 (vvw)		*C–C, Al–O ν(Fe–C) A_1
		425 (vvw)							δ(Fe–C) B_2
		449 (vvw)							ν(Fe–C) B_1
						467 (vvw)	467 (vvw)		δ(Fe–C) E
					490 (w)		526 (vw)		ν(Fe–N) A_1
	499 (vvw)	524 (vvw)	524 (vw)						ν(Fe–N) A_1
	540 (vw)				540 (vw)				C–C, C–O
568 (w)	572 (vw)			567 (w)	569 (w)	569 (vvw)	569 (vvw)	572 (m)	*Al–O, C–C δ(Fe–N) E
592 (w)		625 (vw)							δ(Fe–N) B_1
605 (m)	606 (vw)	646 (vw)	642 (vvw)						δ(Fe–C) B_2 ν(Fe–N) A_1
				628 (w)	629 (vvw)	625 (vvw)	625 (vvw)		δ(Fe–N) E
634 (vw)				639 (vw)				639 (m)	Al–F–Al
					683 (vvw)	683 (vvw)	683 (vvw)		δ(Fe–N) A_1
726 (vvs)				727 (vvs)				728 (s)	C–C, C–O
751 (vvw)	754 (ms)				753 (m)				- [Anion]
									C–C, C–O
760 (vvw)				760 (vvw)					C–C, C–O
	814 (w)			810 (vvw)	817 (vw)				- [Anion]
860 (vw)				862 (vw)				865 (w)	Al–O, Al–F–Al
972 (vvs)				972 (vvs)	977 (vvw)			975 (s)	C–C, C–F
					1134 (vvw)				C–C, C–F
				1176 (vw)				1183 (m)	C–C, C–F
1209 (vvs)				1213 (vvs)				1218 (s)	C–C, C–F
1243 (vvs)				1244 (w)				1249 (s)	C–C, C–F
1277 (ms)	1269 (vw)			1266 (vvw)	1272 (vvw)			1268 (m)	C–C, C–F
1301 (mw)				1301 (vvw)	1308 (vvw)			1301 (m)	C–C, C–F
1353 (vw)				1354 (w)				1355 (m)	C–C, C–F
				1876 (s)**	1881 (vw)	1919 (vvw)	1919 (vvw)		ν(N–O) E
1904 (m)	1905 (w)	1941 (vvs)	1941 (vvw)						ν(N–O) A_1
				1971 (vw)	1972 (vw)	1986 (vw)	1986 (vvw)		ν(N–O) A_1
2083 (vvw)									*$\nu(^{13}C–O)$*
2119 (m)	2121 (vvs)	2096 (vvs)	2096 (vw)						ν(C–O) B_2
2137 (mw)		2114 (vvs)	2114 (w)						ν(C–O) B_1***
2144 (vw, sh)	2145 (vvs)								ν(C–O) A_1***
2183 (vvw)	2183 (vvs)	2168 (vvw)	2169 (w)						ν(C–O) A_1
				2189 (vw)	2190 (s)	2139 (vw)	2139 (vvw)		ν(C–O) A_1

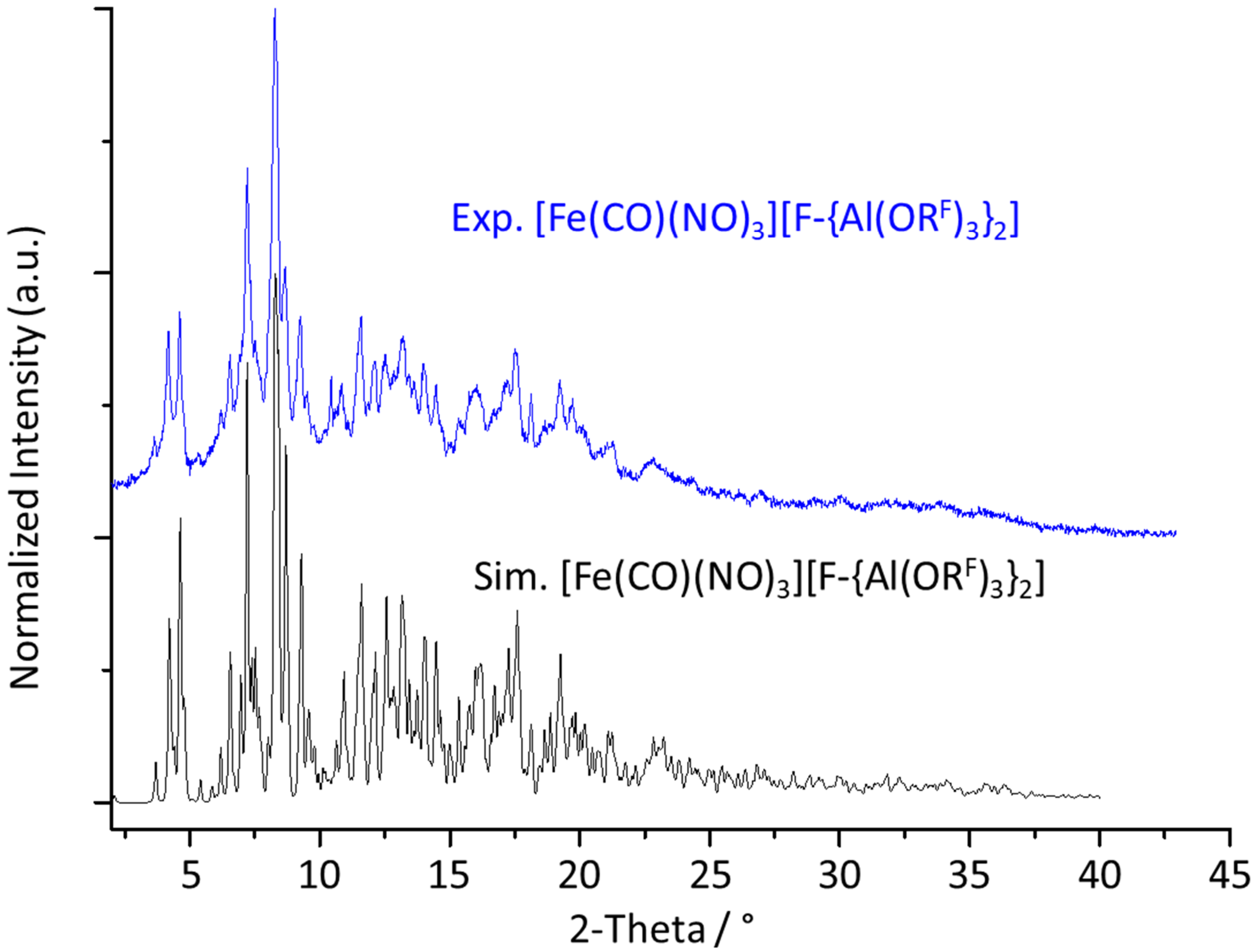
a) BP86-D3BJ/def2-TZVPP, C_{2v} symmetry, **no scale factor was applied**. w: weak, m: medium, s: strong, v: very, sh: shoulder, br: broad.
b) BP86-D3BJ/def2-TZVPP, C_{3v} symmetry, **no scale factor was applied**. w: weak, m: medium, s: strong, v: very, sh: shoulder, br: broad.
c) The assignments of the respective anion bands and their intensities are based on $[CBr_3][F\text{-}\{Al(OR^F)_3\}_2]$ (IR only) in ref.[21].
* *Note*: Due to partial overlap with the anion bands, the ν(Fe–C) A_1/E vibrations cannot be assigned unambiguously.
** Sometimes a possible unknown impurity can be seen as a shoulder (see Supplementary Figure 15) although the powder-XRD of the same sample appears to be phase-pure (Supplementary Figure 22).
*** The assignment of the shoulder is ambiguous.

5. Powder XRD Data

In order to evaluate the phase purity of the bulk materials **1** and **2** powder XRD measurements were conducted at 100K. They confirm the absence of crystalline impurities for both bulk materials.

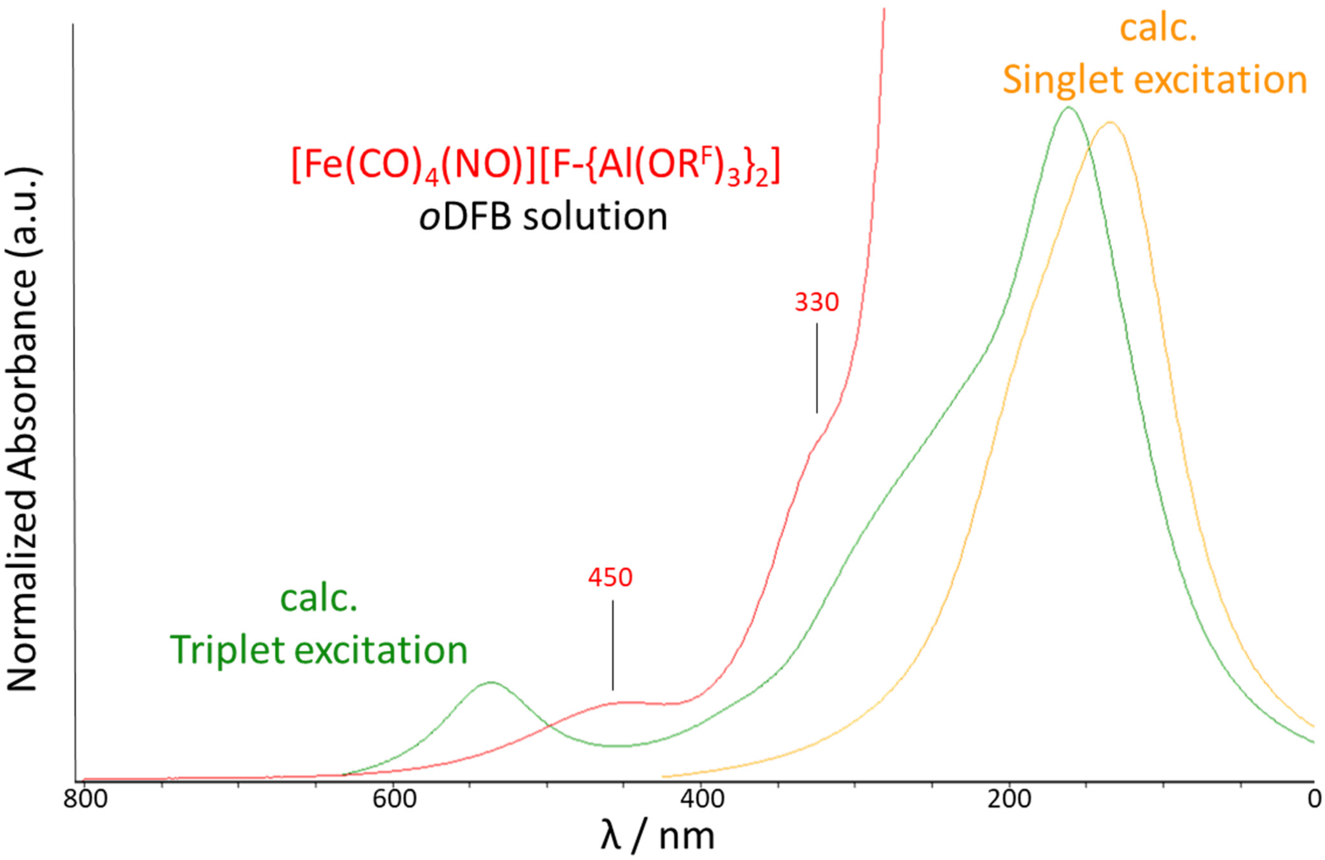


Supplementary Figure 21. Experimental (red) and simulated (black) powder diffractograms of **1.**

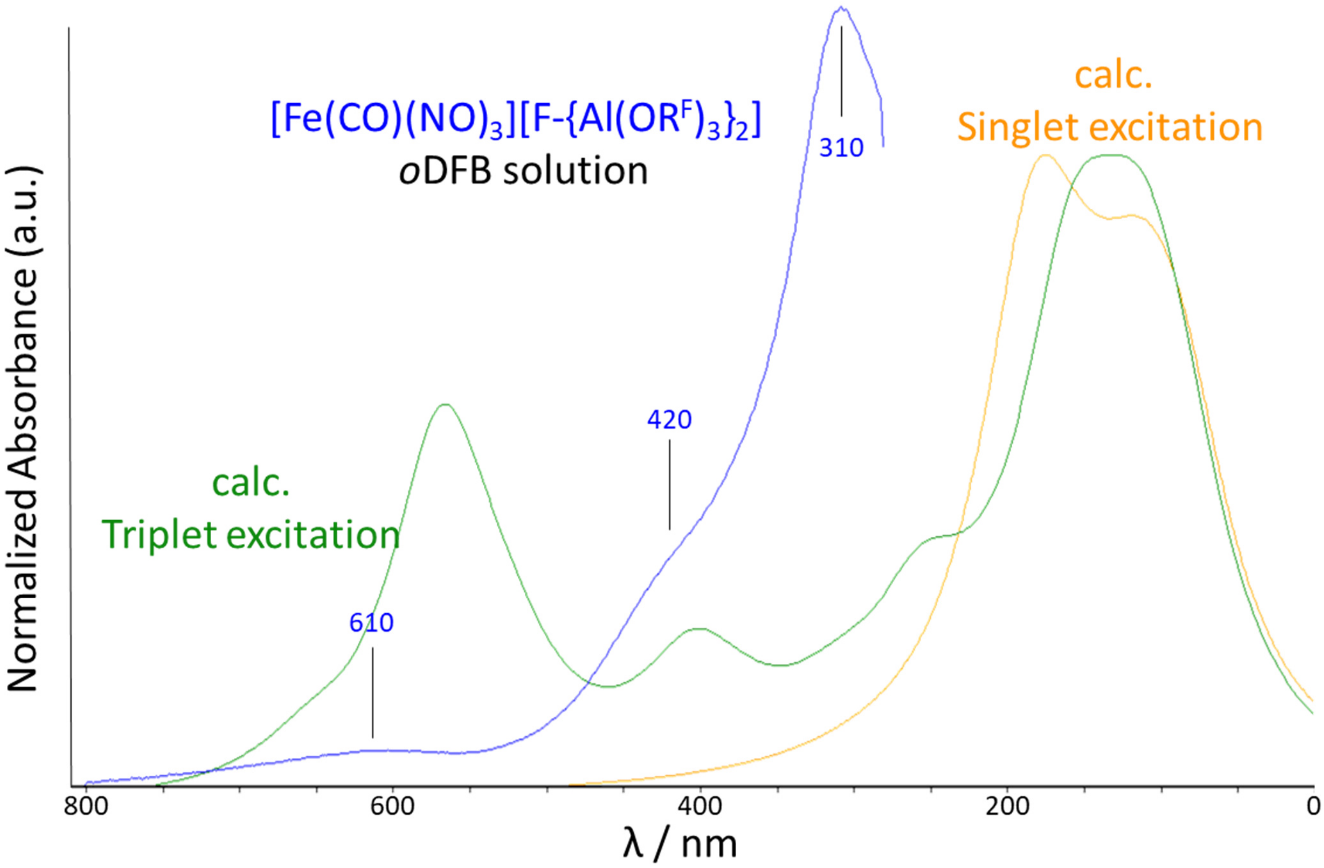


Supplementary Figure 22. Experimental (blue) and simulated (black) powder diffractograms of **2.**

6. UV/VIS Spectra



Supplementary Figure 23. Solution (*o*DFB) UV/VIS absorbance spectrum of **1** (red) with absorption maxima at λ_{max} = 450 nm, 330 nm and calculated (BP86-D3BJ/def2-TZVPP, C_{2v} symmetry, 100 nm line width) UV/VIS spectra of $[Fe(CO)_4(NO)]^+$ with triplet (green) and singlet (orange) excitations.



Supplementary Figure 24. Solution (*o*DFB) UV/VIS absorbance spectrum of **2** (blue) with absorption maxima at λ_{max} = 610 nm, 420 nm, 310 nm and calculated (BP86-D3BJ/def2-TZVPP, C_{3v} symmetry, 100 nm line width) UV/VIS spectra of $[Fe(CO)(NO)_3]^+$ with triplet (green) and singlet (orange) excitations.

7. Discussion of the Existence of "[Fe(CO)$_5$(NO)]Cl"

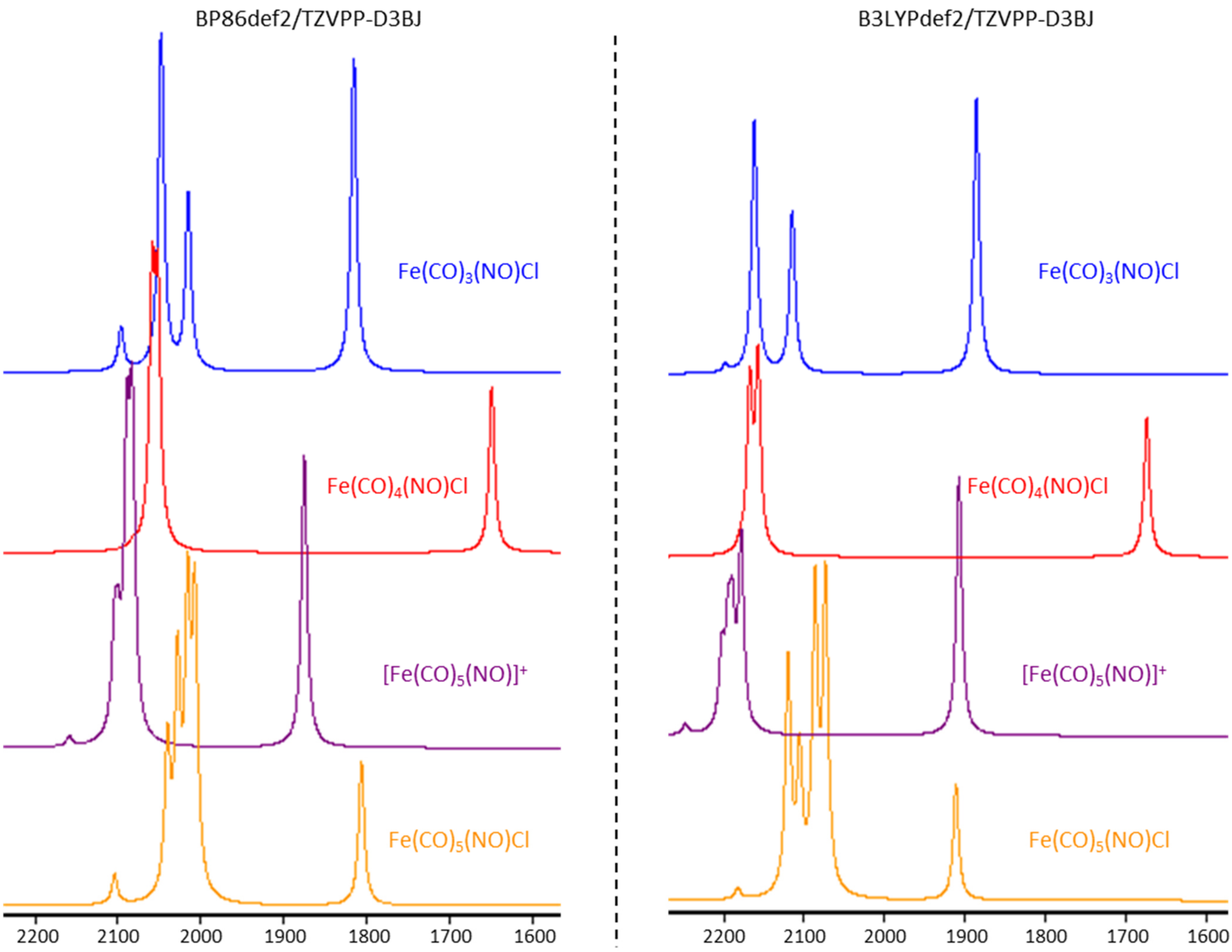
In order to evaluate the existence of the curious [Fe(CO)$_5$(NO)]Cl species[22], we conducted DFT calculations in regard to vibrational spectroscopy and reaction energetics. Although the exotic reaction conditions (liquid HCl as solvent, low temperatures) might stabilize exotic species, several points in the publication raised our doubts.

- *Attempts to prepare the tetrachloroborate complex failed, probably because of a side-reaction between nitrosyl chloride and boron trichloride*."

Another possible conclusion could be the incompatibility of BCl_3 with "[Fe(CO)$_5$(NO)]Cl" if the Cl^- would be bound to the iron in an inner-sphere fashion. Abstraction of the chloride would very likely lead to the decomposition of the labile complex. Furthermore, it also seems curious why an electron deficient cation would not react with an excess of chloride anions in the reaction medium. Furthermore, the fact that "*The solid decomposed very slowly on standing at room temperature, giving off nitrosyl chloride."* also hints at a molecular compound and not a salt with a chloride counterion.

So we calculated the structures several reasonable Fe(CO)$_x$(NO)Cl species (Supplementary Figure 26) and their IR spectra (Supplementary Figure 25). It strikes that the postulated species [Fe(CO)$_5$(NO)]$^+$ and [Fe(CO)$_5$(NO)Cl] (which is rather [Fe(CO)$_5$(NOCl)]) both feature very weak Fe–N bonds as well as NO stretch vibrations in the region of 1800–1900 cm^{-1} (instead of the reported 1610 cm^{-1}). The only species with a NO vibration in the range of 1650 cm^{-1} would be Fe(CO)$_4$(NO)Cl. However, the best agreement with the reported CO stretches (2200w, 2145s, 2125m) shows Fe(CO)$_3$(NO)Cl. The calculated reaction enthalpies (Supplementary Table 2) do not give a significant trend which species is preferred especially since some reactions are not isodesmic.

