

Ground Water Quality Standard for 2,4,6-Trinitrotoluene (TNT)

February 2008

CASRN# 118-96-7

NJDEP

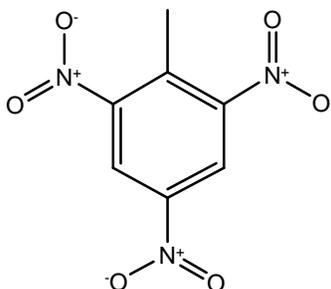
Summary of Decision: In accordance with the New Jersey Ground Water Quality Standards rules at N.J.A.C. 7:9C-1.7, the Department of Environmental Protection (Department) has developed an interim specific ground water quality criterion of 1 µg/L and PQL of 0.3 µg/L (ppb) for 2,4,6-Trinitrotoluene (TNT). The basis for this criterion and PQL are discussed below. Pursuant to N.J.A.C. 7:9C-1.9(c), **the applicable constituent standard is 1 µg/L.**

2,4,6-Trinitrotoluene (TNT)

1-methyl-2,4,6-trinitrobenzene

Molecular Formula: C₇H₅N₃O₆

Molecular Structure:



Background: Nitroaromatic explosives contain three NO₂ groups in various positions on the ring. TNT is the most extensively used explosive. TNT has been evaluated by USEPA and both a Reference Dose for noncarcinogenic effects and a cancer slope factor are available on the [USEPA IRIS database](#). TNT is classified as a Group C, Possible Human Carcinogen, with a cancer slope factor of 0.03 (mg/kg/day)⁻¹ (USEPA, 2002).

Reference Dose: The IRIS Reference Dose for 2,4,6-trinitrotoluene of 0.0005 mg/kg/day was developed in 1988 (USEPA, 2002) based on liver effects in a 26-week feeding study in dogs (US DOD, 1983). In this study, liver histopathology (trace to mild) was observed at the lowest dose, 0.5 mg/kg/day, and more severe liver effects (increased liver weight, effects on liver enzymes, and more severe liver pathology) were seen at higher doses. Therefore, 0.5 mg/kg/day was considered to be the Lowest Observed Adverse Effect Level (LOAEL) and a No Observed Adverse Effect Level (NOAEL) was not identified.

An uncertainty factor of 1000 was applied by USEPA to account for inter-individual sensitivity, interspecies extrapolation, subchronic-to-chronic extrapolation, and LOAEL-to-NOAEL extrapolation, to derive a Reference Dose of 0.0005 mg/kg/day. However, the Department applied a total uncertainty factor of 3000 to account for inter-individual sensitivity (10), interspecies variability (10), subchronic to chronic extrapolation (10), and for extrapolation from a LOAEL to a NOAEL (3).

Uncertainty factor (UF) adjustment:

UF _{inter-individual sensitivity}	= 10
UF _{interspecies variability}	= 10
UF _{subchronic to chronic extrapolation}	= 10
UF _{LOAEL to NOAEL extrapolation}	= 3

$$UF = UF_{\text{total}} = 10 \times 10 \times 10 \times 3 = 3000$$

$$RfD = LOAEL/UF = 0.5 \text{ mg/kg/day}/3000$$

$$RfD = \mathbf{0.00017 \text{ mg/kg/day}}$$

A dose-related increased incidence of urinary bladder papilloma and carcinoma were observed in female, but not male, Fischer 344 rats in a 24 month dietary study (US DOD, 1984a). No statistically significant increase in tumors was seen in male or female mice in a similar chronic study (US DOD, 1984b). Furthermore, 2,4,6-trinitrotoluene was mutagenic in four strains of Salmonella typhimurium with and without metabolic activation (USEPA, 2002). A cancer slope factor of $0.03 \text{ (mg/kg/day)}^{-1}$ was derived based on the urinary bladder carcinomas and papillomas in female rats.

Derivation of Ground Water Quality Criterion: The ground water quality criterion based on the cancer slope factor was derived as follows, using standard default assumptions:

$$\frac{(10^{-6} / 0.03 \text{ (mg/kg/day)}^{-1}) \times 70 \text{ kg}}{2 \text{ L/day}} = 0.0012 \text{ mg/L or } 1.2 \text{ } \mu\text{g/L (which rounds to } 1 \text{ } \mu\text{g/L)}$$

Where:

