Committee of Experts on the Transport of Dangerous Goods and on the Globally Harmonized System of Classification and Labelling of Chemicals

15 June 2021

Sub-Committee of Experts on the Transport of Dangerous Goods

Fifty-eighth session
Geneva, 28 June-2 July 2021
Item 2 (i) of the provisional agenda
Explosives and related matters: miscellaneous

Introduction of a new entry for 5-Trifluoromethyltetrazole, sodium salt (TFMT-Na) in acetone as a desensitized explosive in the Dangerous Goods List of the Model Regulations

Transmitted by the European Chemical Industry Council (Cefic)

Introduction

1. The title compound is a precursor of a new insecticide entering the market. Due to the explosive properties of the dry substance, it is only handled and transported as a homogenous solution in acetone. As sourcing involves international transport from different countries, Cefic proposes the creation of an entry as a desensitized explosive in the Dangerous Goods List in section 3.2.2 of the UN Model Regulations.

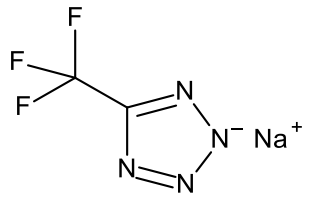


Figure 1: 5-Trifluoromethyltetrazole, sodium salt (TFMT-Na)

2. By request from industry, the German competent authorities have issued a temporary approval for the transport of the compound classified as UN 3379 DESENSITZED EXPLOSIVE, LIQUID, N.O.S. For a permanent solution, Cefic invites the Sub-Committee to create an entry for a corresponding classification in the Dangerous Goods List.

3. A detailed test report and the data sheet to be submitted to the United Nations for new classification of substances can be found in annexes I though V. The Sub-Committee is invited to review the data and to forward any comments to the Cefic delegation.

Test data

4. All tests were performed according to the methods specified in the Manual of Tests and Criteria, sixth revised edition.

5. Dry 5-Trifluoromethyltetrazole, sodium salt (TFMT-Na) is thermally stable (decomposition onset above 230 °C in differential scanning calorimetry (DSC) measurement), not sensitive to mechanical stimuli (impact, friction) and gives a positive result in test series 2.

➡ Provisionally accepted in the Class of Explosives.

6. The solution of TFMT-Na in acetone (concentrations 27.3 % and 53 % (saturated)) gives a negative result in test series 2 (too insensitive for acceptance into this class).

➡ Not an Explosive.

7. In a burning rate test of a TFMT-Na solution (30 %) in acetone according to chapter 51 of the UN Manual of Tests and Criteria, a corrected burning rate of 35 - 41 kg/min was determined for a quantity of 10000 kg. This result corresponds to a classification as Desensitized Explosive, Cat. 4 in GHS.

8. Details are specified in the test reports and flow charts in the annexes to this document, Annexes I and II for pure (crystalline) TFMT-Na and Annexes III and IV for the solution in acetone. Annex V contains the data sheet.

9. So far, studies about harmful biological effects have been initiated. The results will be submitted as soon as they become available along with a formal proposal. However, some difficulties have been encountered due to the explosive character of the main compound. Members of the Sub-Committee are requested to share their corresponding experiences or advice with the Cefic delegation.

Proposal

10. In the Dangerous Goods List of section 3.2.2, create an entry as follows:

UN No.	Name and description	Class or division	Subsi-diary hazard	UN packing group	Special provi-sions	Limited and exepted quantities		Packagings and IBCs		Portable tanks and bulk containers	
								Packing instruction	Special packing provisions	Instructions	Special provisions
(1)	(2)	(3)	(4)	(5)	(6)	(7a)	(7b)	(8)	(9)	(10)	(11)
XX	TRIFLUORO METHYLTET RAZOLE-SODIUM SALT IN ACETONE, with not less than 68 % acetone, by mass	3		I	28, 132, 266	0	E0	PYYY	PP26		

11. Amend the last sentence in 2.3.1.4 to read (new text in **bold underlined**): “Entries in the Dangerous Goods List for liquid desensitized explosives are: UN 1204, UN2059, UN3064, UN3343, UN3357**,** ~~and~~ UN3379 **and UN XX**.”

12. Modify special provision 28 to read: “This substance may be transported **as a desensitized explosive** under the provisions of **class 3 or** division 4.1**, respectively** only if it is so packed that the percentage of diluent will not fall below that stated, at any time during transport (see **2.3.4.1 and** 2.4.2.4).”