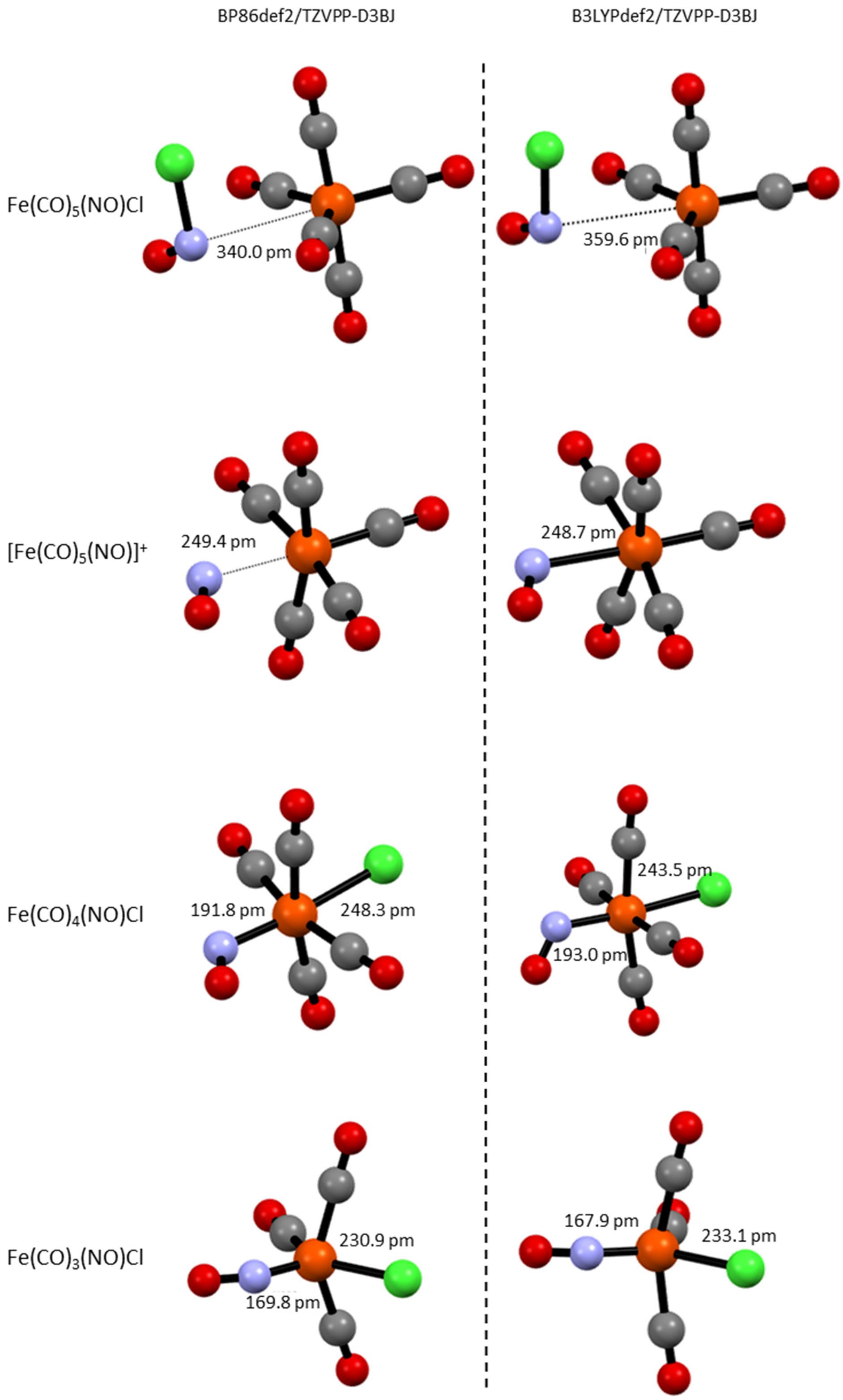
In summary, our DFT calculations do not proof which species was formed in the literature reaction. But however, they show that [Fe(CO)$_5$(NO)]$^+$ and Fe(CO)$_5$(NO)Cl both feature not only very weak Fe–N bonds but also NO stretch vibrations far off from the observed 1610 cm^{-1} as well as a poor agreement in the CO region. Therefore, in addition to the fact that the species was never reproduced in literature, we think it is reasonable to doubt that the species that was observed in 1968 was [Fe(CO)$_5$(NO)]$^+$.



Supplementary Figure 25. Comparison of the calculated (BP86def2/TZVPP-D3BJ left, B3LYPdef2/TZVPP-D3BJ right) IR spectra of $Fe(CO)_3(NO)Cl$ (blue), $Fe(CO)_4(NO)Cl$ (red), $[Fe(CO)_5(NO)]^+$ (purple) and $Fe(CO)_5(NO)Cl$ (orange).

Supplementary Table 2. Calculated reaction enthalpies (@BP86def2/TZVPP-D3BJ, B3LYPdef2/TZVPP-D3BJ) for the reaction of $Fe(CO)_5$ with NOCl.

Reaction	$\Delta H°_{(gas)}$ / kJ mol^{-1}		$\Delta G°_{(gas)}$ / kJ mol^{-1}	
	BP86	B3LYP	BP86	B3LYP
$Fe(CO)_5$ + NOCl ⟶ $Fe(CO)_5(NO)Cl$	-14	-12	+20	+21
$Fe(CO)_5$ + NOCl ⟶ $Fe(CO)_4(NO)Cl$ + CO	+56	+13	+53	+11
$Fe(CO)_5$ + NOCl ⟶ $Fe(CO)_3(NO)Cl$ + 2CO	+42	+7	-3	-37



Supplementary Figure 26. Calculated (BP86def2/TZVPP-D3BJ left, B3LYPdef2/TZVPP-D3BJ right) structures and Fe–N/Fe–Cl bond lengths of $Fe(CO)_3(NO)Cl$, $Fe(CO)_4(NO)Cl$, $[Fe(CO)_5(NO)]^+$ and $Fe(CO)_5(NO)Cl$.

8. Single-Crystal XRD Data of Compounds 1 and 2

$[Fe(CO)_4(NO)][F\text{-}[Al(OR^F)_3\}_2]$ (1)

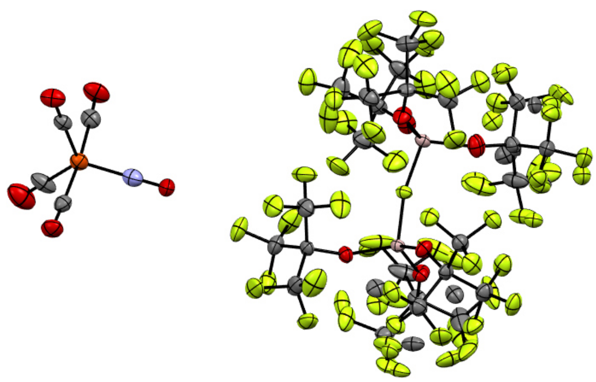


Table 1 Crystal data and structure refinement for p21c_a.

Identification code	p21c_a
Empirical formula	$C_{28}NO_{11}F_{55}Al_2Fe$
Formula weight	1681.10
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	11.4973(5)
b/Å	17.8240(7)
c/Å	24.6741(9)
α/°	90
β/°	95.896(2)
γ/°	90
Volume/Å^3	5029.7(3)
Z	4
ρ_{calc}g/cm^3	2.220
μ/mm^{-1}	0.595
F(000)	3240.0
Crystal size/mm^3	0.15 × 0.08 × 0.08
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.824 to 52.832
Index ranges	$-14 \leq h \leq 14$, $-19 \leq k \leq 22$, $-30 \leq l \leq 30$
Reflections collected	53880
Independent reflections	10282 [R_{int} = 0.0211, R_{sigma} = 0.0243]
Data/restraints/parameters	10282/8037/1125
Goodness-of-fit on F^2	1.057
Final R indexes [I>=2σ (I)]	R_1 = 0.0421, wR_2 = 0.1064
Final R indexes [all data]	R_1 = 0.0640, wR_2 = 0.1186
Largest diff. peak/hole / e Å^{-3}	1.32/-0.51

Table 2 Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for p21c_a. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C3	8865(2)	8916.0(16)	6462.9(10)	29.6(6)
Fe1	7540.1(4)	8452.1(2)	6634.2(2)	34.28(12)
N1	7565(2)	7445.7(17)	6658.5(9)	40.6(6)
Al1	7172.4(6)	2528.0(4)	6513.5(3)	20.44(16)
O1	6674(2)	8485.7(14)	5453.3(8)	52.8(6)
C1	6996(3)	8458.0(17)	5895.6(12)	38.2(7)
O2	5467(3)	9294.1(18)	6852.2(11)	75.6(8)
C2	6252(3)	8974(2)	6767.0(12)	48.7(9)
Al2	7787.6(7)	2591.2(4)	5153.0(3)	22.55(17)
O3	9687.6(19)	9202.8(14)	6354.0(8)	46.3(5)
F004	7388.5(12)	2670.9(8)	5822.6(5)	26.0(3)
O4	8379(2)	8595.8(12)	7814.4(8)	44.6(5)
C4	8073(3)	8530.9(16)	7374.6(12)	34.1(6)
O5	7597.3(19)	6809.3(12)	6673.6(8)	40.6(5)
O1_8	6067(17)	2000(20)	6574(12)	25.0(8)
C1_8	4925(16)	1940(8)	6659(6)	31(3)
C2_8	4164(12)	2296(10)	6179(6)	62(4)
F1_8	4060(18)	1845(12)	5740(7)	77(7)
F2_8	3096(15)	2428(16)	6309(10)	78(8)
F3_8	4630(30)	2897(13)	5980(12)	77(7)
C3_8	4719(13)	2337(7)	7198(5)	36(3)
F4_8	5540(30)	2162(15)	7591(10)	37(5)
F5_8	4639(13)	3072(7)	7121(7)	48(4)
F6_8	3700(20)	2149(17)	7376(15)	49(6)
C4_8	4605(13)	1101(8)	6706(7)	59(4)
F7_8	5040(20)	850(11)	7196(7)	81(6)
F8_8	3469(14)	970(16)	6661(11)	92(8)
F9_8	5130(30)	701(16)	6353(11)	75(9)
O1_6	6976.1(16)	3388.5(10)	6779.8(7)	27.2(4)
C1_6	7365(2)	4088.4(14)	6921.1(9)	24.7(5)
C2_6	7709(3)	4109.1(16)	7545.0(11)	41.5(7)
F1_6	6952.0(19)	3729.5(10)	7807.0(6)	54.4(5)
F2_6	7773(2)	4803.0(10)	7740.2(7)	59.6(6)
F3_6	8756.7(19)	3790.0(12)	7668.2(8)	64.8(6)
C3_6	8438(3)	4300.4(17)	6622.7(12)	39.2(7)
F4_6	8107.0(19)	4479.1(12)	6108.2(7)	58.8(5)
F5_6	9150.3(16)	3711.4(11)	6614.1(10)	63.1(6)
F6_6	9043.8(16)	4869.8(10)	6851.2(8)	51.0(5)
C4_6	6367(3)	4648.6(15)	6771.9(12)	36.9(7)
F7_6	5843.5(17)	4512.6(11)	6286.0(8)	55.7(5)
F8_6	6755.6(17)	5356.9(9)	6782.2(8)	51.1(5)
F9_6	5563.8(16)	4605.6(10)	7125.5(9)	54.1(5)
O1_5	8417.6(16)	2050.8(10)	6738.9(7)	31.5(4)
C1_5	8985(2)	1559.5(14)	7090.6(10)	26.6(5)
C2_5	9065(3)	1870.8(16)	7680.8(11)	37.0(7)
F1_5	9903.2(15)	2401.5(10)	7756.8(7)	42.7(4)
F2_5	9324.8(18)	1335.8(10)	8051.4(6)	50.7(5)
F3_5	8063.9(15)	2184.1(10)	7777.0(7)	44.4(4)
C3_5	8325(3)	799.4(16)	7076.5(11)	37.0(7)
F4_5	7953.0(16)	611.5(9)	6563.2(7)	44.8(4)
F5_5	7396.4(16)	834.5(10)	7353.0(8)	48.9(5)
F6_5	9005.2(17)	234.9(9)	7282.5(7)	46.4(4)
C4_5	10229(3)	1445.0(16)	6925.2(11)	34.1(6)
F7_5	10209.4(16)	998.9(9)	6488.3(6)	43.5(4)
F8_5	10947.5(15)	1140.0(10)	7323.9(7)	44.6(4)
F9_5	10696.5(14)	2097.3(9)	6797.2(7)	37.6(4)
O1_4	5918(3)	1989(4)	6499(2)	25.0(8)
C1_4	4789(4)	1964(2)	6623.9(14)	23.3(8)
C2_4	4770(3)	1801(2)	7241.5(12)	37.0(9)
F1_4	4998(4)	1090(2)	7356.0(13)	57.6(11)
F2_4	3729(5)	1951(4)	7412(3)	49.8(13)
F3_4	5570(6)	2229(4)	7527(2)	52.8(16)
C3_4	4135(3)	2708(2)	6487.7(14)	35.6(8)

F4_4	4441(6)	3000(2)	6036(3)	52.7(12)
F5_4	4375(3)	3222.7(16)	6873.2(14)	48.8(8)
F6_4	2975(3)	2620(2)	6430.6(18)	43.4(8)
C4_4	4168(3)	1320(2)	6290.4(14)	35.3(8)
F7_4	3917(4)	1515(2)	5778.3(16)	52.0(10)
F8_4	3172(3)	1119(3)	6486.6(18)	46.6(8)
F9_4	4835(5)	721(3)	6291.0(19)	45.1(10)
O1_3	6669.3(17)	2955.4(11)	4736.7(7)	36.9(5)
C1_3	6081(2)	3533.7(15)	4475.0(10)	29.9(6)
C2_3	4892(3)	3629(2)	4706.3(13)	51.6(8)
F1_3	4394.2(19)	2977.1(12)	4776.0(10)	70.9(6)
F2_3	4150.9(16)	4052.2(12)	4388.1(9)	62.0(6)
F3_3	5060(3)	3950.6(13)	5197.4(8)	81.4(8)
C3_3	6777(3)	4269.8(18)	4546.1(14)	48.7(8)
F4_3	7656.3(18)	4260.5(12)	4223.4(11)	74.1(7)
F5_3	7271(2)	4342.6(11)	5047.0(9)	76.3(7)
F6_3	6139.3(17)	4874.4(10)	4417.8(8)	54.9(5)
C4_3	5872(3)	3338.5(18)	3862.2(11)	42.6(7)
F7_3	6797.4(17)	3033.9(11)	3685.8(7)	53.4(5)
F8_3	5571.1(19)	3935.4(11)	3559.8(7)	59.3(6)
F9_3	5006.3(17)	2825.5(12)	3773.4(8)	59.3(5)
O1_2	9074.3(16)	3061.7(11)	5176.8(8)	37.9(5)
C1_2	10200(2)	3100.8(15)	5063.6(10)	28.9(6)
C2_2	10832(3)	2344.0(18)	5179.8(11)	39.4(7)
F1_2	10507(2)	2028.9(11)	5623.0(7)	59.4(5)
F2_2	11992.7(16)	2420.3(12)	5240.5(8)	59.4(5)
F3_2	10574.8(16)	1863.5(10)	4769.9(7)	47.3(4)
C3_2	10257(3)	3313.0(18)	4457.0(11)	41.0(7)
F4_2	10052.6(18)	4031.2(11)	4368.2(8)	58.1(5)
F5_2	9460.7(18)	2920.9(11)	4145.8(7)	57.3(5)
F6_2	11300.2(18)	3155.4(13)	4295.4(8)	61.9(6)
C4_2	10817(3)	3719.6(18)	5434.4(12)	42.0(7)
F7_2	10151.5(17)	4324.1(10)	5440.5(8)	52.2(5)
F8_2	11830.4(16)	3925.3(12)	5262.0(9)	61.6(6)
F9_2	11027.5(19)	3474.2(12)	5940.3(7)	59.3(5)
O1_1	7937(6)	1656(3)	5073(2)	34.0(6)
C1_1	7516(4)	1028(2)	4813.6(17)	30.5(10)
C2_1	7310(4)	1139(2)	4183.4(13)	38.0(9)
F1_1	6302(3)	1489.7(19)	4044.4(11)	45.0(8)
F2_1	7264(6)	495(4)	3919(3)	57.8(18)
F3_1	8140(7)	1558(3)	4009(3)	43.4(13)
C3_1	8427(3)	399.5(18)	4945.5(14)	40.1(9)
F4_1	8832(4)	413(5)	5467(3)	45.0(13)
F5_1	9328(4)	490(3)	4655.2(16)	54.0(11)
F6_1	7994(4)	-287.5(16)	4836.1(14)	60.3(10)
C4_1	6352(3)	799(3)	5023.2(14)	48.1(11)
F7_1	6534(5)	488(4)	5517(2)	57.4(16)
F8_1	5767(4)	308(2)	4686.1(18)	72.6(15)
F9_1	5672(6)	1380(5)	5078(2)	66(2)
O1_7	7870(30)	1617(15)	5026(10)	34.0(6)
C1_7	7372(12)	976(9)	4823(6)	28(3)
C2_7	7553(11)	322(7)	5230(5)	33(3)
F1_7	8593(17)	340(20)	5508(11)	36(5)
F2_7	7469(14)	-327(7)	4963(6)	47(3)
F3_7	6740(20)	298(14)	5579(9)	35(4)
C3_7	6057(11)	1088(8)	4648(5)	42(3)
F4_7	5858(11)	1487(8)	4199(5)	37(3)
F5_7	5640(20)	1498(18)	5041(10)	46(5)
F6_7	5454(16)	464(9)	4579(10)	67(6)
C4_7	8022(13)	820(8)	4318(5)	39(3)
F7_7	8190(30)	1460(15)	4060(15)	46(6)
F8_7	7490(20)	347(16)	3962(12)	47(6)
F9_7	9089(15)	540(13)	4468(7)	45(4)

Table 3 Bond Lengths for p21c_a.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C3	Fe1	1.821(3)	C3_4	F4_4	1.310(6)
C3	O3	1.131(3)	C3_4	F5_4	1.330(4)
Fe1	N1	1.795(3)	C3_4	F6_4	1.336(5)
Fe1	C1	1.865(3)	C4_4	F7_4	1.314(5)
Fe1	C2	1.807(3)	C4_4	F8_4	1.338(5)
Fe1	C4	1.872(3)	C4_4	F9_4	1.314(5)
N1	O5	1.135(3)	O1_3	Al2	1.6906(19)
Al1	F004	1.7662(14)	O1_3	C1_3	1.359(3)
O1	C1	1.117(3)	C1_3	C2_3	1.544(4)
O2	C2	1.106(4)	C1_3	C3_3	1.538(4)
Al2	F004	1.7654(14)	C1_3	C4_3	1.546(3)
O4	C4	1.112(3)	C2_3	F1_3	1.314(4)
O1_8	Al1	1.60(2)	C2_3	F2_3	1.332(4)
O1_8	C1_8	1.355(11)	C2_3	F3_3	1.337(4)
C1_8	C2_8	1.536(12)	C3_3	F4_3	1.349(4)
C1_8	C3_8	1.544(12)	C3_3	F5_3	1.312(4)
C1_8	C4_8	1.547(12)	C3_3	F6_3	1.324(3)
C2_8	F1_8	1.343(13)	C4_3	F7_3	1.309(3)
C2_8	F2_8	1.322(12)	C4_3	F8_3	1.325(3)
C2_8	F3_8	1.314(13)	C4_3	F9_3	1.352(4)
C3_8	F4_8	1.319(13)	O1_2	Al2	1.696(2)
C3_8	F5_8	1.325(12)	O1_2	C1_2	1.354(3)
C3_8	F6_8	1.340(13)	C1_2	C2_2	1.545(4)
C4_8	F7_8	1.337(13)	C1_2	C3_2	1.552(4)
C4_8	F8_8	1.320(13)	C1_2	C4_2	1.557(4)
C4_8	F9_8	1.318(13)	C2_2	F1_2	1.317(3)
O1_6	Al1	1.6929(18)	C2_2	F2_2	1.335(3)
O1_6	C1_6	1.358(3)	C2_2	F3_2	1.335(3)
C1_6	C2_6	1.550(3)	C3_2	F4_2	1.316(4)
C1_6	C3_6	1.548(4)	C3_2	F5_2	1.331(3)
C1_6	C4_6	1.537(4)	C3_2	F6_2	1.332(3)
C2_6	F1_6	1.322(3)	C4_2	F7_2	1.322(4)
C2_6	F2_6	1.327(3)	C4_2	F8_2	1.332(3)
C2_6	F3_6	1.338(4)	C4_2	F9_2	1.321(3)
C3_6	F4_6	1.326(3)	O1_1	Al2	1.689(6)
C3_6	F5_6	1.333(4)	O1_1	C1_1	1.354(4)
C3_6	F6_6	1.324(3)	C1_1	C2_1	1.561(5)
C4_6	F7_6	1.308(3)	C1_1	C3_1	1.546(5)
C4_6	F8_6	1.339(3)	C1_1	C4_1	1.538(5)
C4_6	F9_6	1.336(3)	C2_1	F1_1	1.331(5)
O1_5	Al1	1.7085(19)	C2_1	F2_1	1.318(5)
O1_5	C1_5	1.353(3)	C2_1	F3_1	1.318(7)
C1_5	C2_5	1.552(4)	C3_1	F4_1	1.322(6)
C1_5	C3_5	1.552(4)	C3_1	F5_1	1.328(5)
C1_5	C4_5	1.541(4)	C3_1	F6_1	1.339(4)
C2_5	F1_5	1.349(3)	C4_1	F7_1	1.336(6)
C2_5	F2_5	1.334(3)	C4_1	F8_1	1.341(5)
C2_5	F3_5	1.323(3)	C4_1	F9_1	1.313(7)
C3_5	F4_5	1.337(3)	O1_7	Al2	1.77(2)
C3_5	F5_5	1.326(3)	O1_7	C1_7	1.353(11)
C3_5	F6_5	1.342(3)	C1_7	C2_7	1.539(12)
C4_5	F7_5	1.338(3)	C1_7	C3_7	1.542(12)
C4_5	F8_5	1.334(3)	C1_7	C4_7	1.541(12)
C4_5	F9_5	1.332(3)	C2_7	F1_7	1.316(13)
O1_4	Al1	1.730(5)	C2_7	F2_7	1.331(12)
O1_4	C1_4	1.365(4)	C2_7	F3_7	1.333(13)
C1_4	C2_4	1.554(4)	C3_7	F4_7	1.316(12)
C1_4	C3_4	1.544(5)	C3_7	F5_7	1.342(13)
C1_4	C4_4	1.544(5)	C3_7	F6_7	1.312(13)
C2_4	F1_4	1.319(5)	C4_7	F7_7	1.329(13)
C2_4	F2_4	1.334(6)	C4_7	F8_7	1.321(13)
C2_4	F3_4	1.339(7)	C4_7	F9_7	1.341(13)

