SUMMARY OF DATA FOR CHEMICAL SELECTION

Undecane
1120-21-4

BASIS OF NOMINATION TO THE NTP

Undecane is brought to the attention of the Chemical Selection Working Group as an environmental pollutant with widespread human exposure but limited toxicological information.

Undecane was selected from a group of hydrocarbons found in fuels and solvents, but it is also a ubiquitous air pollutant in outdoor and indoor environments, and in water. The National Institute for Occupational Safety and Health (NIOSH) estimated that approximately 1,129 workers are exposed to undecane based on a 1980s survey. However, its main uses as a solvent and as a component of diesel fuels and kerosene do not appear to be reflected in the NIOSH survey.

No adequate 2-year carcinogenicity study of undecane was found in the available literature. Undecane was a tumor promoter in the classical skin tumor promotion model using benzo[a]pyrene as the initiator. In *in vitro* studies, undecane was not mutagenic in *Salmonella typhimurium*.

Undecane may have a considerable human toxicological impact since it is found in many situations where proven carcinogenic hydrocarbons such as fuel combustion products or cigarette smoke are also present.

INPUT FROM GOVERNMENT AGENCIES/INDUSTRY

According to the NTP reviewers of the summary sheets on decane and undecane, a draft report (TR-519) of a 2-year carcinogenicity study of Stoddard solvent is tentatively scheduled for peer review in May 2003. Male Fischer 344 rats inhaled Stoddard solvent at doses of 0, 188, 550, or 1100 mg/m^3 and female Fischer 344 rats and male and female B6C3F$_1$ mice were exposed at 0, 550, 1100, or 2200 mg/m^3. Stoddard solvent is a widely used chemical mixture, with production in 1990 exceeding 38 million pounds. Stoddard solvent contains hydrocarbons ranging from C7 to C12, with the majority in the C9 to C11 range. The hydrocarbons are 30-50% alkanes, 30-

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40% cycloalkanes, and 10-20% aromatics. Both decane and undecane are present in Stoddard Solvent. Although Stoddard solvent was negative in the micronucleus assay, pathologic studies on the mice have been completed. These studies indicate treatment-related effects in the liver in both sexes of mice. The pathologic results in the rats were not available for the CSWG's evaluation.

SELECTION STATUS: Selected
ACTION BY CSWG: 12/17/02
Studies Requested:
Carcinogenicity
Priority: High
Rationale/Remarks:

- Consider nomination with decane and select one of these chemicals for testing.
- Consider also testing in an initiation/promotion protocol.
- Test pure compound rather than a complex mixture of alkanes.
- Ubiquitous air pollutant with widespread human exposure.
- Some evidence that this class of chemicals act as tumor promoters.
- HPV chemical; industry is sponsoring a mixture of alkanes

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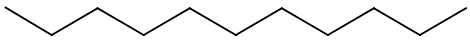
CHEMICAL IDENTIFICATION

CAS Registry No.:1120-21-4

Synonyms:Hendecane, *n*-undecane, alkane C_{11} (ChemID, 2002; Lide, 2000; Sigma-Aldrich, 2002a)

Structure, Molecular Formula, and Molecular Weight:



$C_{11}H_{24}$ Mol. wt: 156.31

Structural Class: Aliphatic alkane

Chemical and Physical Properties:

Description: Colorless liquid (Lewis, 2002; Verschueren, 2001)

Melting Point: 25.5 °C (Lide, 2002)

Boiling Point: 195.9 °C (Lide, 2002)

Flash Point: 65 °C (Lewis, 2002)

Solubility: Sol. in ethyl alcohol and ethyl ether, insol. in water (Lide, 2002)

Density: 0.74 g/mL at 20 °C (Lide, 2002)

Reactivity: Combustible (NTP, 2001); combustion products include CO and CO_2; incompatible with bases, oxidizing agents, and reducing agents (Sigma-Aldrich, 2002b)

Technical Products and Impurities: Undecane (≥99.8%, 99%, 99+%, or ≥97.0%) is available from Sigma-Aldrich (Sigma-Aldrich, 2002a).

