



Fluorides Hot Paper

How to cite: *Angew. Chem. Int. Ed.* **2021**, 60, 6391–6394

International Edition: doi.org/10.1002/anie.202015501

German Edition: doi.org/10.1002/ange.202015501

# Searching for Monomeric Nickel Tetrafluoride: Unravelling Infrared Matrix Isolation Spectra of Higher Nickel Fluorides

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Dedicated to Prof. Dieter Lentz on the occasion of his 70th birthday

**Abstract:** Binary transition metal fluorides are textbook examples combining complex electronic features with most fundamental molecular structures. High-valent nickel fluorides are among the strongest known fluorinating and oxidizing agents, but there is a lack of experimental structural and spectroscopic investigations on molecular  $\text{NiF}_3$  or  $\text{NiF}_4$ . Apart from their demanding synthesis, also their quantum-chemical description is difficult due to their open shell nature and low-lying excited electronic states. Distorted tetrahedral  $\text{NiF}_4$  ( $D_{2d}$ ) and trigonal planar  $\text{NiF}_3$  ( $D_{3h}$ ) molecules were produced by thermal evaporation and laser ablation of nickel atoms in a fluorine/noble gas mixture and spectroscopically identified by a joint matrix-isolation and quantum-chemical study. Their vibrational band positions provide detailed insights into their molecular structures.

**B**inary fluorides of the late 1<sup>st</sup> row transition metals (TM) are among the most efficient oxidative fluorinating agents, especially for the production of perfluorinated organic

compounds.<sup>[1]</sup>  $\text{CoF}_3$  is of industrial importance in the Flutec or Fowler processes,<sup>[2]</sup> and higher nickel fluorides are considered to be the active fluorinating agents in the electrochemical fluorination of organic substrates (Simons process).<sup>[3]</sup> Despite numerous attempts to elucidate this latter process the active species are still unknown.<sup>[3,4]</sup>

Clearly, these particular properties are related to the peculiar electronic structure of these late TM fluorides, such as high ionization energies, the occupation of M–F antibonding molecular orbitals, and the lack of the so-called “primogenic repulsion”, caused by the absence of radial nodes in the 3d valence orbitals.<sup>[5]</sup> Nickel is one of the most electro-negative metallic elements.<sup>[6]</sup> This implies a considerable covalent character of the Ni–F bonds, which increases with the oxidation state of nickel.<sup>[7,8]</sup> Particularly for high-valent 3d TM complexes the similar radial extent of the 3d valence and the 3p core shell leads to repulsion between core 3p and ligand valence electrons, which ultimately results in weakened metal-ligand bonds,<sup>[5]</sup> a weak ligand-field, and the presence of several low-lying excited electronic (spin) states.<sup>[9]</sup> Taken together, these circumstances represent a challenge for quantum-chemical predictions and a major impediment for the spectral analysis of the still elusive high-valent molecular nickel fluorides.

In addition to the trifluorides, the tetrafluorides of the 1<sup>st</sup> row TM are particularly interesting. Solid  $\text{MnF}_4$  releases elemental fluorine at temperatures  $> 170^\circ\text{C}$ .<sup>[10]</sup> It can be used for storage and purification of elemental fluorine.<sup>[2]</sup> In contrast to solid  $\text{MnF}_4$  and  $\text{NiF}_4$ , solid  $\text{FeF}_4$  or solid  $\text{CoF}_4$  are unknown, while the monomeric  $\text{FeF}_4$  and  $\text{CoF}_4$  species have been investigated by high-temperature vapor-phase mass spectrometry and cryogenic matrix-isolation spectroscopy.<sup>[11–13]</sup>

Solid  $\text{NiF}_4$  is one of the strongest known fluorinating oxidizing agents,<sup>[2]</sup> but it is poorly characterized spectroscopically and even its solid-state structure is unknown. We have not found any report on molecular or gaseous  $\text{NiF}_4$ .<sup>[4]</sup> Fluorination of solid  $\text{NiF}_2$  provides thermally unstable higher nickel fluorides such as  $\text{Ni}_2\text{F}_5$  ( $\text{Ni}^{\text{II}}_3\text{Ni}^{\text{IV}}\text{F}_{10}$ )<sup>[14]</sup> or  $\text{R-NiF}_3$  ( $\text{Ni}^{\text{II}}\text{Ni}^{\text{IV}}\text{F}_6$ ),<sup>[15]</sup> and neutral  $\text{NiF}_4$  is claimed to be formed at about  $-60^\circ\text{C}$  by treating  $[\text{NiF}_6]^{2-}$  salts in anhydrous HF with strong Lewis acids such as  $\text{AsF}_5$ ,  $\text{SbF}_5$ , or  $\text{BF}_3$ .<sup>[16]</sup>  $\text{NiF}_4$  releases  $\text{F}_2$  above  $-55^\circ\text{C}$  and forms  $\text{NiF}_3$ , which again releases fluorine above  $20^\circ\text{C}$  to form  $\text{NiF}_2$ .<sup>[17]</sup> As far as we know molecular  $\text{NiF}_3$  has not yet been studied spectroscopically, but it has attracted the interest of a theoretical study because of

