This is an electronic reprint of the original article.
This reprint may differ from the original in pagination and typographic detail.

Scheibe, Benjamin; Rudel, Stefan S.; Buchner, Magnus R.; Karttunen, Antti J.; Kraus, Florian
A 1D Coordination Polymer of UF₅ with HCN as a Ligand

Published in:
CHEMISTRY: A EUROPEAN JOURNAL

DOI:
[10.1002/chem.201605293](https://doi.org/10.1002/chem.201605293)

Published: 05/01/2017

Document Version
Peer reviewed version

Published under the following license:
CC BY-NC-ND

Please cite the original version:
Scheibe, B., Rudel, S. S., Buchner, M. R., Karttunen, A. J., & Kraus, F. (2017). A 1D Coordination Polymer of UF₅ with HCN as a Ligand. *CHEMISTRY: A EUROPEAN JOURNAL*, 23(2), 291-295.
<https://doi.org/10.1002/chem.201605293>

This material is protected by copyright and other intellectual property rights, and duplication or sale of all or part of any of the repository collections is not permitted, except that material may be duplicated by you for your research use or educational purposes in electronic or print form. You must obtain permission for any other use. Electronic or print copies may not be offered, whether for sale or otherwise to anyone who is not an authorised user.

A 1D Coordination Polymer of UF₅ with HCN as a Ligand – ¹[UF₅(HCN)₂]^{**}

Benjamin Scheibe, Stefan S. Rudel, Magnus R. Buchner, Antti J. Karttunen, and Florian Kraus*

Dedicated to Professor Karl O. Christe on the occasion of his 80th birthday

Abstract: We have reacted β -uranium(V) fluoride with liquid anhydrous hydrogen cyanide and obtained a 1D coordination polymer with the composition [UF₅(HCN)₂], ¹[UF_{4/1}F_{2/2}(HCN)_{2/1}], revealed by single crystal X-ray structure determination. The reaction system was furthermore studied by means of vibrational and NMR spectroscopy, as well as by quantum chemical calculations. The compound presents the first described polymeric HCN Lewis adduct and the first HCN adduct of a uranium fluoride.

While f-element coordination chemistry with the cyanide ion (CN[−]) as a ligand is quite well established, there is a noteworthy lack of compounds with its conjugated acid, namely hydrogen cyanide (HCN), as a ligand.^[1] This may be attributed to the more difficult handling of HCN in comparison to cyanide salts and its quite high toxicity for human beings.^[2,3] Nonetheless, Wöhler probably described the first Lewis adduct of a transition metal halide with HCN, [TiCl₄(HCN)₂], revealed by chemical analysis, in 1850.^[4,5]

Only a few more HCN Lewis adducts have been described to date, mainly of transition metal and main group element compounds. Most of them are halides and covered in a review by Corain in 1982.^[6] Furthermore, HCN can act as a ligand towards the XeF⁺ cation, as observed in [Xe(NCH)F][AsF₆].^[7] A selection of compounds known from the literature is shown in Scheme 1. These can be categorized into room temperature stable and unstable towards the loss of HCN, which indicates the strength of interaction. For example, the beryllium chloride adduct, BeCl₂·4HCN, easily loses HCN upon warming, whilst pnictogen fluoride HCN adducts, [EF₅(HCN)] (E = As, Sb) are thermally quite stable solids, which degrade at temperatures of 85 °C or higher.^[8,9]

Scheme 1. Selection of known transition metal and main group halide Lewis adducts with HCN as a ligand: a) beryllium chloride HCN adduct;^[8] b) boron halide HCN adducts;^[10–12] c) hexafluoronitroiron(II) bis-tetrachloroferrate(III);^[13] d) titanium(IV) halide HCN adducts;^[14] e) niobium(V) halide cyanide acids;^[15] f) pnictogen(V) fluoride HCN adducts.^[9]

Regarding the reactivity of HCN towards uranium halides, little is known: The reported attempts of chemical conversion, these are UCl₄ by Bagnall and coworkers and UF₆ by Klapötke and coworkers, did only result in the formation of an adduct in the first case, which was however not further characterized.^[16,17] In the latter case it was assumed, that the formation of a heptacoordinated uranium(VI) species does not occur due to kinetic reasons.