Table 4 Bond Angles for p21c_a.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O3	C3	Fe1	179.7(3)	F1_4	C2_4	F3_4	108.9(4)
C3	Fe1	C1	88.58(12)	F2_4	C2_4	C1_4	112.0(4)
C3	Fe1	C4	89.70(12)	F2_4	C2_4	F3_4	108.1(5)
N1	Fe1	C3	116.78(12)	F3_4	C2_4	C1_4	109.4(4)
N1	Fe1	C1	92.35(12)	F4_4	C3_4	C1_4	111.0(4)
N1	Fe1	C2	121.28(15)	F4_4	C3_4	F5_4	106.3(4)
N1	Fe1	C4	92.28(11)	F4_4	C3_4	F6_4	108.0(4)
C1	Fe1	C4	175.35(14)	F5_4	C3_4	C1_4	112.1(3)
C2	Fe1	C3	121.93(16)	F5_4	C3_4	F6_4	106.8(3)
C2	Fe1	C1	88.59(13)	F6_4	C3_4	C1_4	112.3(3)
C2	Fe1	C4	88.66(13)	F7_4	C4_4	C1_4	111.1(3)
O5	N1	Fe1	179.1(2)	F7_4	C4_4	F8_4	107.9(4)
O1_8	Al1	F004	111.5(11)	F7_4	C4_4	F9_4	106.7(4)
O1_8	Al1	O1_6	111.0(12)	F8_4	C4_4	C1_4	111.9(3)
O1_8	Al1	O1_5	108.8(12)	F9_4	C4_4	C1_4	111.5(4)
O1_6	Al1	F004	106.35(8)	F9_4	C4_4	F8_4	107.6(4)
O1_6	Al1	O1_5	117.73(10)	C1_3	O1_3	Al2	152.88(19)
O1_6	Al1	O1_4	111.5(2)	O1_3	C1_3	C2_3	108.9(2)
O1_5	Al1	F004	100.94(8)	O1_3	C1_3	C3_3	111.4(2)
O1_5	Al1	O1_4	113.5(2)	O1_3	C1_3	C4_3	108.3(2)
O1_4	Al1	F004	105.09(18)	C2_3	C1_3	C4_3	109.3(2)
O1	C1	Fe1	177.8(3)	C3_3	C1_3	C2_3	109.5(2)
O2	C2	Fe1	179.5(3)	C3_3	C1_3	C4_3	109.3(2)
F004	Al2	O1_7	105.6(7)	F1_3	C2_3	C1_3	111.4(3)
O1_3	Al2	F004	106.45(9)	F1_3	C2_3	F2_3	108.5(3)
O1_3	Al2	O1_2	115.93(11)	F1_3	C2_3	F3_3	106.6(3)
O1_2	Al2	F004	103.73(9)	F2_3	C2_3	C1_3	112.4(3)
O1_2	Al2	O1_7	115.3(10)	F2_3	C2_3	F3_3	108.4(3)
O1_1	Al2	F004	103.18(17)	F3_3	C2_3	C1_3	109.3(3)
O1_1	Al2	O1_3	112.8(3)	F4_3	C3_3	C1_3	109.6(3)
O1_1	Al2	O1_2	113.2(2)	F5_3	C3_3	C1_3	111.2(3)
Al2	F004	Al1	165.37(10)	F5_3	C3_3	F4_3	106.2(3)
O4	C4	Fe1	178.2(3)	F5_3	C3_3	F6_3	108.7(3)
C1_8	O1_8	Al1	148(3)	F6_3	C3_3	C1_3	113.5(3)
O1_8	C1_8	C2_8	109.4(16)	F6_3	C3_3	F4_3	107.4(3)
O1_8	C1_8	C3_8	109.6(16)	F7_3	C4_3	C1_3	111.6(2)
O1_8	C1_8	C4_8	109.1(17)	F7_3	C4_3	F8_3	108.7(2)
C2_8	C1_8	C3_8	110.5(11)	F7_3	C4_3	F9_3	106.0(3)
C2_8	C1_8	C4_8	109.6(12)	F8_3	C4_3	C1_3	112.1(2)
C3_8	C1_8	C4_8	108.6(11)	F8_3	C4_3	F9_3	107.9(2)
F1_8	C2_8	C1_8	111.8(13)	F9_3	C4_3	C1_3	110.4(2)
F2_8	C2_8	C1_8	110.9(14)	C1_2	O1_2	Al2	150.14(19)
F2_8	C2_8	F1_8	107.1(15)	O1_2	C1_2	C2_2	111.0(2)
F3_8	C2_8	C1_8	113.9(16)	O1_2	C1_2	C3_2	110.3(2)
F3_8	C2_8	F1_8	101.1(16)	O1_2	C1_2	C4_2	107.6(2)
F3_8	C2_8	F2_8	111.5(18)	C2_2	C1_2	C3_2	109.0(2)
F4_8	C3_8	C1_8	111.3(14)	C2_2	C1_2	C4_2	109.4(2)
F4_8	C3_8	F5_8	111.9(16)	C3_2	C1_2	C4_2	109.4(2)
F4_8	C3_8	F6_8	106.6(18)	F1_2	C2_2	C1_2	111.0(2)
F5_8	C3_8	C1_8	110.1(11)	F1_2	C2_2	F2_2	108.4(2)
F5_8	C3_8	F6_8	104.1(15)	F1_2	C2_2	F3_2	107.2(3)
F6_8	C3_8	C1_8	112.7(17)	F2_2	C2_2	C1_2	112.2(3)
F7_8	C4_8	C1_8	108.8(13)	F2_2	C2_2	F3_2	106.9(2)
F8_8	C4_8	C1_8	113.9(15)	F3_2	C2_2	C1_2	110.9(2)
F8_8	C4_8	F7_8	107.0(16)	F4_2	C3_2	C1_2	111.9(2)
F9_8	C4_8	C1_8	110.3(15)	F4_2	C3_2	F5_2	108.3(2)
F9_8	C4_8	F7_8	105.3(17)	F4_2	C3_2	F6_2	107.8(2)
F9_8	C4_8	F8_8	111.1(17)	F5_2	C3_2	C1_2	109.5(2)
C1_6	O1_6	Al1	151.43(17)	F5_2	C3_2	F6_2	107.7(3)
O1_6	C1_6	C2_6	108.7(2)	F6_2	C3_2	C1_2	111.5(2)
O1_6	C1_6	C3_6	111.1(2)	F7_2	C4_2	C1_2	110.8(2)
O1_6	C1_6	C4_6	108.5(2)	F7_2	C4_2	F8_2	107.8(3)
C3_6	C1_6	C2_6	109.4(2)	F8_2	C4_2	C1_2	111.6(2)
C4_6	C1_6	C2_6	109.3(2)	F9_2	C4_2	C1_2	110.4(3)

C4_6 C1_6 C3_6	109.9(2)	F9_2 C4_2 F7_2	108.0(2)
F1_6 C2_6 C1_6	111.1(2)	F9_2 C4_2 F8_2	108.1(3)
F1_6 C2_6 F2_6	108.3(2)	C1_1 O1_1 Al2	146.7(6)
F1_6 C2_6 F3_6	107.1(2)	O1_1 C1_1 C2_1	112.1(4)
F2_6 C2_6 C1_6	112.4(2)	O1_1 C1_1 C3_1	107.3(5)
F2_6 C2_6 F3_6	107.4(2)	O1_1 C1_1 C4_1	109.9(4)
F3_6 C2_6 C1_6	110.3(2)	C3_1 C1_1 C2_1	109.3(3)
F4_6 C3_6 C1_6	110.5(2)	C4_1 C1_1 C2_1	108.7(3)
F4_6 C3_6 F5_6	106.9(2)	C4_1 C1_1 C3_1	109.3(3)
F5_6 C3_6 C1_6	109.7(2)	F1_1 C2_1 C1_1	110.8(3)
F6_6 C3_6 C1_6	113.3(2)	F2_1 C2_1 C1_1	112.2(4)
F6_6 C3_6 F4_6	108.1(2)	F2_1 C2_1 F1_1	106.9(4)
F6_6 C3_6 F5_6	108.3(2)	F2_1 C2_1 F3_1	109.0(5)
F7_6 C4_6 C1_6	111.2(2)	F3_1 C2_1 C1_1	110.9(5)
F7_6 C4_6 F8_6	108.3(2)	F3_1 C2_1 F1_1	106.9(4)
F7_6 C4_6 F9_6	107.7(2)	F4_1 C3_1 C1_1	110.8(4)
F8_6 C4_6 C1_6	111.6(2)	F4_1 C3_1 F5_1	107.8(4)
F9_6 C4_6 C1_6	110.8(2)	F4_1 C3_1 F6_1	107.4(4)
F9_6 C4_6 F8_6	107.1(2)	F5_1 C3_1 C1_1	110.3(3)
C1_5 O1_5 Al1	149.79(18)	F5_1 C3_1 F6_1	107.3(4)
O1_5 C1_5 C2_5	110.4(2)	F6_1 C3_1 C1_1	113.0(4)
O1_5 C1_5 C3_5	110.4(2)	F7_1 C4_1 C1_1	110.9(4)
O1_5 C1_5 C4_5	108.4(2)	F7_1 C4_1 F8_1	108.4(5)
C3_5 C1_5 C2_5	108.3(2)	F8_1 C4_1 C1_1	111.3(3)
C4_5 C1_5 C2_5	109.2(2)	F9_1 C4_1 C1_1	112.0(5)
C4_5 C1_5 C3_5	110.1(2)	F9_1 C4_1 F7_1	105.8(5)
F1_5 C2_5 C1_5	110.7(2)	F9_1 C4_1 F8_1	108.2(5)
F2_5 C2_5 C1_5	112.0(2)	C1_7 O1_7 Al2	150(3)
F2_5 C2_5 F1_5	107.4(2)	O1_7 C1_7 C2_7	111.9(17)
F3_5 C2_5 C1_5	110.5(2)	O1_7 C1_7 C3_7	111.3(18)
F3_5 C2_5 F1_5	107.5(2)	O1_7 C1_7 C4_7	103.2(11)
F3_5 C2_5 F2_5	108.4(2)	C2_7 C1_7 C3_7	110.1(10)
F4_5 C3_5 C1_5	110.4(2)	C2_7 C1_7 C4_7	110.2(10)
F4_5 C3_5 F6_5	106.7(2)	C4_7 C1_7 C3_7	109.9(11)
F5_5 C3_5 C1_5	111.4(2)	F1_7 C2_7 C1_7	112.2(16)
F5_5 C3_5 F4_5	107.7(2)	F1_7 C2_7 F2_7	107.2(17)
F5_5 C3_5 F6_5	108.0(2)	F1_7 C2_7 F3_7	108.7(16)
F6_5 C3_5 C1_5	112.4(2)	F2_7 C2_7 C1_7	109.7(11)
F7_5 C4_5 C1_5	110.7(2)	F2_7 C2_7 F3_7	105.8(15)
F8_5 C4_5 C1_5	112.3(2)	F3_7 C2_7 C1_7	113.0(12)
F8_5 C4_5 F7_5	108.1(2)	F4_7 C3_7 C1_7	112.7(11)
F9_5 C4_5 C1_5	110.8(2)	F4_7 C3_7 F5_7	105.6(17)
F9_5 C4_5 F7_5	107.6(2)	F5_7 C3_7 C1_7	106.3(13)
F9_5 C4_5 F8_5	107.2(2)	F6_7 C3_7 C1_7	114.6(12)
C1_4 O1_4 Al1	145.5(5)	F6_7 C3_7 F4_7	107.8(13)
O1_4 C1_4 C2_4	109.7(4)	F6_7 C3_7 F5_7	109.4(17)
O1_4 C1_4 C3_4	112.1(4)	F7_7 C4_7 C1_7	109.8(17)
O1_4 C1_4 C4_4	107.6(4)	F7_7 C4_7 F9_7	106.2(18)
C3_4 C1_4 C2_4	108.6(3)	F8_7 C4_7 C1_7	115.2(16)
C4_4 C1_4 C2_4	109.4(3)	F8_7 C4_7 F7_7	107.8(18)
C4_4 C1_4 C3_4	109.6(3)	F8_7 C4_7 F9_7	106.9(16)
F1_4 C2_4 C1_4	111.5(3)	F9_7 C4_7 C1_7	110.6(11)
F1_4 C2_4 F2_4	106.8(4)		

P–1 structure of 1

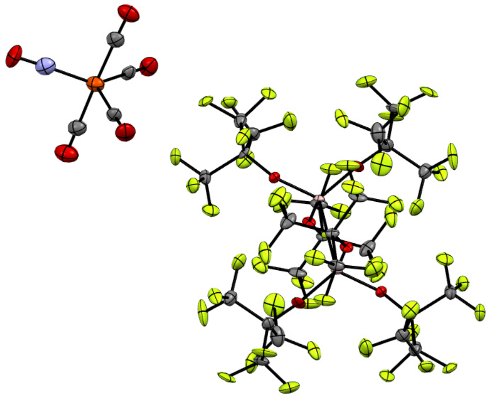


Table 1 Crystal data and structure refinement for p-1_a.

Identification code	p-1_a
Empirical formula	$C_{28}NO_{11}F_{55}Al_2Fe$
Formula weight	1681.10
Temperature/K	100.01
Crystal system	triclinic
Space group	P-1
a/Å	10.296(5)
b/Å	22.904(14)
c/Å	23.622(10)
α/°	109.683(17)
β/°	100.670(16)
γ/°	100.491(7)
Volume/Å^3	4971(4)
Z	4
ρ_{calc}g/cm^3	2.246
μ/mm^{-1}	0.602
F(000)	3240.0
Crystal size/mm^3	0.2 × 0.15 × 0.1
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	1.9 to 55.754
Index ranges	$-13 \leq h \leq 13$, $-30 \leq k \leq 30$, $-31 \leq l \leq 31$
Reflections collected	127020
Independent reflections	23725 [R_{int} = 0.0400, R_{sigma} = 0.0334]
Data/restraints/parameters	23725/32297/2361
Goodness-of-fit on F^2	1.063
Final R indexes [I>=2σ (I)]	R_1 = 0.0461, wR_2 = 0.1046
Final R indexes [all data]	R_1 = 0.0685, wR_2 = 0.1161
Largest diff. peak/hole / e Å^{-3}	1.52/-0.67

Table 2 Fractional Atomic Coordinates (×10[4]) and Equivalent Isotropic Displacement Parameters (Å[2]×10[3]) for p-1_a. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Fe1	-2742.0(5)	7843.5(2)	1590.4(2)	32.96(11)
N1	-4090(3)	7247.2(14)	948.8(14)	39.0(7)
F1	365.5(15)	5221.9(7)	2574.4(6)	16.4(3)
Al1	276.3(7)	5180.3(3)	3297.6(3)	11.37(14)
O1	-1466(3)	9136.5(11)	1650.2(12)	41.9(6)
C1	-1955(3)	8648.7(14)	1627.9(14)	26.5(6)
O3	-4923(3)	6855.1(13)	553.3(12)	48.1(7)
F3	5000	10000	10000	17.4(4)
Al3	5639.6(7)	9645.3(3)	5516.4(3)	11.02(14)
Fe2	2888.3(5)	2513.6(2)	3493.0(2)	29.70(10)
N2	2544(3)	2848.7(12)	2914.7(13)	31.4(6)
F2	5000	10000	5000	13.5(4)
Al2	356.2(7)	5282.5(3)	1848.3(3)	11.19(14)
O2	-4714(3)	8411.0(12)	2231.8(13)	43.9(6)
C2	-3992(3)	8191.3(15)	1984.6(16)	32.1(7)
O4	-660(3)	7380.1(13)	954.2(14)	51.1(7)
Al4	5944.9(7)	10818.4(3)	10318.6(3)	11.73(14)
C4	-1437(3)	7545.9(16)	1197.5(17)	35.9(7)
O5	-1806(3)	7499.0(12)	2655.3(12)	45.9(6)
C5	-2129(3)	7632.0(14)	2246.4(14)	27.1(6)
O6	2915(2)	3672.0(10)	4567.3(11)	35.9(5)
C6	2908(3)	3247.9(14)	4152.5(15)	27.7(6)
O7	2371(3)	3052.9(11)	2541.6(10)	37.9(6)
O8	759(3)	1800.2(14)	3856.4(14)	57.5(8)
C8	1576(4)	2069.0(16)	3711.0(16)	37.3(8)
O9	2854(3)	1258.4(11)	2541.3(11)	44.8(6)
C9	2886(4)	1732.4(16)	2893.3(15)	33.1(7)
C10	4717(3)	2667.9(13)	3864.2(15)	25.1(6)
O10	5838(2)	2784.9(11)	4096.3(13)	45.7(6)
O1_17	5890(40)	8929(12)	5112(15)	21(9)
C1_17	6193(17)	8512(8)	4627(8)	21(4)
C2_17	6765(16)	8020(7)	4847(8)	24(4)
F1_17	8056(15)	8294(9)	5189(9)	42.9(6)
F2_17	6760(20)	7510(10)	4364(10)	40(6)
F3_17	6070(30)	7837(19)	5203(17)	37(8)
C3_17	4878(16)	8155(9)	4083(8)	26(4)
F4_17	4180(40)	8569(16)	4010(20)	35(8)
F5_17	4100(20)	7706(11)	4201(12)	32(5)
F6_17	5170(30)	7871(10)	3548(9)	44(6)
C4_17	7270(20)	8871(9)	4391(10)	36(5)
F7_17	6670(20)	9175(9)	4072(9)	44(5)
F8_17	7770(40)	8462(18)	3996(16)	36(8)
F9_17	8280(30)	9288(15)	4872(14)	29(7)
O1_16	-1000(30)	4503(11)	3063(15)	19.8(6)
C1_16	-1521(14)	3995(7)	3196(6)	22(3)
C2_16	-2906(12)	3624(6)	2696(6)	35(3)
F1_16	-2650(20)	3315(12)	2162(7)	49(5)
F2_16	-3650(20)	3206(8)	2867(10)	43(5)
F3_16	-3630(30)	4025(13)	2616(16)	43(7)
C3_16	-1757(14)	4219(6)	3856(6)	31(3)
F4_16	-660(30)	4664(16)	4268(15)	37.0(6)
F5_16	-2833(15)	4463(8)	3869(7)	49(4)
F6_16	-2010(30)	3727(12)	4032(15)	49(6)
C4_16	-534(12)	3553(6)	3163(6)	32(3)
F7_16	484(15)	3804(9)	3679(6)	37(4)
F8_16	-1168(15)	2966(6)	3106(7)	42(3)
F9_16	-50(30)	3481(11)	2668(10)	30(6)
O1_15	-20(30)	5889(10)	3707(13)	18.3(10)
C1_15	-808(12)	6309(6)	3831(5)	17(3)
C2_15	-1344(9)	6288(4)	4395(4)	29(2)
F1_15	-360(20)	6295(12)	4845(10)	47(5)
F2_15	-1863(11)	6784(5)	4622(6)	36(3)
F3_15	-2343(9)	5756(4)	4222(5)	50(2)

C3_15	-2025(11)	6122(5)	3248(5)	37(3)
F4_15	-1539(11)	6290(5)	2821(3)	62(3)
F5_15	-2611(15)	5495(6)	3043(8)	50(4)
F6_15	-2960(30)	6433(14)	3385(15)	45(5)
C4_15	112(11)	6988(5)	3992(5)	35(3)
F7_15	874(11)	6942(5)	3591(5)	48(3)
F8_15	-509(19)	7442(8)	3993(11)	53(5)
F9_15	945(8)	7206(3)	4569(4)	55(2)
O1_14	7090(20)	10200(13)	6032(11)	13.7(7)
C1_14	8132(15)	10399(6)	6558(7)	16(3)
C2_14	7968(12)	9881(6)	6848(6)	24(3)
F1_14	7710(40)	9301(9)	6403(12)	42(8)
F2_14	9137(15)	9971(11)	7265(7)	30(4)
F3_14	7001(10)	9926(6)	7146(5)	31(3)
C3_14	8065(14)	11051(5)	7021(6)	22(3)
F4_14	8519(10)	11522(4)	6838(5)	26(2)
F5_14	6790(20)	11022(14)	7061(17)	31(5)
F6_14	8890(40)	11213(15)	7589(10)	31(5)
C4_14	9521(12)	10485(6)	6391(6)	25(3)
F7_14	9510(30)	10795(11)	6002(10)	29(4)
F8_14	10590(20)	10826(11)	6888(10)	27(5)
F9_14	9756(11)	9917(5)	6120(5)	31(3)
O1_13	4560(20)	9607(11)	5979(10)	15.7(10)
C1_13	3476(10)	9251(4)	6071(4)	14.9(8)
C2_13	2726(7)	9724(4)	6436(3)	23.8(14)
F1_13	1983(4)	9920(2)	6046(2)	37.3(13)
F2_13	1868(15)	9438(6)	6684(8)	32(3)
F3_13	3607(8)	10231(4)	6884(4)	31.8(18)
C3_13	4008(6)	8890(3)	6481(3)	23.1(13)
F4_13	4975(15)	8632(11)	6265(9)	32(3)
F5_13	4563(5)	9287(2)	7070.0(19)	33.9(11)
F6_13	3015(6)	8416(3)	6464(3)	31.0(13)
C4_13	2492(7)	8759(3)	5443(3)	28.6(15)
F7_13	2988(6)	8250(3)	5217(3)	39.0(14)
F8_13	1253(10)	8545(8)	5505(6)	39(3)
F9_13	2342(17)	9029(7)	5026(5)	41(2)
O1_12	1574.5(18)	5991.3(9)	2079.5(9)	20.1(4)
C1_12	2236(3)	6454.7(12)	1919.0(12)	17.5(5)
C2_12	1815(3)	6282.9(13)	1205.0(13)	26.3(6)
F1_12	1710(2)	5664.9(8)	903.6(8)	37.0(4)
F2_12	2695(2)	6629.4(9)	1020.0(9)	42.6(5)
F3_12	585(2)	6372.1(9)	1025.7(9)	41.6(5)
C3_12	1895(3)	7097.9(13)	2250.8(14)	26.4(6)
F4_12	2465(2)	7332.0(9)	2858.0(8)	38.3(5)
F5_12	546.7(19)	7005.9(9)	2165.8(10)	39.9(5)
F6_12	2324(2)	7546.3(8)	2033.9(10)	41.0(5)
C4_12	3797(3)	6528.1(14)	2131.2(14)	25.4(6)
F7_12	4165.2(18)	6556.8(10)	2708.8(9)	39.3(5)
F8_12	4559.5(18)	7069.7(8)	2125.7(9)	34.4(4)
F9_12	4145.1(19)	6042.3(9)	1760.2(10)	42.7(5)
O1_11	-1229.8(18)	5361.6(9)	1582.9(8)	20.0(4)
C1_11	-2451(2)	5090.5(12)	1147.5(11)	16.6(5)
C2_11	-3412(3)	4630.4(14)	1337.8(13)	25.4(6)
F1_11	-2710.5(19)	4288.9(9)	1566.6(9)	38.6(4)
F2_11	-4451.3(17)	4220.6(9)	860.1(9)	35.0(4)
F3_11	-3952.4(18)	4956.9(9)	1776.5(8)	34.7(4)
C3_11	-3092(3)	5642.9(14)	1104.3(14)	26.3(6)
F4_11	-2456(2)	5956.3(10)	803.3(11)	44.4(5)
F5_11	-2943.1(18)	6077.3(8)	1671.6(9)	36.0(4)
F6_11	-4415.2(17)	5437.0(9)	811.7(8)	33.8(4)
C4_11	-2266(3)	4706.5(14)	497.4(12)	23.2(6)
F7_11	-1137.4(17)	5009.9(9)	413.9(8)	31.7(4)
F8_11	-3326.6(18)	4624.4(10)	32.4(8)	37.8(5)
F9_11	-2140.6(17)	4124.2(8)	452.1(8)	30.3(4)
O1_10	639.7(18)	4599.4(8)	1381.9(8)	18.2(4)
C1_10	1346(2)	4145.4(12)	1275.2(11)	15.5(5)