13. Create a new packing instruction PYYY as follows:

PYYY	PACKING INSTRUCTION	PYYY
This instruction applies to UN No. XX		
The following packagings are authorized, provided that the general provisions of 4.1.1 and 4.1.3 as well as 4.1.5.12 are met: (1) Plastics drum non-removeable head (1H1) of maximum capacity 250 l (2) Combination packagings Outer packagings: 4C2, 4D, 4F, 4G[a], 4H1, 4H2 with a maximum net mass of 2 kg Inner packagings: glass inner packagings cushioned on all sides with dry, absorbent, non-combustible material in a quantity sufficient to absorb the entire contents with a maximum net mass of 1 kg. [a] Packagings shall be siftproof		
Additional requirements: Packagings shall be designed and constructed to prevent the loss of the content of the phlegmatizer. The packagings shall be transported in an upright position.		
Special packing provisions: **PP26** For UN No. XX packagings shall be lead free.		

Justification

14. The fact that the product is carried in increasing quantities between different countries justifies a new entry in the Dangerous Goods List. The test results are clear, and a formal temporary approval has been issued for road and sea transport by the German competent authorities.

Annex I

Test report: Pure compound: Procedure for provisional acceptance in the Class of Explosives acc. to Fig. 10.2 of the Test Manual

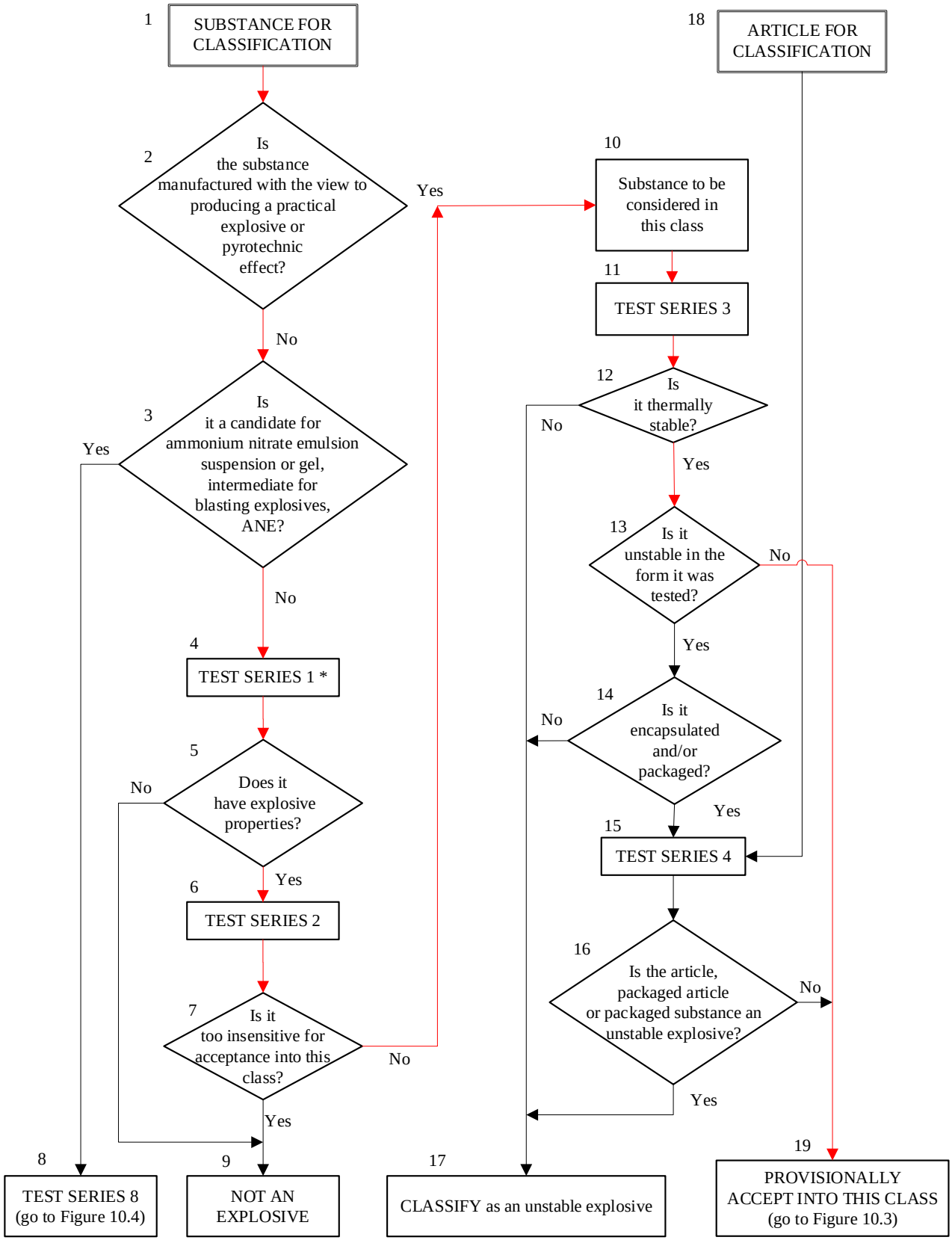
1.	**Name of substance**	:	5-Trifluoromethyltetrazole, sodium salt (TFMT-Na)
2.	**General data**		