The reported solubility of β -UF₅ in acetonitrile and benzonitrile, as well as in other organic solvents, drew our interest to the β -UF₅/HCN system.^[18] The action of liquid anhydrous HCN (aHCN) onto pale green β -UF₅ immediately leads to a color change of the solid to olive green (see SI for photographs). After only a few minutes of reaction time at 0 °C the liquid phase turns turquoise and already after a few hours turquoise needle-shaped crystals separate. The crystallized compound was identified as [UF₅(HCN)₂] (**1**) by means of SCXRD. Scheme 2 shows the reaction equation.

Scheme 2. Formation of coordination compound **1** from β -UF₅ in liquid HCN.

Compound **1** crystallizes in the orthorhombic crystal system in space group type *Pca*2₁ (No. 29) with Z = 4 (see exp. section for further crystallographic details). A section of the crystal structure is shown in Figure 1. Each uranium atom is coordinated by five fluorine atoms, of which two are μ_2 -bridging, and two adjacent HCN molecules, forming a coordination polyhedron shaped like a trigonal-dodecahedron. The compound can thus be regarded as a one-dimensional coordination polymer described with the Niggli representation ¹[UF_{4/1}F_{2/2}(HCN)_{2/1}].^[19]

The U–F (2.014(5)–2.071(6) Å) and U–F_μ (2.227(6)–2.330(5) Å) atomic distances of compound **1** in the crystal structure are comparable to those of both known pure uranium(V) fluorides, showing only minor increases of the atomic distances due to the coordination of HCN molecules (α -UF₅, ¹[UF_{4/1}F_{2/2}], T = n.a., distances [Å]: U–F 2.020(5), U–F_μ 2.236(1); β -UF₅, ²[UF_{2/1}F_{6/2}], T = RT, distances [Å]: U–F 1.96(2), U–F_μ 2.27(2)).^[20,21] The C–F interchain atomic distances (2.963(2)–3.212(2) Å) are in the range of possible, however quite weak hydrogen bonding with resulting $\angle$ CHF angles in the range of 110.1–156.3°. This may promote the

[*] B. Scheibe, S. S. Rudel, Dr. M. R. Buchner, Prof. Dr. F. Kraus
 Fachbereich Chemie, Philipps-Universität Marburg
 Hans-Meerwein-Straße 4, 35032 Marburg (Germany)
 E-Mail: florian.kraus@chemie.uni-marburg.de
 Homepage: <https://www.uni-marburg.de/fb15/ag-kraus>
 Prof. Dr. A. J. Karttunen

Department of Chemistry, Aalto University, 00076 Aalto (Finland)

[**] We thank the Deutsche Forschungsgemeinschaft (DFG) for generous funding, Prof. Dr. Willner, Wuppertal, for the donation of UF₆, Solvay for the donation of fluorine, Dr. Harms, Marburg, for X-ray measurement time, Dr. Kuzu, Marburg, for Raman measurement time. F.K. thanks the DFG for a Heisenberg professorship. A.J.K. thanks the Academy of Finland (grant 294799), CSC, the Finnish IT Center for Science, for computational resources and Dr. Lorenzo Maschio, Turin, for helping with the computational Raman spectrum. Supporting information for this article is given via a link at the end of the document.

