3. CHEMICAL AND PHYSICAL INFORMATION

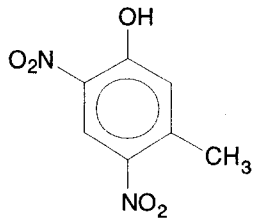
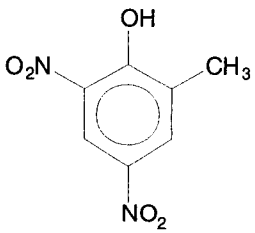
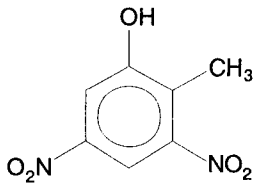
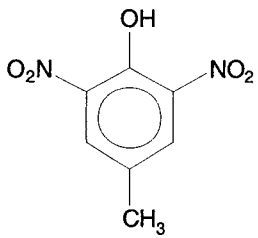
3.1 CHEMICAL IDENTITY

Information regarding the chemical identity of the selected dinitrocresols is given in Table 3-l. According to the current numbering system used in the United States, the phenolic OH substituent to the benzene ring is assigned the number one position. In the older literature, the methyl group is sometimes assigned the number one position. As a result, the compound referred to as 3,.5dinitroo-cresol is synonymous with 4,6-dinitro-*o*-cresol or DNOC (Bailey and White 1965).

3.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of the selected dinitrocresols is located in Table 3-2. Like dinitrophenols, the dinitrocresols are pseudoacids and readily form water soluble sodium, potassium, ammonium, and calcium salts (HSDB 1994; Metcalf 1978). Of the theoretically possible 18 isomers of dinitrocresols (Harvey 1953), the isomer 4,6-dinitro-*o*-cresol is the most commercially important (HSDB 1994). At a pH of 4.4, ≈50% of the DNOC in water exists as the dissociated compound (see pK_a value in Table 3-2). The concentration of the ionized form increases as the pH increases. Essentially, 100% of the DNOC at pH 7 or above will be in the ionized form. Thus, in a whole animal all of the DNOC exists in the ionized form or is associated with a macromolecule such as albumin (King and Harvey 1953b).

TABLE 3-1. Chemical Identity of Selected Isomers of Dinitrocresols

Characteristic	4,6-Dinitro-*m*-cresol	4,6-Dinitro-*o*-cresol[a]	3,5-Dinitro-*o*-cresol	2,6-Dinitro-*p*-cresol[a]
Synonym(s)	4,6-Dinitro-*m*-cresol	4,6-Dinitro-*o*-cresol; DNOC; DNC; 3,5-dinitro-2-hydroxy-toluene, 2-methyl-4,6-dinitrophenol[b]	3,5-Dinitro-*o*-cresol	2,6-Dinitro-*p*-cresol; DNPC; 3,5-Dinitro-4-hydroxy toluene
Registered trade name(s)	No data	Antinonnin; Detal; Dinitrol; Effusan; Selinon; others[b]	No data	Victoria Orange; Victoria Yellow
Chemical formula	$C_7H_6N_2O_5$	$C_7H_6N_2O_5$	$C_7H_6N_2O_5$	$C_7H_6N_2O_5$
Chemical structure				
Identification numbers:				
CAS registry	616–73–9	534–52–1	497–56–3	609–93–8
NIOSH RTECS[c]	G09400000	G09625000	G09500000	G09800000
EPA hazardous waste	No data	P047	No data	No data
OHM/TADS	No data	8100073	No data	No data
DOT/UN/NA/IMCO shipping	No data	UN 1598; IMO 6.1	No data	No data
HSDB	No data	1596	No data	No data
NCI	No data	No data	No data	No data

[a]All information obtained from ChemID 1993 and HSDB 1994 except where noted
[b]Merck 1989
[c]NIOSH 1987

CAS = Chemical Abstracts Services; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substances Data Bank; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data System; RTECS = Registry to Toxic Effects of Chemical Substances

TABLE 3-2. Physical and Chemical Properties of Selected Isomers of Dinitrocresols

Property	4,6-Dinitro-*m*-cresol	4,6-Dinitro-*o*-cresol[a]	3,5-Dinitro-*o*-cresol[b]	2,6-Dinitro-*p*-cresol[c]
Molecular weight	198.13	198.13	198.13	198.13
Color	No data	Yellow	Yellow	Yellow
Physical state	No data	Solid	Solid	Solid
Melting point	No data	87.5 °C; 86.5 °C[d]	85.8 °C	80–81 °C; 85 °C[d]
Boiling point	No data	312 °C[e]	No data	No data
Density	No data	No data	1.49 g/cm^3 [f]	No data
Odor	No data	Odorless[g]	No data	No data
Odor threshold:				
Water	No data	No data	No data	No data
Air	No data	No data	No data	No data
pK_a	No data	4.46[h]; 4.38[i]; 4.35[j]	No data	No data
Solubility:				
Water	No data	130 mg/L at 15 °C[k]	No data	290 mg/L
Organic solvent(s)	No data	Soluble in ethanol (4.3g/100g), acetone (100g/100g), and benzene (37g/100g)[g]	Soluble in ether, ethanol, and acetone	Soluble in ether, ethanol, and acetone[d]
Partition coefficients:				
Log K_{ow}	No data	2.12[l], 2.56[m], 2.16[i], 2.85[n]	No data	No data
Log K_{oc}	No data	2.35–2.77[a,o]	No data	No data
Vapor pressure	No data	1.05x10^{-4} mmHg at 25 °C[p] 3.6x10^{-4} mmHg at 35 °C[r,s]	5.2x10^{-5} mmHg at 20 °C[q]	No data
Henry's law constant	No data	1.4x10^{-6} atm-m^3/mol at 25 °C[t,u]	No data	No data
Autoignition temperature	No data	No data	No data	No data
Flashpoint	No data	No data	No data	No data
Flammability limits	No data	No data	No data	No data
Conversion factors at 25 °C	1 mg/m^3 = 0.12 ppm	1 mg/m^3 = 0.12 ppm	1 mg/m^3 = 0.12 ppm	1 mg/m^3 = 0.12 ppm
Explosive limits	No data	No data	No data	No data

[a]All information obtained from Merck 1989 unless otherwise noted
[b]All information obtained from Lide 1993 unless otherwise noted
[c]All information obtained from EPA 1988a unless otherwise noted
[d]Lide 1993
[e]ACGIH 1986
[f]Bailey and White 1965 (no temperature value given)
[g]Metcalf 1978
[h]Cessna and Grover 1978
[i]Jafvert et al. 1990
[j]Weber 1972
[k]Meister 1991
[l]Schwarzanbach et al. 1988
[m]GEMS 1986
[n]Loehr and Krishnamoorthy 1988
[o]Kenaga 1980
[p]Suntio et al. 1988
[q]EPA 1979
[r]Plimmer 1976
[s]Hamaker and Kerlinger 1969
[t]Shen 1982a
[u]Shen 1982b