C2_10	2511(3)	4296.9(13)	1867.2(12)	20.9(5)
F1_10	3148.6(17)	4918.9(8)	2118.1(8)	30.1(4)
F2_10	3432.5(17)	3965.9(9)	1757.9(9)	31.8(4)
F3_10	1977.0(18)	4160.7(8)	2298.6(8)	28.3(4)
C3_10	347(3)	3477.8(13)	1102.1(13)	25.0(6)
F4_10	-400.2(19)	3249.5(8)	510.5(8)	36.2(4)
F5_10	-518.3(18)	3523.0(9)	1454.2(9)	36.2(4)
F6_10	1012(2)	3049.0(8)	1177.6(10)	38.3(4)
C4_10	1971(3)	4140.3(13)	725.0(12)	21.9(5)
F7_10	1059.6(18)	4164.5(9)	263.3(8)	31.9(4)
F8_10	2399.2(19)	3609.0(9)	498.1(8)	34.3(4)
F9_10	3041.0(17)	4644.5(8)	906.8(8)	28.9(4)
O1_9	-1050(7)	4517(3)	3090(4)	19.8(6)
C1_9	-1618(4)	3989(2)	3189.4(18)	14.8(8)
C2_9	-942(4)	4031.4(16)	3852.8(15)	21.8(7)
F1_9	263(3)	3890(2)	3878.6(16)	33.0(9)
F2_9	-1720(6)	3629(3)	4026(3)	26.8(8)
F3_9	-719(7)	4627(4)	4264(4)	37.0(6)
C3_9	-3175(3)	3929.4(17)	3111.8(17)	24.7(8)
F4_9	-3708(8)	4062(4)	2632(4)	43.0(18)
F5_9	-3375(3)	4338.6(16)	3621.6(17)	38.7(8)
F6_9	-3888(5)	3342.4(19)	3025(2)	33.4(9)
C4_9	-1422(3)	3380.9(16)	2702.9(16)	24.2(8)
F7_9	-2240(5)	3237(3)	2144.5(17)	35.2(10)
F8_9	-1691(4)	2869.3(13)	2857.7(15)	32.9(7)
F9_9	-127(7)	3487(3)	2667(3)	39.1(17)
O1_8	1805.2(17)	5065.6(8)	3604.1(8)	15.3(3)
C1_8	3040(2)	5367.1(11)	4034.8(11)	15.3(5)
C2_8	3628(3)	6049.8(13)	4059.6(13)	23.3(6)
F1_8	3316(2)	6061.0(9)	3494.4(8)	36.4(4)
F2_8	4982.2(17)	6258.6(8)	4293.6(9)	32.3(4)
F3_8	3090.6(18)	6477.2(8)	4416.5(8)	30.9(4)
C3_8	2877(3)	5423.6(13)	4690.2(12)	19.6(5)
F4_8	2696.6(17)	4858.3(8)	4746.0(7)	25.4(3)
F5_8	1791.0(17)	5636.4(8)	4788.4(7)	26.7(4)
F6_8	3976.5(17)	5830.1(8)	5149.9(7)	26.5(4)
C4_8	4038(3)	4947.9(13)	3852.9(12)	20.9(5)
F7_8	3426.7(17)	4326.1(7)	3679.9(8)	26.9(4)
F8_8	5142.9(16)	5104.3(8)	4319.8(7)	26.0(4)
F9_8	4439.9(17)	5016.5(9)	3367.0(8)	28.7(4)
O1_7	157(10)	5908(4)	3766(5)	18.3(10)
C1_7	-573(6)	6347(3)	3886(2)	16.2(11)
C2_7	-2115(5)	6038(2)	3531(2)	34.2(11)
F1_7	-2200(6)	5636(3)	2952(3)	54.4(16)
F2_7	-2790(12)	6464(6)	3481(6)	50(2)
F3_7	-2715(3)	5706.4(16)	3816(2)	55.1(11)
C3_7	-418(4)	6631(2)	4595.0(19)	25.2(9)
F4_7	835(3)	7008.9(15)	4903.9(14)	44.3(8)
F5_7	-611(9)	6162(5)	4809(4)	40.6(16)
F6_7	-1307(5)	6972(2)	4745(3)	39.5(12)
C4_7	6(6)	6897(3)	3682(3)	34.4(12)
F7_7	1364(4)	7093(2)	3882(2)	47.2(11)
F8_7	-499(10)	7396(4)	3896(4)	50.2(19)
F9_7	-358(4)	6690(2)	3062.6(16)	59.1(12)
O1_6	5812(5)	8919.7(16)	5071(2)	15.5(10)
C1_6	6096(3)	8535.7(15)	4556.0(16)	14.4(6)
C2_6	5213(3)	8562.2(14)	3964.1(14)	21.9(6)
F1_6	3925(5)	8518(2)	3994(3)	32.5(9)
F2_6	5208(3)	8093.5(12)	3438.9(11)	31.2(6)
F3_6	5685(3)	9119.8(9)	3915.3(9)	32.5(5)
C3_6	7639(3)	8749.2(16)	4587.5(16)	26.2(7)
F4_6	8396(2)	8566.8(12)	4980.9(11)	42.9(6)
F5_6	8050(4)	9388.8(19)	4791(2)	33.3(10)
F6_6	7893(5)	8504(2)	4039(2)	44.3(14)
C4_6	5745(3)	7834.2(14)	4524.3(15)	23.1(7)
F7_6	6190(5)	7818(2)	5084(2)	36.7(9)

F8_6	6305(3)	7459.7(12)	4133.5(13)	33.2(7)
F9_6	4405(3)	7578.6(14)	4332.3(18)	36.2(8)
O1_5	4460(15)	9552(8)	5925(8)	15.7(10)
C1_5	3338(8)	9171(3)	5967(3)	14.9(8)
C2_5	3044(5)	9524(3)	6599(2)	24.2(11)
F1_5	3951(4)	9499.6(19)	7068.5(15)	33.7(9)
F2_5	1795(11)	9261(4)	6623(6)	25.9(17)
F3_5	3145(7)	10140(3)	6709(4)	34.7(15)
C3_5	2090(5)	9041(3)	5416(3)	23.2(11)
F4_5	2479(13)	8907(5)	4888(4)	33.1(16)
F5_5	1612(3)	9559.8(18)	5506.9(19)	37.4(10)
F6_5	1069(8)	8550(5)	5343(4)	30.6(16)
C4_5	3584(5)	8516(2)	5948(2)	20.0(10)
F7_5	3478(4)	8125.7(19)	5375.1(19)	27.5(9)
F8_5	2712(5)	8214(2)	6174(2)	25.9(9)
F9_5	4854(11)	8609(8)	6297(6)	29(2)
O1_4	7119(5)	10222(3)	5967(2)	13.7(7)
C1_4	8165(4)	10402.2(19)	6488(2)	15.0(8)
C2_4	8644(3)	9813.9(16)	6545.2(16)	23.4(8)
F1_4	7543(8)	9322(2)	6419(3)	31.9(11)
F2_4	9429(4)	9934(3)	7108.6(16)	31.8(9)
F3_4	9340(3)	9604.8(14)	6134.2(12)	34.0(6)
C3_4	9368(4)	10874.3(18)	6429.6(18)	26.8(8)
F4_4	9126(3)	11446.6(11)	6537.0(13)	43.5(8)
F5_4	9553(8)	10651(3)	5862(2)	33.9(12)
F6_4	10556(6)	10964(3)	6840(3)	36.5(14)
C4_4	7722(4)	10738(2)	7083.6(16)	29.2(9)
F7_4	6993(5)	11137(3)	6998(4)	43.1(13)
F8_4	8801(9)	11080(4)	7578(2)	37.6(15)
F9_4	6959(3)	10307.4(19)	7230.8(12)	43.7(8)
O1_3	6746(2)	10942.3(10)	9789.7(8)	27.3(5)
C1_3	6858(3)	10883.4(12)	9213.1(12)	18.7(5)
C2_3	7307(4)	11563.3(15)	9199.0(14)	34.1(7)
F1_3	6248(3)	11820.1(10)	9158.3(11)	53.8(6)
F2_3	7805(2)	11540.0(10)	8710.7(9)	49.4(6)
F3_3	8281(2)	11946.1(9)	9709.2(9)	46.2(5)
C3_3	7944(3)	10511.8(15)	9060.6(14)	29.8(6)
F4_3	7772(2)	10010.8(9)	9229.2(9)	42.3(5)
F5_3	9207.0(18)	10893.9(10)	9374.8(9)	40.7(5)
F6_3	7865(2)	10287.6(11)	8452.4(8)	44.5(5)
C4_3	5455(3)	10507.8(15)	8717.5(13)	28.8(6)
F7_3	5210(2)	9884.5(9)	8613.5(9)	38.9(4)
F8_3	5424(2)	10580.2(9)	8179.1(8)	36.5(4)
F9_3	4456.4(19)	10722.6(11)	8928.5(10)	48.7(6)
O1_2	4653.5(19)	11183.9(9)	10427.7(9)	21.1(4)
C1_2	4328(3)	11733.9(12)	10717.8(12)	18.7(5)
C2_2	4366(3)	11817.9(14)	11402.1(14)	30.8(7)
F1_2	3773(3)	11269.2(10)	11426.4(10)	59.2(7)
F2_2	3721(2)	12248.6(11)	11666.9(10)	53.0(6)
F3_2	5646(2)	12011.5(9)	11753.9(8)	35.8(4)
C3_2	5361(3)	12327.5(14)	10724.7(14)	30.5(7)
F4_2	5105(3)	12353.4(10)	10158.9(10)	54.1(6)
F5_2	6630.5(19)	12266.7(9)	10858.9(9)	39.4(5)
F6_2	5307(2)	12874.8(8)	11132.1(10)	45.0(5)
C4_2	2864(3)	11684.1(15)	10358.4(15)	35.3(7)
F7_2	2730(2)	11477.2(9)	9748.4(9)	42.8(5)
F8_2	2566(2)	12249.3(11)	10533.6(12)	66.4(8)
F9_2	1937.4(19)	11270.9(11)	10452.5(11)	52.7(6)
O1_1	7066.6(18)	10927.9(9)	10998.1(8)	17.5(4)
C1_1	8357(2)	10996.9(12)	11323.4(11)	16.6(5)
C2_1	8927(3)	10430.0(13)	10988.4(13)	23.3(6)
F1_1	7945.0(19)	9880.7(8)	10751.4(9)	35.5(4)
F2_1	9953.5(19)	10360.8(10)	11370.9(9)	38.4(4)
F3_1	9364.2(18)	10508.2(9)	10518.8(8)	30.4(4)
C3_1	9324(3)	11638.9(13)	11400.8(13)	25.0(6)
F4_1	9088(2)	12134.2(8)	11817.2(9)	41.7(5)

F5_1	9158.6(18)	11721.9(8)	10868.3(8)	32.1(4)
F6_1	10652.2(17)	11659.6(9)	11598.8(9)	35.9(4)
C4_1	8286(3)	11002.0(14)	11976.4(13)	24.5(6)
F7_1	7501.1(19)	11357.5(9)	12212.4(8)	34.7(4)
F8_1	9536.3(18)	11230.8(10)	12386.9(8)	37.8(4)
F9_1	7787.3(18)	10409.4(9)	11944.4(8)	31.6(4)

Table 3 Bond Lengths for p-1_a.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Fe1	N1	1.796(3)	C2_11	F1_11	1.331(3)
Fe1	C1	1.840(3)	C2_11	F2_11	1.331(3)
Fe1	C2	1.864(4)	C2_11	F3_11	1.336(3)
Fe1	C4	1.871(4)	C3_11	F4_11	1.340(3)
Fe1	C5	1.814(3)	C3_11	F5_11	1.334(3)
N1	O3	1.128(4)	C3_11	F6_11	1.324(3)
F1	Al1	1.7608(17)	C4_11	F7_11	1.325(3)
F1	Al2	1.7654(17)	C4_11	F8_11	1.333(3)
O1	C1	1.118(4)	C4_11	F9_11	1.334(3)
F3	Al4[1]	1.7722(12)	O1_10	Al2	1.694(2)
F3	Al4	1.7722(12)	O1_10	C1_10	1.357(3)
Al3	F2	1.7739(9)	C1_10	C2_10	1.554(4)
Fe2	N2	1.791(3)	C1_10	C3_10	1.554(4)
Fe2	C6	1.862(3)	C1_10	C4_10	1.551(3)
Fe2	C8	1.799(4)	C2_10	F1_10	1.326(3)
Fe2	C9	1.870(3)	C2_10	F2_10	1.328(3)
Fe2	C10	1.838(3)	C2_10	F3_10	1.341(3)
N2	O7	1.130(3)	C3_10	F4_10	1.335(3)
O2	C2	1.117(4)	C3_10	F5_10	1.322(3)
O4	C4	1.118(4)	C3_10	F6_10	1.335(3)
O5	C5	1.119(4)	C4_10	F7_10	1.324(3)
O6	C6	1.121(4)	C4_10	F8_10	1.344(3)
O8	C8	1.125(4)	C4_10	F9_10	1.326(3)
O9	C9	1.114(4)	O1_9	Al1	1.706(4)
C10	O10	1.121(4)	O1_9	C1_9	1.358(4)
O1_17	Al3	1.694(14)	C1_9	C2_9	1.555(5)
O1_17	C1_17	1.349(13)	C1_9	C3_9	1.554(5)
C1_17	C2_17	1.552(12)	C1_9	C4_9	1.552(5)
C1_17	C3_17	1.549(12)	C2_9	F1_9	1.335(5)
C1_17	C4_17	1.553(13)	C2_9	F2_9	1.329(5)
C2_17	F1_17	1.330(13)	C2_9	F3_9	1.330(7)
C2_17	F2_17	1.329(13)	C3_9	F4_9	1.318(7)
C2_17	F3_17	1.323(13)	C3_9	F5_9	1.332(5)
C3_17	F4_17	1.329(13)	C3_9	F6_9	1.338(5)
C3_17	F5_17	1.327(13)	C4_9	F7_9	1.324(5)
C3_17	F6_17	1.331(13)	C4_9	F8_9	1.338(4)
C4_17	F7_17	1.332(13)	C4_9	F9_9	1.335(6)
C4_17	F8_17	1.334(13)	O1_8	Al1	1.7111(19)
C4_17	F9_17	1.324(13)	O1_8	C1_8	1.363(3)
O1_16	Al1	1.687(13)	C1_8	C2_8	1.548(4)
O1_16	C1_16	1.350(13)	C1_8	C3_8	1.553(3)
O1_16	C1_9	1.385(18)	C1_8	C4_8	1.552(3)
C1_16	C2_16	1.553(12)	C2_8	F1_8	1.324(3)
C1_16	C3_16	1.550(12)	C2_8	F2_8	1.331(3)
C1_16	C4_16	1.554(12)	C2_8	F3_8	1.338(3)
C1_16	O1_9	1.326(19)	C3_8	F4_8	1.328(3)
C1_16	C2_9	1.524(15)	C3_8	F5_8	1.326(3)
C1_16	C3_9	1.650(14)	C3_8	F6_8	1.345(3)
C1_16	C4_9	1.529(14)	C4_8	F7_8	1.334(3)
C2_16	F1_16	1.322(12)	C4_8	F8_8	1.326(3)
C2_16	F2_16	1.334(12)	C4_8	F9_8	1.336(3)
C2_16	F3_16	1.325(13)	O1_7	Al1	1.702(5)
C2_16	C1_9	1.478(13)	O1_7	C1_7	1.349(6)
C2_16	C3_9	1.113(14)	C1_7	C2_7	1.557(6)
C2_16	F4_9	1.438(17)	C1_7	C3_7	1.543(6)
C2_16	F6_9	1.560(13)	C1_7	C4_7	1.556(7)
C2_16	C4_9	1.718(14)	C2_7	F1_7	1.343(7)

C2_16	F7_9	1.652(15)	C2_7	F2_7	1.321(8)
F1_16	C4_9	1.57(2)	C2_7	F3_7	1.317(7)
F2_16	C3_9	1.508(17)	C3_7	F4_7	1.328(5)
F2_16	F6_9	0.527(18)	C3_7	F5_7	1.332(8)
F3_16	C3_9	1.28(3)	C3_7	F6_7	1.331(5)
C3_16	F4_16	1.328(13)	C4_7	F7_7	1.328(6)
C3_16	F5_16	1.328(12)	C4_7	F8_7	1.325(7)
C3_16	F6_16	1.328(13)	C4_7	F9_7	1.330(6)
C3_16	C1_9	1.527(14)	O1_6	Al3	1.703(3)
C3_16	C2_9	1.010(13)	O1_6	C1_6	1.357(4)
C3_16	F2_9	1.539(15)	C1_6	C2_6	1.546(4)
C3_16	F3_9	1.262(16)	C1_6	C3_6	1.555(4)
C3_16	C3_9	1.890(14)	C1_6	C4_6	1.554(4)
C3_16	F5_9	1.756(14)	C2_6	F1_6	1.328(5)
F4_16	C2_9	1.39(3)	C2_6	F2_6	1.338(4)
F5_16	C3_9	1.718(16)	C2_6	F3_6	1.332(4)
F5_16	F5_9	0.666(14)	C3_6	F4_6	1.326(4)
F6_16	C2_9	1.40(2)	C3_6	F5_6	1.335(5)
C4_16	F7_16	1.323(12)	C3_6	F6_6	1.324(5)
C4_16	F8_16	1.333(11)	C4_6	F7_6	1.332(5)
C4_16	F9_16	1.327(12)	C4_6	F8_6	1.328(4)
C4_16	C1_9	1.623(14)	C4_6	F9_6	1.322(4)
C4_16	C2_9	1.803(13)	O1_5	Al3	1.713(8)
C4_16	F1_9	1.582(14)	O1_5	C1_5	1.355(8)
C4_16	C4_9	1.177(13)	C1_5	C2_5	1.555(8)
C4_16	F8_9	1.623(12)	C1_5	C3_5	1.554(8)
C4_16	F9_9	1.288(15)	C1_5	C4_5	1.554(8)
F7_16	C2_9	1.718(16)	C2_5	F1_5	1.334(7)
F7_16	F1_9	0.553(15)	C2_5	F2_5	1.337(9)
F8_16	C4_9	1.576(14)	C2_5	F3_5	1.328(8)
F8_16	F8_9	0.659(13)	C3_5	F4_5	1.334(7)
F9_16	C4_9	1.41(2)	C3_5	F5_5	1.333(6)
O1_15	Al1	1.702(12)	C3_5	F6_5	1.332(9)
O1_15	C1_15	1.360(12)	C4_5	F7_5	1.318(6)
C1_15	C2_15	1.543(11)	C4_5	F8_5	1.331(6)
C1_15	C3_15	1.556(11)	C4_5	F9_5	1.348(10)
C1_15	C4_15	1.548(11)	O1_4	Al3	1.708(4)
C2_15	F1_15	1.322(12)	O1_4	C1_4	1.360(4)
C2_15	F2_15	1.335(10)	C1_4	C2_4	1.555(5)
C2_15	F3_15	1.328(10)	C1_4	C3_4	1.549(5)
C3_15	F4_15	1.339(11)	C1_4	C4_4	1.554(5)
C3_15	F5_15	1.331(11)	C2_4	F1_4	1.352(6)
C3_15	F6_15	1.324(12)	C2_4	F2_4	1.332(4)
C4_15	F7_15	1.327(11)	C2_4	F3_4	1.324(4)
C4_15	F8_15	1.315(12)	C3_4	F4_4	1.328(5)
C4_15	F9_15	1.340(11)	C3_4	F5_4	1.327(5)
O1_14	Al3	1.708(13)	C3_4	F6_4	1.346(5)
O1_14	C1_14	1.360(13)	C4_4	F7_4	1.325(6)
C1_14	C2_14	1.556(12)	C4_4	F8_4	1.341(6)
C1_14	C3_14	1.550(12)	C4_4	F9_4	1.328(5)
C1_14	C4_14	1.549(12)	O1_3	Al4	1.690(2)
C2_14	F1_14	1.330(13)	O1_3	C1_3	1.351(3)
C2_14	F2_14	1.339(12)	C1_3	C2_3	1.555(4)
C2_14	F3_14	1.321(11)	C1_3	C3_3	1.548(4)
C3_14	F4_14	1.333(11)	C1_3	C4_3	1.562(4)
C3_14	F5_14	1.322(13)	C2_3	F1_3	1.333(4)
C3_14	F6_14	1.335(13)	C2_3	F2_3	1.335(4)
C4_14	F7_14	1.337(13)	C2_3	F3_3	1.322(4)
C4_14	F8_14	1.335(13)	C3_3	F4_3	1.329(4)
C4_14	F9_14	1.332(12)	C3_3	F5_3	1.341(4)
O1_13	Al3	1.708(10)	C3_3	F6_3	1.334(3)
O1_13	C1_13	1.354(10)	C4_3	F7_3	1.331(4)
C1_13	C2_13	1.562(9)	C4_3	F8_3	1.332(3)
C1_13	C3_13	1.559(9)	C4_3	F9_3	1.326(3)
C1_13	C4_13	1.548(9)	O1_2	Al4	1.709(2)
C2_13	F1_13	1.334(8)	O1_2	C1_2	1.351(3)

