



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

Sub-Committee of Experts on the Transport of Dangerous Goods

Fifty-seventh session

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Item 3 of the provisional agenda

Listing, classification and packing

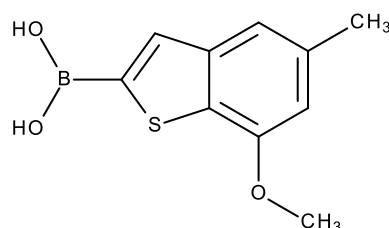
Introduction of a new entry for (7-Methoxy-5-methyl- benzothiophen-2-yl) boronic acid as a self-reactive substance in section 2.4.2.3.2.3 of the Model Regulations

Transmitted by the European Chemical Industry Council (CEFIC)*

Introduction

1. The title compound is a precursor of a new active pharmaceutical ingredient in the approval process. As sourcing involves international transport from different countries, CEFIC proposes the creation of an entry in the list of self-reactive substances under 2.4.2.3.2.3 of the Model Regulations.

Figure 1: Chemical structure of (7-Methoxy-5-methyl-benzothiophen-2-yl) boronic acid



2. By request from industry, the German competent authorities issued a temporary approval for the transport of the compound classified as UN 3230 SELF-REACTIVE SOLID TYPE F. For a permanent solution, CEFIC invites the Sub-Committee to create a corresponding entry in 2.4.2.3.2.3.

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

* 2020 (A/74/6 (Sect.20) and Supplementary, Subprogramme 2

Test data

4. All tests were performed according to the methods specified in the Manual of Tests and Criteria, fifth revised edition.
5. The classification procedure led to the following final result according to Figure 20.1 of the Manual of Tests and Criteria:

Exit F, may be considered for transport in IBCs or tanks.
6. Details are specified in the test report in Annex I to this document, Annex II shows the resulting flow chart and Annex III contains the data sheet.

Proposal

7. In 2.4.2.3.2.3, create an entry in the list of self-reactive substances as follows

SELF-REACTIVE SUBSTANCE	Concentration (%)	Packing method	Control temperature (°C)	Emergency temperature (°C)	UN generic entry	Remarks
(7-Methoxy-5-methyl-benzothiophen-2-yl) boronic acid	88-100	OP 7			3230	(11)

8. Add the following new remark (11) under the table in 2.4.2.3.2.3:
“(11) The technical compound with the specified concentration limits may contain up to 12 % water and up to 1 % organic impurities.”.

Justification

9. The fact that the product is carried in increasing quantities between different countries justifies a new entry in the list of self-reactive substances. The test results are clear, and a formal temporary approval has been issued for all modes by the German authorities.

