

Project: 3M Novec 649 as a replacement of C₆F₁₄ in liquid cooling systems

Abstract

3M Novec 649 is a fluid with thermo-physical properties similar to C₆F₁₄, and a very low global warming potential. This memo represents a compilation of published information about Novec 649, with the stress on applications as a heat transfer fluid in cooling systems. A draft plan for validation of Novec 649 at CERN is proposed, for a possible replacement of C₆F₁₄ or as the baseline solution in new cooling applications.

Contents:

1. Perfluorocarbon (PFC) liquids: properties and impact on the environment
2. Alternative heat transfer fluids (HTF)
3. Novec 649
4. Draft plan for validation of Novec 649 at CERN (contributions by M.Battistin, R.Setnescu)

1. Perfluorocarbon liquids: brief overview

Perfluorocarbon¹ (PFC) liquids, especially perfluoroalkanes², have been traditionally used in the semiconductor manufacture, as refrigerants and in some fire extinguishing systems. Despite their relatively low thermal conductivity compared to water and *heat transfer fluids* (HTFs), they possess other properties that make them useful as refrigerants: a wide range of boiling points, high densities, low viscosities, low pour points, low surface tension, and high thermal and chemical stability. They evaporate cleanly and are practically non-toxic, which results in easier safe usage and storage [2,3]. A comprehensive review of PFC heat transfer fluids (HTF) and their environmental effects is given by F. Tuma of 3M Company [3].

Long the standard for inert dielectric HTFs in cooling applications, PFC liquids have faced scrutiny due to their very high Global Warming Potentials (GWPs)³: 5,000 to 10,000 times that of CO₂, see Figure 1. The major release of PFCs to the environment (CF₄, C₂F₆) is from primary

¹ Compounds containing just fluorine and carbon. They are generally colourless, odourless, nonconducting, non-flammable gases/liquids at environmental temperatures. Most of PFCs are chemically un-reactive, totally or almost insoluble in water and are not or little metabolized in body tissues. The C-F bond is the strongest single bond encountered in organic chemistry[1f], and its strength is further increased when several fluorine atoms are present on the same carbon atom. The presence of fluorine also reinforces the C-C bonds[1d]. This makes PFC fluids among the most chemically inert [1d,e][3]. PFCs are produced by fluorination of corresponding hydrocarbons, residuals of which represent the main contaminant in commercial PFCs, like 3M FluorinertsTM [xx].

² Fully saturated PFC having an empirical formula C_nF_{2n+2}, like CF₄, C₆F₁₄ etc

³ The concept of GWP provides a common scale to compare the ability of different gases to trap heat in the atmosphere, relative to carbon dioxide [1a,b].

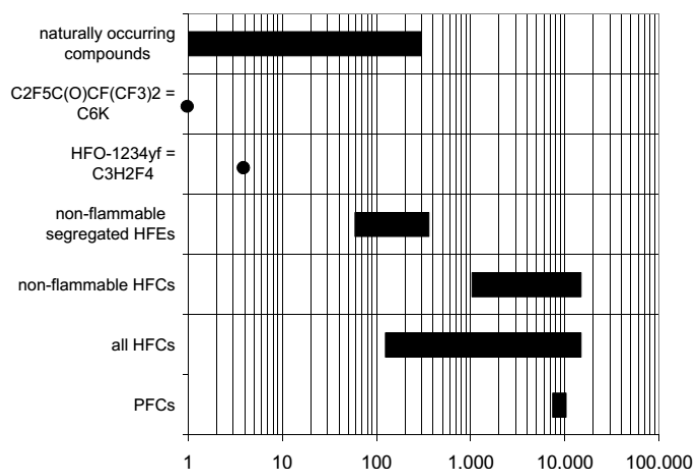


Figure 1: GWP of PFCs compared to other commercially available refrigerants and naturally occurring compounds (from [7])⁴. Based upon 100 year integration time horizon (ITH).

used in three sub-detectors (TT, IT and RICH [4c,d]). The proposed upgrade of the LHCb Outer Tracker, the SciFi Tracker [5], foresees the use of a single-phase cooling for the SiPM photo-detectors, in order to operate them at the temperatures down to -40°C . A search for a refrigerant alternative to PFC was undertaken at an early conceptual design stage.

