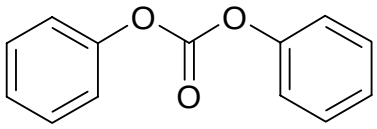
SIDS INITIAL ASSESSMENT PROFILE

CAS No.	102-09-0
Chemical Name	Diphenyl carbonate
Structural Formula	

SUMMARY CONCLUSIONS OF THE SIAR

Human Health

The acute dermal toxicity of diphenyl carbonate is relatively low with LD_{50} values exceeding 2000 mg/kg bw in rats and rabbits (no clinical signs noted). The acute oral LD_{50} in rats was 1500 mg/kg bw, with clonic convulsions as main clinical sign appearing at doses near to or exceeding the LD_{50} value. There are no acute inhalation studies available.

Diphenyl carbonate was not irritating to the skin and eye of rabbits (OECD TG 404, 405). Diphenyl carbonate showed no skin sensitisation potential in a Buehler patch test on 10 guinea pigs, limited by the small number of treated animals.

Repeated oral dosing of rats with diphenyl carbonate over 11 weeks (males) or 18 weeks (females) led to increases in liver weight and to hepatocellular hypertrophy and histopathological changes in the adrenals in males at a dietary concentration of 5000 ppm (about 427 mg/kg bw/day), and in females of 1500 ppm (about 219 mg/kg bw/day). At 1500 ppm, females exhibited also morphological changes in the ovaries (increased number and mononuclear infiltration of corpora lutea, granulated luteal cells, hypertrophic ovarian interstitial cells). The NOAEL in males was 1500 ppm (about 132 mg/kg bw/day) and in females about 50 mg/kg bw/day.

Diphenyl carbonate showed no mutagenic properties in bacterial and mammalian cell gene mutation assays performed according to current guidelines. In the *in vitro* chromosome aberration assay diphenyl carbonate led to increased frequencies of structural chromosomal aberrations in V79 cells both in the absence and in the presence of metabolic activation. This positive result could not be confirmed *in vivo* by two mouse bone marrow micronucleus assays performed according to current guidelines and with evidence of target cell exposure. An *in vivo/in vitro* UDS assay on rat liver, also performed according to current guidelines with oral doses up to the MTD, gave negative results. It is concluded that the genotoxic properties observed *in vitro* are not expressed *in vivo.*

In repeated dose toxicity studies on rats, diphenyl carbonate led to increased organ weights and morphological alterations in adrenals and ovaries. These effects did not influence reproductive performance in a one-generation dietary study on rats (OECD TG 415/416; NOAEL for fertility: 15 000 ppm = about 1561/2432 mg/kg bw/day for males/females; highest tested dose).

In a developmental toxicity study on rats according to OECD TG 414, daily gavage administration of 750 mg diphenyl carbonate/kg bw/day to pregnant rats on gestation days 6 to 19, led to severe maternal toxicity (mortality, convulsions, piloerection, body weight loss). Fetuses of this dose group showed reduced body weights and increased incidences of unspecific malformations (mainly dysplastic forelimb bones). The NOAEL for maternal toxicity and developmental toxicity of diphenyl carbonate in rats was 50 mg/kg bw/day. At 200 mg/kg bw/day slight maternal toxicity occurred and a retarding effect on fetal skeletal ossification of toes and cervical vertebral bodies could not be

completely excluded.

Environment

Diphenyl carbonate is a white solid (flakes) with a melting point of 78.8 °C, and a boiling point of 302 °C. The density of the solid is 1.272 g/cm^3 at 14 °C. The vapour pressure is 0.014 Pa at 20 °C. The log K_{ow} is 3.21 - 3.28. The solubility of the substance in water is ca. 13 mg/l at 20 °C. The flash point is 168 °C.

Diphenyl carbonate hydrolyses under environmental conditions forming phenol and carbon dioxide. A study on the abiotic degradation of diphenyl carbonate in water predicted that the test substance has a $t_{1/2}$ of 39.9 h at pH 7 and 25 °C.

According to a Mackay Level I calculation the favourite target compartment of the substance is water with 72.2 % (soil 11 %, sediment 11 % and air 6 %). Henry's law constants of 8.59 Pa × m^3 mol^{-1} (calculated according to the Bond method) and 0.23 Pa × m^3 mol^{-1} respectively (derived from water solubility and vapour pressure) indicate that the compound has a slight to moderate potential for volatilization from surface waters. These results should only be considered of theoretical interest since the calculation programs are adequate for substances which show stability in water. The calculated half-life of diphenyl carbonate in air due to indirect photodegradation is $t_{1/2}$ = 4.0 days. Due to the low absorption in the UV-B range, no direct photodegradation is expected.

Diphenyl carbonate is not readily biodegradable but biodegraded by adapted microorganisms. After 28 days 37 % of the test substance had been degraded in a closed bottle test (Directive 92/69/EEC, C.4-E). With adapted domestic sewage, more than 99 % of the test substance had been degraded after 20 days in another closed bottle test (OECD TG 301 D).

