

**Safety Data Sheet**

according to Regulation (EC) No 1907/2006

**BOP**

Revision date: 29.06.2021

Product code: RL-5096

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**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1. Product identifier**

BOP

**Further trade names**

Benzotriazol-1-yl-oxy-tris-(dimethylamino)-phosphonium hexafluorophosphate  
Benzotriazol-1-yloxytris(dimethylamino)phosphonium hexafluorophosphate  
Tri(dimethylamino)benzotriazol-1-yloxyphosphonium hexafluorophosphate  
1H-Benzotriazol-1-yloxytris(dimethylamino)phosphonium Hexafluorophosphate  
Castros reagent

Substance name: (Benzotriazol-1-yloxy)tris(dimethylamino)phosphonium hexafluorophosphate  
(BOP)

CAS No: 56602-33-6

EC No: 260-279-1

**1.2. Relevant identified uses of the substance or mixture and uses advised against****Use of the substance/mixture**

Laboratory chemical. Manufacture of the substance

**Uses advised against**

Do not use for private purposes (household).

Restrictions on use: Pharmaceutical substance

**1.3. Details of the supplier of the safety data sheet**

Company name: Iris Biotech GmbH  
Street: Adalbert-Zoellner-Straße 1  
Place: D-95615 Marktredwitz, Germany  
Post-office box: 568  
D-95605 Marktredwitz, Germany

Telephone: +49 9231 97121 0

Telefax: +49 9231 97121 99

e-mail: info@iris-biotech.de

Contact person: Compliance Department

Telephone: +49 9231 97121 0

e-mail: sds@iris-biotech.de

Internet: www.iris-biotech.de

Responsible Department: Only available during office hours.

**1.4. Emergency telephone number:** +49 (0)89 19240 (POISON CENTER Munich: 24 h)

**SECTION 2: Hazards identification****2.1. Classification of the substance or mixture****Regulation (EC) No. 1272/2008**

Hazard categories:

Flammable solid: Flam. Sol. 1

Skin corrosion/irritation: Skin Irrit. 2

Serious eye damage/eye irritation: Eye Irrit. 2

Specific target organ toxicity - single exposure: STOT SE 3

Hazard Statements:

Flammable solid.

Causes skin irritation.

Causes serious eye irritation.

May cause respiratory irritation.

**2.2. Label elements****Regulation (EC) No. 1272/2008**

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**Signal word:** Danger

**Pictograms:**

**Hazard statements**

H228 Flammable solid.  
 H315 Causes skin irritation.  
 H319 Causes serious eye irritation.  
 H335 May cause respiratory irritation.

**Precautionary statements**

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.  
 P240 Ground and bond container and receiving equipment.  
 P241 Use explosion-proof electrical/ventilating/lighting equipment.  
 P261 Avoid breathing dust/fume/gas/mist/vapours/spray.  
 P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.  
 P302+P352 IF ON SKIN: Wash with plenty of water.  
 P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.  
 P337+P313 If eye irritation persists: Get medical advice/attention.

**Special labelling of certain mixtures**

EUH044 Risk of explosion if heated under confinement.

**Additional advice on labelling**

Warning - substance not yet tested completely.

**2.3. Other hazards**

May form explosible dust-air mixture if dispersed. This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

**SECTION 3: Composition/information on ingredients**
**3.1. Substances**
**Chemical characterization**

Benzotriazol-1-yl-oxy-tris-(dimethylamino)-phosphonium hexafluorophosphate

Sum formula: C<sub>12</sub>H<sub>22</sub>N<sub>6</sub>OP\*PF<sub>6</sub>

Molecular weight: 297,32\*144,96 g/mol

**Hazardous components**

CAS No	Chemical name			Quantity
	EC No	Index No	REACH No	
	GHS Classification			
56602-33-6	(Benzotriazol-1-yloxy)tris(dimethylamino)phosphonium hexafluorophosphate (BOP)			100 %
	260-279-1			
	Flam. Sol. 1, Skin Irrit. 2, Eye Irrit. 2, STOT SE 3; H228 H315 H319 H335 EUH044			

Full text of H and EUH statements: see section 16.

