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**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 GoodsTwenty-eighth session, 28 November-7 December 2005
Item 5 of the provisional agenda

LISTING, CLASSIFICATION AND PACKING

Classification of 1-hydroxybenzotriazole, anhydrous (HOBt), under Division 1.1DTransmitted by the expert from Germany**1. Background and properties**

For many years, the substance 1-Hydroxybenzotriazole, anhydrous (HOBt), has been placed on the market all over the world and is used as a peptide-coupling reagent. However, people are not often aware that this compound shows explosive properties when heated under defined confinement or when subjected to mechanical stimulus. 1-Hydroxybenzotriazole (HOBt) is able to propagate a detonation when a stronger booster is used. The most hazardous property of HOBt is the ability to propagate a deflagration very rapidly according to UN Test C.1 of the Manual of Tests and Criteria. Currently, there is the situation that this substance is mostly not classified correctly on the basis of test results and, consequently, not classified according to the principles of the UN Recommendations on the Transport of Dangerous Goods.

1-Hydroxybenzotriazole can already be found in catalogues of commercial fine chemicals mostly without any references to the above-mentioned properties.

The compound was tested at the Federal Institute for Materials Research and Testing (BAM) according to the UN test methods for explosive substances of Class 1. The data obtained are presented on the following pages (Annex 1). In the opinion of the German expert, the outcome of the tests is, that 1-Hydroxybenzotriazole, anhydrous, is doubtless a substance of Class 1.1D. It is not necessary to perform tests of Test Series 6 because the test results of test Series 1 and 2 show the high sensitivity of the substance to shock, the violent effect of heating under confinement and the ability to propagate a deflagration rapidly. In all probability, a single package test (test 6(a)) with an igniter leads to a mass explosion. The data sheet (Annex 2) gives further information necessary for classification.

2. Proposal

Considering the test results obtained (Annex 1), it is proposed to assign the substance 1-Hydroxybenzotriazole, anhydrous, to Division 1.1D.

Proper shipping name : 1-Hydroxybenzotriazole, anhydrous

Class or Division : 1.1D

UN number : xxxx

Concentration : 100 %

Subsidiary Risks : (-)

Special Provisions : (-)

Packing Method : Packing instruction 112(c).

Special packing instruction PP48:

For UN Nos. 0504 and xxxx, metal packagings shall not be used

Annex 1 (English only)**Test Report**

- 1. Name of substance** : 1-Hydroxybenzotriazole, anhydrous
- 2. General data**
- 2.1 Composition : 100 % 1-hydroxybenzotriazole, anhydrous
- 2.2 Molecular formula : C₆H₅N₃O
- 2.3 Physical form : Fine crystalline powder
- 2.4 Colour : White to light beige
- 2.5 Apparent density : 454 kg/m³, when crystalline
- 2.6 Particle size : not determined
- 3. Box 2** : 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** : Test Series 1
- 4.1 Propagation of Detonation : UN test A.1
- 4.2 Sample conditions : Ambient temperature, 425 g
- 4.3 Observations : Fragmentation into 4 pieces, no substance remains
- 4.4 Result : “+”, propagation of detonation
- 4.5 Effect of heating under confinement : Koenen test (test 1(b))
- 4.6 Sample conditions : Mass 13 g
- 4.7 Observations : Limiting diameter 10.0 mm
Fragmentation type “F” (time to reaction 12 s, duration of reaction 0 s)
- 4.8 Result : “+”, shows some explosive effects on heating under confinement
- 4.9 Effect of ignition under confinement : Time/pressure test (test 1(c)(i))
- 4.10 Sample conditions : Ambient temperature
- 4.11 Observations : Time for a pressure rise from 690 to 2070 kPa < 0.5 ms!
- 4.12 Result : “+”, propagation of deflagration
- 4.13 Exit : Go to box 4
- 5. Box 4** : Is it an explosive substance?
- 5.1 Answer from Test Series 1 : Yes
- 5.2 Exit : Go to box 5
- 6. Box 5** : Test Series 2
- 6.1 Sensitivity to shock : BAM 1“ steel tube test, standard detonator
0.6 g PETN
- 6.2 Sample conditions : Ambient temperature, mass 63.5 g

