SECTION 2: CHEMISTRY ASSESSMENT

1. Overview

Aldicarb is an oxime carbamate insecticide. It structurally resembles acetycholine and is a potent cholinesterase inhibitor.

1.1 Mode of Action

The mode of aldicarb action is systemic (contact and stomach action), and exposure of pests to this active constituent affects the nervous system by inhibiting the activity of acetyl cholinesterase. Aldicarb is metabolically transformed to aldicarb sulfoxide and aldicarb sulfone. Aldicarb sulfoxide has similar toxicity to aldicarb; aldicarb sulfone (also known as aldoxycarb) is considerably less toxic (approximately 4% of that of aldicarb).

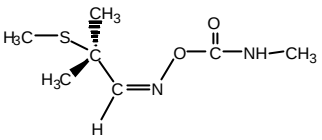
Aldicarb is an acutely toxic pesticide and is included in Schedule 7 of the SUSDP.

The physico-chemical properties of aldicarb are given in below, along with the relevant chemistry details.

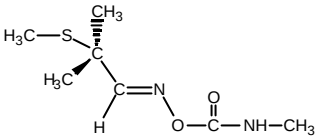
2. ACTIVE CONSTITUENT

2.1 Chemistry Identity

Common name	Aldicarb (BSI, E-ISO, ANSI, SA)
IUPAC Name	2-methyl-2-(methylthio)propionaldehyde *O*-methylcarbamoyloxime
CA Name	2-methyl-2-(methylthio)propanal *O*-[(methylamino)carbonyl]oxime
CAS Registry Number	116-06-3
Empirical formula	$C_7H_{14}N_2O_2S$
Molecular weight	190.25 daltons
Development code/official codes	UC 21 149; OMS 771; ENT 27 093; AI3-27 093
Principal tradename	'Temik' (Rhone-Poulenc)
Structural formula	Since the carbon – nitrogen double bond prevents both rotation and ammonia like inversion, two geometrical isomers of aldicarb are possible. The commercial product is a mixture of these two isomers. It is not certain which isomer is the more biologically active form.



Anti-aldicarb



Syn-aldicarb

Chemical family	Aldicarb is a systemic pesticide belonging to the carbamate ester family

2.2 Physical and Chemical Properties

2.2.1 Physical and chemical properties of the pure active constituent

Colour	White/colourless crystals	
Odour	Odourless, or slight sulphurous smell	
Physical state	Crystalline solid	
Melting point	98 to 100 ^{o}C	
Boiling point	Unknown; decomposes above 100 ^{o}C	
Vapour pressure	1 x 10^{-5} mm Hg at 0 ^{o}C 1 x 10^{-4} mm Hg (13 mPa) at 25 ^{o}C 7 x 10^{-4} mm Hg at 50 ^{o}C 4 x 10^{-3} mm Hg at 75 ^{o}C	
Relative density/Specific gravity	1.195 at 25/20 ^{o}C	
Octanol/water partition coefficient	Log P = 1.359	
Solubility in water	Moderately soluble in water; 6 g/L at 20 ^{o}C (WHO, 1991); 4.93 g/L (pH 7, 20 ^{o}C) (The Pesticide Manual, 1994)	
pH (1% aqueous suspension)	5 to 8	
Solvent solubility (at 20 to 25 ^{o}C)	Acetone	350 g/L
	Benzene	150 g/L
	Chlorobenzene	150 g/L
	Chloroform	350 g/L
	Dichloromethane	300 g/L
	DMSO	= 100 g/L
	Ethanol (95%)	= 100 g/L
	Ether	200 g/L
	Heptane	Insoluble
	Isopropane	200 g/L
	Methylene chloride	300 g/L
	Mineral oils	Insoluble
	Toluene	100 g/L
	Xylene	50 g/L
Stability	Pure crystalline aldicarb is stable when stored under ambient temperature. Aldicarb decomposes above 100 ^{o}C. It is stable in neutral, acidic and weakly alkaline media, but is rapidly hydrolysed by concentrated alkalis. Hydrolysis of the carbamate	

	ester group, which inactivates the pesticide, is pH dependent, half-lives in distilled water varies from a few minutes at a pH > 12 to 560 days at pH of 6.0. In the presence of oxidising agents, aldicarb is rapidly converted by to the sulfoxide, which is then (more slowly) oxidised to the sulfone.
Corrosiveness	Aldicarb is non-corrosive to metals.
Flash point	Non-flammable

2.2.2 Physical and chemical properties of the TGAC

The physical properties of aldicarb TGAC are identical to the pure active constituent.

Impurities	• dimethylamine • 2-methyl-2-(methylthio)propionitrile • 2-methyl-2-(2-methylthiopropylenaminoxy)-propinaldehyde *O*-(methylcarbamoyl)oxime • 2-methyl-2-(methylthio)propionaldehyde oxime
Flammability	The flashpoint is over 170 ^{o}C by open cup
Ignition temperature	360 ^{o}C
Suitable extinguishing agent	Powder, foam, CO_2, or water spray (do not use direct jet of water). Combustion products are toxic and/or irritant.
Hazard rating	Explosiveness – not explosive Health hazard – high Occupational toxicity – high Fire hazard – fumes would be expected to be moderately to highly toxic

2.3 Chemistry Aspects

The chemistry aspects (manufacturing process, quality control procedures, batch analysis results, and analytical methods) of aldicarb TGAC were evaluated and found acceptable. The levels of aldicarb and its impurities are quantified using reverse-phase HPLC with UV detection.

3. FORMULATION OF THE END-USE PRODUCT

Aldicarb is formulated as a granular form (10 to 15% active ingredient) because of its toxicity. This reduces the generation of dust and the risk from occupational exposure. It is applied below the soil surface to be absorbed by the plant roots. Soil moisture is essential for release of aldicarb from the granules. The mode of aldicarb action is systemic (contact and stomach action), and exposure of pests affects the nervous system by inhibiting the activity of acetyl cholinesterase.

4. DECLARATION OF COMPOSITION

The FAO monograph specifications for aldicarb technical and aldicarb technical concentrate are listed below:

4.1 Aldicarb Technical

Active Constituent		
	Aldicarb content	Minimum 920 g/kg
Impurities		
	Aldicarb oxime	Maximum 4.0 g/kg
	Methyl isocyanate	Maximum 12.5 g/kg
	Trimethylamine	Maximum 12.5 g/kg
	Aldicarb nitrile	Maximum 35.0 g/kg
	Dimethylurea + Triethylbiuret	Maximum 50.0 g/kg
	Water	Maximum 2.5 g/kg

4.2 Aldicarb Technical Concentrate

Active Constituent		
	Aldicarb content	Shall be declared. Minimum 356 g/kg
Impurities		
	Aldicarb oxime	Maximum 1.0 g/kg
	Methyl isocyanate	Maximum 5.0 g/kg
	Trimethylamine	Maximum 5.0 g/kg
	Aldicarb nitrile	Maximum 15.0 g/kg
	Dimethylurea + Triethylbiuret	Maximum 20.0 g/kg
	Water	Maximum 1.0 g/kg

The NRA Minimum Compositional Standard for technical aldicarb is listed below:

Active Constituent		
	Aldicarb content	Minimum 920 g/kg
Impurity		
	Methyl isocyanate	Maximum 12.5 g/kg

Aldicarb Manufacturing Concentrates from the approved sources comply with the FAO specifications for the active constituent and the impurities.

5. CONCLUSION

The currently approved sources of aldicarb manufacturing concentrate comply with both the NRA Minimum Compositional Standard and the FAO specifications for this chemical.