2. Alternative heat transfer liquids

The utility of hydrocarbon alternatives to PFC, like Polyalphaolefin [25b] (PAO), is limited by flammability and high viscosity at low temperature. Segregated Hydrofluoroether (HFE) and Fluoroketone (FK) fluids are non-flammable and have much lower GWPs than PFCs. They compare favorably with the PAO fluids for single phase applications, and may be suitable also for evaporative (2-phase) applications. Table 1 shows properties of representative PFC, PAO, FK and segregated HFE fluids.

Table 1 A comparison of properties of representative heat transfer fluids (from [3])

Molecular Formula ¹	C_6F_{14}	R_FOR_H	$\text{R}_F\text{C}(\text{O})\text{R}_F$	$\text{CH}_3(\text{CH}_2)_n\text{CH}_3$
Fluid Type	PFC	HFE	FK	PAO
Tradename	Fluorinert FC-77	Novec 7200	Novec 649	Various
Normal Boiling Point [$^{\circ}\text{C}$]	100	76	49	>200
Freezing Point [$^{\circ}\text{C}$]	<-100	<-100	<-100	<-60
Flashpoint [$^{\circ}\text{C}$]	None	None	None	163
Thermal Conductivity [W/m-K]	0.057	0.063-0.075	0.059	0.136
Liquid Specific Heat [J/kg-K]	1050	1130-1320	1100	2200
Liquid Density [kg/m^3]	1680	1400-1660	1610	785
Kinematic Viscosity, 25 $^{\circ}\text{C}$ [cSt]	0.40	0.32-1.1	0.42	8.8
Kinematic Viscosity, -40 $^{\circ}\text{C}$ [cSt]	0.90	0.6-2.5	1.3	>300
Vapor Pressure at 25 $^{\circ}\text{C}$ [kPa]	30.9	0.96-65	40	<1
Resistivity [Gohm-cm]	1,000,000	0.1	10,000	
Dielectric Constant	1.76	7.4	1.84	2.1
Dielectric Strength [kV@2.54mm]	~40	~40	~40	~40

¹ R_F and R_H refer to fully fluorinated and fully hydrogenated alkyl groups, respectively.

2.1 Fluoroketones as a possible replacement of PFCs in cooling and other applications

⁴ HFC = hydrofluorocarbons (hydrocarbon molecules in which hydrogen is partially or mostly replaced with fluor); HFE = hydrofluoroethers, FK - fluoroketones (molecules containing at least one ketone $\text{RC}(\text{=O})\text{R}'$ group, with R/R' being fully fluorinated, that is containing no hydrogen).

aluminium production [1c]. The semiconductor industry and the refrigeration sector (leakage during operation and the end-of-life destruction of equipment) represent a relatively small source of emissions. However, the environmentally responsible industries and institutions, like CERN, have plans to reduce and, eventually, deprecate the use of PFCs [Ref for CERN?]. At CERN, the LHC experiments use significant quantities of such fluids (C3F8, C6F14) as refrigerants in mono- and two-phase cooling systems [4]. In LHCb alone, C6F14 is currently

PFC liquids were selected for particle detector cooling because of their high radiation hardness [6],[4c]. An essential requirement for the fluids used in the radiation environment is the absence, or very low content, of hydrogen which, as a result of the fluid radiolysis, can form the hydrofluoric acid HF that would cause corrosion of thin pipes and capillaries. This consideration excludes PAOs and HFEs and leaves *fluoroketones* [7] as the only alternative to PFCs. Fluoroketone (FK) fluids have among the lowest GWPs of manmade compounds (see again Figure 1) and the thermo-physical and dielectric properties nearly indistinguishable from PFCs. At least one such fluid, FK 5-1-12 or C6K, is commercially available in bulk quantities from 3M as Novec 1230 [9a,b], an agent for clean gaseous fire-suppressing systems intended for data centers, museums etc. The electrical resistivity of FK, though lower than PFCs, is well above that of deionized water. FKs also share the low dielectric constant of PFCs. Under a different trade name Novec 649, C6K is being promoted by 3M as a fluid for the ORC⁵ and immersion cooling applications [10].