- 6.3 Observations : No fragmentation, no substance remains, deflagration
- 6.4 Result : “-“, not sensitive to shock
- 6.5 Effect of heating under confinement : Koenen test (test 2(b))
- 6.6 Sample conditions : Mass 13 g
- 6.7 Observations : Limiting diameter 10.0 mm
Fragmentation type “F” (time to reaction 12 s, duration of reaction 0 s)
- 6.8 Result : “+”, violent effect on heating under confinement
- 6.9 Effect of ignition under confinement : Time/pressure test (test 2(c)(i))
- 6.10 Sample conditions : Ambient temperature
- 6.11 Observations : Time for a pressure rise from 690 to 2070 kPa < 0.5 ms!
- 6.12 Result : “+”, propagation of deflagration
- 6.13 Exit : Go to box 6
- 7. Box 6** : Is the substance too insensitive for acceptance into Class 1?
- 7.1 Answer from Test Series 2 : No
- 7.2 Conclusion : Substance to be considered for Class 1 (box 8)
- 7.3 Exit : Go to box 9
- 8. Box 9** : Test Series 3
- 8.1 Thermal stability : 75 °C/48 hour test (test 3(c))
- 8.2 Remark : Test not performed
- 8.3 Observations : Melting point 158 °C (DSC, 5 K/min); decomposition above the melting point
- 8.4 Result : “-“, thermally stable
- 8.5 Impact sensitivity : BAM fallhammer test (test 3(a)(ii))
- 8.6 Sample conditions : as received
- 8.7 Observations : Limiting impact energy 10 J
- 8.8 Result : “-“, not too dangerous to transport in form tested
- 8.9 Friction sensitivity : BAM friction test (test 3(b)(i))
- 8.10 Sample conditions : as received
- 8.11 Observations : Limiting load > 360 N
- 8.12 Result : “-“, not too dangerous to transport in form tested
- 8.13 Exit : Go to box 10
- 9. Box 10** : Is the substance thermally stable?
- 9.1 Answer from test 3(c) : Yes
- 9.2 Exit : Go to box 11
- 10. Box 11** : Is the substance too dangerous for transport in the form in which it was tested?
- 10.1 Answer from Test Series 3 : No
- 10.2 Exit : Go to box 18

- 11. Conclusion** : PROVISIONALLY ACCEPT INTO CLASS 1
11.1 Exit : Apply the Class 1 assignment procedure

It should not be necessary to perform tests of Test Series 6 because the test results of Test Series 1 and 2 show the high sensitivity of the substance to shock, the violent effect of heating under confinement and the ability to propagate a deflagration very rapidly. In all probability, a single package test (test 6(a)) with an igniter leads to a mass explosion. Therefore, the substance 1-Hydroxybenzotriazole, anhydrous, should be a candidate of Division 1.1D.

Proposed assignment

Proper shipping name : 1-Hydroxybenzotriazole, anhydrous

Class or Division : 1.1D

UN number : xxxx

Concentration : 100 %

Subsidiary Risks : (-)

Special Provisions : (-)

Packing Method : Packing instruction 112(c).
*Special packing instruction PP48:
For UN Nos. 0504 and xxxx, metal packagings shall not be used*

Annex 2 (English only)**Figure 1****DATA SHEET TO BE SUBMITTED TO THE UNITED NATIONS
FOR NEW OR AMENDED CLASSIFICATION OF SUBSTANCES**

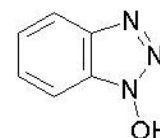
Submitted by Germany

August 2005

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 1-Hydroxybenzotriazole

1.2 Chemical formula $C_6H_5N_3O$ 

1.3 Other names/synonyms 1-Hydroxy-1H-benzotriazole; 1-Hydroxybenzotriazole anhydrous; HOBt; N-Hydroxybenzotriazole; N-Hydroxy-1,2,3-benzotriazole; 1H-Benzotriazole, 1-hydroxy-

1.4.1 UN number 1.4.2 CAS number 2592-95-2

1.5 Proposed classification for the Recommendations

1.5.1 proper shipping name (3.1.21) 1-Hydroxybenzotriazole, anhydrous (HOBt)