2.1	Composition	:	5-Trifluoromethyltetrazole, sodium salt (TFMT-Na), technically pure
2.2	Molecular formula	:	$C_2N_4F_3Na$
2.3	Available oxygen content	:	Not aplicable
2.4	Activator content	:	Not applicable
2.5	Physical form	:	Solid, crystalline
2.6	Colour	:	White
2.7	Apparent density	:	Not known
2.8	Particle size	:	Not determined
3.	**Box 2 of the flow chart**	:	Is the substance manufactured with the view to producing a practical explosive or pyrotechnic effect?
3.1	Answer	:	No
3.2	Exit	:	Go to Box 3
4.	**Box 3**	:	Is it a candidate for ammonium nitrate emulsion suspension or gel, intermediate for blasting explosives, ANE?
4.1	Answer	:	No
4.2	Exit	:	Go to Box 4
5.	**Box 4**	:	Test series 1
5.1	Propagation of detonation	:	Trauzl test (UN F.3) with initiation by detonator No. 8 acc. to 11.3.5 UN-MTC
5.2	Sample conditions	:	Ambient temperature
5.3	Observations	:	Lead block expansion 120-124 ml/10 g Not low
5.4	Result	:	"+", propagation of detonation in test 1 (a)
5.5	Effect of heating under confinement	:	Koenen test (test 1(b))
5.6	Sample conditions	:	Mass 24.0-24.2 g
5.7	Observations	:	Limiting diameter > 16 mm Fragmentation type "F" (time to reaction 16 s; duration of reaction 0 s)
5.8	Result	:	"+", shows some explosive effects on heating under confinement
5.9	Effect of ignition under confinement	:	Time/pressure test (test 1 (c) (i))
5.10	Sample conditions	:	Ambient temperature
5.11	Observations	:	Maximum pressure: 3560 kPa
5.12	Result	:	"+", substance is able to deflagrate
5.13	Exit	:	Go to Box 5