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EXPOSURE INFORMATION

Production and Producers:

Manufacturing Processes: Petroleum is the most abundant source of saturated hydrocarbons. Petroleum is separated into individual fractions by distillation in a refinery; these fractions can be processed further to obtain many organic chemicals. N-Alkanes having more than six carbons, such as undecane, are not fractionated individually but as mixtures of several homologues. These mixtures are isolated in high isomeric purity from higher boiling petroleum, gas-oil, and wax distillate fractions by selective separation techniques, such as molecular sieve separation or urea extractive crystallization (Griesbaum *et al.*, 1989; HSDB, 2002).

Before natural gas and petroleum became essential raw materials for organic chemicals, the most important source of saturated hydrocarbons was coal. Coal liquefaction provided the greatest variety of saturated hydrocarbons, the Fischer-Tropsch synthesis producing alkanes in the range of C_1 to C_{30} or higher (Griesbaum *et al.*, 1989).

Production/Import Level: Undecane is listed in the US Environmental Protection Agency's (EPA's) Toxic Substances Control Act (TSCA) Inventory (ChemID, 2002).

Undecane is a high production volume (HPV) chemical with production exceeding 1 million pounds annually in the US. It has no sponsor in the HPV Challenge Program (EPA, 2002).

Producers and Importers: According to Chemical Sources International, there are 18 US suppliers of undecane (Chemical Sources International, 2002).

Undecane is currently manufactured or distributed by Alfa Aesar/Johnson Matthey; Dow Chemical Company; Roper Thermals; and Spectrum Chemical Manufacturing Corporation (Chemcyclopedia, 2002; Hunter, 2002; Tilton, 2001).

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Use Pattern: Undecane is a constituent of diesel oil and kerosene (Verschueren, 2001). Major uses include:

- jet-fuel and petroleum research
- distillation chaser
- chemical intermediate in the manufacture of chlorinated paraffins, linear alkylbenzenes, primary detergent alcohols, C_{11}-C_{14} paraffins, olefins, and sulfonates
- feedstock for citric acid production by fermentation
- solvent, especially for printing inks and degreasing applications (HSDB, 2002; Lewis, 2002).

Undecane was listed as a synthetic flavoring agent in a Japanese report (Yoo, 1986).

Undecane is also found in several widely used petroleum distillates, such as Stoddard solvent and jet fuel. Undecane represents 2.7-17.5 % of white spirits, a mixture of saturated aliphatic and alicyclic, and alkyl aromatic C_7-C_{12} hydrocarbons. Stoddard solvent, a form of white spirit, is a mixture containing 30-50% linear and branched alkanes (ATSDR, 1995a; World Health Organization, 1996). The source used to prepare JP-4 jet fuel apparently affects the amount of decane present. Undecane was found at a percentage of 16.62 or 4.17 in JP-4 fuel when the source was shale or petroleum, respectively (Irwin, 1997).

In 1985, the US consumption of aliphatic hydrocarbon-based solvents in the paint industry was 433,000 tons. The annual sale of white spirits in the US was 717,000 tons in 1985 (World Health Organization, 1996).

Human Exposure:

Occupational Exposure: The National Occupational Exposure Survey (NOES), which was conducted by the National Institute for Occupational Safety and Health (NIOSH) between 1981 and 1983, estimated that 1,129 workers in 51 facilities were potentially exposed to undecane in the workplace (Sigma-Aldrich, 2002). The NOES database does not contain information on the frequency, level, or duration of exposure to

workers of any chemical listed therein. Apparently the NOES survey does not address the presence of undecane in other solvents since NOES estimates, for example, that 1,922,235 employees in 142,653 facilities are exposed to Stoddard solvent (RTECS, 2000).

Exposure to undecane has been documented in a wide variety of occupational settings.

In a 1996 report, the possibility that the exposure of office workers to 0.3 ppb of undecane was associated with the use of carbonless copy paper was raised (NIOSH, 2000). Undecane was released from an idle photocopy machine and from a printing photocopy machine at a rate of 36 and 2,000 µg/hour (HSDB, 2002).