1.5.2 class/division 1.1 D subsidiary risk(s)
packing group

1.5.3 proposed special provisions, if any

1.5.4 proposed packing instruction(s) P112(c), PP48

Section 2. PHYSICAL PROPERTIES

2.1 Melting point or range 157-158 °C

2.2 Boiling point or range °C not applicable (n. a.)

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

- 2.3 Relative density at :
- 2.3.1 15 °C
- 2.3.2 20 °C Apparent density about 454 kg/m³
- 2.3.3 50 °C
- 2.4 Vapour pressure at :
- 2.4.1 50 °C n. a kPa
- 2.4.2 65 °C n. a kPa
- 2.5 Viscosity at 20 °C² n. a m²/s
- 2.6 Solubility in water at 20 °C < 1 mg/l
- 2.7 Physical state at 20°C (2.2.1.1¹) solid/~~liquid~~/gas²
- 2.8 Appearance at normal transport temperatures, including colour and odour
crystalline powder; white to light beige; nearly odourless
- 2.9 Other relevant physical properties
danger of deflagration and dust explosion

Section 3. FLAMMABILITY

- 3.1 Flammable vapour
- 3.1.1 Flash point (2.3.3¹) n. a °C oc/cc
- 3.1.2 Is combustion sustained? (2.3.1.3¹) ~~yes~~/no
- 3.2 Autoignition temperature °C
- 3.3 Flammability range (LEL/UEL) %
- 3.4 Is the substance a flammable solid? (2.4.2¹) ~~yes~~/no

3.4.1 If yes, give details

The substance propagates a deflagration very rapidly and shows therefore also the properties of a flammable solid but on the basis of the test results (see test report) this substance should be classified as an explosive substance of class 1

Section 4. CHEMICAL PROPERTIES

- 4.1 Does the substance require inhibition/stabilization or other treatment such as nitrogen blanket to prevent hazardous reactivity? ~~yes~~/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

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

- 4.2 Is the substance an explosive according to paragraph 2.1.1.1? (2.1¹) ~~yes/no~~
4.2.1 If yes, give details see Test Report
- 4.3 Is the substance a desensitized explosive? (2.4.2.4¹) ~~yes~~/no
4.3.1 If yes, give details
- 4.4 Is the substance a self-reactive substance? (2.4.1¹) ~~yes~~/no
If yes, state:
4.4.1 exit box of flow chart
What is the self-accelerating decomposition temperature (SADT) for a 50 kg package? °C
Is the temperature control required? (2.4.2.3.4¹) ~~yes~~/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) ~~yes~~/no
4.5.1 If yes, give details
- 4.6 Is the substance liable to self-heating? (2.4.3.1) ~~yes~~/no
4.6.1 If yes, give details
- 4.7 Is the substance an organic peroxide (2.5.11) ~~yes~~/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) ~~yes~~/no
4.8.1 If yes, give details
- 4.9 Does the substance have oxidizing properties (2.5.11) ~~yes~~/no
4.9.1 If yes, give details
- 4.10 Corrosivity (2.81) to: no data available, metal packagings should not be used
4.10.1 mild steel mm/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): > 2000 mg/kg, Animal species: rat
- 5.2 LD50, dermal (2.6.2.1.2¹): no data available mg/kg, Animal species
- 5.3 LC50, inhalation (2.6.2.1.3¹): no data available mg/litre Exposure time hours
or ml/m³ Animal species
- 5.4 Saturated vapour concentration at 20 °C (2.6.2.2.4.3¹): no data available ml/m³
- 5.5 Skin exposure (2.8¹) results: “mild” Exposure time hours/minutes 24 hours (500 mg)
Animal species rabbit
- 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)
compatible with all established extinguishing agents
- 6.1.2 Spillage cover spilled substance with water
- 6.2 Is it proposed to transport the substance in:
- 6.2.1 Bulk Containers (6.8¹) *yes/no*
- 6.2.2 Intermediate Bulk Containers (6.5¹)? *yes/no*
- 6.2.3 Portable tanks (6.7¹)? *yes/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)

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
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