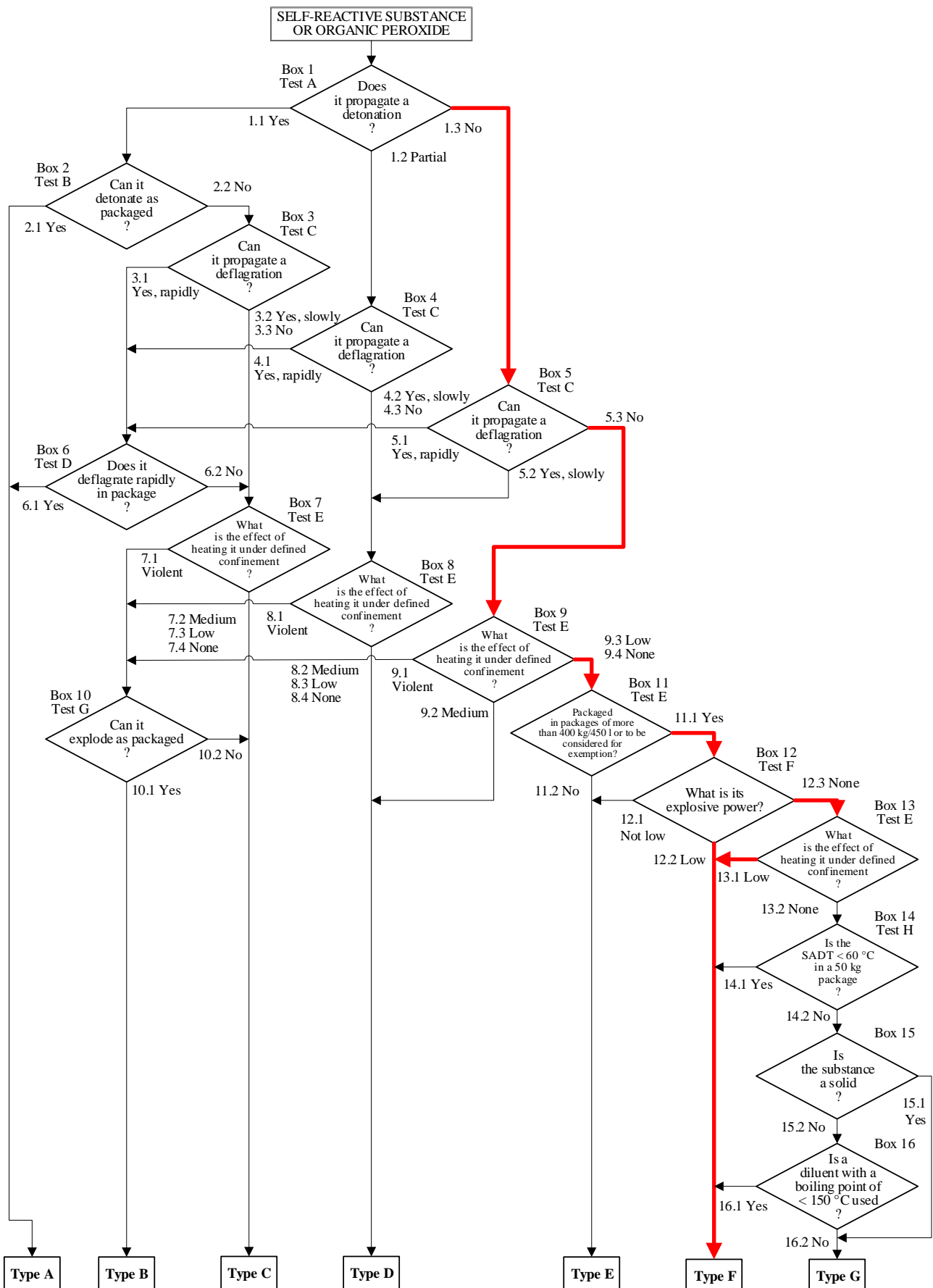
Annex I

Test report

1.	Name of substance	:	(7-Methoxy-5-methyl-benzothiophen-2-yl) boronic acid
2.	General data		
2.1	Composition	:	88.6 % (7-Methoxy-5-methyl-benzothiophen-2-yl) boronic acid 0.8 % organic impurities 10.6 % water
2.2	Molecular formula	:	C ₁₀ H ₁₁ BO ₃ S
2.3	Available oxygen content	:	Not applicable
2.4	Activator content	:	Not applicable
2.5	Physical form	:	Solid
2.6	Colour	:	White
2.7	Apparent density	:	Not known
2.8	Particle size	:	Not applicable
3.	Detonation (test series A)		
	Box 1 of the flow chart	:	Does the substance propagate a detonation?
3.1	Method	:	Combination of UN F.3 (BAM Trauzl test) with E.1 (Koenen test) and E.2 (Dutch pressure vessel test) acc. to UN MTC, section 21.2.2
3.2	Sample conditions	:	Ambient temperature
3.3	Observations	:	Low in UN E.1 (see below) No in UN E.2 No in UN F.3 → No in test series A
3.4	Result	:	No
3.5	Exit	:	1.3
4.	Deflagration (test series C)		
	Box 5 of the flow chart	:	Does the substance propagate a deflagration?
4.1	Method 1	:	Time/pressure test (test C.1)
4.2	Sample conditions	:	Ambient temperature
4.3	Observations	:	3 tests; maximum pressures: 343 kPa; 375 kPa; 375 kPa
4.4	Result	:	No
4.5	Method 2	:	Deflagration test (test C.2)
4.6	Sample conditions	:	Temperature 47 – 50 °C (2 tests)
4.7	Observations	:	No deflagration observed in either test
4.8	Result	:	No
4.9	Overall result	:	No
4.10	Exit	:	5.3
5.	Heating under confinement (test series E)		
	Box 9 of the flow chart	:	What is the effect of heating it under defined confinement?
5.1	Method 1	:	Koenen test (test E.1)
5.2	Sample conditions	:	Mass 13.2; 13.3; 13.5 g (3 tests)
5.3	Observations	:	Limiting diameter: less than 1.0 mm (time to reaction 21 s; 16 s; 19 s) Effect types: “O”; “A”; “A”
5.4	Result	:	Low
5.5	Method 2	:	Dutch pressure vessel test (test E.2)
5.6	Sample conditions	:	10.0 g; 50.0 g