Undecane concentrations in the vulcanization area of a shoe-sole factory ranged from 1-170 $\mu g/m^3$. The observed undecane levels were probably due to the use of raw materials, curing temperatures, and high production rates (Cocheo *et al.*, 1983).

Workers employed in drilling operations that use low-aromatic oil-based drilling fluids may be exposed to undecane as these oils contain aliphatic hydrocarbons in the range of C_9-C_{15} (Eide, 1990).

Individuals working with jet fuel used in commercial or military aircrafts may be exposed to undecane since it is a prevalent component of these kerosene-based fuels (Riviere *et al.*, 1999).

Undecane was detected in gas samples emitted during the germination phase in malting and beer manufacture using a pilot-scale brewery (Gibson *et al.*, 1995).

Environmental Exposure: The general population is exposed to undecane via inhalation of ambient air, ingestion of food and drinking water, and dermal contact with products containing undecane (HSDB, 2002).

Undecane was detected in the breast milk of 7 of 12 samples from mothers living in four US urban areas. It was also identified in the breath and personal air samples collected from 50 individuals living in Los Angeles, California (HSDB, 2002).

Consumer Exposure: Undecane is found in pesticides, waxes and cleansers, building materials, adhesives, and paints used by consumers (Wallace *et al.*, 1985).

Undecane was detected in the interior of new cars as a component of volatile organic compounds (VOCs). A car that was on the market for 3 weeks had undecane concentrations of 870 $\mu g/m^3$. After 9 weeks, undecane levels decreased to 310 $\mu g/m^3$. VOC concentrations in new car interiors decreased approximately 20% per week (Brown & Cheng, 2000).

Dry cleaning solvents that remain on clothing are a source of undecane exposure. The total amount of undecane that evaporated from a pair of trousers was 1.09 mg in 5 days after dry cleaning. The undecane level on the fifth day was 32% of the first day's concentration and it was determined that the half time of undecane on this article of clothing was 2.7 days (Tashiro *et al.*, 1999).

Undecane was identified as a volatile component of peanut oil (heated between 150 and 200 °C), cheese, fried bacon, fried chicken, and raw beef (HSDB, 2002). It was also detected in coupons from food packages, contributing an off-flavor to foods such as breakfast cereals (Reineccius, 1991).

Undecane was detected in extracts of the plant species *Hypericum perforatum* (St. Johns wort) (European Commission, 2002), a popular dietary supplement used to treat mild to moderate depression.

The general population is also exposed to undecane through the inhalation of vapors from paints and lacquers containing white spirits (World Health Organization, 1996).

Environmental Occurrence: Undecane is found in crude oil, a naturally occurring substance found trapped among sedimentary rocks below the earth's surface (Chevron, 2002; NETLAB, 1997).

Air Pollution: Undecane has been detected among VOCs in several studies analyzing indoor air quality.

- Undecane was one of the most frequently reported chemicals in indoor air as mentioned in a review of the literature from 1979 to 1990 (Samfield, 1992).

- An EPA study of seven volunteers who performed 25 common activities found that painting and removing paint for 4 hours resulted in exposure to undecane at a concentration of 150 $\mu g/m^3$. A home where paint, solvents, paint thinners, kerosene, gasoline, and pesticides were stored had undecane levels as high as 290 $\mu g/m^3$ (Wallace *et al.*, 1989).

- In a Finnish study, the concentrations of 48 VOCs, including undecane, exceeded normal levels more often in sick houses than in normal houses. Sick houses were defined as dwellings in which inhabitants show symptoms such as headache, nausea, irritation of the eyes, and general malaise, among others (Kostiainen, 1995).

- Indoor concentrations of *n*-alkanes (C_8-C_{11}) and other organic solvents were significantly elevated in newly painted Swedish dwellings. *n*-Alkanes were emitted from both solvent- and water-based paints, the emissions being 100 times higher with solvent-based paints (Wieslander *et al*.,1997).