2.2 Materials compatibility of FKs

FKs will often function as drop-in replacements for PFCs and are compatible with all metals, hard plastics, and a variety of inexpensive hydrocarbon elastomers like Ethylene Propylene (EP) and butyl. All fluorocarbon fluids feature some hydrocarbon solvency, so heavily plasticized elastomers may shrink or become brittle while relatively pure elastomeric polymers perform well. For this reason, no sweeping statements can be made about the compatibility of FKs with different materials. FKs far are less studied than PFCs in that respect, therefore general recommendations are based on the experience with PFCs [3, 11]:

- a) O-rings and seals should be made of elastomers previously used successfully in a PFC systems (i.e. butyl, nitrile, EPDM, silicone, etc.) or hydrocarbon elastomers specifically tested or otherwise known to be low in extractable material. 3M maintains databases of compatible materials and also *provide free testing services* (to be confirmed!)
- b) FC fluids, including C6K, are incompatible with fluoroelastomers, because they are similar in composition and have an affinity for each other. Thus, Teflon and Viton should be avoided.
- c) Thermoplastic hoses that have been used in PFC systems generally perform well with HFEs. Elastomeric or “rubbery” tubing/hoses should be low in extractable material and, preferably graded as “no-plasticizer” products (examples: ...).

2.3 FK stability

Though FKs hydrolyse to form an organic acid when dissolved in liquid water, they are very stable in its absence. FK fluids (like PFCs) are only minimally soluble in water and, due to the big difference in the density and surface tension, are very difficult to mix with it. This limits the potential hazards. Nonetheless, this “FK hydrolysis factor” should be kept in mind, together with the unknown radiation hardness, for cooling applications in HEP. See more in Section 3.

2.4 FK safety and handling

FK fluids are non-flammable and have no flash point. They are nonirritating, have low acute toxicity, and high inhalation exposure guidelines as would be expected for materials used in fire extinguishing applications. Like with PFCs (and unlike PAO and silicon oils), FK fluids evaporate cleanly and quickly if spilled and will not trap grime that must be cleaned from hardware components.

⁵ “Organic” Rankine Cycle, using an organic fluid to drive a turbine at a temperature lower than water-steam phase change, thereby giving a possibility to recuperate heat from low-temperature heat sources.

3. C6-fluoroketone (C6K) fluid (3M Novec 1230 and 3M Novec 649)

The rest of this memo is devoted to C6-fluoroketone, or *Perfluoro (2-methyl-3-pentan-one, CAS 756-13-8)*, the chemical with the molecular formula $C_2F_5C(O)CF(CF_3)_2$ ($C_6F_{12}O$ for short) and the structure illustrated by Figure 2. It is sold by 3M Corp. as Novec 1230 (since 2003) and Novec 649 (since ??). The Ref. [9] gives links to all relevant 3M documents about these fluids. Ref. [12] contains a very complete compilation of documents related to the environmental and health safety issues. Ref. [10] discusses the aspects of C6K applications as a heat transfer fluid (HTF) for 2-phase applications and contains a comprehensive general description of this fluid.

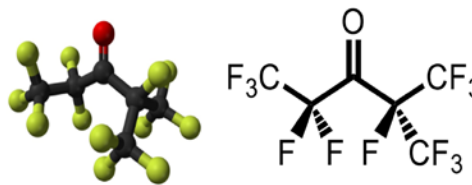


Figure 2 The molecular structure of C6-fluoroketone (from [9e] and [13e]).

Novec 1230 and Novec 649 are different brand names of the *same chemical* (further referred to as C6K), intended for different industrial applications: the 1230 – as a clean fire extinguishing agent, the 649 - as a heat transfer fluid. According to the MSDSs [14], they have different purity grades (>99% and >99.9%, respectively) and are sold via different channels. The literature on the 1230, mostly focused on the environmental and health safety aspects, is fully applicable to the 649, positioned by 3M as a *thermal management fluid*. The 649 is covered mostly with thermal applications in mind, especially for ORC and “open bath immersion” (or “pool boiling”) cooling [10], because of its relatively low normal boiling point (49°C).