adjacent coordination mode of the HCN ligands and strengthen the interchain bonding interaction. The U–N atomic distances (2.643(8)–2.735(8) Å) and $\angle$ CNU angles (168.1(9)–178.4(8)°) of compound **1** are different due to space group symmetry and this different bonding of HCN ligands is further supported by the Raman and IR spectra. There, two bands for C–N stretching modes are present (see Figure 2 and 3). If one compares the C–N atomic distances (1.113(1)–1.145(1) Å) of compound **1** with other HCN Lewis adducts like $\text{VCl}_4 \cdot 2\text{HCN}$ (1.13(1) Å, $T = \text{n.a.}$), $[\text{TiCl}_4(\text{HCN})_2]$ (1.11(1) Å, $T = \text{n.a.}$), or $[\text{H}(\text{NbCl}_5\text{CN})]$ (1.090(4) Å, $T = \text{n.a.}$), only a significant difference can be seen for the latter one.^[5,22,23] This can be attributed to the quite strong interaction in the niobium compound, leading to a rise in the acidity and thus the formation of the $[\text{NbCl}_5\text{CN}]^-$ anion.^[15] The comparison with the C–N atomic distance in the gas phase (1.157 Å) also speaks for a rather weak interaction of HCN with UF_5 .^[24]

Figure 1. Section of the crystal structure of compound **1**. Infinite chains are truncated (dots) and an exemplary coordination polyhedron around an uranium atom is shown. Displacement ellipsoids are shown at the 70% probability level at 100 K, hydrogen atoms are depicted isotropic with arbitrary radii.

To verify the coordination of the HCN molecules via the N atoms, which in this case could not be unambiguously shown by the X-ray structure determination, Raman and ATR-IR spectra of compound **1** were collected. The Raman spectrum of turquoise crystals of compound **1** shows three distinct bands at 2135, 2131 and 599 cm^{-1} beneath the lattice modes, which can be attributed to C–N and U–F stretching modes (Table 1 and Figure 2).^[25,26] The first two bands are shifted hypsochromic in comparison to the mode of liquid HCN and the latter U–F mode is shifted bathochromic with regard to α - and β - UF_5 . The initial ATR-IR spectrum of time dependent measurements of a powdered sample of compound **1**, which were measured in a glovebox under an Ar atmosphere, shows characteristic bands of HCN at 3222, 2137 and 781 cm^{-1} , respectively (Table 2 and Figure 3). One could come up with the idea that HNC would form and coordinate via the carbon atom. However, the bands of a HNC molecule in an Ar matrix appear at 3620, 2029 and 477 cm^{-1} . Also, there is an enthalpy difference of approx. 62 kJ/mol to the HCN molecule, thus making the formation and coordination of HNC molecules very unlikely.^[27,28] We also calculated the Raman and IR spectra using quantum chemical methods (DFT-PBE0), and the calculated peak positions listed in Table 1 are in very good agreement with the experimental data (full spectral figures and assignment are available in the Supporting Information). The computationally calculated spectra also make it possible to distinguish between U–F (non-bridging) and U– F_μ (bridging F) stretching vibrations. The latter occur at about 70–100 cm^{-1} lower energy in comparison to the former, thus lying in the far IR range, which was not measured. This is in

line with the results from a population analysis, which suggests that the U– F_μ (bridging) bonds are slightly more ionic in comparison to the non-bridging U–F bonds.

Table 1. Raman spectroscopic data of α - and β - UF_5 in comparison to compound **1**. All values are given in $[\text{cm}^{-1}]$.

Species	$\nu(\text{C–N})$	$\nu(\text{U–F})$	Ref.
α - UF_5	-	628	[26]
β - UF_5	-	614	
1	2135, 2131	599	(exptl)
	2190	589	(theory)

Table 2. IR spectroscopic data of HCN, α - and β - UF_5 in comparison to compound **1** (initial measurement). All values are given in $[\text{cm}^{-1}]$.