C2_13	F2_13	1.337(10)	C1_2	C2_2	1.554(4)
C2_13	F3_13	1.313(9)	C1_2	C3_2	1.560(4)
C3_13	F4_13	1.340(12)	C1_2	C4_2	1.550(4)
C3_13	F5_13	1.325(7)	C2_2	F1_2	1.318(4)
C3_13	F6_13	1.334(7)	C2_2	F2_2	1.336(3)
C4_13	F7_13	1.344(9)	C2_2	F3_2	1.325(4)
C4_13	F8_13	1.334(10)	C3_2	F4_2	1.337(4)
C4_13	F9_13	1.328(11)	C3_2	F5_2	1.331(4)
O1_12	Al2	1.707(2)	C3_2	F6_2	1.317(3)
O1_12	C1_12	1.356(3)	C4_2	F7_2	1.328(4)
C1_12	C2_12	1.552(4)	C4_2	F8_2	1.331(3)
C1_12	C3_12	1.556(4)	C4_2	F9_2	1.322(4)
C1_12	C4_12	1.552(4)	O1_1	Al4	1.706(2)
C2_12	F1_12	1.326(3)	O1_1	C1_1	1.358(3)
C2_12	F2_12	1.327(3)	C1_1	C2_1	1.554(4)
C2_12	F3_12	1.334(4)	C1_1	C3_1	1.551(4)
C3_12	F4_12	1.321(3)	C1_1	C4_1	1.554(4)
C3_12	F5_12	1.332(3)	C2_1	F1_1	1.331(3)
C3_12	F6_12	1.336(3)	C2_1	F2_1	1.328(3)
C4_12	F7_12	1.322(3)	C2_1	F3_1	1.325(3)
C4_12	F8_12	1.347(3)	C3_1	F4_1	1.323(3)
C4_12	F9_12	1.319(3)	C3_1	F5_1	1.319(3)
O1_11	Al2	1.702(2)	C3_1	F6_1	1.348(3)
O1_11	C1_11	1.353(3)	C4_1	F7_1	1.314(3)
C1_11	C2_11	1.548(4)	C4_1	F8_1	1.350(3)
C1_11	C3_11	1.554(4)	C4_1	F9_1	1.332(3)
C1_11	C4_11	1.558(4)			

[1]1-X,2-Y,2-Z

Table 4 Bond Angles for p-1_a.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	Fe1	C1	124.64(13)	O1_10	C1_10	C4_10	108.9(2)
N1	Fe1	C2	92.03(15)	C2_10	C1_10	C3_10	109.7(2)
N1	Fe1	C4	90.04(15)	C4_10	C1_10	C2_10	109.6(2)
N1	Fe1	C5	117.18(13)	C4_10	C1_10	C3_10	109.5(2)
C1	Fe1	C2	88.28(14)	F1_10	C2_10	C1_10	110.3(2)
C1	Fe1	C4	88.13(15)	F1_10	C2_10	F2_10	108.6(2)
C2	Fe1	C4	176.40(14)	F1_10	C2_10	F3_10	106.7(2)
C5	Fe1	C1	118.19(13)	F2_10	C2_10	C1_10	113.4(2)
C5	Fe1	C2	89.37(14)	F2_10	C2_10	F3_10	107.7(2)
C5	Fe1	C4	92.30(15)	F3_10	C2_10	C1_10	109.8(2)
O3	N1	Fe1	177.4(3)	F4_10	C3_10	C1_10	110.7(2)
Al1	F1	Al2	176.18(10)	F4_10	C3_10	F6_10	108.4(2)
O1_16	Al1	F1	100.7(11)	F5_10	C3_10	C1_10	110.6(2)
O1_16	Al1	O1_15	117.9(17)	F5_10	C3_10	F4_10	107.1(2)
O1_16	Al1	O1_9	3.1(17)	F5_10	C3_10	F6_10	107.9(2)
O1_16	Al1	O1_8	110.5(12)	F6_10	C3_10	C1_10	111.9(2)
O1_15	Al1	F1	104.6(11)	F7_10	C4_10	C1_10	110.8(2)
O1_15	Al1	O1_9	115.0(11)	F7_10	C4_10	F8_10	108.0(2)
O1_15	Al1	O1_8	115.2(9)	F7_10	C4_10	F9_10	107.9(2)
O1_9	Al1	F1	102.8(3)	F8_10	C4_10	C1_10	111.8(2)
O1_9	Al1	O1_8	111.8(3)	F9_10	C4_10	C1_10	110.6(2)
O1_8	Al1	F1	105.96(9)	F9_10	C4_10	F8_10	107.6(2)
O1_7	Al1	F1	107.5(4)	C1_16	O1_9	Al1	145.9(8)
O1_7	Al1	O1_8	108.6(3)	C1_16	O1_9	C1_9	3.9(7)
O1	C1	Fe1	179.3(3)	C1_9	O1_9	Al1	149.0(5)
Al4[1]	F3	Al4	180.00(5)	O1_16	C1_9	C2_16	108.8(14)
O1_17	Al3	F2	110.4(13)	O1_16	C1_9	C3_16	110.4(15)
O1_17	Al3	O1_14	114.1(19)	O1_16	C1_9	C4_16	104.7(16)
O1_17	Al3	O1_13	114.4(16)	O1_16	C1_9	C2_9	112.6(12)
O1_14	Al3	F2	105.9(10)	O1_16	C1_9	C3_9	111.2(15)
O1_13	Al3	F2	108.7(10)	O1_16	C1_9	C4_9	105.8(17)
O1_13	Al3	O1_14	102.7(14)	C2_16	C1_9	C3_16	115.6(8)
O1_6	Al3	F2	107.17(18)	C2_16	C1_9	C4_16	110.2(8)
O1_6	Al3	O1_5	110.9(6)	C2_16	C1_9	C2_9	137.3(6)
O1_6	Al3	O1_4	116.6(3)	C2_16	C1_9	C3_9	43.0(6)
O1_5	Al3	F2	107.4(8)	C2_16	C1_9	C4_9	69.0(6)

O1_4	Al3	F2	100.8(2)	C3_16	C1_9	C4_16	106.5(7)
O1_4	Al3	O1_5	112.9(6)	C3_16	C1_9	C2_9	38.2(5)
N2	Fe2	C6	94.47(13)	C3_16	C1_9	C3_9	75.7(6)
N2	Fe2	C8	123.78(15)	C3_16	C1_9	C4_9	138.5(6)
N2	Fe2	C9	91.77(13)	O1_9	C1_9	O1_16	4(2)
N2	Fe2	C10	114.51(13)	O1_9	C1_9	C2_16	109.0(6)
C6	Fe2	C9	173.73(13)	O1_9	C1_9	C3_16	107.3(7)
C8	Fe2	C6	88.11(15)	O1_9	C1_9	C4_16	107.8(7)
C8	Fe2	C9	87.87(16)	O1_9	C1_9	C2_9	111.5(4)
C8	Fe2	C10	121.70(15)	O1_9	C1_9	C3_9	108.7(4)
C10	Fe2	C6	86.79(13)	O1_9	C1_9	C4_9	109.4(5)
C10	Fe2	C9	91.23(14)	C2_9	C1_9	C4_16	69.1(5)
O7	N2	Fe2	177.1(3)	C3_9	C1_9	C4_16	140.7(5)
Al3	F2	$Al3^{2}$	180.00(3)	C3_9	C1_9	C2_9	109.4(3)
O1_12	Al2	F1	100.70(9)	C4_9	C1_9	C4_16	43.4(5)
O1_11	Al2	F1	104.88(9)	C4_9	C1_9	C2_9	108.4(3)
O1_11	Al2	O1_12	110.86(10)	C4_9	C1_9	C3_9	109.3(3)
O1_10	Al2	F1	107.47(9)	C1_16	C2_9	C4_16	54.9(5)
O1_10	Al2	O1_12	118.67(10)	C1_16	C2_9	F7_16	93.0(7)
O1_10	Al2	O1_11	112.57(10)	C1_16	C2_9	C1_9	3.4(6)
O2	C2	Fe1	178.3(3)	C3_16	C2_9	C1_16	72.2(8)
O1_3	Al4	F3	107.27(8)	C3_16	C2_9	F4_16	64.9(14)
O1_3	Al4	O1_2	115.78(11)	C3_16	C2_9	F6_16	64.3(10)
O1_3	Al4	O1_1	112.54(11)	C3_16	C2_9	C4_16	125.3(9)
O1_2	Al4	F3	100.25(8)	C3_16	C2_9	F7_16	162.9(10)
O1_1	Al4	F3	106.06(8)	C3_16	C2_9	C1_9	69.4(8)
O1_1	Al4	O1_2	113.47(10)	C3_16	C2_9	F1_9	169.9(9)
O4	C4	Fe1	178.0(3)	C3_16	C2_9	F2_9	81.0(8)
O5	C5	Fe1	177.0(3)	C3_16	C2_9	F3_9	63.5(9)
O6	C6	Fe2	176.5(3)	F4_16	C2_9	C1_16	108.6(19)
O8	C8	Fe2	178.8(3)	F4_16	C2_9	F6_16	101.3(18)
O9	C9	Fe2	177.9(3)	F4_16	C2_9	C4_16	141.1(18)
O10	C10	Fe2	177.5(3)	F4_16	C2_9	F7_16	113.9(14)
C1_17	O1_17	Al3	154(3)	F4_16	C2_9	C1_9	108.4(19)
O1_17	C1_17	C2_17	108.2(15)	F6_16	C2_9	C1_16	107.9(13)
O1_17	C1_17	C3_17	109.6(19)	F6_16	C2_9	C4_16	117.0(13)
O1_17	C1_17	C4_17	110.7(18)	F6_16	C2_9	F7_16	130.5(11)
C2_17	C1_17	C4_17	110.1(12)	F6_16	C2_9	C1_9	104.8(13)
C3_17	C1_17	C2_17	109.7(11)	F7_16	C2_9	C4_16	44.1(5)
C3_17	C1_17	C4_17	108.4(12)	C1_9	C2_9	C4_16	57.2(5)
F1_17	C2_17	C1_17	109.3(13)	C1_9	C2_9	F7_16	96.1(5)
F2_17	C2_17	C1_17	111.0(14)	F1_9	C2_9	C1_16	108.0(6)
F2_17	C2_17	F1_17	107.8(15)	F1_9	C2_9	F4_16	106.1(13)
F3_17	C2_17	C1_17	111.6(17)	F1_9	C2_9	F6_16	123.9(9)
F3_17	C2_17	F1_17	107.2(18)	F1_9	C2_9	C4_16	58.3(5)
F3_17	C2_17	F2_17	109.9(18)	F1_9	C2_9	F7_16	15.1(5)
F4_17	C3_17	C1_17	110.1(18)	F1_9	C2_9	C1_9	111.1(3)
F4_17	C3_17	F6_17	107.7(19)	F2_9	C2_9	C1_16	114.8(7)
F5_17	C3_17	C1_17	110.2(14)	F2_9	C2_9	F4_16	111.5(19)
F5_17	C3_17	F4_17	109.3(19)	F2_9	C2_9	F6_16	16.7(9)
F5_17	C3_17	F6_17	108.0(16)	F2_9	C2_9	C4_16	107.3(5)
F6_17	C3_17	C1_17	111.5(14)	F2_9	C2_9	F7_16	113.8(7)
F7_17	C4_17	C1_17	109.5(13)	F2_9	C2_9	C1_9	112.1(4)
F7_17	C4_17	F8_17	106.0(18)	F2_9	C2_9	F1_9	107.4(4)
F8_17	C4_17	C1_17	111.4(17)	F2_9	C2_9	F3_9	108.6(5)
F9_17	C4_17	C1_17	109.7(17)	F3_9	C2_9	C1_16	110.0(8)
F9_17	C4_17	F7_17	110.2(17)	F3_9	C2_9	F4_16	3(2)
F9_17	C4_17	F8_17	110(2)	F3_9	C2_9	F6_16	98.5(14)
C1_16	O1_16	Al1	145(2)	F3_9	C2_9	C4_16	144.0(6)
C1_16	O1_16	C1_9	3.7(7)	F3_9	C2_9	F7_16	116.0(7)
C1_9	O1_16	Al1	148(2)	F3_9	C2_9	C1_9	109.6(5)
O1_16	C1_16	C2_16	106.4(13)	F3_9	C2_9	F1_9	107.8(5)
O1_16	C1_16	C3_16	111.0(18)	F7_16	F1_9	C4_16	52.8(16)
O1_16	C1_16	C4_16	110.4(18)	F7_16	F1_9	C2_9	125.9(18)
O1_16	C1_16	C2_9	116.7(16)	C2_9	F1_9	C4_16	75.8(5)
O1_16	C1_16	C3_9	107.6(15)	C2_9	F2_9	C3_16	40.4(5)

O1_16	C1_16	C4_9	108.9(17)	C3_16	F3_9	C2_9	45.8(6)
C2_16	C1_16	C4_16	110.0(10)	C1_16	C3_9	C3_16	51.4(5)
C2_16	C1_16	C3_9	40.5(6)	C1_16	C3_9	F5_16	90.0(6)
C3_16	C1_16	C2_16	110.1(10)	C2_16	C3_9	C1_16	65.0(7)
C3_16	C1_16	C4_16	108.9(10)	C2_16	C3_9	F2_16	58.9(8)
C3_16	C1_16	C3_9	72.4(7)	C2_16	C3_9	F3_16	66.7(12)
C4_16	C1_16	C3_9	138.1(11)	C2_16	C3_9	C3_16	113.1(8)
O1_9	C1_16	O1_16	4(2)	C2_16	C3_9	F5_16	154.9(8)
O1_9	C1_16	C2_16	106.5(11)	C2_16	C3_9	C1_9	64.8(7)
O1_9	C1_16	C3_16	107.7(11)	C2_16	C3_9	F4_9	71.9(9)
O1_9	C1_16	C4_16	113.7(11)	C2_16	C3_9	F5_9	174.2(7)
O1_9	C1_16	C2_9	115.4(10)	C2_16	C3_9	F6_9	78.5(7)
O1_9	C1_16	C3_9	105.0(10)	F2_16	C3_9	C1_16	97.8(9)
O1_9	C1_16	C4_9	112.6(11)	F2_16	C3_9	C3_16	108.6(10)
C2_9	C1_16	C2_16	133.3(12)	F2_16	C3_9	F5_16	127.5(9)
C2_9	C1_16	C3_16	38.3(6)	F2_16	C3_9	C1_9	97.6(8)
C2_9	C1_16	C4_16	71.7(8)	F3_16	C3_9	C1_16	107.3(15)
C2_9	C1_16	C3_9	106.1(9)	F3_16	C3_9	F2_16	100.2(15)
C2_9	C1_16	C4_9	111.3(9)	F3_16	C3_9	C3_16	145.6(16)
C4_9	C1_16	C2_16	67.8(8)	F3_16	C3_9	F5_16	126.8(13)
C4_9	C1_16	C3_16	138.5(12)	F3_16	C3_9	C1_9	107.3(15)
C4_9	C1_16	C4_16	44.9(6)	F3_16	C3_9	F4_9	5.3(15)
C4_9	C1_16	C3_9	105.6(8)	F3_16	C3_9	F5_9	113.3(12)
C1_16	C2_16	F6_9	106.8(10)	F3_16	C3_9	F6_9	106.4(15)
C1_16	C2_16	C4_9	55.5(6)	F5_16	C3_9	C3_16	42.9(4)
C1_16	C2_16	F7_9	96.0(8)	C1_9	C3_9	C1_16	0.2(8)
F1_16	C2_16	C1_16	108.5(12)	C1_9	C3_9	C3_16	51.5(5)
F1_16	C2_16	F2_16	109.8(15)	C1_9	C3_9	F5_16	90.2(5)
F1_16	C2_16	F3_16	109.0(17)	F4_9	C3_9	C1_16	111.0(7)
F1_16	C2_16	C1_9	110.8(12)	F4_9	C3_9	F2_16	103.1(10)
F1_16	C2_16	F4_9	111.2(14)	F4_9	C3_9	C3_16	145.3(6)
F1_16	C2_16	F6_9	127.4(14)	F4_9	C3_9	F5_16	122.2(7)
F1_16	C2_16	C4_9	60.4(10)	F4_9	C3_9	C1_9	111.0(4)
F1_16	C2_16	F7_9	14.2(10)	F4_9	C3_9	F5_9	108.2(4)
F2_16	C2_16	C1_16	110.9(13)	F4_9	C3_9	F6_9	107.6(5)
F2_16	C2_16	C1_9	109.9(13)	F5_9	C3_9	C1_16	110.0(5)
F2_16	C2_16	F4_9	106.1(14)	F5_9	C3_9	F2_16	126.1(7)
F2_16	C2_16	F6_9	19.0(9)	F5_9	C3_9	C3_16	63.3(4)
F2_16	C2_16	C4_9	102.1(12)	F5_9	C3_9	F5_16	20.7(4)
F2_16	C2_16	F7_9	109.8(12)	F5_9	C3_9	C1_9	110.2(3)
F3_16	C2_16	C1_16	110.8(15)	F5_9	C3_9	F6_9	106.8(3)
F3_16	C2_16	F2_16	107.7(17)	F6_9	C3_9	C1_16	113.1(6)
F3_16	C2_16	C1_9	109.5(16)	F6_9	C3_9	F2_16	20.2(6)
F3_16	C2_16	F4_9	2.3(19)	F6_9	C3_9	C3_16	107.0(5)
F3_16	C2_16	F6_9	93.1(17)	F6_9	C3_9	F5_16	112.1(6)
F3_16	C2_16	C4_9	150.2(17)	F6_9	C3_9	C1_9	112.9(3)
F3_16	C2_16	F7_9	121.0(17)	C3_9	F4_9	C2_16	47.4(6)
C1_9	C2_16	C1_16	2.3(6)	F5_16	F5_9	C3_16	41.1(12)
C1_9	C2_16	F6_9	105.1(8)	F5_16	F5_9	C3_9	114.5(13)
C1_9	C2_16	C4_9	57.5(5)	C3_9	F5_9	C3_16	74.1(5)
C1_9	C2_16	F7_9	98.3(8)	F2_16	F6_9	C2_16	55.5(17)
C3_9	C2_16	C1_16	74.4(8)	F2_16	F6_9	C3_9	98.5(19)
C3_9	C2_16	F1_16	171.7(16)	C3_9	F6_9	C2_16	44.3(5)
C3_9	C2_16	F2_16	75.5(11)	C1_16	C4_9	C2_16	56.8(5)
C3_9	C2_16	F3_16	62.9(17)	C1_16	C4_9	F1_16	98.1(8)
C3_9	C2_16	C1_9	72.2(7)	C1_16	C4_9	F8_16	100.9(8)
C3_9	C2_16	F4_9	60.7(8)	C1_16	C4_9	C1_9	3.5(6)
C3_9	C2_16	F6_9	57.1(6)	F1_16	C4_9	C2_16	47.2(5)
C3_9	C2_16	C4_9	125.7(10)	F1_16	C4_9	F8_16	133.2(11)
C3_9	C2_16	F7_9	170.4(10)	C4_16	C4_9	C1_16	68.7(7)
F4_9	C2_16	C1_16	110.2(11)	C4_16	C4_9	C2_16	122.0(8)
F4_9	C2_16	C1_9	108.8(10)	C4_16	C4_9	F1_16	166.4(10)
F4_9	C2_16	F6_9	91.2(9)	C4_16	C4_9	F8_16	55.7(7)
F4_9	C2_16	C4_9	151.6(10)	C4_16	C4_9	F9_16	60.8(9)
F4_9	C2_16	F7_9	123.3(10)	C4_16	C4_9	C1_9	71.5(7)
F6_9	C2_16	C4_9	115.7(9)	C4_16	C4_9	F7_9	169.1(7)