Table 2 gives a more detailed overview of C6K (3M Novec 649) properties in comparison with C6F14 (3M Fluorinert FC-72, aka PF-5060 [8]). Apart from a strikingly different GWP, the two fluids have very similar physical properties. In particular, both have relatively low boiling points and very low vaporization heat (25 times lower than that of water), which makes them extremely volatile under normal conditions. There is, however, an important difference at the level of chemistry: the reactivity with water that is reportedly much higher with C6K than with pFCs. Further aspect in which C6K might potentially differ is its compatibility with different materials, especially elastomers. Finally, of particular interest for CERN applications is the radiation hardness of the C6K itself and the contaminants present in the commercial fluid.

3.1 Atmospheric chemistry, GWP

The atmospheric chemistry and the environmental fate of C6F have been extensively studied because of the massive application of Novec-1230 as one of “next-generation” alternatives to halon. All relevant publications are assembled in Ref. [13]. Containing no chlorine or bromine, C6K, like PFCs, has no effect on the atmospheric ozone (its Ozone Depletion Potential is zero). The striking difference between C6K and PFCs regards the atmospheric lifetime, which is very short, only 1-2 weeks, for C6K, because of strong UV absorption at ~307 nm. The photolysis results in cleavage of one the C-C bonds alpha to the carbonyl group [13c]. The carbonyl group remains intact through the entire C6K decomposition chain till the final incorporation into water and hydrolyzation to $CF_3C(O)OH$, CO_2 and HF. The degradation products of C6F are short-lived, resulting in negligible GWP. The “indirect” GWP calculated on a mass basis, is comparable with that of CO_2 , because the release of 1 kg of Novec 1230 fluid to the atmosphere produces 0.56 kg of CO_2 [13a].

In PFCs all C-C bonds are strengthened by F and their energies are beyond most of the solar UV spectrum at higher atmosphere, which makes these fluids potent greenhouse gases.

Table 2 : Comparison of C6K and C6F14 properties (from [7a]). ⁽¹⁾ For 100 years ITH

Molecular Formula	$C_2F_5C(O)CF(CF_3)_2$	C_6F_{14}
Fluid Type	fluoroketone	perfluorocarbon
Abbreviation	C6K	-
Normal Boiling Point [°C]	49	56
Critical Temperature [°C]	169	178
Critical Pressure [MPa]	1.87	1.83
Freezing Point [°C]	<-100	<-100
Closed Cup Flashpoint [°C]	None	None
Open Cup Flashpoint [°C]	None	None
Surface Tension [dynes/cm]	11.4	12.0
Thermal Conductivity [W/m-K]	0.059	0.057
Liquid Specific Heat [J/kg-K]	1103	1050
Liquid Density [kg/m ³]	1610	1680
Kinematic Viscosity [cSt]	0.42	0.40
Latent Heat [kJ/kg]	88	88
Vapor Pressure at 25°C [kPa]	40.4	30.9
Vapor Pressure at 100°C [kPa]	441	350
Resistivity [Gohm-cm]	10,000	1,000,000
Dielectric Constant	1.84	1.76
Dielectric Strength [kV@2.54mm]	~40	~40
Solub. H ₂ O in Fluid [ppmw]	21	10
Atmospheric Lifetime [year]	0.014	3200
Global Warming Potential ¹	1	9300
Ozone Depletion Potential	0	0

3.3 Hydraulic and Cooling properties, cavitation

As mentioned above, the thermo-physical properties of C6K and C6F14 are very similar. Fig. 3 shows the comparison of kinematic viscosity, density, heat capacity and thermal conductivity as function of temperature. Both fluids have very small heat conductivity and though it gets higher at low temperatures, they remain rather “insulators” than heat conductors. Below -10°C, C6K has a bit better characteristics as a coolant than C6F14: a lower viscosity, a higher and more stable specific heat, a higher thermal conductivity. This means that with C6K one can expect smaller temperature drops along and across the cooling pipe and the turbulent flow regime will be achieved at smaller fluid velocities than with C6F14.

Both fluids are heavy and have high vapour pressure. An addition, their fluid/vapour density ratio is two to three orders of magnitude smaller than that of water. These factors favour erosion and cavitation [14] in the pipes, so the cooling system design should aim at lower fluid velocities and lower overall flow rate (mind the pumps!). A very high thermal expansion coefficient of these fluids (~1%/10K) must also be taken into account.

In summary, as a coolant, C6K seem to be a good drop-in replacement candidate for C6F14.