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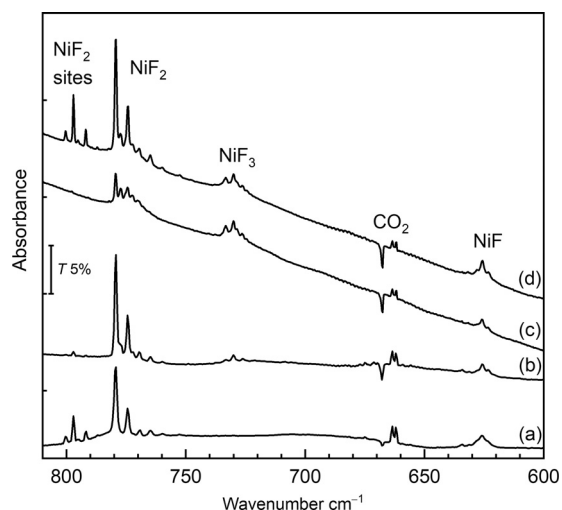
Supporting information and the ORCID identification number(s) for the author(s) of this article can be found under:  
<https://doi.org/10.1002/anie.202015501>.

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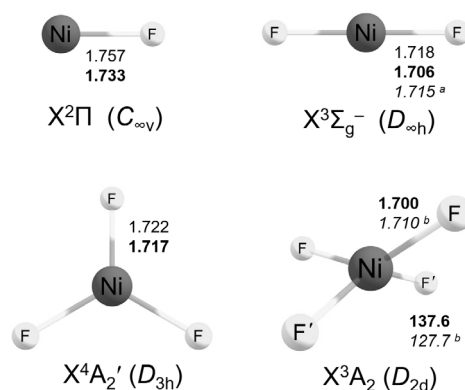
its low-lying electronically degenerate excited states, which are prone to Jahn–Teller (JT) effects.<sup>[18]</sup>

We carried out spectroscopic investigations on molecular NiF<sub>3</sub> and NiF<sub>4</sub> for the first time. Different methods were applied to produce these species which were subsequently isolated in cryogenic rare-gas matrices. First, nickel atoms were vaporized by heating a nickel wire and allowed to react with elemental fluorine diluted in argon prior to deposition on a matrix support at 10 K. Vaporization of atomic nickel was also achieved by laser ablation using the 1064 nm fundamental of a Nd:YAG laser focused onto a rotating nickel target and trapping the products at 6–15 K. The laser ablation process is associated with a hot plasma plume and a bright broad-band radiation, where excited nickel atoms can react with elemental fluorine and atomic fluorine radicals seeded in excess of noble gases (neon or argon). This method is particularly useful for the generation of highly fluorinated species.<sup>[13,19]</sup> For example, laser ablation from a metallic cobalt target in a fluorine/argon gas mixture clearly produces not only molecular CoF, CoF<sub>2</sub> and CoF<sub>3</sub> but also CoF<sub>4</sub> (for experimental details see the Supporting Information), which could be detected using its known IR band in solid argon reported in a previous study,<sup>[12]</sup> in which CoF<sub>4</sub> was obtained at 650 K from solid mixtures of CoF<sub>3</sub> and TbF<sub>4</sub> as atomic fluorine source in a perfluorinated nickel effusion cell.<sup>[12]</sup> The wavenumber ordering of the  $\nu_{\text{Co-F}}$  modes is CoF<sub>4</sub> > CoF<sub>3</sub> > CoF<sub>2</sub> > CoF, see the Supporting Information.