F6_9	C2_16	F7_9	128.7(9)	C4_16	C4_9	F8_9	80.1(6)
F7_9	C2_16	C4_9	46.2(4)	C4_16	C4_9	F9_9	61.3(7)
C2_16	F1_16	C4_9	72.4(10)	F8_16	C4_9	C2_16	115.1(8)
C2_16	F2_16	C3_9	45.6(8)	F9_16	C4_9	C1_16	107.0(11)
F6_9	F2_16	C2_16	106(2)	F9_16	C4_9	C2_16	150.5(9)
F6_9	F2_16	C3_9	61.3(18)	F9_16	C4_9	F1_16	123.3(11)
C3_9	F3_16	C2_16	50.5(9)	F9_16	C4_9	F8_16	91.0(9)
C1_16	C3_16	C3_9	56.3(6)	F9_16	C4_9	C1_9	110.4(10)
C1_16	C3_16	F5_9	95.4(8)	C1_9	C4_9	C2_16	53.4(5)
F4_16	C3_16	C1_16	110.5(18)	C1_9	C4_9	F1_16	95.4(7)
F4_16	C3_16	F5_16	108.4(18)	C1_9	C4_9	F8_16	101.4(6)
F4_16	C3_16	F6_16	109.0(19)	F7_9	C4_9	C1_16	113.1(6)
F4_16	C3_16	C1_9	113.6(19)	F7_9	C4_9	C2_16	64.2(5)
F4_16	C3_16	F2_9	103(2)	F7_9	C4_9	F1_16	17.1(6)
F4_16	C3_16	C3_9	150(2)	F7_9	C4_9	F8_16	132.0(6)
F4_16	C3_16	F5_9	125.9(18)	F7_9	C4_9	F9_16	109.1(9)
F5_16	C3_16	C1_16	111.5(11)	F7_9	C4_9	C1_9	110.7(3)
F5_16	C3_16	C1_9	108.5(11)	F7_9	C4_9	F8_9	108.1(4)
F5_16	C3_16	F2_9	120.6(12)	F7_9	C4_9	F9_9	108.5(4)
F5_16	C3_16	C3_9	61.6(8)	F8_9	C4_9	C1_16	112.8(7)
F5_16	C3_16	F5_9	19.2(7)	F8_9	C4_9	C2_16	102.7(5)
F6_16	C3_16	C1_16	110.6(14)	F8_9	C4_9	F1_16	109.0(10)
F6_16	C3_16	F5_16	106.7(14)	F8_9	C4_9	F8_16	24.4(4)
F6_16	C3_16	C1_9	110.4(15)	F8_9	C4_9	F9_16	106.5(8)
F6_16	C3_16	F2_9	13.9(12)	F8_9	C4_9	C1_9	111.8(3)
F6_16	C3_16	C3_9	101.0(15)	F9_9	C4_9	C1_16	106.3(7)
F6_16	C3_16	F5_9	104.4(13)	F9_9	C4_9	C2_16	149.2(6)
C1_9	C3_16	C1_16	3.5(6)	F9_9	C4_9	F1_16	122.5(8)
C1_9	C3_16	F2_9	102.8(8)	F9_9	C4_9	F8_16	92.2(7)
C1_9	C3_16	C3_9	52.8(4)	F9_9	C4_9	F9_16	1.4(10)
C1_9	C3_16	F5_9	92.2(7)	F9_9	C4_9	C1_9	109.7(4)
C2_9	C3_16	C1_16	69.5(9)	F9_9	C4_9	F8_9	107.9(4)
C2_9	C3_16	F4_16	71.5(19)	C4_9	F7_9	C2_16	69.5(5)
C2_9	C3_16	F5_16	179.0(15)	F8_16	F8_9	C4_16	52.9(11)
C2_9	C3_16	F6_16	72.4(14)	F8_16	F8_9	C4_9	98.4(12)
C2_9	C3_16	C1_9	72.4(7)	C4_9	F8_9	C4_16	45.6(5)
C2_9	C3_16	F2_9	58.6(7)	C4_16	F9_9	C4_9	53.3(6)
C2_9	C3_16	F3_9	70.7(10)	C1_8	O1_8	Al1	143.51(16)
C2_9	C3_16	C3_9	118.9(10)	O1_8	C1_8	C2_8	112.1(2)
C2_9	C3_16	F5_9	161.2(11)	O1_8	C1_8	C3_8	109.4(2)
F2_9	C3_16	C1_16	102.3(10)	O1_8	C1_8	C4_8	107.5(2)
F2_9	C3_16	C3_9	106.2(8)	C2_8	C1_8	C3_8	108.6(2)
F2_9	C3_16	F5_9	117.1(9)	C2_8	C1_8	C4_8	109.7(2)
F3_9	C3_16	C1_16	112.3(12)	C4_8	C1_8	C3_8	109.5(2)
F3_9	C3_16	F4_16	3(3)	F1_8	C2_8	C1_8	110.3(2)
F3_9	C3_16	F5_16	109.2(13)	F1_8	C2_8	F2_8	108.7(2)
F3_9	C3_16	F6_16	106(2)	F1_8	C2_8	F3_8	107.0(2)
F3_9	C3_16	C1_9	115.5(11)	F2_8	C2_8	C1_8	112.7(2)
F3_9	C3_16	F2_9	100.5(10)	F2_8	C2_8	F3_8	106.9(2)
F3_9	C3_16	C3_9	152.7(12)	F3_8	C2_8	C1_8	111.0(2)
F3_9	C3_16	F5_9	127.0(11)	F4_8	C3_8	C1_8	111.6(2)
F5_9	C3_16	C3_9	42.6(3)	F4_8	C3_8	F6_8	107.3(2)
C3_16	F4_16	C2_9	43.6(8)	F5_8	C3_8	C1_8	110.3(2)
C3_16	F5_16	C3_9	75.5(8)	F5_8	C3_8	F4_8	107.4(2)
F5_9	F5_16	C3_16	119.7(18)	F5_8	C3_8	F6_8	107.8(2)
F5_9	F5_16	C3_9	44.9(11)	F6_8	C3_8	C1_8	112.2(2)
C3_16	F6_16	C2_9	43.3(8)	F7_8	C4_8	C1_8	111.0(2)
C1_16	C4_16	C1_9	2.4(7)	F7_8	C4_8	F9_8	107.0(2)
C1_16	C4_16	C2_9	53.4(6)	F8_8	C4_8	C1_8	112.0(2)
C1_16	C4_16	F1_9	95.2(8)	F8_8	C4_8	F7_8	108.0(2)
C1_16	C4_16	F8_9	97.6(9)	F8_8	C4_8	F9_8	108.5(2)
F7_16	C4_16	C1_16	109.6(11)	F9_8	C4_8	C1_8	110.1(2)
F7_16	C4_16	F8_16	108.0(13)	C1_7	O1_7	Al1	148.6(7)
F7_16	C4_16	F9_16	110.4(15)	O1_7	C1_7	C2_7	111.1(6)
F7_16	C4_16	C1_9	111.2(11)	O1_7	C1_7	C3_7	108.6(6)
F7_16	C4_16	C2_9	64.6(9)	O1_7	C1_7	C4_7	109.1(7)

F7_16	C4_16	F1_9	19.4(7)	C3_7	C1_7	C2_7	109.7(4)
F7_16	C4_16	F8_9	131.1(12)	C3_7	C1_7	C4_7	108.9(4)
F8_16	C4_16	C1_16	111.9(11)	C4_7	C1_7	C2_7	109.3(4)
F8_16	C4_16	C1_9	109.5(10)	F1_7	C2_7	C1_7	108.4(5)
F8_16	C4_16	C2_9	100.0(10)	F2_7	C2_7	C1_7	113.1(7)
F8_16	C4_16	F1_9	103.2(10)	F2_7	C2_7	F1_7	107.8(7)
F8_16	C4_16	F8_9	23.2(6)	F3_7	C2_7	C1_7	110.0(4)
F9_16	C4_16	C1_16	110.2(12)	F3_7	C2_7	F1_7	108.7(5)
F9_16	C4_16	F8_16	106.7(14)	F3_7	C2_7	F2_7	108.6(7)
F9_16	C4_16	C1_9	111.0(12)	F4_7	C3_7	C1_7	111.3(4)
F9_16	C4_16	C2_9	152.8(12)	F4_7	C3_7	F5_7	106.8(5)
F9_16	C4_16	F1_9	129.0(14)	F4_7	C3_7	F6_7	107.8(4)
F9_16	C4_16	F8_9	96.2(13)	F5_7	C3_7	C1_7	110.3(6)
C1_9	C4_16	C2_9	53.7(4)	F6_7	C3_7	C1_7	112.8(4)
F1_9	C4_16	C1_9	96.2(7)	F6_7	C3_7	F5_7	107.6(6)
F1_9	C4_16	C2_9	45.9(4)	F7_7	C4_7	C1_7	111.2(4)
F1_9	C4_16	F8_9	124.1(8)	F7_7	C4_7	F9_7	108.8(5)
C4_9	C4_16	C1_16	66.4(8)	F8_7	C4_7	C1_7	111.3(6)
C4_9	C4_16	F7_16	174.4(13)	F8_7	C4_7	F7_7	108.8(6)
C4_9	C4_16	F8_16	77.5(9)	F8_7	C4_7	F9_7	107.0(5)
C4_9	C4_16	F9_16	68.4(13)	F9_7	C4_7	C1_7	109.7(5)
C4_9	C4_16	C1_9	65.1(6)	C1_6	O1_6	Al3	150.6(4)
C4_9	C4_16	C2_9	113.8(9)	O1_6	C1_6	C2_6	109.9(3)
C4_9	C4_16	F1_9	159.7(11)	O1_6	C1_6	C3_6	110.8(3)
C4_9	C4_16	F8_9	54.3(5)	O1_6	C1_6	C4_6	108.5(3)
C4_9	C4_16	F9_9	65.4(8)	C2_6	C1_6	C3_6	109.5(3)
F8_9	C4_16	C1_9	95.2(7)	C2_6	C1_6	C4_6	109.1(3)
F8_9	C4_16	C2_9	106.8(7)	C4_6	C1_6	C3_6	109.0(3)
F9_9	C4_16	C1_16	107.3(10)	F1_6	C2_6	C1_6	110.5(3)
F9_9	C4_16	F7_16	113.2(12)	F1_6	C2_6	F2_6	108.1(3)
F9_9	C4_16	F8_16	106.8(12)	F1_6	C2_6	F3_6	107.6(3)
F9_9	C4_16	F9_16	3.3(13)	F2_6	C2_6	C1_6	112.9(3)
F9_9	C4_16	C1_9	108.0(9)	F3_6	C2_6	C1_6	110.3(3)
F9_9	C4_16	C2_9	151.9(9)	F3_6	C2_6	F2_6	107.3(3)
F9_9	C4_16	F1_9	131.6(10)	F4_6	C3_6	C1_6	110.7(3)
F9_9	C4_16	F8_9	95.2(8)	F4_6	C3_6	F5_6	107.9(3)
C4_16	F7_16	C2_9	71.4(8)	F5_6	C3_6	C1_6	109.7(3)
F1_9	F7_16	C4_16	108(2)	F6_6	C3_6	C1_6	112.5(3)
F1_9	F7_16	C2_9	39.0(15)	F6_6	C3_6	F4_6	107.7(4)
C4_16	F8_16	C4_9	46.8(7)	F6_6	C3_6	F5_6	108.2(4)
F8_9	F8_16	C4_16	103.9(15)	F7_6	C4_6	C1_6	110.9(3)
F8_9	F8_16	C4_9	57.2(11)	F8_6	C4_6	C1_6	112.1(3)
C4_16	F9_16	C4_9	50.8(8)	F8_6	C4_6	F7_6	107.8(3)
C1_15	O1_15	Al1	153.6(19)	F9_6	C4_6	C1_6	110.5(3)
O1_15	C1_15	C2_15	109.1(15)	F9_6	C4_6	F7_6	107.8(3)
O1_15	C1_15	C3_15	109.5(13)	F9_6	C4_6	F8_6	107.5(3)
O1_15	C1_15	C4_15	107.5(14)	C1_5	O1_5	Al3	147.9(12)
C2_15	C1_15	C3_15	110.5(8)	O1_5	C1_5	C2_5	108.0(7)
C2_15	C1_15	C4_15	109.9(8)	O1_5	C1_5	C3_5	110.1(10)
C4_15	C1_15	C3_15	110.3(9)	O1_5	C1_5	C4_5	111.0(10)
F1_15	C2_15	C1_15	111.1(13)	C3_5	C1_5	C2_5	110.3(5)
F1_15	C2_15	F2_15	108.7(14)	C4_5	C1_5	C2_5	108.8(5)
F1_15	C2_15	F3_15	108.2(12)	C4_5	C1_5	C3_5	108.6(5)
F2_15	C2_15	C1_15	111.4(9)	F1_5	C2_5	C1_5	110.3(5)
F3_15	C2_15	C1_15	110.1(8)	F1_5	C2_5	F2_5	107.5(7)
F3_15	C2_15	F2_15	107.1(8)	F2_5	C2_5	C1_5	112.3(7)
F4_15	C3_15	C1_15	108.3(9)	F3_5	C2_5	C1_5	111.6(6)
F5_15	C3_15	C1_15	108.5(10)	F3_5	C2_5	F1_5	107.1(5)
F5_15	C3_15	F4_15	112.7(11)	F3_5	C2_5	F2_5	107.7(6)
F6_15	C3_15	C1_15	111.4(15)	F4_5	C3_5	C1_5	109.4(7)
F6_15	C3_15	F4_15	107.9(15)	F5_5	C3_5	C1_5	110.5(5)
F6_15	C3_15	F5_15	108.1(16)	F5_5	C3_5	F4_5	108.1(5)
F7_15	C4_15	C1_15	108.1(9)	F6_5	C3_5	C1_5	112.2(6)
F7_15	C4_15	F9_15	108.5(9)	F6_5	C3_5	F4_5	108.3(8)
F8_15	C4_15	C1_15	117.1(11)	F6_5	C3_5	F5_5	108.2(6)
F8_15	C4_15	F7_15	108.6(13)	F7_5	C4_5	C1_5	111.6(4)

F8_15 C4_15 F9_15	104.6(12)	F7_5	C4_5	F8_5	107.7(4)
F9_15 C4_15 C1_15	109.7(9)	F7_5	C4_5	F9_5	107.8(6)
C1_14 O1_14 Al3	150(2)	F8_5	C4_5	C1_5	112.7(5)
O1_14 C1_14 C2_14	108.5(15)	F8_5	C4_5	F9_5	106.8(9)
O1_14 C1_14 C3_14	109.0(16)	F9_5	C4_5	C1_5	110.0(8)
O1_14 C1_14 C4_14	109.6(15)	C1_4	O1_4	Al3	143.5(4)
C3_14 C1_14 C2_14	110.4(10)	O1_4	C1_4	C2_4	111.3(4)
C4_14 C1_14 C2_14	110.1(10)	O1_4	C1_4	C3_4	107.2(3)
C4_14 C1_14 C3_14	109.2(10)	O1_4	C1_4	C4_4	110.8(4)
F1_14 C2_14 C1_14	109.4(15)	C3_4	C1_4	C2_4	109.1(3)
F1_14 C2_14 F2_14	107.4(17)	C3_4	C1_4	C4_4	110.0(3)
F2_14 C2_14 C1_14	110.1(12)	C4_4	C1_4	C2_4	108.5(3)
F3_14 C2_14 C1_14	110.6(10)	F1_4	C2_4	C1_4	109.8(4)
F3_14 C2_14 F1_14	111.9(17)	F2_4	C2_4	C1_4	113.7(3)
F3_14 C2_14 F2_14	107.4(11)	F2_4	C2_4	F1_4	107.5(4)
F4_14 C3_14 C1_14	110.1(10)	F3_4	C2_4	C1_4	111.0(3)
F4_14 C3_14 F6_14	105.2(16)	F3_4	C2_4	F1_4	106.8(4)
F5_14 C3_14 C1_14	109.8(15)	F3_4	C2_4	F2_4	107.8(3)
F5_14 C3_14 F4_14	110.6(14)	F4_4	C3_4	C1_4	110.8(3)
F5_14 C3_14 F6_14	109.2(19)	F4_4	C3_4	F6_4	107.2(4)
F6_14 C3_14 C1_14	111.9(17)	F5_4	C3_4	C1_4	110.6(4)
F7_14 C4_14 C1_14	109.8(14)	F5_4	C3_4	F4_4	108.5(4)
F8_14 C4_14 C1_14	113.2(14)	F5_4	C3_4	F6_4	107.5(5)
F8_14 C4_14 F7_14	107.2(16)	F6_4	C3_4	C1_4	112.0(4)
F9_14 C4_14 C1_14	110.7(10)	F7_4	C4_4	C1_4	111.1(4)
F9_14 C4_14 F7_14	109.0(13)	F7_4	C4_4	F8_4	107.5(5)
F9_14 C4_14 F8_14	106.9(14)	F7_4	C4_4	F9_4	107.9(4)
C1_13 O1_13 Al3	147.1(16)	F8_4	C4_4	C1_4	112.1(5)
O1_13 C1_13 C2_13	107.6(11)	F9_4	C4_4	C1_4	110.7(3)
O1_13 C1_13 C3_13	109.1(14)	F9_4	C4_4	F8_4	107.4(4)
O1_13 C1_13 C4_13	111.3(12)	C1_3	O1_3	Al4	155.64(19)
C3_13 C1_13 C2_13	108.4(6)	O1_3	C1_3	C2_3	109.4(2)
C4_13 C1_13 C2_13	110.8(7)	O1_3	C1_3	C3_3	108.5(2)
C4_13 C1_13 C3_13	109.7(7)	O1_3	C1_3	C4_3	110.5(2)
F1_13 C2_13 C1_13	109.4(6)	C2_3	C1_3	C4_3	109.0(2)
F1_13 C2_13 F2_13	107.5(9)	C3_3	C1_3	C2_3	110.0(2)
F2_13 C2_13 C1_13	111.4(8)	C3_3	C1_3	C4_3	109.4(2)
F3_13 C2_13 C1_13	111.1(7)	F1_3	C2_3	C1_3	110.7(3)
F3_13 C2_13 F1_13	108.5(7)	F1_3	C2_3	F2_3	107.7(3)
F3_13 C2_13 F2_13	108.9(10)	F2_3	C2_3	C1_3	111.4(2)
F4_13 C3_13 C1_13	108.8(11)	F3_3	C2_3	C1_3	110.3(2)
F5_13 C3_13 C1_13	111.3(5)	F3_3	C2_3	F1_3	109.1(3)
F5_13 C3_13 F4_13	108.1(9)	F3_3	C2_3	F2_3	107.6(3)
F5_13 C3_13 F6_13	108.3(5)	F4_3	C3_3	C1_3	110.5(2)
F6_13 C3_13 C1_13	112.2(6)	F4_3	C3_3	F5_3	107.7(2)
F6_13 C3_13 F4_13	108.1(12)	F4_3	C3_3	F6_3	107.4(3)
F7_13 C4_13 C1_13	110.6(6)	F5_3	C3_3	C1_3	110.2(2)
F8_13 C4_13 C1_13	111.8(8)	F6_3	C3_3	C1_3	112.0(2)
F8_13 C4_13 F7_13	108.0(9)	F6_3	C3_3	F5_3	108.9(2)
F9_13 C4_13 C1_13	110.3(9)	F7_3	C4_3	C1_3	110.0(2)
F9_13 C4_13 F7_13	108.3(7)	F7_3	C4_3	F8_3	108.9(2)
F9_13 C4_13 F8_13	107.8(10)	F8_3	C4_3	C1_3	112.1(2)
C1_12 O1_12 Al2	147.78(17)	F9_3	C4_3	C1_3	109.6(2)
O1_12 C1_12 C2_12	112.2(2)	F9_3	C4_3	F7_3	108.3(3)
O1_12 C1_12 C3_12	109.3(2)	F9_3	C4_3	F8_3	107.8(2)
O1_12 C1_12 C4_12	107.8(2)	C1_2	O1_2	Al4	146.01(18)
C2_12 C1_12 C3_12	108.4(2)	O1_2	C1_2	C2_2	109.6(2)
C2_12 C1_12 C4_12	108.8(2)	O1_2	C1_2	C3_2	110.9(2)
C4_12 C1_12 C3_12	110.3(2)	O1_2	C1_2	C4_2	107.9(2)
F1_12 C2_12 C1_12	109.8(2)	C2_2	C1_2	C3_2	108.7(2)
F1_12 C2_12 F2_12	108.8(2)	C4_2	C1_2	C2_2	110.1(2)
F1_12 C2_12 F3_12	106.5(2)	C4_2	C1_2	C3_2	109.7(2)
F2_12 C2_12 C1_12	112.9(2)	F1_2	C2_2	C1_2	110.6(2)
F2_12 C2_12 F3_12	107.8(2)	F1_2	C2_2	F2_2	107.1(3)
F3_12 C2_12 C1_12	110.9(2)	F1_2	C2_2	F3_2	108.0(3)
F4_12 C3_12 C1_12	111.1(2)	F2_2	C2_2	C1_2	112.9(3)

F4_12	C3_12	F5_12	107.5(2)	F3_2	C2_2	C1_2	110.9(2)
F4_12	C3_12	F6_12	107.9(2)	F3_2	C2_2	F2_2	107.1(2)
F5_12	C3_12	C1_12	110.4(2)	F4_2	C3_2	C1_2	109.8(2)
F5_12	C3_12	F6_12	107.4(2)	F5_2	C3_2	C1_2	109.7(2)
F6_12	C3_12	C1_12	112.3(2)	F5_2	C3_2	F4_2	107.2(3)
F7_12	C4_12	C1_12	111.3(2)	F6_2	C3_2	C1_2	112.8(2)
F7_12	C4_12	F8_12	106.3(2)	F6_2	C3_2	F4_2	108.5(2)
F8_12	C4_12	C1_12	112.5(2)	F6_2	C3_2	F5_2	108.7(3)
F9_12	C4_12	C1_12	110.9(2)	F7_2	C4_2	C1_2	111.0(2)
F9_12	C4_12	F7_12	108.7(2)	F7_2	C4_2	F8_2	107.7(3)
F9_12	C4_12	F8_12	107.0(2)	F8_2	C4_2	C1_2	111.8(2)
C1_11	O1_11	Al2	146.33(17)	F9_2	C4_2	C1_2	110.8(3)
O1_11	C1_11	C2_11	110.4(2)	F9_2	C4_2	F7_2	107.2(3)
O1_11	C1_11	C3_11	107.5(2)	F9_2	C4_2	F8_2	108.1(3)
O1_11	C1_11	C4_11	111.1(2)	C1_1	O1_1	Al4	149.89(17)
C2_11	C1_11	C3_11	109.8(2)	O1_1	C1_1	C2_1	110.9(2)
C2_11	C1_11	C4_11	108.9(2)	O1_1	C1_1	C3_1	110.4(2)
C3_11	C1_11	C4_11	109.1(2)	O1_1	C1_1	C4_1	107.5(2)
F1_11	C2_11	C1_11	109.8(2)	C2_1	C1_1	C4_1	109.3(2)
F1_11	C2_11	F2_11	107.9(2)	C3_1	C1_1	C2_1	109.2(2)
F1_11	C2_11	F3_11	108.0(2)	C3_1	C1_1	C4_1	109.5(2)
F2_11	C2_11	C1_11	112.6(2)	F1_1	C2_1	C1_1	110.1(2)
F2_11	C2_11	F3_11	107.2(2)	F2_1	C2_1	C1_1	112.4(2)
F3_11	C2_11	C1_11	111.2(2)	F2_1	C2_1	F1_1	107.5(2)
F4_11	C3_11	C1_11	110.7(2)	F3_1	C2_1	C1_1	111.2(2)
F5_11	C3_11	C1_11	110.8(2)	F3_1	C2_1	F1_1	107.2(2)
F5_11	C3_11	F4_11	106.4(2)	F3_1	C2_1	F2_1	108.2(2)
F6_11	C3_11	C1_11	112.8(2)	F4_1	C3_1	C1_1	111.0(2)
F6_11	C3_11	F4_11	108.0(2)	F4_1	C3_1	F6_1	107.0(2)
F6_11	C3_11	F5_11	107.9(2)	F5_1	C3_1	C1_1	111.2(2)
F7_11	C4_11	C1_11	110.2(2)	F5_1	C3_1	F4_1	108.2(2)
F7_11	C4_11	F8_11	108.6(2)	F5_1	C3_1	F6_1	107.5(2)
F7_11	C4_11	F9_11	107.3(2)	F6_1	C3_1	C1_1	111.8(2)
F8_11	C4_11	C1_11	112.1(2)	F7_1	C4_1	C1_1	111.7(2)
F8_11	C4_11	F9_11	107.3(2)	F7_1	C4_1	F8_1	107.7(2)
F9_11	C4_11	C1_11	111.1(2)	F7_1	C4_1	F9_1	107.9(2)
C1_10	O1_10	Al2	151.62(17)	F8_1	C4_1	C1_1	111.9(2)
O1_10	C1_10	C2_10	110.2(2)	F9_1	C4_1	C1_1	110.9(2)
O1_10	C1_10	C3_10	109.0(2)	F9_1	C4_1	F8_1	106.5(2)

[1]1-X,2-Y,2-Z; [2]1-X,2-Y,1-Z

[Fe(CO)(NO)$_3$][F-{Al(OR^F)$_3$}$_2$] (2)

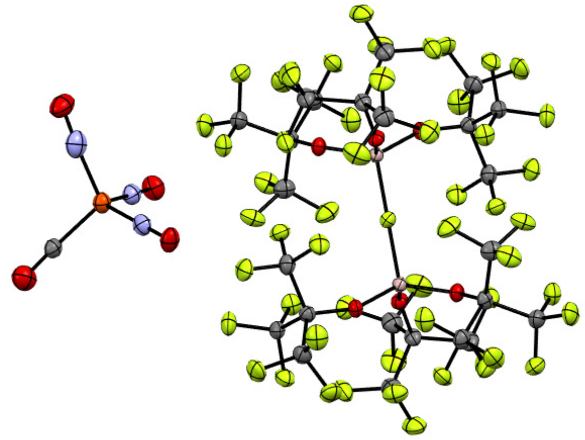


Table 1 Crystal data and structure refinement for p-1_b_a.