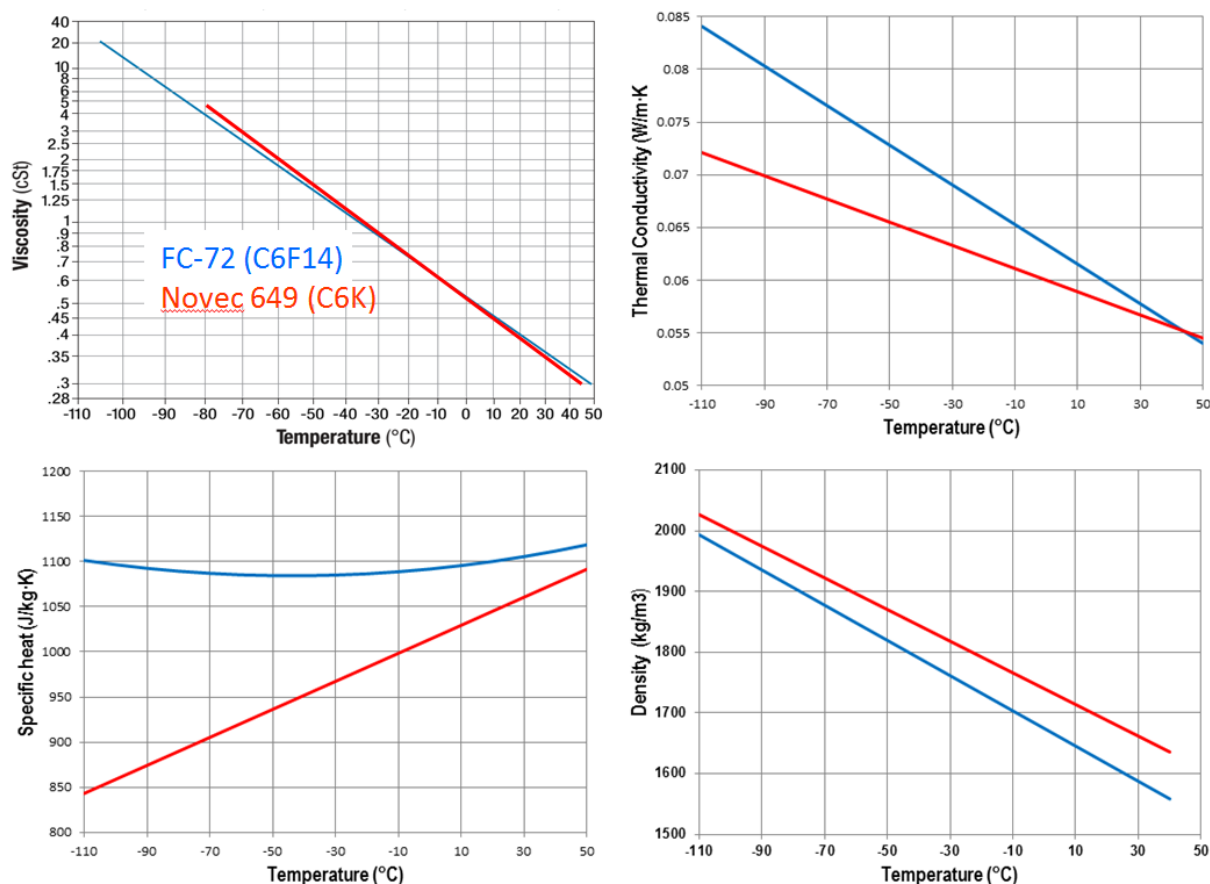


Figure 3 A comparison of some thermo-physical properties of C6K and C6F14 (from [8a] and [9c]).

3.4 Expected radiation resistance

The presence of weaker bonds in C6K molecules might imply its lower radiation resistance than with C6F14 [15], because the release of energy following the excitation by ionizing radiation will easier break the weak bonds. A direct comparison of the two compounds in dedicated irradiation tests is absolutely needed. The comparison with PEEK, the solid ketone known to be radiation hard, is not legitimate.

As to formation of long-lived isotopes by neutron radiation, there are no a priori reasons to expect a difference between C6K and C6F14.

