GDCh-Advisory Committee
on Existing Chemicals (BUA)

tert-Butylbenzene

BUA Report 234

(June 2001)

S. Hirzel
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on Existing Chemicals (BUA, Status June 2001)

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S. Hirzel
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Preface

The Advisory Committee on Existing Chemicals, BUA for short, was established in May 1982 to help the German federal government cope with the large task of dealing with existing chemicals. In an agreement between federal government, scientific community, and the chemical industry, it was associated with the German Chemical Society (GDCh, Gesellschaft Deutscher Chemiker) to ensure objective work, carried out in accordance with scientific principles. Since the beginning of 2001 the BUA has been composed of a new constellation of cooperating scientists from the research areas of chemistry, chemical analysis, monitoring, toxicology, primary and secondary exposition, aquatic and terrestrial toxicology as well as the fate and behaviour of compounds in water, soil, air. In addition the BUA is supported by experts within the national government agencies and the German Chemical Industry Association (VCI, Verband der Chemischen Industrie).

No other national or international body has dealt with the ecological and health-related effects of so many existing chemicals as the BUA. Upon the recommendation of the national government, since 2000, the BUA has participated as Peer-Review-Group in the pilot phase of the evaluation of ICCA-compounds (ICCA, International Council of Chemical Associations) and, in addition, acts as the national 'Contact Point' in this OECD existing chemicals program. The goal of the initiative is, on the one hand to create a more expansive database to evaluate the HPV chemicals and on the other to screen these chemicals for potential hazards.

In 1997 BUA began an additional national project, which also selects and assesses existing chemicals with a lower production volume in the range of 100 - 1000 tonnes/year. Comprehensive reports are published on chemicals suspected of having a hazardous potential. If the data available for substance assessment are insufficient, the gaps in knowledge are documented and, if necessary, investigations recommended. On the national level, the BUA has produced comprehensive reports on about 300 substances and carried out preliminary evaluation and classification (priority setting) for approximately 200 more. Publication of the process leading to priority setting, in addition to the BUA reports, lends transparency to the Committee's work.

Moreover, BUA is increasingly addressing scientific questions and problems such as "Endocrine Disruptors", selection criteria for "Persistent Organic Pollutants" (POPs), "Risk Assessment of Substances in Soils", "Evaluation Criteria for the Marine Sector" and "Safety Factors Within the Framework of Toxicological Risk Assessment". The aim of BUA is to develop assessment concepts, determine data gaps, point out the need for further research and, last but not least, also to reduce information deficits in the general population.

Weihenstephan, April 2001

Helmut Greim
BUA Chairman

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Ecological Aspect

A total of 130 tonnes of tert-butylbenzene (TBB) was produced by the chemical industry in Germany in 1999.

In manufactured mineral oil products, the following quantities can be determined for 1999: 25 500 tonnes in gasoline and 26 100 tonnes in diesel and heating oils and jet aviation fuel. TBB exports in 1999 amounted to 3390 tonnes in gasoline, 1190 tonnes in diesel and heating oils, and 280 tonnes in jet fuel. TBB imports into Germany in 1999 amounted to 6770 tonnes in gasoline, 5040 tonnes in diesel and heating oils, and 8500 tonnes in jet aviation fuel.

Environmental emissions through industrial manufacturing and processing are estimated as follows:

Through production, 2.6 tonnes enter the wastewater, 2.34 tonnes of which are stripped and incinerated with the exhaust. Of the remainder, 0.14 tonnes are emitted into the atmosphere, 0.10 tonnes into sewage sludge, and 0.02 tonnes into the hydrosphere.

For the processing to aromas (about 129 tonnes/year) a calculation according to the TGD indicates that 1.40 tonnes are emitted into the atmosphere, 1.0 tonnes into the sewage sludge, and 0.15 tonnes into the hydrosphere.

Emissions from oil production in Germany cannot be quantified, as data on crude oil deposits are missing. Emissions from refineries (which cannot be differentiated by target compartments) are estimated by the hydrocarbon emission factor and the TBB contents of the products to total about 10 tonnes for 1999.