- Undecane was identified in 2 of 7 samples of household waste headspace at a concentration of 0.1-1 mg/m^3 in a Danish study (Wilkins, 1994).

- Undecane was detected in smoking and nonsmoking households or workplaces. The highest concentration of undecane, found in workplaces that allowed smoking, was a maximum value of 155 $\mu g/m^3$ (Heavner *et al.*, 1996).

- Indoor samples taken from 49 Columbus, Ohio homes in 1991 showed an average concentration of undecane in nonsmoking and smoking households of 3.86 and 14.5 $\mu g/m^3$, respectively (HSDB, 2002).

- Undecane concentrations ranged from 48.3 to 115.6 $\mu g/m^3$ in air samples collected in a new building during 1987-1988. A separate study reported concentrations of undecane between 5.5 and 14 $\mu g/m^3$ during a 1987-1988 sampling period, 2 to 3 years after the facility opened (HSDB, 2002).

- According to a 1987 EPA report, glued carpets, wallpapers, and cleaning agents and pesticides emit undecane. The highest concentration measured was for painted sheetrock with a value of 228 µg/m^3 (Wallace *et al.*, 1987). Undecane has also been detected after carpet installation, during application of acrylic floor wax, and during renovation (Chang & Guo, 1992; Shields & Weschler, 1990; Tharr, 1996).

- The indoor concentration of undecane in Dutch homes, 3-9 μg/m^3 (1981-1983) was dependent on their construction date (pre-war-<6 yrs old). Outdoor air concentrations were 0.4 μg/m^3 (median) with a maximum of 3 μg/m^3 (Verscheuren, 2001).

- The mean annual undecane concentration inside British homes was 14 µg/m^3 (MRC Institute for Environment and Health, 2000).

- In a 1983-1984 Italian study, the indoor and outdoor mean concentration of undecane was 80 and <2 μg/m^3, respectively (Verscheuren, 2001).

Undecane has been measured in the atmosphere of several US and European cities. Undecane was detected in roadway air, airfield air, and aircraft air in concentrations of 0.242, 1.7, and 4.89 ppb, respectively. The mean concentration of undecane in the Caldecott Tunnel (San Francisco, California) was 2.43 ppb (HSDB, 2002).

Undecane emissions from gasoline- and diesel-fueled cars passing through the Tuscarora Mountain Tunnel on the Pennsylvania Turnpike were 0.58 mg/mi and 4.27 mg/mi, respectively (Gertler *et al.*, 2002). Undecane emissions from light-duty gasoline vehicles were calculated to be 428 tons per year in a 1994 study conducted in Washington State (Brady *et al.*, 1998).

Soil Accumulation: In a 1986 study, hydrocarbon characterization of soils containing spilled crude oil (>3 yr) showed the presence of *n*-alkanes, including undecane, in some soil samples. The abundance of *n*-alkanes decreased in contaminated soils because of biological transformation and volatilization (Saterbak *et al*., 1998).

Water Pollution: Undecane was detected in groundwater at 0.22-0.70 µg/L according to a 1980 US study. It has also been identified in US drinking water and in water samples from European rivers, lakes, and marine coastal waters. The concentration of undecane in surface water at an offshore oil production operation in the Gulf of Mexico was 310

μg/L (HSDB, 2002).

Industrial wastewater generated from publicly owned treatment facilities contained undecane in concentrations from 10 to 15 ppb (HSDB, 2002).

Undecane was one of over 300 compounds detected in neutral extracts of 24-hr composite samples from petroleum refinery wastewaters in a 1978 study (Burks, 1982).

Biodegradation and Ecotoxicity: Undecane can be degraded by naturally occurring marine microorganisms within 20 days when present in diesel oil. Anaerobic biodegradation can occur under methanogenic conditions (Verscheuren, 2001).

The EC_{50} in methanogens was 0.61 mg/L (Verscheuren, 2001). Undecane also inhibited bacterial spore germination on certain growth media (Cavender, 1994).

Regulatory Status: No standards or guidelines have been set by NIOSH or OSHA for occupational exposure to or workplace allowable levels of undecane. Undecane was not on the American Conference of Governmental Industrial Hygienists (ACGIH) list of compounds for which recommendations for a Threshold Limit Value (TLV) or Biological Exposure Index (BEI) are made.