6.	**Box 5**	:	Does it have explosive properties?
6.1	Answer from Test Series 1	:	Yes
6.2	Exit	:	Go to Box 6
7.	**Box 6**	:	Test Series 2
7.1	Sensitivity to shock	:	Trauzl test (UN F.3) with initiation by detonator No. 8 acc. to 12.3.4 UN-MTC
7.2	Sample conditions	:	Ambient temperature
7.3	Observations	:	Lead block expansion 120-124 ml/10 g Not low
7.4	Result	:	"+", sensitive to shock in test 2 (a)
7.5	Effect of heating under confinement	:	Koenen test (test 2(b))
7.6	Sample conditions	:	Mass 24.0-24.2 g
7.7	Observations	:	Limiting diameter > 16 mm Fragmentation type "F" (time to reaction 16 s; duration of reaction 0 s)
7.8	Result	:	"+", violent effects on heating under confinement
7.9	Effect of ignition under confinement	:	Time/pressure test (test 2 (c) (i))
7.10	Sample conditions	:	Ambient temperature
7.11	Observations	:	Time for pressure rise from 690 to 2070 kPa: 1.9 – 3.9 ms
7.12	Result	:	"+", substance is able to deflagrate rapidly
7.13	Exit	:	Go to Box 7
8.	**Box 7**	:	Is it too insensitive for acceptance into this class?
8.1	Answer from Test Series 2	:	No
8.2	Conclusion	:	Substance to be considered in this class (box 10)
8.3	Exit	:	Go to Box 11
9.	**Box 11**	:	Test Series 3
9.1	Thermal stability	:	DSC (UN MTC section 20.3.3.3) Screening test as alternative to test 3 (c)
9.2	Sample conditions	:	Heating rate 1 K/min in closed Hastelloy crucible) Sample mass 101 mg
9.3	Observations	:	Decomposition onset > 230 °C
9.4	Result	:	"-", thermally stable
9.5	Impact sensitivity	:	BAM Fallhammer test (test 3 (a) (ii))
9.6	Sample conditions	:	as above
9.7	Observations	:	Limiting impact energy 40 J
9.8	Result	:	"-", not unstable in the form it was tested
9.9	Friction sensitivity	:	BAM friction test (test 3 (b) (i))
9.10	Sample conditions	:	as above
9.11	Observations	:	Limiting load > 360 N
9.12	Result	:	"-", not unstable in the form it was tested
9.13	Ease of deflagration to detonation transition	:	Small scale burning test (test 3 (d))
9.14	Observations	:	Not performed
9.15	Result	:	n/a

9.16	Exit	:	Go to box 12
10.	**Box 12**	:	Is it thermally stable?
10.1	Answer from test 3(c)	:	Yes
10.2	Exit	:	Go to box 13
11.	**Box 13**	:	Is it unstable in the form it was tested?
11.1	Answer from Test Series 3	:	No
11.2	Exit	:	Go to box 19
12.	**Conclusion**	:	PROVISIONALLY ACCEPT INTO THIS CLASS

Annex II

Resulting flow chart for pure (dry) compound



Annex III

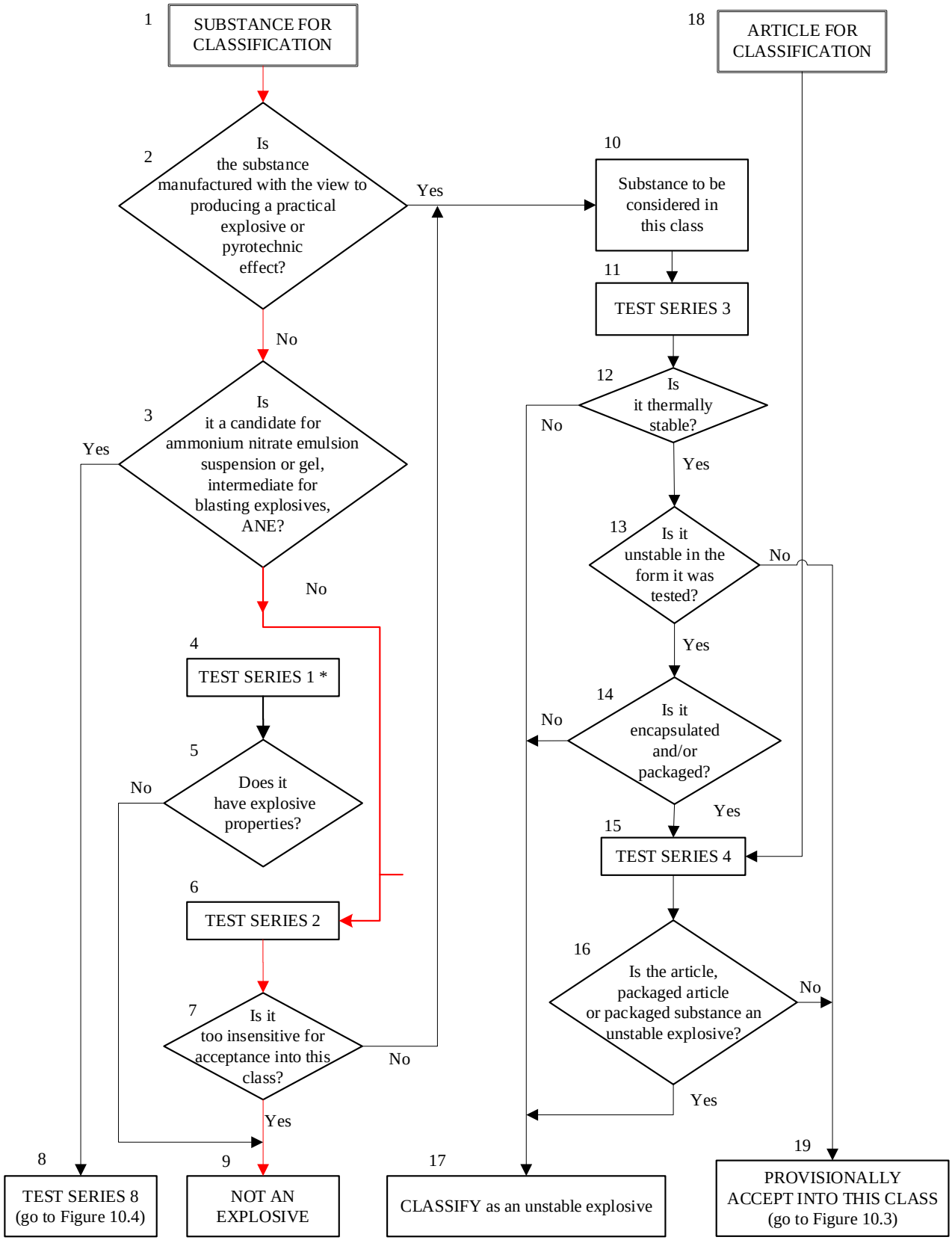
Test report: Solution of TFMT-Na in Acetone (27.3 % and 53 % (saturated)) Procedure for provisional acceptance in the Class of Explosives acc. to Fig. 10.2 of the Test Manual