The emissions through application (as a solvent) are estimated according to the TGD to be 1.2 tonnes, of which 1.04 tonnes are emitted into the atmosphere, 0.13 tonnes into the hydrosphere, and 0.03 tonnes into the soil.

For 1999, the following TBB emissions into the environment from mineral oil products during handling, storage, filling, and evaporation from fuel tanks and heating oil tanks, as well as through their combustion, were determined:

Emissions in t/y (1999)	Gasoline	Diesel Oil	Heating Oil	Jet Aviation Fuel
Handling and Storage	0.015	0.17	0.18	0.41
Filling	3.6	1.11	0.22	0.51
Evaporation	0.62	---	---	---
Combustion	242	0.18	3.6	1.14
Total	246.2	1.46	4.0	2.1

Additional emissions of 0.8 tonnes occur through running losses from automobiles and Otto engines.

Overall TBB emissions from gasoline, diesel oil, heating oil, and jet aviation fuel in 1999 were thus about 254 tonnes.

Total atmospheric emissions from the combustion of coal and coal products in the year 2000 are estimated at 11 tonnes; 0.8 tonnes were emitted through garbage incineration in 1994.

Emissions through the decomposition of other products (bitumen, expanded polystyrene, sunscreens) cannot be quantified.

TBB has been detected in the atmosphere: In the vicinity of London's Gatwick Airport up to 10 µg TBB/m^3 were measured in 1979. At the workplace (processing of thermoplastics) up to 120 µg TBB/m^3 were detected (1995 publication).

No data are available on the occurrence in surface waters. TBB concentrations of up to 93 µg/l (TBB and 1,2,4-trimethylbenzene combined) were detected in seepage waters below contaminated areas, a maximum of 1.1 µg/l being detected in groundwater in the USA. The 4234 µg/l detected in polluted groundwater in Milan is the sum of TBB and 1,2,4-trimethylbenzene.

TBB has also been detected in many plants and plant extracts (Siberian pine, tomato, Chinese plants incl. ginseng), animals (olive fruit fly, American white-tailed deer), and food (ham, cheese, ready-to-serve meals).

The following results on the biodegradation of TBB have been determined:

In an experimental sewage plant 0.1 ppm TBB was degraded “after a few days” to within the “lower ppb range”. With sewage sludge from a municipal sewage plant 45.7 mg TBB/l was degraded by 29 % in 28 days.

TBB in refinery water (starting concentration unknown) was degraded by natural microflora to 80 % after 23 days without aeration and completely degraded after 15 days with aeration; after inoculation with a bacterial culture (*Pseudomonas aeruginosa*) it was completely degraded after 15 days (without aeration) or 7 days (with aeration).

The metabolism of TBB was investigated in bacteria and the rainbow trout (*Oncorhynchus mykiss)*. The bacteria *Pseudomonas sp.* and *Achromobacter sp.* led to the occurrence of 2,3-dihydrodiol (as primary product), 2,3-diol, and ring cleavage products (e.g. 2,2-dimethylpropanic acid). In the bile of the rainbow trout, two monohydroxylation products were detected, as well as two diols and traces of a carboxylic acid.

A half-life of 3.5 days was found for the photochemical degradation by OH radicals.

According to a Mackay Level 1 calculation, more than 90 % is distributed in the atmosphere, 5 – 8 % in the geosphere, and less than 1 % in the hydrosphere.

The adsorption to sandy clay is weakened by even small amounts of water (0.8 %) by a factor of 3 – 4. TBB evaporates from such a soil to nearly 100 % within 16 hours. After modification by quaternary ammonium ions, stratified silicate minerals can adsorb up to 4 g TBB/kg mineral, and are suited for the adsorption of TBB, e.g. in wastewater.

Toxic threshold concentrations (EC_3) > 100 mg/l were determined in bacteria (*Pseudomonas putida*) and unicellular algae (*Scenedesmus quadricauda*). A study on ciliates gave 30.9 mg/l as the concentration at which all cells are immediately destroyed.