5.7	Observations	:	Limiting diameter <1.0 mm (shortest time to reaction 118 s)
5.8	Result	:	No
5.9	Overall result	:	Low
5.10	Exit	:	9.3
<hr/>			
6.	Packages of more than 400 kg/450 l or considered for exemption?		
	Box 11 of the flow chart	:	Packaged in packages of more than 400 kg/450 l or to be considered for exemption?
6.1	Result	:	Yes
6.2	Exit	:	11.1
<hr/>			
7.	Explosive Power		
	Box 12 of the flow chart	:	What is its explosive power?
7.1	Method	:	BAM Trauzl test (test F.3)
7.2	Sample conditions	:	Mass 4.36 g; 4.34 g (2 tests)
7.3	Observations	:	Volume increase 8.7 ml and 8.1 ml per 10 g sample Expansion of lead block is less than 10 ml per 10 g of sample
7.4	Result	:	No (none)
7.5	Exit	:	12.3
<hr/>			
8.	Heating under confinement (test series E)		
	Box 13 of the flow chart	:	What is the effect of heating it under defined confinement?
8.1	see number 5 above		
8.2	Overall result	:	Low
8.3	Exit	:	13.1 → TYPE F
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9.	Thermal stability (test series H)		
9.1	Method	:	Heat accumulation storage test (test H.4)
9.2	Sample conditions	:	Tests performed at 76 °C, 61 °C and 51 °C Sample mass 140-148 g Heat loss of Dear vessel 34 – 42 mW/(kg K)
9.3	Observations	:	Auto-accelerating decomposition at 76 °C, borderline (6 K rise) at 61 °C, no auto-accelerating decomposition at 51 °C
9.4	Result	:	60 °C ≤ SADT < 75 °C No temperature control required
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10.	Proposed assignment		
10.1	Proper shipping name	:	SELF-REACTIVE SOLID TYPE F
10.2	UN number	:	3230
10.3	Division	:	4.1
10.4	Technical name	:	(7-Methoxy-5-methyl-benzothiophen-2-yl) boronic acid
10.5	Concentration	:	88 - 100%
10.6	Diluent(s)	:	0 - 12 % water
10.7	Subsidiary hazards	:	None
10.8	Packing group	:	
10.9	Packing method	:	OP7
10.10	Control temperature	:	Not required
10.11	Emergency temperature	:	Not required

Annex II Resulting flow chart



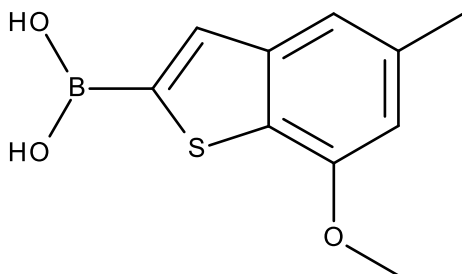
Annex III**Data sheet to be submitted to the United Nations for new or amended classification of substances**

Submitted by..... CEFIC.....Date 11 March 2020

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 (7-Methoxy-5-methyl-benzothiophen-2-yl) boronic acid
 1.2 Chemical formula



- 1.3 Other names/synonyms not known
 1.4.1 UN number 3230 1.4.2 CAS number 1443531-60-9
 1.5 Proposed classification for the Recommendations
 1.5.1 proper shipping name (3.1.2¹) SELF-REACTIVE SOLID TYPE F
 1.5.2 class/division 4.1 subsidiary risk(s) not applicable
 packing group not applicable
 1.5.3 proposed special provisions, if any
 1.5.4 proposed packing instruction(s) P520 OP 7

Section 2. PHYSICAL PROPERTIES

- 2.1 Melting point or range > 70 °C
 2.2 Boiling point or range not applicable
 2.3 Relative density at :
 2.3.1 15 °C
 2.3.2 20 °C
 2.3.3 50 °C
 2.4 Vapour pressure at:

