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On the explosive properties of 1*H*-benzotriazole and 1*H*-1,2,3-triazole

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Abstract—For 1*H*-benzotriazole, no explosive properties are observable, but the relative high exothermic decomposition energy of 1590 J/g should be kept in mind. Nevertheless, an endothermic melting barrier at 100 °C ensures safe handling at lower temperatures. For 1*H*-1,2,3-triazole, the exothermic decomposition energy is as high as 2600 J/g, but explosive properties are also not detectable. Therefore, both reagents are hazardous with regard to the exothermic decomposition potential and can be handled safely with precautions.

In a recent Letter the thermal and potential explosive properties of 1*H*-benzotriazole and 1*H*-1,2,3-triazole have been discussed on the basis of DSC, TGA and DTA measurements.[1] This was because in a former paper[2] 1*H*-benzotriazole was referred as an explosive reagent based on a report,[3] and that 1,2,3-triazole afforded better yields in Bruylants reaction than 1*H*-benzotriazole. To evaluate the thermal stability of energetic substances DSC measurements are of course well suited, but for a discussion of explosive properties additional tests should be carried out.

As BAM is the competent authority in Germany for testing, classification and assignment of substances showing explosive properties, those of 1*H*-benzotriazole[†] have been investigated. Some of the necessary test procedures to characterize explosive properties are already described in a former paper where the explosive properties of 1-hydroxybenzotriazole and some derivatives[4] have been investigated on the basis of the criteria given in the UN Recommendations on the Transport of Dangerous Goods.[5]

Differential scanning calorimetry (DSC) was used to describe the thermal behaviour of 1*H*-benzotriazole and 1*H*-1,2,3-triazole[‡] in the same way as described in an other recent paper.[6] According to the standards DIN 51007 and ASTM E 473, a positive deflection in the DSC curve corresponds to an endothermic effect, and a negative deflection corresponds to an exothermic one. The exothermic decomposition energy of 1*H*-benzotriazole as determined from our DSC measurements is 1590 J/g as shown in Figure 1. This is about 1000 J/g higher than the value reported.[1] This discrepancy may be due to the fact that our pans are made from stainless steel and, when hermetically sealed, withstanding an inner pressure as high as 15 MPa. This is obviously in contrast to the sealed aluminium pans used by Katritzky et al.[1] As no leakage was observed in our tests, disturbing effects like mass loss did not interfere with decomposition energy. Therefore, it is strongly recommended to use particularly suitable pans, which guarantee to measure the heats of decomposition effectively.

The thermal stability of 1*H*-1,2,3-triazole was investigated using DSC as well. Figure 2 shows the corresponding curve. We did not detect an endothermic peak in contrast to the work of Katritzky et al.[1] This again might be due to the fact that we use closed pressure tight stainless steel cylinders. The result of our DSC measurement

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† Merck, purity grade >99%.
‡ Aldrich, purity grade >97%.

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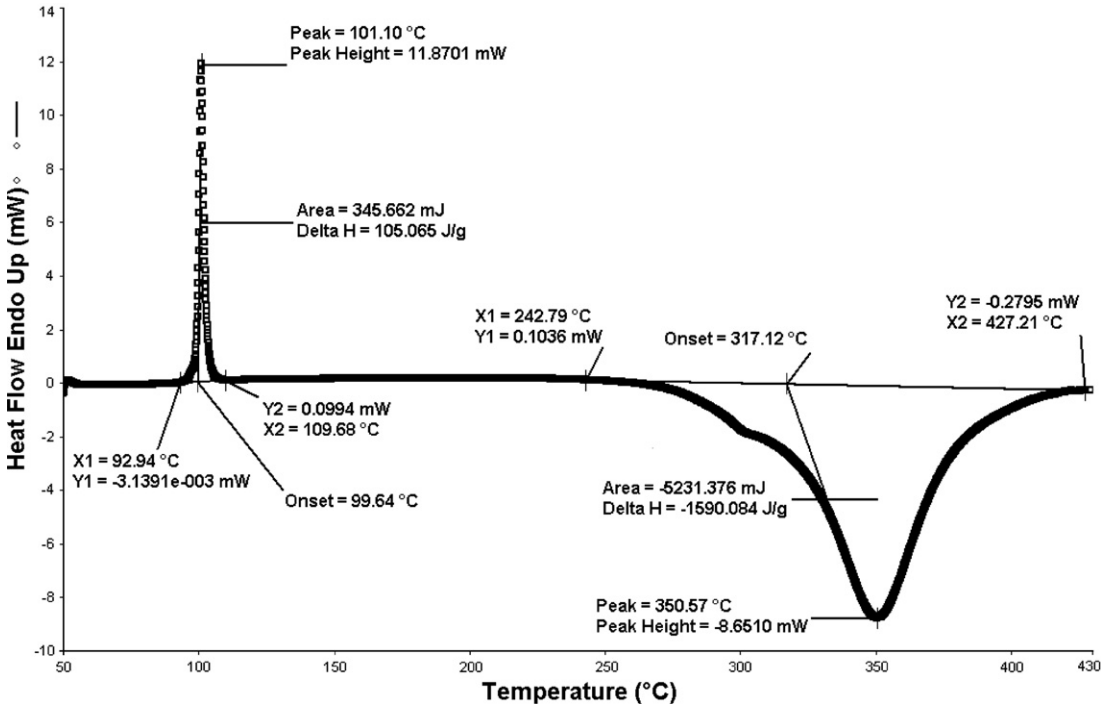

Figure 1. DSC curve for 1*H*-benzotriazole.