Acute daphniae tests gave the following results:

1) 24h LC_0 = 19 mg/l, 24h LC_{50} = 41 mg/l

2) 24h LC_0 = 20 mg/l, 24h LC_{50} = 63 mg/l (95% confidence range: 47 – 84 mg/l),
   24h LC_{100} = 75 mg/l

3) 24h EC_{50} = 11 mg/l (95% confidence range: 9 – 13 mg/l)

4) 24h EC_{50} = 1.9 mg/l, 48h EC_{50} = 2.1 mg/l.

The following results are available for the fish test with the golden orfe (*Leuciscus idus melanotus*):

1) 48h LC_0 = 8,0 mg/l, 48h LC_{50} = 9,1 mg/l, (95% confidence range: 7.9 – 11 mg/l)
   48h LC_{100} = 13 mg/l

2) 48h LC_0 = 44.0 mg/l, 48h LC_{50} = 65 mg/l,
   48h LC_{100} = 87 mg/l.

All of the above data should be viewed critically for several reasons: The effective values were determined in open systems, usually with aeration and without a solubilizer. Therefore, the actual concentration sinks rapidly to a level below the starting value. The effective concentrations determined are usually far above the water solubility and thus not valid. Where solubilizers were employed, no information is available on their concentration (MARLOWET EF) or they were used at excessively high doses (acetone; a control experiment without acetone was not performed). The above experimental results thus provide only very rough indications of the acute toxic effects of TBB.

No data are available on the effects on terrestrial organisms or ecosystems.

Toxicological Aspect

No quantitative data are available on the absorption of TBB. Due to its lipophilic nature, the compound concentrates mainly in adipose tissue, being rapidly eliminated via the kidney, however. In *in vitro* investigations on the rabbit liver, 2,2-dimethyl-phenylethanol was identified as a metabolite.

The acute toxicity of TBB is slight after oral and dermal exposure, being pronounced after inhalation exposure. In mice, an RD_{50} of 760 ml/m^3 is given for sensory irritation, but no pulmonary irritation was observed. Animal experiments on the repeated administration of TBB are not available. TBB is severely irritating to the skin and causes weak eye irritation. It does not have a sensitizing effect in animal experiments after dermal administration. No studies on pulmonary sensitization are available.

TBB is not mutagenic in *S. typhimurium* or *E. coli.* It did not induce an increased incidence of mitotic gene conversions in *Saccharomyces cerevisiae* JD1 or chromosome aberrations in RL_1 rat liver cells in a screening test. TBB does not cause increased cell transformations of SHE cells or affect the transformation rate induced by benzo[a]pyrene. Studies are not available on in vivo genotoxicity, carcinogenicity, or reproduction toxicity.

Data Gaps

Ecological Aspect

The following data are needed in order to determine TBB emissions into the environment more exactly: up-do-date, representative data on emissions through the production of fuels, the occurrence in mineral oil products, especially Otto fuels, diesel and heating oils, and jet aviation fuel, the emission behavior of diesel and jet engines, and the emission factors of brown and hard coal.

Environmental measurements are missing or incomplete on the following: polluted surface waters, groundwater in the vicinity of contaminated sites, and the atmosphere in industrial and urban areas.

The available acute tests on aquatic organisms were determined by unsuitable methods. Valid tests are missing on bacteria, algae, daphniae, and fish in systems in which TBB is not eliminated by either photolysis (with the exception of algae) or evaporation. Particularly those endpoints lying above the water solubility should be examined critically. Data are missing on the toxicity to terrestrial organisms.

Toxicological Aspect

Data gaps still exist with respect to the toxicity after repeated administration to determine the target organs and NOEL, on the reproduction toxicity, the clastogenicity in vitro (only a screening test is available), the genotoxicity in vivo, and carcinogenicity.

The product database of the BgVV does not mention emissions from consumer products. Due to the known deficiencies of this database (not all consumer products are included) consumer exposure cannot be ruled out. Widespread environmental and consumer exposure exists in the automobile and fuel sector, however.

While no measurements are available on workplace exposure, TBB is produced in a closed system according to the German manufacturer (Degussa-Hüls AG 2000). In filling areas, contact with TBB must be avoided by safety measures (the wearing of breathing masks, protective goggles/face masks, hand savers and protective clothing).