Species	$\nu(\text{C–H})$	$\nu(\text{C–N})$	$\delta(\text{H–C–N})$	$\nu(\text{U–F})$	Ref.
$\text{HCN}_{(l)}$	3215	2096	794	-	[29]
α - UF_5	-	-	-	580	
β - UF_5	-	-	-	573	[26]
1	3222	2137	781	511	(exptl)
	3210	2190	790	530	(theory)

Figure 2. Room temperature Raman spectrum of turquoise crystals of compound **1** under liquid HCN. The band at 2094 cm^{-1} is assigned to $\nu(\text{C–N})$ of liquid HCN by comparison to the literature.

Figure 3. Time dependent room temperature ATR-IR spectra of compound **1** measured under Ar atmosphere. For comparison, the ATR-IR spectrum of β -UF₅ is also shown (top).

The applicability of NMR spectroscopy for the analysis of uranium(V) is limited due to its paramagnetism. Therefore, the chemical shift is unpredictable and the signals are broadened, sometimes to an extent that they are not observable.^[30,31] To the best of our knowledge there is currently only one solution NMR spectroscopic investigation on UF₅ and its derivatives in acidic media (anhydrous HF) and only one solid state NMR spectroscopic characterization of α -UF₅.^[32,33] The number of NMR spectroscopic studies with aHCN as solvent is very small and focus mainly on the physicochemical properties.^[34,35]

To gain insight into the solution state of β -UF₅ we recorded ¹H and ¹⁹F NMR spectra of solutions in aHCN. The solvent signal (aHCN solutions of UF₅) is observed at 6.63 ppm with a line width of 8.4 Hz in the ¹H NMR spectrum. In comparison, the signal of neat HCN is observed at 5.95 ppm with a line width of 9.0 Hz. This distinctive paramagnetic down field shift of 0.68 ppm is evidence for the interaction of UF₅ with HCN as well as for the rapid exchange of free and coordinated HCN molecules on the NMR time scale. The fast exchange is further supported by the narrow line width and the lack of further signals in the ¹H NMR spectrum (−30 – 20 ppm).

However, no signals could be observed by ¹⁹F NMR spectroscopy in a range of −345 to 595 ppm. This might be caused by the direct interaction of the ¹⁹F nuclei with the paramagnetic uranium(V) atoms, which can cause extreme line broadening. Additionally, the fluorine nuclei are probably chemically inequivalent due to a coordination polyhedron which we assume to be related to or derived from the one in the crystal structure. We suppose that five fluorine nuclei and an unknown number of HCN molecules are coordinated. This leads to smaller signals, since several individual signals rather than one mutual signal are present, and to even further broadening, if site exchange occurs. Due to the induced polymerization of HCN at ambient temperature no larger spectroscopic windows could be explored, while the high melting point of −13 °C HCN paired with the relatively low solubility of β -UF₅ excluded variable temperature NMR experiments.

We took insight into the β -UF₅/HCN system and found that a coordination polymer, $[\text{UF}_5(\text{HCN})_2]_n$, is formed, which was an unknown structural feature for HCN Lewis adducts. The interaction of HCN is only weak, thus the compound easily gives off HCN *in vacuo* and Ar. The calculated IR and Raman spectra show a good agreement with experimental data and allow a full assignment of bands. Further studies regarding aHCN as a solvent for uranium compounds are underway.

Experimental Section

Caution! The toxicity of hydrogen cyanide or its solutions should not be underestimated.^[2,3] Working under a well ventilated fume hood is mandatory, a HCN-detector and butyl rubber gloves are recommended. Furthermore we cannot yet recommend the advice of Gattermann to smoke cigars during the work with HCN. We could not recognize the described 'special' taste whilst smoking near an open bottle full of KCN beyond doubt but further studies are underway.^[36]

General: All operations with UF₆ were performed either in stainless steel (316L) or in Monel metal Schlenk lines, which were passivated with 100% fluorine at various pressures before use. Preparations were carried out in an atmosphere of dry and purified argon (5.0, Praxair). UF₆ was prepared by reacting UF₄ and F₂ and was used after sublimation. β -UF₅ was prepared by photoreduction of UF₆ with CO in a fused quartz apparatus, according to a literature procedure.^[37] Anhydrous HCN was prepared from KCN and H₂SO₄ and purified by several distillation steps and finally stored over Sicapent (Merck).^[38]