3.5 Reactivity with water

Fluorinated ketones (e.g. hexafluoroacetone) are known to hydrolyze quite vigorously. Although C6K does not exhibit this highly exothermic reaction with water, it has been found to undergo hydrolysis [13c]. It reacts with water to form heptafluoropropane (HFC-227ea) and pentafluoropropionic acid (PFPA). This fact was used by 3M opponents to criticize the Novec 1230-based fire suppression systems [9b, 16]. According to 3M [9b], “Novec 1230 fluid reacts with water only when dissolved in water and it is only minimally soluble in water. Accordingly, only a very small amount of acid is formed when Novec 1230 fluid contacts liquid water and no

acid is formed when Novec 1230 fluid contacts water vapor. This has been verified through numerous laboratory and full-scale tests in which Novec 1230 fluid was discharged into a humid atmosphere and monitored via methods such as FTIR. No formation of PFPA has been detected.”. The PFPA is very corrosive to a variety of metals, including stainless steel. I can confirm this by my experience with the chiller: the visible trace of corrosion which appeared on the cold SS drain valve after a long period of running with C6F14 rapidly deteriorated when I switched to Novec 649. The drain suffered because it was there that the coolant met with liquid condensation water when the coolant was drained. As a partial solution, I usually drain the coolant at -5...-10°C and try to wipe the residual drops of the coolant before the valve warms up.

The cooling systems used at CERN are closed circulation circuits, equipped with moisture and acid filters. Therefore, under normal running conditions there should be no risk of corrosion. Special procedures for filling and draining should be designed, similar to those applied at Novec 1230 filling stations.

However, the reactivity with water might become the principal objection by the CERN safety and the detector people, because in the case of leaks the coolant may get in contact with condensation moisture and cause the corrosion of the affected area.

3.6 Compatibility with materials

The only information about the compatibility of Novec fluids comes from 3M [16]. “Novec 649 fluid is compatible with a wide range of materials of construction and requires no special piping or handling systems, and is very stable in storage.” [9d]. B. Kaiser of 3M also presented the C6K-specific summary shown in Table 3 (it also appeared in [7a]). A very good compatibility with all materials used in power electronics (including copper) can be assumed, following successful applications in immersion cooling [10]. Corrosion testing in presence of O₂ [7a] showed no significant corrosion, as well.

Elastomere compatibility in 6-month tests at 75°C showed good results for EPDM rubber. B.Kaiser [16c] claimed that the best elastomer for C6K is natural rubber, but its low-temperature performance is questionable. IMO, potential materials for flexible hoses with C6K would be ultra-pure plasticizer-free silicone rubber (e.g. Tygon formulations 2075, 2001) or PU rubber (e.g. Tygotan C-555-A, known to be very radiation-hard and to withstand low-temperatures down to -73°C) [16d].

3.7 Safety

This topic, especially in application to Novec 1230, had been extensively addressed by the 3M Company [18,19]. Novec 1230 fluid is very low in toxicity, with NOAEL of >10% v/v, and is acceptable for use in occupied areas. It has shown a very low potential for irritation to the eyes, skin, and mucous membranes. The acute and repeat dose toxicity of Novec 1230 fluid are also very low. The toxicity of Novec 1230 fluid has been also independently assessed by several competent institutions and consulting firms [19h]. There is general consensus that Novec 1230 Fire Protection Fluid is not only safe for its intended use but provides a large margin of safety relative to anticipated design concentrations of fire protection systems and during the manufacture of those systems [19c]. All this, of course, regards a massive release of C6K in the event of fire. Given the intended applications in close-circuit cooling systems at CERN, only minor release in case of leaks can be anticipated. In any case, the safety arrangements for C6K should be similar to those for C6F14.

Leak detection: C6K is easy to detect (WL for IR measurement is 6.84 μm).

Table 3 Novec 649 compatibility with materials (from [16c] and [7a])

Materials Compatibility				
Compatibility of "O" Rings with Novec 649				
Exposure Time: 1 Week@ 25°C, 100°C				
Elastomer Type	Exposure Temperature	Change in Shore A Hardness	% Change in Weight	% Change in Volume
Neoprene	25°C	-1.8	-.06	-1.2
	100°C	-2.2	+2.3	+0.8
Butyl rubber	25°C	-2.7	+0.2	+0.1
	100°C	-4.0	+4.3	+4.2
Fluoroelastomer	25°C	-6.2	+0.7	+0.6
	100°C	-12.6	+9.5	+10.6
EPDM	25°C	-4.7	+0.6	+0.3
	100°C	-5.7	+3.3	+2.4
Silicone	25°C	N/A	+3.1	+2.8
	100°C	-5.4	+6.0	+5.1
Nitrile	25°C	-0.7	-0.3	-0.5
	100°C	+2.5	+4.6	+0.7