EVIDENCE FOR POSSIBLE CARCINOGENIC ACTIVITY

Human Data: No epidemiological studies or case reports investigating the specific association of exposure to undecane and cancer risk in humans were identified in the available literature.

An epidemiological study of chronic workplace exposure to white spirits reported an odds ratio >1 for prostate cancer, Hodgkin's lymphoma, and squamous cell carcinoma of the lung. In addition, several epidemiological studies have shown increased risks of respiratory, pancreatic, kidney, and lung cancer in workers exposed mostly to white spirits. None of the studies mentioned above demonstrated a causal association between cancer and exposure to white spirits (ATSDR, 1995a; World Health Organization, 1996). The role of undecane, if any, was not examined.

Undecane, in solutions as strong as 30%, produced no skin irritation in human subjects when applied for 24 hours (Criteria Group for Occupational Standards, 1983).

Animal Data:

Acute Studies: The LC_{50} for undecane is reported to be >442 ppm/8hr in rats (Sigma-Aldrich, 2002b).

Undecane (0.05 ml) produced only mild irritation in the rabbit skin irritation test (Criteria Group for Occupational Standards, 1983).

Chronic/Carcinogenicity Studies: No 2-year carcinogenicity studies of undecane were identified in the available literature.

Undecane was shown to have tumor promoting activity. In a 1976 study, undecane (25 mg) and benzo[a]pyrene (BP) (5 μg) applied to the skin of female ICR/Ha Swiss mice, 3/wk for 440 days, induced papillomas in 41 of 50 animals. BP alone induced tumors in 12 of 50 animals in the same time, while undecane alone did not produce tumors (Van Duuren & Goldschmidt, 1976).

Several studies that examined the potential carcinogenicity of JP-4 jet fuel have been conducted. No increase in the incidence of tumors was found in rats and mice one year after 8 months of inhalation exposure to JP-4 fuel. In a 1993 study, F344 rats exposed to JP-4 at 5,000 mg/m^3 for 12 months had an increase of interstitial cell tumors in the testis 12 months after the termination of the exposure. However, mice exposed to the same regimen did not show an increase in the incidence of neoplastic lesions. Dermal administration of JP-4 jet fuel (25 mg, 3/wk for 105 wk) increased the incidence of squamous cell carcinomas and fibrosarcomas in mice exposed to shale-derived JP-4 (50% incidence), and in animals exposed to petroleum-derived JP-4 (26% incidence) compared to the appropriate controls (2% and 0%, respectively) (ATSDR, 1995b). The relevance of these studies to undecane has not been determined.

Short-Term Tests: Undecane was not mutagenic when tested in *Salmonella typhimurium* strains TA98, TA100, UTH8413, and UTH8414 at concentrations up to 2,000 μg/plate. Mutagenicity was not enhanced by rodent liver S-9 (Connor *et al.*, 1985). Undecane was negative in the rec-assay with *Bacillus subtilis* strains M45 (rec^-) and H17 (rec^+) (Yoo, 1986).

Undecane did not induce *in vitro* transformation of Syrian hamster embryo cells or Balb/3T3 mouse embryo fibroblasts. Neither did it enhance co-transformation when added with BP in both cell systems. Undecane also had no effect on intercellular communication in a monolayer of Syrian hamster embryo cells (Atchison *et al.*, 1985).

Metabolism:

Absorption and Distribution: Inhaled undecane is rapidly distributed from the blood to different organs and tissues, especially those with high lipid content. The concentrations of undecane in the brains and blood of rats exposed at 100 ppm, 12 hr/day for 3 days were 47.7 and 13.7 μmol/kg (Eide, 1990).

Aliphatic Hydroxylation: This process involves insertion of oxygen into a C-H bond.

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Cleavage of the C-H bond by hydrogen abstraction is the rate-limiting step. In the case of simple, straight chain hydrocarbons, such as undecane, aliphatic hydroxylation occurs at both the terminal methyl groups and the internal methylene groups (Parkison, 1996).