Synthesis: 1: β -UF₅ was placed in a Schlenk tube and cooled with liquid nitrogen. An excess of aHCN was added by vacuum distillation. The mixture was warmed to 0 °C with an ice bath. After a short time the solid turned light green to turquoise and after a few hours turquoise crystals of compound **1** are formed, which are suitable for SCXRD. After storage for several days at 0 °C a brown amorphous product also is formed, which is considered to be a polymerization product of HCN.^[39] Photographs of the reaction mixture can be found in the SI.

Single crystal X-ray diffraction: X-ray structure analysis of a single crystal of compound **1** was carried out with a D8 Quest diffractometer (Bruker) with monochromated molybdenum radiation (MoK α λ = 0.71073 Å) and a PHOTON 100 CMOS detector. Evaluation and integration of the diffraction data was carried out by using the Bruker APEX2 software, and an empirical absorption correction was applied (multi-scan).^[40] The structure was solved by using direct methods (SHELXT) in the space group type *Pca*2₁ (29), and refined against *F*² (SHELXL) as an inversion twin.^[41,42] All atoms were located by difference Fourier synthesis and refined anisotropically, hydrogen atoms were located and refined using a riding model. Representations of the crystal structure were created by using the Diamond software.^[41] Crystallographic data: C₂F₅H₂N₂U (1, *M* = 387.07 g mol^{−1}), crystal size 0.21 × 0.39 × 0.51 mm³, orthorhombic, *Pca*2₁ (No. 29); *a* = 23.047(1), *b* = 8.521(1), *c* = 14.369(1) Å; *V* = 2821.7(3) Å³, *Z* = 4, ρ_{calcd} = 3.645 g cm^{−3}, $\mu(\text{MoK}\alpha)$ = 23.03 mm^{−1}, $\lambda(\text{MoK}\alpha)$ = 0.71073 Å, *T* = 100 K, θ_{max} = 30.60°; Data, parameter, restraints: 8631, 371, 1; *R*_{int}: 0.050; *R*(*F*) (*I* ≥ 2 σ (*I*), all data): 0.034, 0.034; *wR*(*F*²) (*I* ≥ 2 σ (*I*), all data): 0.087, 0.087; $\Delta\rho_{\text{max/min}}$ = 5.58 / −1.88 e Å^{−3}, BASF = 0.21(1). Further details of the crystal structure investigation can be obtained from the Cambridge Structural Database (<http://www.ccdc.cam.ac.uk/>) on quoting the depository number CCDC-1511349.

Computational details: The calculations were carried out with the CRYSTAL14 program package, using the PBE0 hybrid density functional method.^[44,45] Full computational details are given in the Supporting information.

IR and Raman Spectroscopy: The IR spectra were measured on an alpha FTIR spectrometer (Bruker) by using a diamond ATR unit under an Ar atmosphere in a glovebox. The spectra were processed with the OPUS software package.^[46] The Raman spectrum was collected by using a Labram HR800 (JobinYvon) instrument equipped with a 25 mW He/Ne laser tube (λ = 632.817 nm). The sample of compound **1** was prepared in a flame-sealed glass capillary under Ar shortly before the measurement. Turquoise crystals were measured, and the collected data were handled with the LabSpec software.^[47]

NMR spectroscopy: ¹H and ¹⁹F NMR spectra were recorded on an Avance III HD 300 NMR spectrometer (Bruker). ¹H NMR spectroscopy (300.25 MHz) used SiMe₄ and ¹⁹F NMR spectroscopy (282.62 MHz) used neat CFCl₃ as an external reference. Samples were prepared by condensing aHCN onto β -UF₅ at −78 °C in J.-Young NMR tubes. Chemical shifts are given for 300 K at 1.04 bar hydrogen cyanide vapor pressure.^[48]