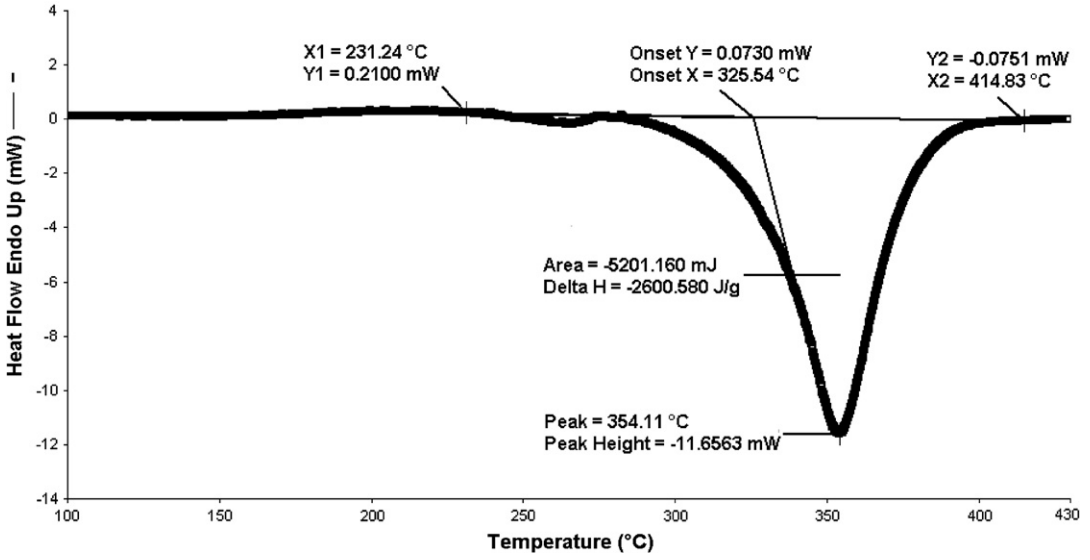

Figure 2. DSC curve for 1*H*-1,2,3-triazole.

shows a decomposition energy of 2600 J/g which is as much as 2474 J/g higher than the reported value.[1]

Due to these considerably high exothermic potentials, the question about the explosive properties of such substances has to be answered. The tests with 1*H*-benzotriazole have been performed at BAM, while the results for 1*H*-1,2,3-triazole have been reported to us.[7] The appropriate test results for 1*H*-benzotriazole and 1*H*-1,2,3-triazole are summarized in Table 1 and will be discussed here very briefly.

In the BAM 50/60 steel tube test where 560 g 1*H*-benzotriazole have been subjected to a detonating booster we did not find a propagation of the detonation at all. Thirty-six centimetres of the steel tube (50 cm) was still intact after the test and a larger amount of the substance remains non-reacted in the tube as well. Also no propagation of the detonation was found for 1*H*-1,2,3-triazole where 1118 g have been tested under equal conditions.

In the time/pressure test 1*H*-benzotriazole was not ignitable.

In the Koenen test no explosions occurred at a diameter of the orifice of 1.0 mm (type of fragmentation 'O') for both substances.

Table 1. Test data for 1*H*-benzotriazole and 1*H*-1,2,3-triazole

	UN test					
	A.1	C.1	E.1	F.3	3(a)(ii)	3(b)(i)
Test name	Detonation test (BAM 50/60 steel tube test)	Time/pressure test	Koenen test	Trauzl test	BAM Fallhammer	BAM friction apparatus
Results for 1*H*-benzotriazole	No	No ignition	No explosion (<1 mm, 'O')	No (9 ml)	>40 J	>360 N
Results for 1*H*-1,2,3-triazole[7]	No	—	No explosion (<1 mm, 'O')	—	>50 J	Not applicable to liquids

The volume of expansion in the Trauzl test was 9 ml for 1*H*-benzotriazole corresponding to a very low explosive power.

1*H*-Benzotriazole and 1*H*-1,2,3-triazole are not sensitive to drop weight impact (UN test 3(a)(ii), limiting impact energy >40 J for 1*H*-benzotriazole and >50 J for 1*H*-1,2,3-triazole) and 1*H*-benzotriazole is not sensitive to friction stimuli (UN test 3(b)(i), limiting load >360 N) as revealed by the mechanical sensitivity tests.

On basis of the above-mentioned test results and in agreement with the international accepted criteria 1*H*-benzotriazole and 1*H*-1,2,3-triazole are neither 'explosives' nor 'explosive reagents' but hazardous with regard to the exothermic decomposition potential.

Concerning the safety in synthesis and general handling the reported DSC values[1] for 1*H*-benzotriazole and 1*H*-1,2,3-triazole are not sufficiently helpful.

Acknowledgments

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