1.	**Name of substance**	:	5-Trifluoromethyltetrazole, sodium salt (TFMT-Na) in Acetone
2.	**General data**		
2.1	Composition	:	5-Trifluoromethyltetrazole, sodium salt (TFMT-Na), in Acetone; concentration 27.3 % and 53 %
2.2	Molecular formula	:	$C_2N_4F_3Na$
2.3	Available oxygen content	:	Not aplicable
2.4	Activator content	:	Not applicable
2.5	Physical form	:	Homogenous solution
2.6	Colour	:	clear, colorless
2.7	Apparent density	:	Not known
2.8	Particle size	:	Not applicable
3.	**Box 2 of the flow chart**	:	Is the substance manufactured with the view to producing a practical explosive or pyrotechnic effect?
3.1	Answer	:	No
3.2	Exit	:	Go to Box 3
4.	**Box 3**	:	Is it a candidate for ammonium nitrate emulsion suspension or gel, intermediate for blasting explosives, ANE?
4.1	Answer	:	No
4.2	Exit	:	Go to Box 6
5.	**Box 6**	:	Test Series 2
5.1	Sensitivity to shock	:	UN gap test (test 2 (a))
5.2	Sample conditions	:	Ambient temperature
5.3	Observations	:	Witness plate slightly domed; no propagation
5.4	Result	:	"-", not sensitive to shock in test 2 (a)
5.5	Effect of heating under confinement	:	Koenen test (test 2(b))
5.6	Sample conditions	:	Mass 26.0 g for 27.3 % solution Mass 28.0 g for 53 % solution
5.7	Observations	:	Limiting diameter < 2 mm Fragmentation type "O" (time to reaction 7 - 9 s; duration of reaction 40 – 42 s) for 27.3 % solution Fragmentation type "A" (time to reaction 9 s; duration of reaction 55 - 59 s) for 53 % solution
5.8	Result	:	"-", no violent effects on heating under confinement
5.9	Effect of ignition under confinement	:	Time/pressure test (test 2 (c) (i))
5.10	Sample conditions	:	Ambient temperature
5.11	Observations	:	Pressure of 2070 kPa gauge not reached for 27.3 % solution Time for pressure rise from 690 to 2070 kPa: 300 – 420 ms for 53 % solution
5.12	Result	:	"-", substance shows no or slow deflagration
5.13	Exit	:	Go to Box 7

6.	**Box 7**	:	Is it too insensitive for acceptance into this class?
6.1	Answer from Test Series 2	:	Yes
6.2	Exit	:	Go to Box 9
7.	**Conclusion**	:	NOT AN EXPLOSIVE

Annex IV

Resulting flow chart for the solution of TFMT-Na in Acetone (27.3 % and 53 %)



Annex V

DATA SHEET TO BE SUBMITTED TO THE UNITED NATIONS FOR NEW OR AMENDED CLASSIFICATION OF SUBSTANCES

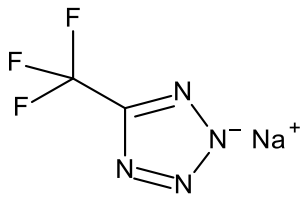
Submitted by....Cefic..... Date May 31, 2021 .....