Keywords: coordination polymer • fluorides • cyanides • uranium • X-ray diffraction

- [2] <http://gestis-en.itrust.de/>, Search Entry: "hydrogen cyanide", 23.10.2016.
- [3] http://gestis-en.itrust.de, Search Entry: "hydrogen cyanide, aqueous solution", 23.10.2016.
- [4] F. Wöhler, *Ann. Chem. Pharm.* **1850**, 73, 226–228.
- [5] G. Constant, J. C. Daran, Y. Jeannin, *Acta Crystallogr. Sect. B* **1971**, 27, 2388–2392.
- [6] B. Corain, *Coord. Chem. Rev.* **1982**, 47, 165–200.
- [7] A. A. A. Emara, G. J. Schrobilgen, *Inorg. Chem.* **1992**, 31, 1323–1332.
- [8] R. Fricke, O. Rode, *Z. Anorg. Allg. Chem.* **1926**, 152, 347–356.
- [9] I. C. Tornieporth-Oetting, T. M. Klapötke, T. S. Cameron, J. Valkonen, P. Rademacher, K. Kowski, *J. Chem. Soc. Dalton Trans.* **1992**, 537–543.
- [10] W. A. Burns, K. R. Leopold, *J. Am. Chem. Soc.* **1993**, 115, 11622–11623.
- [11] K. Kawai, I. Kanesaka, *Spectrochim. Acta Part Mol. Spectrosc.* **1969**, 25, 1265–1273.
- [12] I. Kanesaka, Y. Hase, K. Kawai, *Bull. Chem. Soc. Jpn.* **1972**, 45, 1595–1598.
- [13] G. Constant, J. C. Daran, Y. Jeannin, *J. Solid State Chem.* **1970**, 2, 421–429.
- [14] G. Constant, J.-C. Daran, Y. Jeannin, B. Saperas, *C. R. Acad. Sci. Paris* **1969**, 269, 975–977.
- [15] G. Brauer, H. Walz, *Z. Anorg. Allg. Chem.* **1963**, 319, 236–243.
- [16] K. W. Bagnall, J. L. Baptista, *J. Inorg. Nucl. Chem.* **1970**, 32, 2283–2285.
- [17] I. C. Tornieporth-Oetting, T. M. Klapötke, *Inorg. Chim. Acta* **1994**, 215, 5–7.
- [18] G. W. Halstead, P. G. Eller, M. P. Eastman, *Inorg. Chem.* **1979**, 18, 2867–2872.
- [19] J. Lima-de-Faria, E. Hellner, F. Liebau, E. Makovicky, E. Parthé, *Acta Crystallogr. Sect. A* **1990**, 46, 1–11.
- [20] C. J. Howard, J. C. Taylor, A. B. Waugh, *J. Solid State Chem.* **1982**, 45, 396–398.
- [21] R. R. Ryan, R. A. Penneman, L. B. Asprey, *Acta Crystallogr. Sect. B* **1976**, 32, 3311–3313.
- [22] G. Constant, J.-C. Daran, Y. Jeannin, R. Morancho, *J. Coord. Chem.* **1973**, 2, 303–308.
- [23] C. Chavant, G. Constant, Y. Jeannin, R. Morancho, *Acta Crystallogr. Sect. B* **1975**, 31, 1823–1827.
- [24] J. W. Simmons, W. E. Anderson, W. Gordy, *Phys. Rev.* **1950**, 77, 77–79.
- [25] G. Herzberg, *J. Chem. Phys.* **1940**, 8, 847–848.
- [26] E. Jacob, *Z. Anorg. Allg. Chem.* **1973**, 400, 45–50.
- [27] D. E. Milligan, M. E. Jacox, *J. Chem. Phys.* **1967**, 47, 278–285.
- [28] C. F. Pau, W. J. Hehre, *J. Phys. Chem.* **1982**, 86, 321–322.
- [27] M. Pezolet, R. Savoie, *Can. J. Spectrosc.* **1972**, 17, 34.