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

- 2.4.1 50 °C kPa
- 2.4.2 65 °C kPa
- 2.5 Viscosity at 20 °C² m²/s
- 2.6 Solubility in water at 20 °C not soluble
- 2.7 Physical state at 20°C (2.2.1.1¹) solid
- 2.8 Appearance at normal transport temperatures, including colour and odour
- White crystals, odourless
- 2.9 Other relevant physical properties
-
-

Section 3. FLAMMABILITY

- 3.1 Flammable vapour
- 3.1.1 Flash point (2.3.3¹) not applicable
- 3.1.2 Is combustion sustained? (2.3.1.3¹) not applicable
- 3.2 Autoignition temperature: not applicable
- 3.3 Flammability range (LEL/UEL) not applicable
- 3.4 Is the substance a flammable solid? (2.4.2¹) 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
- 4.1.2 Alternative method
- 4.1.3 Time effective at 55 °C
- 4.1.4 Conditions rendering it ineffective
- 4.2 Is the substance an explosive according to paragraph 2.1.1.1? (2.1¹) no
- 4.2.1 If yes, give details
-
-
-

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.

- 4.3 Is the substance a desensitized explosive? (2.4.2.4¹) no
4.3.1 If yes, give details
- 4.4 Is the substance a self-reactive substance? (2.4.1¹) yes
If yes, state:
4.4.1 exit box of flow chartExit F
What is the self-accelerating decomposition temperature (SADT) for a 50 kg package?
60 °C ≤ SADT < 75 °C
Is the temperature control required? (2.4.2.3.4¹) 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? (2.4.3¹) no
4.5.1 If yes, give details
- 4.6 Is the substance liable to self-heating? (2.4.3¹) no
4.6.1 If yes, give details
- 4.7 Is the substance an organic peroxide (2.5.1¹) no
If yes state:
4.7.1 exit box of flow chart
What is the self accelerating decomposition temperature (SADT) for a 50 kg package? °C
Is temperature control required? (2.5.3.4.1¹) yes/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? (2.4.4¹) no
4.8.1 If yes, give details
- 4.9 Does the substance have oxidizing properties (2.5.1¹) no
4.9.1 If yes, give details

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

- 4.10 Corrosivity (2.8¹) to: not corrosive to metals
- 4.10.1 mild steelmm/year at °C
- 4.10.2 aluminium.....mm/year at °C
- 4.10.3 other packaging materials (specify)
- mm/year at..... °C
- mm/year at..... °C
- 4.11 Other relevant chemical properties
-
-
-

Section 5. HARMFUL BIOLOGICAL EFFECTS

- 5.1 LD₅₀, oral (2.6.2.1.1¹)..... not known mg/kg Animal species
- 5.2 LD₅₀, dermal (2.6.2.1.2¹) not known mg/kg Animal species
- 5.3 LC₅₀, inhalation (2.6.2.1.3¹)not knownmg/litre Exposure time hours
- or ml/m³ Animal species
- 5.4 Saturated vapour concentration at 20 °C (2.6.2.2.4.3¹) not knownml/m³
- 5.5 Skin exposure (2.8¹) results Exposure time not known hours/minutes
- Animal species
- 5.6 Other data
-
-
- 5.7 Human experience
-
-

Section 6. SUPPLEMENTARY INFORMATION

- 6.1 Recommended emergency action
- 6.1.1 Fire (include suitable and unsuitable extinguishing agents)
Use of any extinguishing media possible; wear self-contained breathing apparatus since evolution of hazardous smoke / gases such as boron oxides, sulphur oxides or carbon oxides is possible.
- 6.1.2 Spillage contain spillage, then collect with an electrically protected vacuum cleaner or by wet-brushing; collect in appropriate disposal container.
- 6.2 Is it proposed to transport the substance in:
- 6.2.1 Bulk Containers (6.8¹) no
- 6.2.2 Intermediate Bulk Containers (6.5¹)? no
- 6.2.3 Portable tanks (6.7¹)? no
- If yes, give details in Sections 7, 8 and/or 9.

¹ This and similar references are to chapters and paragraphs in 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.

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

7.1 Proposed type(s)

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

8.1 Proposed type(s)

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)

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