Supply all relevant information including sources of basic classification data. Data should relate to the product in the form to be transported. State test methods. Answer all questions - if necessary, state "not known" or "not applicable" - If data is not available in the form requested, provide what is available with details. Delete inappropriate words.

Section 1. SUBSTANCE IDENTITY

1.1 Chemical name 5-Trifluoromethyltetrazole, sodium salt (TFMT-Na) in Acetone

1.2 Chemical formula $C_2N_4F_3Na$



1.3 Other names/synonyms Sodium-5-trifluormethyl-1H-tetrazolate in Acetone

1.4.1 UN number .....1.4.2 CAS number 1702-15-4.....

1.5 Proposed classification for the Recommendations

1.5.1 proper shipping name (3.1.2[1])... TRIFLUOROMETHYLTETRAZOLE-SODIUM SALT IN ACETONE, with not less than 68 % acetone, by mass

1.5.2 class/division 3.....subsidiary risk(s) ..... packing group I .....

1.5.3 proposed special provisions, if any: SP 28, SP 132, SP 266 (see proposal).....

1.5.4 proposed packing instruction(s): New PXXX suggested, see proposal.

Section 2. PHYSICAL PROPERTIES

2.1 Melting point or range: below -95 °C (Acetone)

2.2 Boiling point or range 56 °C (Acetone)

2.3 Relative density at :

2.3.1 15 °C 0.980 g/ml

2.3.2 20 °C 0.977 g/ml

2.3.3 30 °C 0.955 g/ml

[1] This and similar references are to chapters and paragraphs in the Model Regulations on the Transport of Dangerous Goods.

2.4 Vapour pressure at :

2.4.1 50 °C .....80 kPa

2.4.2 65 °C .....n/a

2.5 Viscosity at 20 °C[2] 0.917 mPas

2.6 Solubility in water at 20 °C: completely miscible;

solubility in acetone: 53 % (w/w) TFMT-Na in acetone

2.7 Physical state at 20°C (2.2.1.1[1])..... liquid[2]

2.8 Appearance at normal transport temperatures, including colour and odour:

Colourless liquid, smell of acetone

2.9 Other relevant physical properties: n/a

.....

.....

Section 3. FLAMMABILITY

3.1 Flammable vapour

3.1.1 Flash point (2.3.3[1]): -18 °C (closed cup)

3.1.2 Is combustion sustained? (2.3.1.3[1]) yes

3.2 Autoignition temperature: 465 °C

3.3 Flammability range (LEL/UEL): 2.5 – 14.3 Vol%

3.4 Is the substance a flammable solid? (2.4.2[1]) no

3.4.1 If yes, give details .....

.....

.....

.....

Section 4. CHEMICAL PROPERTIES

4.1 Does the substance require inhibition/stabilization or other treatment such as nitrogen blanket to prevent hazardous reactivity? no

If yes, state:

4.1.1 Inhibitor/stabilizer used .....n/a

4.1.2 Alternative method ..... n/a

4.1.3 Time effective at 55 °C..... n/a

4.1.4 Conditions rendering it ineffective n/a

4.2 Is the substance an explosive according to paragraph 2.1.1.1? (2.1[1]) no

[2] See definition of "liquid" in 1.2.1 of the Model Regulations on the Transport of Dangerous Goods.

[1] This and similar references are to chapters and paragraphs in the Model Regulations on the Transport of Dangerous Goods.

4.2.1 If yes, give details n/a

.....

.....

.....

4.3 Is the substance a desensitized explosive? (2.4.2.4[1]) yes

4.3.1 If yes, give details: Dry TFMT-Na is provisionally accepted in the Class of Explosives based on test results (see attached report for details).

The solution in acetone passes Test Series 2 and is therefore not to be classified as explosive; see test report. .....

.....