Identification code	p-1_b_a
Empirical formula	$C_{25}N_3O_{10}F_{55}Al_2Fe$
Formula weight	1657.09
Temperature/K	100.0
Crystal system	triclinic
Space group	P-1
a/Å	10.6555(2)
b/Å	12.7849(2)
c/Å	20.0830(4)
α/°	74.6740(10)
β/°	85.0720(10)
γ/°	65.5470(10)
Volume/Å^3	2401.06(8)
Z	2
ρ_{calc}g/cm^3	2.292
μ/mm^{-1}	0.621
F(000)	1596.0
Crystal size/mm^3	0.15 × 0.1 × 0.1
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.104 to 52.736
Index ranges	$-13 \leq h \leq 12$, $-15 \leq k \leq 15$, $-25 \leq l \leq 25$
Reflections collected	42788
Independent reflections	9775 [R_{int} = 0.0313, R_{sigma} = 0.0364]
Data/restraints/parameters	9775/1842/869
Goodness-of-fit on F^2	1.025
Final R indexes [I>=2σ (I)]	R_1 = 0.0429, wR_2 = 0.0978
Final R indexes [all data]	R_1 = 0.0642, wR_2 = 0.1069
Largest diff. peak/hole / e Å^{-3}	0.69/-0.28

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for p-1_b_a. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Al2	757.5(8)	8603.4(7)	-192.9(4)	17.74(17)
O2	6827(2)	7014(2)	8012.6(11)	37.8(5)
N2	7888(3)	6776(2)	7783.3(12)	30.1(6)
F2	0	10000	0	22.7(5)
N4	9591(3)	7813(3)	6984.5(14)	42.6(7)
O4	11741(3)	4893(2)	8392.9(12)	47.5(6)
O3	9607(3)	8716(2)	6716.9(12)	48.4(6)
Al1	5521.5(8)	3432.7(6)	5300.4(4)	17.89(17)
C1	10863(3)	5511(2)	8011.0(14)	26.3(6)
Fe1	9452.2(4)	6435.8(4)	7386.9(2)	28.45(11)
O1	9606(2)	5099.0(19)	6420.1(11)	36.4(5)
N1	9574(2)	5633(2)	6795.2(13)	29.5(5)
F1	5000	5000	5000	20.4(4)
O1_6	-538(2)	8307.3(19)	-412.3(11)	33.3(5)
C1_6	-1814(3)	8324(2)	-363.7(14)	26.1(6)
C2_6	-1700(3)	7066(3)	-334.9(15)	28.9(6)
F1_6	-828.4(17)	6607.0(14)	-799.6(9)	34.5(4)
F2_6	-2903.8(18)	7059.1(15)	-456.4(10)	39.1(4)
F3_6	-1223(2)	6332.7(16)	278.6(9)	45.8(5)
C3_6	-2522(3)	8699(3)	299.7(15)	32.0(7)
F4_6	-2946.7(18)	9868.0(16)	206.7(9)	40.7(4)
F5_6	-1617(2)	8168.5(19)	825.9(9)	50.4(5)
F6_6	-3593.5(19)	8426.1(17)	471.3(10)	44.6(5)
C4_6	-2690(3)	9225(3)	-1009.7(15)	33.1(7)
F7_6	-2462(2)	10204.1(15)	-1167.9(10)	44.9(5)
F8_6	-4032.6(18)	9529.8(16)	-925.6(10)	44.7(5)
F9_6	-2350(2)	8764.9(15)	-1561.0(9)	40.2(4)
O1_5	1825.4(19)	8726.1(16)	-858.6(9)	24.6(4)
C1_5	2112(3)	8800(2)	-1536.6(13)	21.2(6)
C2_5	922(3)	9838(2)	-2007.3(14)	28.9(6)
F1_5	-114.9(16)	9526.8(16)	-2052.4(9)	35.9(4)
F2_5	1331.1(18)	10154.6(15)	-2643.2(9)	39.2(4)
F3_5	423.0(19)	10771.0(15)	-1743.0(10)	44.4(5)
C3_5	3448(3)	9013(2)	-1673.7(13)	24.1(6)
F4_5	4391.3(16)	8312.8(15)	-1178.0(8)	32.9(4)
F5_5	3205.0(17)	10131.4(14)	-1694.8(8)	31.8(4)
F6_5	4000.4(16)	8797.3(15)	-2272.7(8)	30.8(4)
C4_5	2344(3)	7616(2)	-1710.9(14)	26.0(6)
F7_5	3569.3(17)	6767.0(14)	-1477.7(9)	35.2(4)
F8_5	2262.7(17)	7731.6(15)	-2387.7(8)	31.7(4)
F9_5	1392.4(18)	7232.5(15)	-1415.4(9)	34.5(4)
O1_4	1619(2)	7750.8(16)	570.9(9)	28.0(4)
C1_4	2612(3)	6703(2)	896.4(13)	24.6(6)
C2_4	2558(3)	5659(2)	654.6(15)	30.5(7)
F1_4	1510.7(19)	5396.5(15)	941.7(10)	42.6(5)
F2_4	3704.7(17)	4673.9(13)	819.0(9)	34.7(4)
F3_4	2343(2)	5962.8(15)	-23.9(9)	45.0(5)
C3_4	4049(3)	6724(3)	744.5(17)	38.0(7)
F4_4	4033(2)	7748.2(17)	773.8(14)	62.8(6)
F5_4	4436(2)	6565.1(17)	119.5(11)	52.9(5)
F6_4	5022.8(19)	5872.5(17)	1196.0(11)	53.1(6)
C4_4	2344(3)	6521(3)	1678.2(14)	34.1(7)
F7_4	2649(2)	7248.1(16)	1930.0(9)	50.0(5)
F8_4	3095(2)	5408.7(15)	2030.1(9)	54.2(6)
F9_4	1031(2)	6740.6(16)	1807.6(9)	46.8(5)
O1_3	4830.9(18)	2991.9(15)	4747.7(9)	21.6(4)
C1_3	4983(3)	2584(2)	4171.8(13)	22.3(6)
C2_3	4733(3)	3622(2)	3521.8(14)	30.1(6)
F1_3	3387.9(17)	4323.1(14)	3432.9(8)	33.7(4)
F2_3	5159.3(18)	3258.0(15)	2945.5(8)	35.9(4)
F3_3	5377.4(19)	4278.7(15)	3592.4(9)	39.6(4)
C3_3	6440(3)	1582(2)	4156.3(14)	27.8(6)
F4_3	6834.4(17)	859.6(14)	4782.9(8)	33.6(4)

F5_3	7376.0(17)	2038.0(15)	3958.2(9)	35.8(4)
F6_3	6492.6(18)	932.5(14)	3725.4(9)	37.2(4)
C4_3	3874(3)	2072(2)	4182.5(14)	28.9(6)
F7_3	4239.2(19)	1016.9(14)	4615.7(9)	37.6(4)
F8_3	3687.9(18)	1963.8(15)	3554.5(8)	37.3(4)
F9_3	2667.4(16)	2779.2(14)	4373.6(8)	32.4(4)
O1_2	4760.2(18)	3287.2(15)	6084.9(9)	21.2(4)
C1_2	4388(3)	2529(2)	6588.5(13)	23.6(6)
C2_2	3231(3)	2293(3)	6322.0(15)	30.9(7)
F1_2	2318.0(17)	3282.6(15)	5925.9(9)	37.1(4)
F2_2	2553.4(18)	1864.1(16)	6833.8(9)	40.3(4)
F3_2	3756(2)	1510.9(16)	5935.5(9)	41.4(4)
C3_2	5636(3)	1327(3)	6850.0(15)	32.0(7)
F4_2	6463.3(17)	1422.6(15)	7271.4(9)	38.3(4)
F5_2	6382.6(18)	987.5(14)	6314.3(9)	36.3(4)
F6_2	5261.7(18)	455.7(14)	7184.7(9)	39.7(4)
C4_2	3848(3)	3121(3)	7197.3(15)	32.9(7)
F7_2	4659.9(19)	3589.6(15)	7335.4(8)	36.6(4)
F8_2	3734(2)	2359.2(17)	7775.5(8)	42.4(5)
F9_2	2586.7(19)	4006.8(16)	7034.2(9)	44.1(5)
O1_1	7277.8(17)	2827.8(15)	5281.3(9)	21.1(4)
C1_1	8503(3)	2776(2)	5463.0(13)	21.8(6)
C2_1	8678(3)	3912(2)	5051.3(14)	26.3(6)
F1_1	8283.5(17)	4181.1(14)	4394.4(8)	32.6(4)
F2_1	9975.2(16)	3805.5(15)	5061.7(9)	33.3(4)
F3_1	7891.0(17)	4832.0(13)	5307.8(8)	30.6(4)
C3_1	8575(3)	2657(2)	6252.0(14)	24.3(6)
F4_1	8794.1(17)	1557.3(14)	6609.8(8)	31.5(4)
F5_1	7391.1(16)	3382.3(14)	6451.7(8)	29.6(4)
F6_1	9578.4(17)	2911.7(15)	6424.3(8)	33.3(4)
C4_1	9685(3)	1674(2)	5286.8(15)	28.6(6)
F7_1	9366.3(18)	736.8(14)	5474.8(9)	36.6(4)
F8_1	10872.8(16)	1389.0(15)	5602.4(9)	37.4(4)
F9_1	9888.0(18)	1864.1(15)	4607.8(9)	37.7(4)

Table 3 Bond Lengths for p-1_b_a.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Al2	F2	1.7631(7)	C3_4	F5_4	1.328(4)
O2	N2	1.133(3)	C3_4	F6_4	1.337(3)
N2	Fe1	1.719(3)	C4_4	F7_4	1.324(3)
N4	O3	1.143(4)	C4_4	F8_4	1.336(3)
N4	Fe1	1.794(3)	C4_4	F9_4	1.325(4)
O4	C1	1.131(3)	O1_3	Al1	1.7046(18)
Al1	F1	1.7846(7)	O1_3	C1_3	1.361(3)
C1	Fe1	1.816(3)	C1_3	C2_3	1.545(4)
Fe1	N1	1.729(2)	C1_3	C3_3	1.555(4)
O1	N1	1.133(3)	C1_3	C4_3	1.566(4)
O1_6	Al2	1.693(2)	C2_3	F1_3	1.336(3)
O1_6	C1_6	1.347(3)	C2_3	F2_3	1.335(3)
C1_6	C2_6	1.548(4)	C2_3	F3_3	1.324(3)
C1_6	C3_6	1.562(4)	C3_3	F4_3	1.330(3)
C1_6	C4_6	1.552(4)	C3_3	F5_3	1.335(3)
C2_6	F1_6	1.329(3)	C3_3	F6_3	1.333(3)
C2_6	F2_6	1.330(3)	C4_3	F7_3	1.316(3)
C2_6	F3_6	1.326(3)	C4_3	F8_3	1.344(3)
C3_6	F4_6	1.335(3)	C4_3	F9_3	1.325(3)
C3_6	F5_6	1.327(3)	O1_2	Al1	1.7103(19)
C3_6	F6_6	1.320(3)	O1_2	C1_2	1.361(3)
C4_6	F7_6	1.325(3)	C1_2	C2_2	1.550(4)
C4_6	F8_6	1.326(3)	C1_2	C3_2	1.551(4)
C4_6	F9_6	1.342(3)	C1_2	C4_2	1.552(4)
O1_5	Al2	1.698(2)	C2_2	F1_2	1.327(3)
O1_5	C1_5	1.357(3)	C2_2	F2_2	1.335(3)
C1_5	C2_5	1.553(4)	C2_2	F3_2	1.337(3)
C1_5	C3_5	1.547(4)	C3_2	F4_2	1.334(3)
C1_5	C4_5	1.558(4)	C3_2	F5_2	1.339(3)

C2_5	F1_5	1.337(3)	C3_2	F6_2	1.333(3)
C2_5	F2_5	1.327(3)	C4_2	F7_2	1.320(3)
C2_5	F3_5	1.322(3)	C4_2	F8_2	1.337(3)
C3_5	F4_5	1.326(3)	C4_2	F9_2	1.347(3)
C3_5	F5_5	1.333(3)	O1_1	Al1	1.7050(19)
C3_5	F6_5	1.338(3)	O1_1	C1_1	1.356(3)
C4_5	F7_5	1.329(3)	C1_1	C2_1	1.546(4)
C4_5	F8_5	1.334(3)	C1_1	C3_1	1.557(4)
C4_5	F9_5	1.333(3)	C1_1	C4_1	1.553(4)
O1_4	Al2	1.7068(19)	C2_1	F1_1	1.331(3)
O1_4	C1_4	1.351(3)	C2_1	F2_1	1.334(3)
C1_4	C2_4	1.560(4)	C2_1	F3_1	1.335(3)
C1_4	C3_4	1.545(4)	C3_1	F4_1	1.330(3)
C1_4	C4_4	1.545(4)	C3_1	F5_1	1.324(3)
C2_4	F1_4	1.337(3)	C3_1	F6_1	1.335(3)
C2_4	F2_4	1.328(3)	C4_1	F7_1	1.330(3)
C2_4	F3_4	1.327(3)	C4_1	F8_1	1.331(3)
C3_4	F4_4	1.320(3)	C4_1	F9_1	1.335(3)

Table 4 Bond Angles for p-1_b_a.

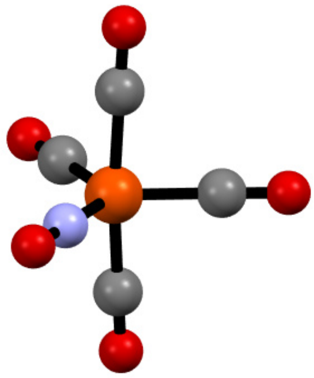
Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1_6	Al2	F2	107.31(8)	F4_4	C3_4	C1_4	110.8(2)
O1_6	Al2	O1_5	112.02(10)	F4_4	C3_4	F5_4	108.5(3)
O1_6	Al2	O1_4	116.60(11)	F4_4	C3_4	F6_4	107.1(3)
O1_5	Al2	F2	106.54(7)	F5_4	C3_4	C1_4	110.4(2)
O1_5	Al2	O1_4	113.12(10)	F5_4	C3_4	F6_4	107.4(2)
O1_4	Al2	F2	99.83(7)	F6_4	C3_4	C1_4	112.5(3)
O2	N2	Fe1	176.5(2)	F7_4	C4_4	C1_4	110.9(3)
Al2[1]	F2	Al2	180.0	F7_4	C4_4	F8_4	108.1(2)
O3	N4	Fe1	176.3(3)	F7_4	C4_4	F9_4	107.1(2)
O1_3	Al1	F1	107.96(7)	F8_4	C4_4	C1_4	111.6(2)
O1_3	Al1	O1_2	110.14(9)	F9_4	C4_4	C1_4	111.5(2)
O1_3	Al1	O1_1	111.03(9)	F9_4	C4_4	F8_4	107.4(3)
O1_2	Al1	F1	102.71(7)	C1_3	O1_3	Al1	147.78(18)
O1_1	Al1	F1	105.80(7)	O1_3	C1_3	C2_3	109.6(2)
O1_1	Al1	O1_2	118.32(9)	O1_3	C1_3	C3_3	111.5(2)
O4	C1	Fe1	176.9(3)	O1_3	C1_3	C4_3	107.8(2)
N2	Fe1	N4	107.14(12)	C2_3	C1_3	C3_3	110.0(2)
N2	Fe1	C1	110.96(12)	C2_3	C1_3	C4_3	109.2(2)
N2	Fe1	N1	110.72(11)	C3_3	C1_3	C4_3	108.8(2)
N4	Fe1	C1	109.75(13)	F1_3	C2_3	C1_3	110.1(2)
N1	Fe1	N4	111.82(12)	F2_3	C2_3	C1_3	112.9(2)
N1	Fe1	C1	106.50(11)	F2_3	C2_3	F1_3	107.4(2)
O1	N1	Fe1	177.0(2)	F3_3	C2_3	C1_3	110.3(2)
Al1[2]	F1	Al1	180.0	F3_3	C2_3	F1_3	107.6(2)
C1_6	O1_6	Al2	154.26(18)	F3_3	C2_3	F2_3	108.3(2)
O1_6	C1_6	C2_6	108.6(2)	F4_3	C3_3	C1_3	110.6(2)
O1_6	C1_6	C3_6	110.9(2)	F4_3	C3_3	F5_3	106.9(2)
O1_6	C1_6	C4_6	108.9(2)	F4_3	C3_3	F6_3	108.2(2)
C2_6	C1_6	C3_6	109.5(2)	F5_3	C3_3	C1_3	110.7(2)
C2_6	C1_6	C4_6	109.7(2)	F6_3	C3_3	C1_3	112.7(2)
C4_6	C1_6	C3_6	109.2(2)	F6_3	C3_3	F5_3	107.5(2)
F1_6	C2_6	C1_6	111.0(2)	F7_3	C4_3	C1_3	111.4(2)
F1_6	C2_6	F2_6	107.4(2)	F7_3	C4_3	F8_3	107.7(2)
F2_6	C2_6	C1_6	112.6(2)	F7_3	C4_3	F9_3	107.9(2)
F3_6	C2_6	C1_6	110.9(2)	F8_3	C4_3	C1_3	111.3(2)
F3_6	C2_6	F1_6	106.9(2)	F9_3	C4_3	C1_3	110.9(2)
F3_6	C2_6	F2_6	107.8(2)	F9_3	C4_3	F8_3	107.6(2)
F4_6	C3_6	C1_6	110.1(2)	C1_2	O1_2	Al1	143.62(17)
F5_6	C3_6	C1_6	109.6(2)	O1_2	C1_2	C2_2	110.9(2)
F5_6	C3_6	F4_6	107.4(2)	O1_2	C1_2	C3_2	111.2(2)
F6_6	C3_6	C1_6	113.0(2)	O1_2	C1_2	C4_2	107.5(2)
F6_6	C3_6	F4_6	108.3(2)	C2_2	C1_2	C3_2	109.0(2)
F6_6	C3_6	F5_6	108.4(3)	C2_2	C1_2	C4_2	109.3(2)
F7_6	C4_6	C1_6	110.8(2)	C3_2	C1_2	C4_2	108.9(2)
F7_6	C4_6	F8_6	108.2(2)	F1_2	C2_2	C1_2	110.9(2)

