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COMITÉ D'EXPERTS DU TRANSPORT DES MARCHANDISES
DANGEREUSES ET DU SYSTÈME GÉNÉRAL HARMONISÉ
DE CLASSIFICATION ET D'ÉTIQUETAGE
DES PRODUITS CHIMIQUES

Sous-Comité d'experts du transport des marchandises dangereuses

Vingt-huitième session, 28 novembre-7 décembre 2005
Point 5 de l'ordre du jour provisoire

INSCRIPTION, CLASSEMENT ET EMBALLAGE

Classement du 1-hydroxybenzotriazole, anhydre (HOBt), dans la division 1.1D

Transmis par l'expert de l'Allemagne

1. Historique et propriétés

Depuis de nombreuses années, le 1-hydroxybenzotriazole, anhydre (HOBt), est commercialisé dans le monde entier comme réactif de couplage peptidique. Or, on ignore souvent que ce composé peut exploser lors du chauffage sous confinement ou lorsqu'il est soumis à une sollicitation mécanique. Le 1-hydroxybenzotriazole (HOBt) est capable de propager une détonation lorsqu'on utilise un renforçateur plus actif. Sa propriété la plus dangereuse est sa capacité à propager une déflagration très rapidement selon l'épreuve C.1 du Manuel d'épreuves et de critères de l'ONU. Actuellement, cette matière, le plus souvent, n'est pas classée correctement sur la base des résultats d'épreuve et par conséquent n'est pas classée selon les principes des Recommandations des Nations Unies relatives au transport des marchandises dangereuses.

Le 1-hydroxybenzotriazole figure déjà dans les catalogues de produits de chimie fine des fabricants, le plus souvent sans aucune référence aux propriétés mentionnées ci-dessus.

Ce composé a été testé à l'Institut fédéral de recherche et d'essai des matériaux (BAM) où il a été soumis aux épreuves de l'ONU pour les matières explosives de la classe 1. Les résultats obtenus sont présentés ci-après (annexe 1). Pour l'expert de l'Allemagne, ces résultats montrent que le 1-hydroxybenzotriazole, anhydre, appartient sans aucun doute à la classe 1.1D. Il n'est pas nécessaire d'exécuter les épreuves de la série 6 car les résultats obtenus aux épreuves des séries 1 et 2 font apparaître la forte sensibilité de cette matière aux chocs, l'effet violent du chauffage sous confinement et son aptitude à propager rapidement une déflagration. Selon toute probabilité, l'épreuve sur un seul colis (épreuve 6 a)) avec un inflammateur provoque une explosion en masse. La formule de renseignements (annexe 2) fournit des données supplémentaires nécessaires au classement.

2. Proposition

Au vu des résultats d'épreuve (annexe 1), il est proposé d'affecter le 1-hydroxybenzotriazole, anhydre, à la division 1.1D.

Désignation officielle de transport:	1-hydroxybenzotriazole, anhydre
Classe ou division:	1.1D
Numéro ONU:	Xxxx
Concentration:	100 %
Risques subsidiaires:	(-)
Dispositions spéciales:	(-)
Méthode d'emballage:	Instruction d'emballage 112 c) <i>Disposition spéciale d'emballage PP48: Pour les numéros ONU 0504 et xxxx, on ne doit pas utiliser d'emballages métalliques.</i>

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**

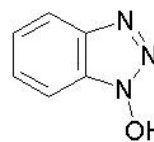
Submitted by Germany

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? (2.4.31) 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