Thermally evaporated Ni atoms react with F<sub>2</sub> on deposition (Figure 1) to yield limited amounts of NiF<sub>2</sub> at 779.4 cm<sup>-1</sup><sup>[20]</sup> and a broad band at 625.8 cm<sup>-1</sup> assigned to molecular NiF on the basis of the gas-phase IR band of <sup>58</sup>NiF (<sup>2</sup>Π<sub>3/2</sub>) at 634.7 cm<sup>-1</sup>,<sup>[21]</sup> and our computed value of 639.1 cm<sup>-1</sup> at the CCSD(T)/AVT(Q)Z-DK level (Table S4.2). UV and broadband photolysis, associated with the formation of F radicals, resulted in the dramatic growth of the bands due to NiF<sub>2</sub> (Figure 1(a,d)), and two additional sets of overlapping bands close to 800 cm<sup>-1</sup>. Like the NiF<sub>2</sub> bands the well resolved



**Figure 1.** IR spectra of reaction products from thermally evaporated Ni atoms in 0.5% F<sub>2</sub>/Ar matrices: a) after deposition and broadband photolysis, b) after annealing to 25 K, c) after deposition and annealing to 25 K, d) after broadband photolysis.

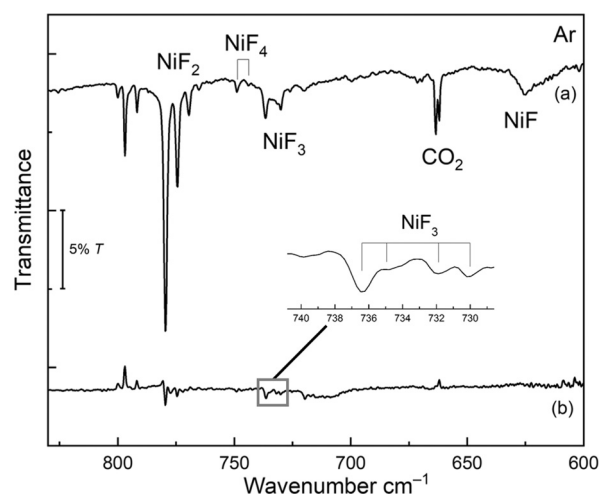


**Scheme 1.** Structures of NiF<sub>n</sub> (*n* = 1–4) species. Values calculated at the RCCSD(T)/AVTZ(NREL) and the RCCSD(T)/AVTZ-DK (in bold) levels of theory. [a] Experimental value from a gas phase electron diffraction study.<sup>[23]</sup> [b] CASPT2/AVTZ-DK.

<sup>58,60</sup>Ni isotopic pattern on the 800 cm<sup>-1</sup> bands is consistent with linear NiF<sub>2</sub> units (Table S3.1).<sup>[22]</sup> These new bands were assigned to matrix sites of NiF<sub>2</sub> in F<sub>2</sub>/Ar matrices (see the Supporting Information).

On annealing (Figure 1(b,c)), the bands due to NiF<sub>2</sub> increased while those close to 800 cm<sup>-1</sup> decreased, and weak bands at 735–724 cm<sup>-1</sup> appeared. These latter bands are assigned to the asymmetric stretch of molecular NiF<sub>3</sub>, trapped in different matrix sites. CCSD(T) calculations predict a <sup>4</sup>A<sub>2</sub>' ground state with D<sub>3h</sub> structure for molecular NiF<sub>3</sub> (Scheme 1, Table S6.3) and a single infrared active E' stretching fundamental about 40 cm<sup>-1</sup> below that of NiF<sub>2</sub> (Table S6.4).

Subsequent nickel laser ablation experiments fully corroborate the assignment of NiF<sub>3</sub> in solid argon (Figure 2). Due to the formation of considerably larger amounts of atomic fluorine radicals in the laser ablation experiment, the yield of NiF<sub>3</sub> increased and further rose by annealing the deposit to 20 K (Figure 2). The NiF<sub>3</sub> region is even more congested in



**Figure 2.** IR spectrum of the reaction products of laser-ablated Ni with F<sub>2</sub> (0.5%) seeded in excess argon: a) co-deposited for 60 min at 15 K, b) difference spectrum after annealing to 20 K.