4.4 Is the substance a self-reactive substance? (2.4.1[1]) no

If yes, state:

4.4.1 exit box of flow chart... n/a

What is the self-accelerating decomposition temperature (SADT) for a 50 kg package? ..... °C

Is the temperature control required? (2.4.2.3.4[1]) no

4.4.2 proposed control temperature for a 50 kg package ..... °C

4.4.3 proposed emergency temperature for a 50 kg package ..... °C

4.5 Is the substance pyrophoric? (2.4.3[1]) no

4.5.1 If yes, give details .....

.....

.....

.....

4.6 Is the substance liable to self-heating? (2.4.3[1]) no

4.6.1 If yes, give details .....

.....

.....

.....

4.7 Is the substance an organic peroxide (2.5.1[1]) no

If yes state:

4.7.1 exit box of flow chart... n/a

What is the self-accelerating decomposition temperature (SADT) for a 50 kg package? ..... °C

Is temperature control required? (2.5.3.4.1[1]) no

4.7.2 proposed control temperature for a 50 kg package ..... °C

4.7.3 proposed emergency temperature for a 50 kg package ..... °C

4.8 Does the substance in contact with water emit flammable gases? (2.4.4[1]) no

4.8.1 If yes, give details .....

[1] This and similar references are to chapters and paragraphs in the Model Regulations on the Transport of Dangerous Goods.

.....

.....

.....

4.9 Does the substance have oxidizing properties (2.5.1[1]) no

4.9.1 If yes, give details .....

.....

.....

.....

4.10 Corrosivity (2.8[1]) to:

4.10.1 mild steel n/a.....mm/year at ..... °C

4.10.2 aluminium n/a .....mm/year at..... °C

.....No corrosivity expected due to chemical structure

4.10.3 other packaging materials (specify)

n/a..... mm/year at..... °C

..... mm/year at..... °C

4.11 Other relevant chemical properties n/a

.....

.....

.....

Section 5. HARMFUL BIOLOGICAL EFFECTS

5.1 LD_{50}, oral (2.6.2.1.1[1])... .....mg/kg Animal species .....

5.2 LD_{50}, dermal (2.6.2.1.2[1]).....mg/kg Animal species .....

5.3 LC_{50}, inhalation (2.6.2.1.3[1]) ... .mg/litre Exposure time..... hours

or ....ml/m^3 Animal species .....

5.4 Saturated vapour concentration at 20 °C (2.6.2.2.4.3[1]) .....ml/m^3

5.5 Skin exposure (2.8[1]) results Exposure time ..... hours/minutes

Animal species.....

5.6 Other data .....

.....

.....

5.7 Human experience .....

.....

.....

[1] This and similar references are to chapters and paragraphs in the Model Regulations on the Transport of Dangerous Goods.

Section 6. SUPPLEMENTARY INFORMATION

6.1 Recommended emergency action

6.1.1 Fire (include suitable and unsuitable extinguishing agents)
Suitable extinguishing media: Water spray jet, alcohol resistant foam, extinguishing powder, carbon dioxide (CO_2);

Unsuitable media: Full water jet.

6.1.2 Spillage: Dilute spilled product with water and absorb with liquid-binding material (e.g. sand, diatomaceous earth, universal binding agents). Take up mechanically and place in appropriate containers for disposal. Keep the content of the container wet with water.

6.2 Is it proposed to transport the substance in:

6.2.1 Bulk Containers (6.8[1]) no

6.2.2 Intermediate Bulk Containers (6.5[1])? no

6.2.3 Portable tanks (6.7[1])? no

If yes, give details in Sections 7, 8 and/or 9.

Section 7. BULK CONTAINERS (only complete if yes in 6.2.1)

7.1 Proposed type(s) n/a

Section 8. INTERMEDIATE BULK CONTAINERS (IBCs) (only complete if yes in 6.2.2)

8.1 Proposed type(s) n/a

Section 9. MULTIMODAL TANK TRANSPORT (only complete if yes in 6.2.3)

9.1 Description of proposed tank (including IMO tank type if known) n/a

9.2 Minimum test pressure .....

9.3 Minimum shell thickness .....

9.4 Details of bottom openings, if any .....

9.5 Pressure relief arrangements .....

9.6 Degree of filling .....

9.7 Unsuitable construction materials .....

[1] This and similar references are to chapters and paragraphs in the Model Regulations on the Transport of Dangerous Goods.