F7_6 C4_6 F9_6	106.9(2)	F1_2 C2_2 F2_2	107.9(2)
F8_6 C4_6 C1_6	112.7(2)	F1_2 C2_2 F3_2	107.0(2)
F8_6 C4_6 F9_6	107.2(2)	F2_2 C2_2 C1_2	112.6(2)
F9_6 C4_6 C1_6	110.6(2)	F2_2 C2_2 F3_2	107.7(2)
C1_5 O1_5 Al2	149.70(17)	F3_2 C2_2 C1_2	110.5(2)
O1_5 C1_5 C2_5	111.3(2)	F4_2 C3_2 C1_2	111.1(2)
O1_5 C1_5 C3_5	107.9(2)	F4_2 C3_2 F5_2	107.5(2)
O1_5 C1_5 C4_5	110.1(2)	F5_2 C3_2 C1_2	109.8(2)
C2_5 C1_5 C4_5	109.0(2)	F6_2 C3_2 C1_2	112.9(2)
C3_5 C1_5 C2_5	109.3(2)	F6_2 C3_2 F4_2	108.0(2)
C3_5 C1_5 C4_5	109.2(2)	F6_2 C3_2 F5_2	107.3(2)
F1_5 C2_5 C1_5	110.5(2)	F7_2 C4_2 C1_2	111.5(2)
F2_5 C2_5 C1_5	112.1(2)	F7_2 C4_2 F8_2	108.1(2)
F2_5 C2_5 F1_5	107.8(2)	F7_2 C4_2 F9_2	107.3(2)
F3_5 C2_5 C1_5	110.3(2)	F8_2 C4_2 C1_2	112.5(2)
F3_5 C2_5 F1_5	107.2(2)	F8_2 C4_2 F9_2	107.3(2)
F3_5 C2_5 F2_5	108.9(2)	F9_2 C4_2 C1_2	110.0(2)
F4_5 C3_5 C1_5	110.9(2)	C1_1 O1_1 Al1	149.47(16)
F4_5 C3_5 F5_5	107.5(2)	O1_1 C1_1 C2_1	109.3(2)
F4_5 C3_5 F6_5	107.5(2)	O1_1 C1_1 C3_1	110.6(2)
F5_5 C3_5 C1_5	111.0(2)	O1_1 C1_1 C4_1	108.9(2)
F5_5 C3_5 F6_5	107.8(2)	C2_1 C1_1 C3_1	109.9(2)
F6_5 C3_5 C1_5	111.8(2)	C2_1 C1_1 C4_1	109.3(2)
F7_5 C4_5 C1_5	111.5(2)	C4_1 C1_1 C3_1	108.8(2)
F7_5 C4_5 F8_5	107.7(2)	F1_1 C2_1 C1_1	110.3(2)
F7_5 C4_5 F9_5	107.3(2)	F1_1 C2_1 F2_1	107.8(2)
F8_5 C4_5 C1_5	112.8(2)	F1_1 C2_1 F3_1	107.5(2)
F9_5 C4_5 C1_5	110.3(2)	F2_1 C2_1 C1_1	112.9(2)
F9_5 C4_5 F8_5	107.1(2)	F2_1 C2_1 F3_1	107.6(2)
C1_4 O1_4 Al2	145.84(17)	F3_1 C2_1 C1_1	110.5(2)
O1_4 C1_4 C2_4	110.9(2)	F4_1 C3_1 C1_1	110.6(2)
O1_4 C1_4 C3_4	110.2(2)	F4_1 C3_1 F6_1	107.8(2)
O1_4 C1_4 C4_4	107.4(2)	F5_1 C3_1 C1_1	110.2(2)
C3_4 C1_4 C2_4	108.9(2)	F5_1 C3_1 F4_1	107.5(2)
C4_4 C1_4 C2_4	109.2(2)	F5_1 C3_1 F6_1	108.1(2)
C4_4 C1_4 C3_4	110.3(2)	F6_1 C3_1 C1_1	112.5(2)
F1_4 C2_4 C1_4	110.8(2)	F7_1 C4_1 C1_1	110.5(2)
F2_4 C2_4 C1_4	112.7(2)	F7_1 C4_1 F8_1	107.9(2)
F2_4 C2_4 F1_4	107.4(2)	F7_1 C4_1 F9_1	107.0(2)
F3_4 C2_4 C1_4	110.4(2)	F8_1 C4_1 C1_1	112.3(2)
F3_4 C2_4 F1_4	106.7(2)	F8_1 C4_1 F9_1	108.0(2)
F3_4 C2_4 F2_4	108.7(2)	F9_1 C4_1 C1_1	111.0(2)

[1]-X,2-Y,-Z; [2]1-X,1-Y,1-Z

9. Additional Information on the DFT Calculations

$[Fe(CO)_4(NO)]^+$ (C_{2v} symmetry @BP86-D3BJ/def2-TZVPP) (NO equatorial)



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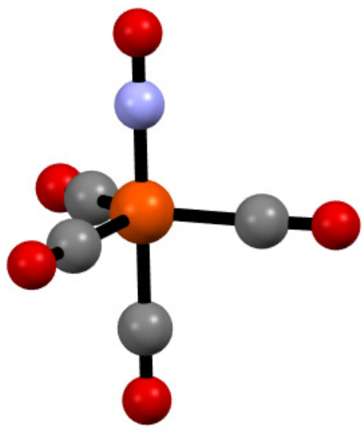
     5                       0.00          0.00000         -        -
     6                       0.00          0.00000         -        -
     7         a1           53.43          0.00008        YES      YES
     8         b2           59.01          0.00715        YES      YES
     9         b1           90.99          0.00039        YES      YES
    10         a2           96.16          0.00000        NO       YES
    11         b2           96.87          0.31360        YES      YES
    12         b1          101.32          0.72918        YES      YES
    13         a1          104.97          0.51102        YES      YES
    14         b2          330.70          0.00284        YES      YES
    15         b1          339.54          0.25727        YES      YES
    16         a2          358.81          0.00000        NO       YES
    17         a1          398.79          3.82138        YES      YES
    18         a1          408.84          0.87373        YES      YES
    19         a1          414.57          0.00137        YES      YES
```

```
     20          b2              424.83           14.26280         YES       YES
     21          b1              449.41            8.71662         YES       YES
     22          b2              514.34            4.39916         YES       YES
     23          b1              522.17            1.51767         YES       YES
     24          a1              523.78           10.23997         YES       YES
     25          a2              532.53            0.00000         NO        YES
     26          b1              624.68          111.56695         YES       YES
     27          a1              641.93           95.26997         YES       YES
     28          b2              646.80          113.49697         YES       YES
     29          a1             1941.25          883.68741         YES       YES
     30          b2             2095.69          680.65338         YES       YES
     31          b1             2114.27          763.42678         YES       YES
     32          a1             2114.31          100.05333         YES       YES
     33          a1             2167.74           42.90675         YES       YES
$end
```

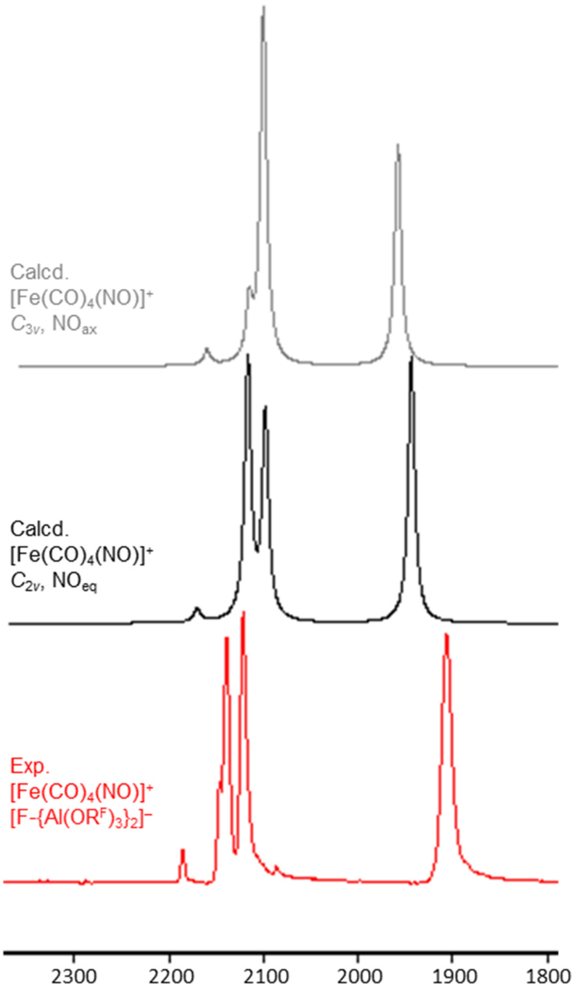
[Fe(CO)₄(NO)]⁺ (*C*₃ᵥ symmetry @BP86-D3BJ/def2-TZVPP) (NO axial)



```
$coord
    0.00000000000000      0.00000000000000      0.25078955674978  fe
    1.74129538649716     -3.01601208039834     -0.04846088545601  c
    1.74129538649716      3.01601208039834     -0.04846088545601  c
    0.00000000000000      0.00000000000000      3.44996681051303  n
   -0.00000000000000      0.00000000000000     -3.23326551166298  c
   -3.48259077299430      0.00000000000000     -0.04846088545601  c
    0.00000000000000      0.00000000000000     -5.38453712056163  o
    0.00000000000000      0.00000000000000      5.59935191883626  o
   -5.63116012160138      0.00000000000000     -0.17897433250214  o
    2.81558006080070     -4.87672771808467     -0.17897433250214  o
    2.81558006080070      4.87672771808467     -0.17897433250214  o

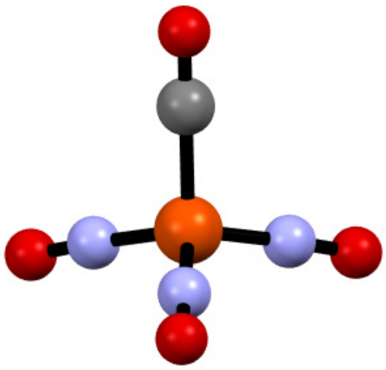

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)       km/mol          IR      RAMAN
     1                      0.00        0.00000         -        -
     2                      0.00        0.00000         -        -
     3                      0.00        0.00000         -        -
     4                      0.00        0.00000         -        -
     5                      0.00        0.00000         -        -
     6                      0.00        0.00000         -        -
     7        e            37.45        0.15171        YES      YES
     8        e            37.45        0.15171        YES      YES
     9        e            94.80        0.06903        YES      YES
    10        e            94.80        0.06903        YES      YES
    11        a1          106.36        0.94866        YES      YES
    12        e           106.45        0.06163        YES      YES
    13        e           106.45        0.06163        YES      YES
    14        a2          342.26        0.00000        NO       NO
    15        e           346.39        0.11886        YES      YES
    16        e           346.39        0.11886        YES      YES
    17        e           378.04        7.18260        YES      YES
    18        e           378.04        7.18260        YES      YES
    19        a1          396.38        0.00075        YES      YES
    20        e           432.65        5.94459        YES      YES
    21        e           432.65        5.94459        YES      YES
    22        a1          437.76        0.96428        YES      YES
    23        a1          493.70       23.35968        YES      YES
    24        e           529.47        5.78819        YES      YES
```

```
     25          e            529.47         5.78819        YES       YES
     26          a1           618.96        82.18842        YES       YES
     27          e            667.59        92.33210        YES       YES
     28          e            667.59        92.33210        YES       YES
     29          a1          1955.56       856.07511        YES       YES
     30          e           2097.55       689.31745        YES       YES
     31          e           2097.55       689.31745        YES       YES
     32          a1          2112.71       216.92820        YES       YES
     33          a1          2157.63        57.80197        YES       YES
$end
```



Supplementary Figure 27. Comparison of calculated and experimental IR spectra of **1**. Only the CO/NO region is shown.

[Fe(CO)(NO)$_3$]$^+$ (C_{3v} symmetry @BP86-D3BJ/def2-TZVPP)



```
$coord
   -0.00000000000000      0.00000000000000      0.24725638522662  fe
   -1.54999255674679     -2.68466585963901      1.09014987083261  n
    0.00000000000000      0.00000000000000     -3.31102864973505  c
   -1.54999255674679      2.68466585963901      1.09014987083261  n
    3.09998511349359      0.00000000000000      1.09014987083261  n
    0.00000000000000      0.00000000000000     -5.45718570748089  o
   -2.57517766763481     -4.46033855886023      1.75016945316387  o
    5.15035533526963      0.00000000000000      1.75016945316387  o
   -2.57517766763481      4.46033855886023      1.75016945316387  o
$end

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol         IR      RAMAN
     1                      -0.00         0.00000        -        -
     2                      -0.00         0.00000        -        -
     3                       0.00         0.00000        -        -
     4                       0.00         0.00000        -        -
     5                       0.00         0.00000        -        -
     6                       0.00         0.00000        -        -
     7         e            68.30         0.09261       YES      YES
     8         e            68.30         0.09261       YES      YES
     9         a1           73.57         0.01693       YES      YES
    10         e            83.91         0.00478       YES      YES
    11         e            83.91         0.00478       YES      YES
    12         a2          283.14         0.00000       NO       NO
    13         e           306.44         0.08598       YES      YES
    14         e           306.44         0.08598       YES      YES
    15         a1          405.12        10.40445       YES      YES
    16         e           467.32        13.60844       YES      YES
    17         e           467.32        13.60844       YES      YES
    18         a1          526.15         4.88199       YES      YES
    19         e           568.63        16.33473       YES      YES
    20         e           568.63        16.33473       YES      YES
    21         e           624.80        91.69973       YES      YES
    22         e           624.80        91.69973       YES      YES
    23         a1          682.98        76.18859       YES      YES
    24         e          1919.39      1179.43145       YES      YES
    25         e          1919.39      1179.43145       YES      YES
    26         a1         1985.82       332.02390       YES      YES
    27         a1         2138.62       308.66085       YES      YES
$end
```

AIM analysis

For the QTAIM calculations (QTAIM = Quantum Theory of Atoms In Molecules) the multifunctional wavefunction analyzer Multiwfn was employed.[23] wfn input files were generated by single-point calculations on the B3LYP-D3BJ/def2-TZVPP level of theory employing TURBOMOLE. A basin analysis (options 17 + 1) has been performed on the electron density (option 1) employing a high quality grid (spacing = 0.06 Bohr, option 3). The electron density has been integrated with atomic-center + uniform grids and with exact refinement of the basin boundaries (options 7 + 2 + 1). As a result, the atomic charges after normalization are given.

The atomic charges after normalization and atomic volumes:

$[Fe(CO)_4(NO)]^+$ (C_{3v}, NO_{ax}, $E_{rel.}$ = +45 kJ/mol)

```
      1 (Fe)     Charge:    0.894687     Volume:    74.304 Bohr^3
      2 (C )     Charge:    1.028693     Volume:    76.441 Bohr^3
      3 (C )     Charge:    1.028693     Volume:    76.441 Bohr^3
      4 (N )     Charge:    0.235497     Volume:    81.211 Bohr^3
      5 (C )     Charge:    1.056015     Volume:    66.588 Bohr^3
      6 (C )     Charge:    1.026304     Volume:    76.436 Bohr^3
      7 (O )     Charge:   -1.012657     Volume:   125.420 Bohr^3
      8 (O )     Charge:   -0.197147     Volume:   103.584 Bohr^3
      9 (O )     Charge:   -1.017820     Volume:   126.436 Bohr^3
     10 (O )     Charge:   -1.021133     Volume:   126.445 Bohr^3
     11 (O )     Charge:   -1.021133     Volume:   126.445 Bohr^3
```

$[Fe(CO)_4(NO)]^+$ (C_{2v}, NO_{eq}, $E_{rel.}$ = 0 kJ/mol)

```
      1 (Fe)     Charge:    0.934523     Volume:    72.439 Bohr^3
      2 (N )     Charge:    0.239864     Volume:    86.543 Bohr^3
      3 (C )     Charge:    1.024855     Volume:    74.863 Bohr^3
      4 (C )     Charge:    1.024855     Volume:    74.863 Bohr^3
      5 (C )     Charge:    1.053088     Volume:    70.277 Bohr^3
      6 (C )     Charge:    1.053088     Volume:    70.277 Bohr^3
      7 (O )     Charge:   -0.258832     Volume:   104.858 Bohr^3
      8 (O )     Charge:   -1.023555     Volume:   126.555 Bohr^3
      9 (O )     Charge:   -1.023554     Volume:   126.555 Bohr^3
     10 (O )     Charge:   -1.012166     Volume:   125.616 Bohr^3
     11 (O )     Charge:   -1.012166     Volume:   125.616 Bohr^3
```

$[Fe(CO)(NO)_3]^+$ (C_{3v})

```
      1 (Fe)     Charge:    1.049618     Volume:    83.258 Bohr^3
      2 (N )     Charge:    0.214417     Volume:    90.453 Bohr^3
      3 (C )     Charge:    1.034258     Volume:    81.994 Bohr^3
      4 (N )     Charge:    0.214416     Volume:    90.453 Bohr^3
      5 (N )     Charge:    0.217405     Volume:    90.415 Bohr^3
      6 (O )     Charge:   -1.024933     Volume:   126.488 Bohr^3
      7 (O )     Charge:   -0.234048     Volume:   104.552 Bohr^3
      8 (O )     Charge:   -0.237085     Volume:   104.552 Bohr^3
      9 (O )     Charge:   -0.234048     Volume:   104.552 Bohr^3
```

$[Co(CO)_5]^+$ (D_{3h})

```
      1 (Co)     Charge:    0.740927     Volume:    75.755 Bohr^3
      2 (C )     Charge:    1.057833     Volume:    75.557 Bohr^3
      3 (C )     Charge:    1.057830     Volume:    75.557 Bohr^3
      4 (C )     Charge:    1.061765     Volume:    75.485 Bohr^3
      5 (C )     Charge:    1.080244     Volume:    68.513 Bohr^3
      6 (C )     Charge:    1.080248     Volume:    68.513 Bohr^3
      7 (O )     Charge:   -1.011064     Volume:   125.358 Bohr^3
      8 (O )     Charge:   -1.016972     Volume:   126.282 Bohr^3
      9 (O )     Charge:   -1.019874     Volume:   126.370 Bohr^3
```

10	(O)	Charge:	-1.019870	Volume:	126.370	Bohr^3
11	(O)	Charge:	-1.011067	Volume:	125.358	Bohr^3

$[Mn(NO)_4]^+$ (T_d)

1	(Mn)	Charge:	1.227927	Volume:	79.894	Bohr^3
2	(N)	Charge:	0.181712	Volume:	92.564	Bohr^3
3	(N)	Charge:	0.181714	Volume:	92.564	Bohr^3
4	(N)	Charge:	0.181712	Volume:	92.564	Bohr^3
5	(N)	Charge:	0.181712	Volume:	92.564	Bohr^3
6	(O)	Charge:	-0.238695	Volume:	104.799	Bohr^3
7	(O)	Charge:	-0.238696	Volume:	104.799	Bohr^3
8	(O)	Charge:	-0.238693	Volume:	104.799	Bohr^3
9	(O)	Charge:	-0.238693	Volume:	104.799	Bohr^3

$[Co(CO)_2(NO)_2]^+$ (C_{2v})

1	(Co)	Charge:	0.872674	Volume:	87.764	Bohr^3
2	(N)	Charge:	0.258136	Volume:	89.636	Bohr^3
3	(N)	Charge:	0.258123	Volume:	89.636	Bohr^3
4	(C)	Charge:	1.056014	Volume:	81.222	Bohr^3
5	(C)	Charge:	1.056015	Volume:	81.222	Bohr^3
6	(O)	Charge:	-0.227424	Volume:	103.865	Bohr^3
7	(O)	Charge:	-0.227423	Volume:	103.865	Bohr^3
8	(O)	Charge:	-1.023057	Volume:	126.406	Bohr^3
9	(O)	Charge:	-1.023057	Volume:	126.406	Bohr^3

Gas Phase and Solution Reaction Enthalpies

Supplementary Table 3. Gas phase and COSMO solution thermodynamics in CH_2Cl_2 (ε = 8.93) and oDFB (ε = 13.8).

Reaction	BP86 ΔH°(gas)	BP86 ΔG°(solv) CH_2Cl_2	BP86 ΔG°(solv) *o*DFB	B3LYP ΔH°(gas)	B3LYP ΔG°(solv) CH_2Cl_2	B3LYP ΔG°(solv) *o*DFB
$Fe(CO)_5 + NO^+ \longrightarrow [Fe(CO)_4(NO)]^+ + CO$	–213	–103	–96	–219	–110	–103
$Fe(CO)_5 + NO^+ + 2NO \longrightarrow [Fe(CO)(NO)_3]^+ + 4CO$	–260	–190	–183	–197	–127	–120
$[Fe(CO)_4(NO)]^+ + 2NO \longrightarrow [Fe(CO)(NO)_3]^+ + 3CO$	–47	–87	–87	+22	–18	–18

Molecule	BP86 energies (kJ mol^{-1}) Enthalpy H	freeH energy	freeH entropy	CH_2Cl_2, ε = 8.93 COSMO energy	*o*DFB, ε = 13.8 COSMO energy
$Fe(CO)_5$ (D_{3h})	-4807274.1937358200	139.720	0.445790	-1831.0513838031	-1831.0516380071
CO (C_{6v})	-297620.9347443340	18.910	0.197890	-113.3667511377	-113.3668061814
NO (C_{2v})	-341192.7487023620	17.470	0.199780	-129.9619266897	-129.9619870253
NO^+ (C_{6v})	-340264.7504791870	20.320	0.198440	-129.7224232666	-129.7297605215
$[Fe(CO)_4(NO)]^+$ (C_{2v})	-4850130.8947143500	140.140	0.457830	-1847.4446335846	-1847.4494952486
$[Fe(CO)(NO)_3]^+$ (C_{3v})	-4639700.6116683000	110.480	0.412860	-1767.2852293669	-1767.2900975994

Molecule	B3LYP energies (kJ mol^{-1}) Enthalpy H	freeH energy	freeH entropy	CH_2Cl_2, ε = 8.93 COSMO energy	*o*DFB, ε = 13.8 COSMO energy
$Fe(CO)_5$ (D_{3h})	-4805540.54803954	141.740	0.445290	-1830.3925929252	-1830.3929019448
CO (C_{6v})	-297476.31921281	19.430	0.197720	-113.3119230922	-113.3119815473
NO (C_{2v})	-341010.51564983	18.020	0.199580	-129.8927231012	-129.8927828069
NO^+ (C_{6v})	-340084.09190075	21.050	0.198240	-129.6540344915	-129.6613804183
$[Fe(CO)_4(NO)]^+$ (C_{2v})	-4848366.95541261	142.340	0.458640	-1846.7745986457	-1846.7795209233
$[Fe(CO)(NO)_3]^+$ (C_{3v})	-4637937.31977398	112.850	0.410580	-1766.6156184687	-1766.6205644599

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