Undecane may also directly affect P-450 enzyme activity. Undecane caused reduced recovery of products of liver and lung 7-ethoxycoumarin deethylase and of lung benzo[*a*]pyrene hydroxylase activities in microsome preparations from Sprague-Dawley rats. However, it did not reduce NADPH formation and did not affect P-450 reductase activity when the enzyme was assayed with the substrate, cytochrome *c* (Rabovsky *et al.*, 1986).

Other Biological Effects:

Cellular Damage: In an *in vitro* study, undecane induced the production of interleukin 8, a proinflammatory cytokine, in normal human epidermal keratinocytes (NHEK) (Allen *et al.*, 2001).

Neurological Alterations from Products Containing Undecane: Undecane may be linked to the development of neurological impairment associated with acute exposure to a high level of JP-4 jet fuel (ATSDR, 1995b). Minor neurological effects (dizziness, changes in simple reaction time, and visual-motor coordination) have also been reported in humans from short-term exposure to Stoddard solvent. Similarly, minor neurobehavioral changes were seen in subjects exposed to other white spirits (World Health Organization, 1996). More severe neurological changes were described from chronic exposure to Stoddard solvent, white spirits, and other similar solvents; although a cause-effect relationship could not be established (ATSDR, 1995a).

Several inhalation studies in rats involving various types of white spirits described minor behavioral changes and some neurochemical effects. Dearomatized white spirits (mostly alkanes) induced alterations in sensory-evoked potentials in rats

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(ATSDR, 1995a; World Health Organization, 1996).

Kidney Toxicity from Products Containing Undecane: Animals exposed to vaporized white spirits and Stoddard solvent did not have kidney pathology (ATSDR, 1995a). In contrast, a C_{10}-C_{11} solvent fraction (mainly aliphatic) and JP-4 jet fuel caused the type of renal damage in male rats generally associated with the binding of xenobiotic compounds to α_{2u}-globulin (ATSDR, 1995a; World Health Organization, 1996).

Male Sprague-Dawley rats exposed to a white-spirit-like solvent (99% C_{10}-C_{12} aliphatics) showed a significant decrease in urine osmolality after 9.5 months of exposure. Increased activity of urinary lactate dehydrogenase was further noted as an indication of distal tubular dysfunction (Viau *et al*., 1984).

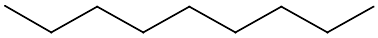
Several human studies showed no association between exposure to Stoddard solvents and kidney dysfunction. However, the studies lacked sufficient exposure data to draw firm conclusions. A man who was exposed to Stoddard solvent by direct dermal contact and inhalation for 1 year developed glomerulonephritis (ATSDR, 1995a).

Hemapoietic System Effects from Stoddard Solvent: Studies of humans with aplastic anemia who were also exposed to Stoddard solvent have been reported, although a causal relationship was not established (ATSDR, 1995a).

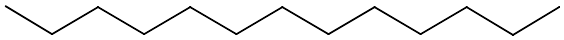
Liver and White Spirits: Studies on humans exposed to white spirits and other chemicals in the workplace reported no histopathological changes in liver biopsies, however, some hepatic enzymes had elevated serum levels (ATSDR, 1995a).

Structure-Activity Relationships: *N*-alkanes are thought to modulate carcinogenesis, especially because of their ubiquitous distribution and their tumor-promoting activity (Baxter *et al*., 1981). Nonane [111-84-2] and tridecane [629-50-5], two hydrocarbons structurally related to undecane, were selected for review.

Nonane



Tridecane



No carcinogenicity bioassays conducted by modern regulatory standards are available for these compounds.

Nonane is a CNS depressant and a primary skin irritant. Chronic inhalation of nonane may cause altered neutrophils but no pulmonary lesions or axonopathies were noted (Cavender, 1994). Nonane was not mutagenic when tested in *Salmonella typhimurium* TA97, TA98, TA100, TA1535, and TA1537 with or without S-9 (CCRIS, 2002b).

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