10^{-6} = Risk Level

$0.03 \text{ (mg/kg/day)}^{-1}$ = Cancer Slope Factor

70 kg = assumed body weight of average person

2 L/day = assumed daily drinking water intake

For comparison, the ground water criterion based on the Reference Dose was also derived, using standard default assumptions, to ensure that the criterion based on carcinogenicity is protective for systemic toxicity:

$$\frac{0.00017 \text{ mg/kg/day} \times 70 \text{ kg} \times 0.2}{2 \text{ L/day}} = 0.0012 \text{ mg/L or } 1.2 \text{ } \mu\text{g/L (which rounds to } 1 \text{ } \mu\text{g/L)}$$

Where:

0.00017 mg/kg/day = Reference Dose (derived by the Department using an uncertainty factor of 3000)

70 kg = assumed body weight of average person

0.2 = Relative Source Contribution from drinking water

2 L/day = assumed daily drinking water intake

As shown above, the ground water criteria derived based on both carcinogenic and systemic endpoints are identical. Therefore, the interim specific ground water quality criterion for TNT is $1 \text{ } \mu\text{g/L}$.

Derivation of PQL: The method detection limit (MDL) and the practical quantitation level (PQL) are performance measures used to estimate the limits of performance of analytic chemistry methods for measuring contaminants. The MDL is defined as "the minimum concentration of a substance that can be measured and reported with 99 percent confidence that the analyte concentration is greater than zero" (40 CFR Part 136 Appendix B). USEPA recommends that the MDL be multiplied by a factor of five or 10 to account for the variability and uncertainty that can occur at the MDL. The Department uses a value of five as the median upper boundary of the inter-laboratory MDL distribution from the New Jersey certified laboratory community and multiplies the MDL by five to derive the PQL. Establishing the PQL at a level that is five times the MDL provides a reliable quantitation level that most laboratories can be expected to meet during day-to-day operations.

No published method was listed for TNT in the [National Environmental Methods Index \(NEMI\)](#). However, there are many analytical method references for the determination of TNT. The best literature detection level that meets the interim specific criterion is a Gas Chromatography Electron Capture Detector method with a reported level of 0.06 ppb (Walsh, M.E. and T. Ranney, 1998). As explained above, a more conservative detection limit is established using a multiplier of five. $0.06 \text{ ppb} \times 5 = 0.3 \text{ ppb}$. Therefore, the Department has established a PQL of 0.3 ppb for TNT.

Conclusion: Based on the information provided above (and cited below), the Department has established an interim specific ground water quality criterion of 1 µg/L and a PQL of 0.3 µg/L (ppb) for TNT. Pursuant to N.J.A.C. 7:9C-1.9(c), since the criterion is higher than the PQL for this constituent, **the applicable constituent standard for 2,4,6-Trinitrotoluene (TNT) is 1 µg/L.**

Technical Support Documents: *Interim Specific Ground Water Quality Criterion Recommendation Report for 2,4,6-Trinitrotoluene (TNT)*, Dr. Gloria Post, NJDEP, [September 7, 2006; *Procedure for Describing Process for Development of Analytical Practical Quantitation Levels (PQLs) for 2,4,6-Trinitrotoluene*, R. Lee Lippincott, Ph.D, NJDEP, September 14, 2006.

References:

Almog, J., Kraus S., and A. Basch. 1983. Determination of TNT metabolites in urine. *Archives Toxicology [Suppl]* 6:351-353.

USDOD. 1983. U.S. Department of Defense. AD-A157 002. Available from Defense Technical Center. Write to Documents, Cameron Station, Alexandria, VA 22314, or call (703)274-7633 (cited in USEPA, 2002).

USDOD. 1984a. U.S. Department of Defense. AD-A168637. Available from Defense Technical Center. Write to Documents, Cameron Station, Alexandria, VA 22314, or call (703) 274-7633. (cited in USEPA, 2002).

USDOD. 1984b. U.S. Department of Defense. AD-A168754. Available from Defense Technical Center. Write to Documents, Cameron Station, Alexandria, VA 22314, or call (703) 274-7633. (cited in USEPA, 2002).

USEPA. 2002. United States Environmental Protection Agency. Integrated Risk

Information System. 2,4,6-Trinitrotoluene (TNT) (CASRN 118-96-7). Last updated 12/03/2002.

Walsh, M.E. and T. Ranney. 1998. Determination of Nitroaromatic, Nitramine, and Nitrate Ester Explosives in Water using Solid-phase Extraction and Gas Chromatography-electron Capture Detection: Comparison with High-performance Liquid Chromatography. *Journal of Chromatographic Science*, 36, pp. 406-416 (1998).



New Jersey Department of Environmental Protection
Water Monitoring and Standards
Bureau of Water Quality Standards and Assessment
www.state.nj.us/dep/wms/bwqsa/
(609) 777-1753