3.8 Suppliers, commercial availability

C6K is immediately available from 3M and its dealers, always with the certificate of analysis. Novec 1230 is exclusively shipped to OEMs specializing in fire protection⁶, so for CERN applications we are, essentially, limited to Novec 649. The current list price of Novec 649 is 62-66 CHF/kg (from 3M Switzerland, quotation of 22.10.2014). As "CAS 756-13-8", this compound is available from numerous Chinese suppliers [20a], in quantities from 1 kg to tons (??), with relatively low ($\leq 98\%$) purity. A research-grade "756-13-8" is also available from standard pure chemicals suppliers, but the price can be astronomical (thousands CHF/kg).

3.9 Purification methods and other information from B.Kaiser of 3M

B.K. claimed that molecular sieve (adsorber) types are not good, because the fluid will be in contact with the increasing amount of H₂O molecules, which will react with fluoroketone. He said that the *absorber type* filters (sodium sulphate or similar anhydrous stuff) are more appropriate and can be even cheaper⁷.

⁶ On 5.11.2014 I received a rectification from B.Kaiser of 3M, quoting the following statement of the European 3M management: "Novec 1230 fluid application can only be restricted to fire protection. *No other application is allowed.* If the test is required for fire protection, than a supply is possible. For the fire fighting installation you have to go to an official OEM. It would make sense to go to one of them also for the test's. For any other application, *we have to decline the supply of this material.* The price is the same as for 3M Novec 649."

⁷ I think that zeolite adsorbents should work with Novec, as well: the pore size is too small for C₆K molecules (comparable in size with C₆F₁₄) to reach H₂O. C₆K can be chemically reactive with activated alumina adsorbents, though [7a], to be verified experimentally.

4. Draft plan for testing C6K at CERN

The EN-CV and TE-VSC-SCC groups were involved in the C6F14 validation project at CERN [6c]; their experience is indispensable for this study. At a preliminary discussion with M. Battistin he also suggested to involve R. Setnescu (currently, a PJAS at TE-VSC-SCC).

Mauro and Michele proposed to perform a quick pilot study to make sure that C6K has a *reasonable* radiation resistance. Should it turn out to be incompatible with the doses in excess of 100 Gy, then the scope of this study will be limited to the SciFi application [5]. Otherwise, a new full-blast Detector Cooling project can be launched to qualify the fluid properly; all LHC experiments can be involved in its funding.

After the first brainstorming meeting with TE-VSC-SCC (November 4, 2014), a more detailed plan will be presented. Topics to be discussed:

- Where to irradiate; the amount of fluid required for irradiations, rough cost estimate for the pilot study?
- Containers: make new or re-use the old one?
- Shall we irradiate C6F14 together with C6K, to compare the effects of the same dose?
- Whether to continue attempts to purchase Novec 1230?
- C6K reactivity with water: can it be a show-stopper for applications at CERN?
- Additional aspects to be studied: rectification methods, compatibility with elastomers.
- Rectification of commercial samples at CERN or elsewhere?

The principal study could be quite similar to the one for C6F14: we take a fresh commercial sample (>99% pure C6K + some unknown impurities), irradiate discrete portions with a wide range of doses and watch the fluid for the appearance of undesirable products of the C6K decomposition products, like acids and water. Appropriate purification methods should be proposed.

Mauro remarked that the price for such an irradiation test in an external firm would be the same for one of more samples if we can irradiate them in the same run. Therefore, it would be beneficial to irradiate samples of different fluids, including C6F14 (and Novec 1230, should we be able to get it).

One factor that differs C6F from heavy fluorocarbons (apart from GWP) is its reported reactivity with liquid water phase (Section 3.5). Though this factor has a lower importance in the closed-loop applications, especially at below-zero temperatures, water-removal methods should be addressed with particular attention in this study.

The time frame is quite limited: from now through May 2015 we want to get some initial results, at least for low-dose irradiation (relevant for the SciFi application).

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