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MEMORANDUM

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DATE: October 27, 2000

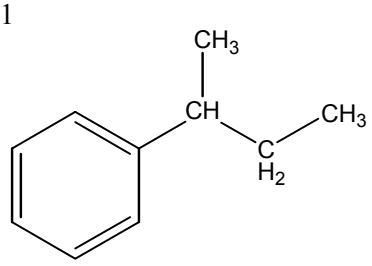
SUBJECT: PROPOSED ACTION LEVELS FOR SEC-BUTYLBENZENE AND TERT-BUTYLBENZENE

Staff of the Office of Environmental Health Hazard Assessment (OEHHA) have reviewed your Department's proposed action levels of 80 µg/L for sec-butylbenzene and tert-butylbenzene. OEHHA recommends action levels of 260 µg/L for sec-butylbenzene and tert-butylbenzene. The toxicological basis is the same, except for the use of an uncertainty factor of three (3) instead of ten (10) for the subchronic to chronic toxicity study extrapolation.

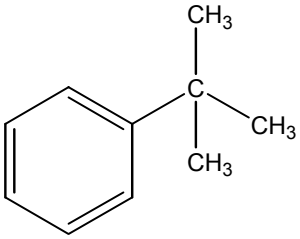
Sec-butylbenzene and tert-butylbenzene (Figure 1) are flammable liquids used in United States commerce for synthetic organic chemistry, as solvents, and tert-butylbenzene is used as a polymer linking agent. Sec-butylbenzene is a component of crude oil (Wang and Fingas, 1995), vehicle emissions (Schroder and Dannecker, 1994; Sigsby et al., 1987), ambient air (Juttner, 1986), and is a possible migrant from microwave heating of thermoset polyester plastics (Gramshaw et al., 1995). Tert-butylbenzene has been identified in landfill gas (Eklund

et al., 1998). Both compounds are on the U.S. Environmental Protection Agency (U.S. EPA) Method 524.2 analyte list for monitoring in groundwater, surface water, and drinking water and, in California, are considered unregulated chemicals requiring monitoring (Title 22, California Code of Regulations §64450).

Figure 1



sec-butylbenzene



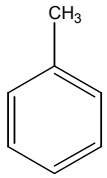
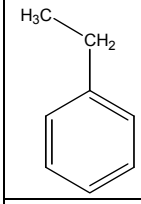
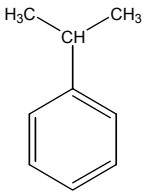
tert-butylbenzene

The routes of exposure to sec-butylbenzene and tert-butylbenzene are ingestion, inhalation, and dermal. These chemicals are known to cause eye and skin irritation, can cause irritation to mucous membranes, and are considered aspiration hazards to the lung. However, their prevalence in the environment is apparently rare, with only one detection of tert-butylbenzene in California water supplies among 9635 tests and no detections of sec-butylbenzene in 9637 tests (California Department of Health Services, 2000). This compilation covered the years 1984-1998. On the other hand, Wisconsin detected sec-butylbenzene 110 times out of 2207 tests of wells (January-December 1997), with a high measurement of 60 µg/L. They also found 66 occurrences of tert-butylbenzene out of 2168 tests, with a high value of 9 µg/L (Wisconsin Department of Natural Resources, 2000).

The toxicology of these isomers has not been thoroughly characterized. Acute oral data have been reported. Eight out of ten rats died after administration of approximately 4.3 g/kg sec-butylbenzene and 7/10 died after the same dose of tert-butylbenzene in olive oil (Gerarde, 1959). Dow Chemical (1954) reported that no deaths occurred among four rats treated orally with 2 g/kg sec-butylbenzene and Sandmeyer (1981) reported an LD_{50} of 2.24 g/kg for this isomer. LD_{50}s in rats for tert-butylbenzene ranged from 2.5 to 5.0 g/kg (U.S. EPA, 1997). These oral toxicity data indicate low acute oral toxicity but are inadequate to derive a no-adverse-effect-level (NOAEL) for either sec-butylbenzene or tert-butylbenzene for long-term exposures.

The U.S. EPA National Center for Environmental Assessment (NCEA) has recommended that a provisional reference dose (RfD) for these compounds be derived from the toxicity data for a closely-related branched-chain alkylbenzene, cumene (isopropylbenzene). NCEA states that

"confidence in this provisional RfD is very low, reflecting low confidence in the RfD for cumene and the lack of suitable data for the branched-chain butylbenzenes"(U.S. EPA, 1997). Confidence can be enhanced somewhat by comparing cumene toxicity with other saturated short-chain alkylbenzenes which are structurally similar. These are summarized below:

Chemical	Critical Effect	NOAEL (mg/kg-day)	LOAEL (mg/kg-day)
Toluene 	Increased liver and kidney weights in rats	223	446
Ethylbenzene 	Histological alterations in the liver and kidneys of rats	97	291
Cumene 	Increased kidney weight in rats	110	331

(Adapted from U.S. EPA, 1997)

Cumene (isopropylbenzene) has a dose-schedule-adjusted NOAEL of 110 mg/kg-day based on 139 gavage doses to female rats in a 194-day period (Wolf et al., 1956). Other data on cumene and similar alkylbenzenes support this as an approximate NOAEL for the chemicals. OEHHA therefore agrees that this NOAEL is appropriate to be used for sec-butylbenzene and tert-butylbenzene. However, the lack of specific data justifies a large uncertainty factor. An uncertainty factor of 3,000 is recommended (three for subchronic to chronic extrapolation, ten for interspecies extrapolation, ten for human variability, and ten for database deficiencies).

A public health protective concentration (C) for sec-butylbenzene and tert-butylbenzene in drinking water can be derived from the equation:

$$C = \frac{NOAEL \times BW \times RSC}{UF \times DWC} = \frac{(110\ mg/kg\text{-}day)(70\ kg)(0.2)}{(3{,}000)(2\ L/day)} = 0.257\ mg/L \cong 260\ \mu g/L$$

where:

NOAEL = no-observed-adverse-effect-level,
BW = body weight (adult),
RSC = relative source contribution,
UF = uncertainty factor, and
DWC = drinking water consumption (adult).

Based on the health protective concentration calculated, OEHHA recommends and supports an action level of 260 ppb (µg/L) for sec-butylbenzene and an action level of 260 ppb (µg/L) for tert-butylbenzene in drinking water.

Should you have any questions about this review, please contact me at (510) 622-3168 or Dr. Robert Haas at (510) 622-3172.

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