the laser ablation experiment due the presence of different matrix sites. UV radiation of  $\lambda = 273$  nm (LED) depletes the NiF<sub>3</sub> bands (band points upwards in Figure S4b) and forms NiF<sub>2</sub>, while  $\lambda = 193$  nm laser radiation destroyed both, NiF<sub>2</sub> and NiF<sub>3</sub> (Figure S4d). More interestingly, in these experiments a new band at 749.1 cm<sup>-1</sup> with a distinct  $\Delta\nu(^{58/60}\text{Ni})$  isotope splitting of 5.1 cm<sup>-1</sup> occurred (Figure 2). This band was very difficult to detect in the thermal evaporation experiment due to its much lower intensity. The carrier of this band appears to be formed by fluorination of NiF<sub>3</sub>, since it can only be observed when a sufficient amount of NiF<sub>3</sub> is available and its intensity grows along with that of the NiF<sub>3</sub> band, i.e. by annealing and with higher fluorine concentrations of the F<sub>2</sub>/Ar mixture (Figure S5). Based on this behavior, the new band is assigned to the strongest IR band of molecular NiF<sub>4</sub>. For a tetrahedral tetrafluoride only a single infrared-active Ni–F stretching mode is expected, however, for the *d*<sup>6</sup> electronic configuration of NiF<sub>4</sub> a Jahn–Teller distorted *D*<sub>2d</sub> structure is predicted at all levels of theory (Figure S7.1).

We are not aware of previous high-level ab initio calculations for molecular NiF<sub>4</sub>. We carried out quantum-chemical investigations of various energetically low-lying electronic states of NiF<sub>4</sub>, especially of the lowest-energy triplet (<sup>3</sup>A<sub>2</sub>) and quintet (<sup>5</sup>B<sub>1</sub>, <sup>5</sup>A<sub>1</sub>) states of *D*<sub>2d</sub> symmetry (Table S3.4). For the triplet ground state (Scheme 1) a strong IR band of E symmetry is predicted for NiF<sub>4</sub> about 11 cm<sup>-1</sup> blue-shifted from the E' band of NiF<sub>3</sub> at the CCSD(T)/AVTZ-DK level (Table 1), which is in excellent agreement with the observation. The much weaker predicted *B*<sub>2</sub> band of NiF<sub>4</sub> (Tables S7.2, S7.4, S7.6) was not detected. All four nickel fluorides are also observed in solid neon matrices (Tables 1, S3.3).

A comparison of experimental M–F stretching bands of high-valent first-row metal fluorides is particularly revealing. The molecular trifluorides of M = Fe, Co, and Ni all adopt *D*<sub>3h</sub> structures, and their stretching fundamentals were found in Ne matrices, in a very narrow range, at 743.6 cm<sup>-1</sup> (Fe),<sup>[13]</sup> 748.2 cm<sup>-1</sup> (Co), and 743.8 cm<sup>-1</sup> (Ni, Table 1). For a series of molecules with similar structures one expects a strong correlation between stretching frequencies and bond lengths, a trend that also applies to the bond length of CoF<sub>3</sub> (1.722 Å) and NiF<sub>3</sub> (1.722 Å, Table S3.5) obtained at the CCSD(T)/AVTZ level. A similar frequency-bond length

correlation (Table S3.5) is expected for the stretching vibrations of the tetrafluorides MF<sub>4</sub> of Fe to Ni observed in solid argon, which also appear in a narrow spectral range (757 cm<sup>-1</sup> (M = Fe),<sup>[13]</sup> 767.8 (Co),<sup>[12]</sup> 749.1 (Ni)). However, this correlation is less accurate due to the Jahn–Teller deformed *D*<sub>2d</sub> molecular structures of FeF<sub>4</sub> and NiF<sub>4</sub> and due to stronger matrix interactions in solid argon.

Apart from these similarities, the higher nickel fluorides are strikingly different from their third-row predecessors. The rule of thumb that higher fluorides have shorter and stronger M–F bonds that applies to ionic metal fluorides does not apply to the higher nickel fluorides. While CCSD(T)/AVTZ calculations predict a successive M–F bond shortening for the ionic iron fluorides FeF<sub>*n*</sub>, with *n* = 1–4,<sup>[13]</sup> and, albeit significantly weakened, also for CoF<sub>*n*</sub>, *n* = 2–4, the bond length in NiF<sub>*n*</sub>, *n* = 2–4, remains almost unchanged (Table S3.5). This different trend for nickel and its predecessors can be traced back to fundamental aspects of their atomic structures, such as a higher nickel ionization energy. This leads to a considerable covalent character of the Ni–F bonds, associated with a low-spin triplet electronic ground-state of NiF<sub>4</sub> and a considerable radical character of the fluorine ligands (Figure S11).<sup>[7,8]</sup>

From these experiments we conclude that NiF<sub>2</sub>, initially formed from the reaction of nickel atoms and elemental fluorine, can be regarded as chemically inert to elemental fluorine, but reacts rapidly with atomic fluorine radicals to