According to the bioconcentration factor BCF = 66.9, calculated from the octanol-water partition coefficient the substance has a low potential to bioaccumulate in aquatic organisms. With a calculated K_{oc} value of 3926, diphenyl carbonate could be regarded as a substance with high geoaccumulation properties. However, due to hydrolysis geoaccumulation is not expected.

For fish (*Danio rerio)* the acute toxicity (LC_{50}, 96 h) of diphenyl carbonate (Directive 92/69/EEC, C.1) was 3.9 mg/l (effective concentration; nominal concentration: 10.0 mg/l). The acute toxicity (EC_{50}, 48 h) of diphenyl carbonate to the invertebrate *Daphnia magna* (Directive 92/69/EEC, C.2) was 6.5 mg/l (effective; nominal: 14.2 mg/l). Concerning the algal toxicity (Directive 92/69/EEC, C.3), for *Desmodesmus subspicatus* a 72 h-E_rC_{50} of 0.9 mg/l (effective; nominal: 2.4 mg/l) for the growth rate and a 72 h-E_bC_{50} 0.5 mg/l (effective; nominal: 1.4 mg/l) for the integral of biomass were determined. The corresponding 72 h-NOEC obtained from growth rate and biomass were 0.22 mg/l and 0.11 mg/l, respectively (effective; nominal 0.63 mg/l and 0.31 mg/l, respectively). The corresponding 72 h-LOEC obtained from growth rate and biomass were 0.44 mg/l and 0.22 mg/l, respectively (effective; nominal 1.25 mg/l and 0.63 mg/l, respectively).

Based on the lowest effect concentration observed for the algae a Predicted No Effect Concentration ($PNEC_{aqua}$) can be calculated with an assessment factor of 1000. Using the effective 72 h-E_rC_{50} of 0.9 mg/l (growth rate) found for the algae species *Desmodesmus subspicatus* a $PNEC_{aqua}$ of 0.9 µg/l was determined.

Exposure

Phosgenation of phenol is the most important method for producing diphenyl carbonate. In 2002, the world wide production capacity of diphenyl carbonate is estimated to be 254 000 metric tonnes (Western Europe 141 000, Japan 61 000, Far East (excl. Japan) 52 000) by about 10 producers. The total manufacturing capacity of the sponsor company amounts to 10 000 - 50 000 tonnes/a in 2002 in Belgium (no production in the Sponsor country).

Diphenyl carbonate is a chemical intermediate mainly used for the synthesis of aromatic polycarbonates. It is also

used for the synthesis of aliphatic polycarbonates and some aliphatic mono-isocyanates. Diphenyl carbonate is listed in the Danish, Finnish, Norwegian, and Swedish product registers as a product with industrial applications. No consumer applications are listed. Based on this data no exposure of the environment due to releases from consumer products occurs.

At the Sponsor company, diphenyl carbonate is manufactured and processed in closed systems. The exhausts from manufacturing and processing of diphenyl carbonate are connected to absorbing units, thermal exhaust purification plants and air washing units, thus virtually no emissions of diphenyl carbonate occurred into the atmosphere.

Due to the water-free processing processes emissions into wastewater may occur only in the case of cleaning procedures. The wastewater of the production plant is treated with activated carbon and subsequently in a biological wastewater treatment plant. For the biological wastewater treatment plant an effluent concentration of < 2 µg/l is calculated. Using the local dilution factor of 554, this results in a local PEC of <0.0036 µg/l. Emissions of diphenyl carbonate from polycarbonate resins were 0.14 - 4.94 mg/m^3 exhaust stream during experimental extrusion.

There are no environmental monitoring data available for diphenyl carbonate.

Occupational exposure at production and processing sites of the Sponsor company is controlled and the concentration of diphenyl carbonate is currently below the detection limit of 0.003 mg/m^3 (time weighted average). Based on data presented by the Sponsor company, consumer exposure to diphenyl carbonate via the environment is anticipated to be low.

Diphenyl carbonate is used for the manufacturing of food contact material. Based on a very low migration from the food contact material into food, and based on the toxicological data, the European Scientific Committee on Food classified diphenyl carbonate in “List 3”, i.e. substances for which an ADI or TDI could not be established, but where the present use could be accepted. In the EU, the use is restricted to a maximum limit of 0.05 mg/kg of food.

No consumer preparations containing diphenyl carbonate are listed in the Nordic product registers.

RECOMMENDATION AND RATIONALE FOR THE RECOMMENDATION AND NATURE OF FURTHER WORK RECOMMENDED

Human Health: The chemical is currently of low priority for further work because of its low hazard profile.

Environment: The chemical possesses properties indicating a hazard for the environment. Based on data presented by the Sponsor country (relating to production by one producer which accounts for approximately 4 % to 20 % of global production and relating to the use pattern in several OECD countries), exposure to the environment is anticipated to be low, and therefore this chemical is currently of low priority for further work. Countries may desire to investigate any exposure scenarios that were not presented by the Sponsor.