- [28] K. E. Schwarzhans, *Angew. Chem.* **1970**, 82, 975–982.
- [29] K. E. Schwarzhans, *Angew. Chem. Int. Ed. Engl.* **1970**, 9, 946–953.
- [30] B. Scheibe, S. Lippert, S. S. Rudel, M. R. Buchner, O. Burghaus, C. Pietzonka, M. Koch, A. J. Karttunen, F. Kraus, *Chem. Eur. J.* **2016**, 22, 12145–12153.
- [31] S. P. Gabuda, V. K. Goncharuk, S. A. Polishchuk, V. N. Ikovskii, *J. Struct. Chem.* **1987**, 27, 894–898.
- [32] C. J. Jameson, *J. Chem. Phys.* **1982**, 76, 152–162.
- [33] R. E. Wasylshen, *Can. J. Chem.* **1987**, 65, 2077–2081.
- [34] L. Gattermann, *Justus Liebigs Ann. Chem.* **1907**, 357, 313–383.
- [35] G. W. Halstead, P. G. Eller, R. T. Paine, in *Inorg. Synth.* (Ed.: J.P. Fackler), John Wiley & Sons, Inc., Hoboken, NJ, USA, **1982**, 162–167.
- [36] K. H. Slotta, *Berichte Dtsch. Chem. Ges. B Ser.* **1934**, 67, 1028–1030.
- [37] D. Koschel, L. Gmelin, R. J. Meyer, E. H. E. Pietsch, E. Fluck, Deutsche Chemische Gesellschaft, Gmelin-Institut für Anorganische Chemie und Grenzgebiete, Eds., *Kohlenstoff-Stickstoff-Verbindungen*, Verl. Chemie, Berlin, **1971**.
- [38] *APEX Suite of Crystallographic Software*, Bruker AXS Inc., Madison, WI, USA, **2008**.
- [39] G. M. Sheldrick, *Acta Crystallogr. Sect. Found. Adv.* **2015**, 71, 3–8.
- [40] G. M. Sheldrick, *Acta Crystallogr. Sect. C* **2015**, 71, 3–8.
- [41] K. Brandenburg, M. Berndt, *Diamond - Visual Crystal Structure Information System*, Crystal Impact GbR, Bonn, **1998**.
- [42] R. Dovesi, R. Orlando, A. Erba, C. M. Zicovich-Wilson, B. Civalieri, S. Casassa, L. Maschio, M. Ferrabone, M. De La Pierre, P. D'Arco, Y. Noël, M. Causà, M. Rérat, B. Kirtman, *Int. J. Quantum Chem.* **2014**, 114, 1287–1317.
- [43] L. Maschio, B. Kirtman, M. Rérat, R. Orlando, R. Dovesi, *J. Chem. Phys.* **2013**, 139, 164101.
- [44] *OPUS*, Bruker Optik GmbH, Ettlingen (Germany), **2009**.
- [45] *Labspec Spectroscopy Suit Software*, HORIBA Scientific, **2000**.
- [46] D. G. Edwards, *UCRL-7167(Rev.1)*, University of California - Lawrence Radiation Laboratory, **1964**.

COMMUNICATION

Entry for the Table of Contents

COMMUNICATION

UF₅/HCN: The system of β -uranium(V) fluoride and HCN was studied. The crystal structure of a polymeric HCN adduct is presented. The compound was studied by means of quantum chemical methods, as well as by vibrational spectroscopy.

*B. Scheibe, S. S. Rudel, M. R. Buchner, A. J. Karttunen, F. Kraus**

Page No. – Page No.

A 1D Coordination Polymer of UF₅ with HCN as a Ligand – ¹[UF₅(HCN)₂]