**Table 2:** Calculated thermochemistry of nickel fluorides in kJ mol<sup>-1</sup>.

	$\Delta E^\circ$ (kJ mol <sup>-1</sup> ), CCSD(T)/AVTZ-DK
Ni + F → NiF	-426.16
NiF + F → NiF <sub>2</sub>	-507.44
NiF + F <sub>2</sub> → NiF <sub>3</sub>	-517.91
NiF <sub>2</sub> + F → NiF <sub>3</sub>	-163.50
NiF <sub>3</sub> + F → NiF <sub>4</sub>	-76.04

form NiF<sub>3</sub> and further to NiF<sub>4</sub>. It has also been shown that the reaction of Ni atoms with elemental F<sub>2</sub> to produce NiF<sub>2</sub> requires UV photolysis to yield appreciable quantities of product under the cryogenic conditions applied here. Given the highly exothermic reaction energy of this reaction

**Table 1:** Vibrational frequencies observed in laser-ablation experiments and computed harmonic frequencies (in cm<sup>-1</sup>) for NiF<sub>*n*</sub> (*n* = 1–4).

Species	Ground State	Sym.		calcd <sup>[a]</sup>		Exp. (Ne Matrix)		Exp. (Ar Matrix)	
				<sup>58</sup> Ni	<sup>60</sup> Ni	<sup>58</sup> Ni	<sup>60</sup> Ni	<sup>58</sup> Ni	<sup>60</sup> Ni
NiF	<sup>2</sup> Π	<i>C</i> <sub>∞v</sub>	NR <sup>[b]</sup>	612.98 (Σ <sup>+</sup> )	610.46	646.2	643.5	625.8 (broad)	
			DK <sup>[b]</sup>	639.13 (Σ <sup>+</sup> )	636.50				
			NR <sup>[c]</sup>	806.42 (Σ <sub>u</sub> <sup>+</sup> )	801.09				
NiF <sub>2</sub>	<sup>3</sup> Σ <sub>g</sub> <sup>-</sup>	<i>D</i> <sub>∞h</sub>	DK <sup>[c]</sup>	819.17 (Σ <sub>u</sub> <sup>+</sup> )	813.75	800.1	794.9	779.5	774.4
			NR <sup>[b]</sup>	810.25 (Σ <sub>u</sub> <sup>+</sup> )	804.89				
			DK <sup>[b]</sup>	824.62 (Σ <sub>u</sub> <sup>+</sup> )	819.17				
NiF <sub>3</sub>	<sup>4</sup> A <sub>2</sub> '	<i>D</i> <sub>3h</sub>	NR <sup>[c]</sup>	762.95 (E)	758.67	743.8	740.0	736.5	731.7
			DK <sup>[c]</sup>	767.83 (E)	763.54				
NiF <sub>4</sub>	<sup>3</sup> A <sub>2</sub>	<i>D</i> <sub>2d</sub>	NR <sup>[c]</sup>	767.24 (E)	762.56	762.3	757.2	749.1	744.0
			DK <sup>[c]</sup>	778.50 (E)	773.71				

[a] Non-relativistic (NR) and with scalar-relativistic Douglas-Kroll-Hess (DK) Hamiltonian; [b] RCCSD(T)/AVQZ; [c] RCCSD(T)/AVTZ.

(Table 2), this observation indicates a considerable reaction barrier and the necessity for fluorine radicals.

To summarize, molecular  $\text{NiF}_4$  ( $D_{2d}$ ) and  $\text{NiF}_3$  ( $D_{3h}$ ) were produced, isolated in solid noble-gas matrices, and spectroscopically identified aided by quantum-chemical calculations. Their weak Ni–F bonds and a considerable fluorine radical character make these molecular species very powerful fluorination and oxidation agents.

### Acknowledgements

We gratefully acknowledge the Zentraleinrichtung für Datenverarbeitung (ZEDAT) of the FU Berlin for the allocation of computer time. We thank the DFG (HA 5639/10) for financial support. L.L. thanks the China Scholarship Council (CSC) for a PhD fellowship. AKS thanks the University of Hull for a PhD studentship. Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation)—Project-ID 387284271—SFB 1349. S.R. thanks the late Dr. B. Schimmelpfennig for fruitful discussions. Open access funding enabled and organized by Projekt DEAL.

### Conflict of interest

The authors declare no conflict of interest.

**Keywords:** IR spectroscopy · matrix isolation · nickel fluorides · tetrafluoride · trifluoride

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Manuscript received: November 20, 2020

Accepted manuscript online: December 10, 2020

Version of record online: January 28, 2021