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**Specific Conc. Limits, M-factors and ATE**

CAS No	EC No	Chemical name	Quantity
		Specific Conc. Limits, M-factors and ATE	
56602-33-6	260-279-1	(Benzotriazol-1-yloxy)tris(dimethylamino)phosphonium hexafluorophosphate (BOP)	100 %
		inhalation: Data lacking (gases); dermal: Data lacking; oral: Data lacking	

**SECTION 4: First aid measures****4.1. Description of first aid measures****General information**

In case of accident or unwellness, seek medical advice immediately (show directions for use or safety data sheet if possible).

In all cases of doubt, or when symptoms persist, seek medical advice.

**After inhalation**

Provide fresh air. Medical treatment necessary. Remove casualty to fresh air and keep warm and at rest. In case of irregular breathing or respiratory arrest provide artificial respiration.

In all cases of doubt, or when symptoms persist, seek medical advice.

**After contact with skin**

After contact with skin, wash immediately with plenty of water and soap. Take off immediately all contaminated clothing and wash it before reuse. If skin irritation occurs: Get medical advice/attention.

In all cases of doubt, or when symptoms persist, seek medical advice.

**After contact with eyes**

After contact with the eyes, rinse with water with the eyelids open for a sufficient length of time, then consult an ophthalmologist immediately.

**After ingestion**

Rinse mouth immediately and drink 1 glass of water. Rinse mouth thoroughly with water. Never give anything by mouth to an unconscious person or a person with cramps.

In all cases of doubt, or when symptoms persist, seek medical advice.

**4.2. Most important symptoms and effects, both acute and delayed**

Refer to chapter 11.

**4.3. Indication of any immediate medical attention and special treatment needed**

Treat symptomatically.

**SECTION 5: Firefighting measures****5.1. Extinguishing media****Suitable extinguishing media**

Water spray jet, Carbon dioxide (CO<sub>2</sub>), Foam, Extinguishing powder. Water spray. alcohol resistant foam. Dry extinguishing powder. Sand.

**Unsuitable extinguishing media**

High power water jet.

**5.2. Special hazards arising from the substance or mixture**

Flammable. Vapours can form explosive mixtures with air. Heating causes rise in pressure with risk of bursting. Thermal decomposition can lead to the escape of irritating gases and vapours.

In case of fire may be liberated: Carbon dioxide (CO<sub>2</sub>). Carbon monoxide (CO). Nitrogen oxides (NO<sub>x</sub>).

Phosphorus oxides. Fluorhydric acid.

**5.3. Advice for firefighters**

Wear a self-contained breathing apparatus and chemical protective clothing. Full protection suit.

**Additional information**

Use water spray jet to protect personnel and to cool endangered containers. Suppress gases/vapours/mists

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with water spray jet. Collect contaminated fire extinguishing water separately. Do not allow entering drains or surface water.

Usual measures for fire prevention.

**SECTION 6: Accidental release measures****6.1. Personal precautions, protective equipment and emergency procedures****General advice**

Remove all sources of ignition. Provide adequate ventilation. Avoid dust formation. Do not breathe dust. Avoid contact with skin, eyes and clothes. Use personal protection equipment. Provide adequate ventilation. Avoid breathing dust/fume/gas/mist/vapours/spray. Avoid contact with skin, eyes and clothes. Wear personal protection equipment. In case of fire: Evacuate area.

**6.2. Environmental precautions**

Do not allow uncontrolled discharge of product into the environment. Explosion risk. Do not allow to enter into soil/subsoil. Do not allow to enter into surface water or drains.

**6.3. Methods and material for containment and cleaning up****For cleaning up**

Take up mechanically. Treat the recovered material as prescribed in the section on waste disposal.

**Other information**

Take up mechanically, placing in appropriate containers for disposal. Avoid dust formation. Clear contaminated areas thoroughly.

**6.4. Reference to other sections**

Safe handling: see section 7  
Personal protection equipment: see section 8  
Disposal: see section 13 Treat the recovered material as prescribed in the section on waste disposal.

**SECTION 7: Handling and storage****7.1. Precautions for safe handling****Advice on safe handling**

If handled uncovered, arrangements with local exhaust ventilation have to be used. Avoid dust formation. Do not breathe dust. Provide adequate ventilation. Avoid dust formation. Take precautionary measures against static discharges. Avoid breathing dust/fume/gas/mist/vapours/spray. Avoid contact with skin, eyes and clothes.

**Advice on protection against fire and explosion**

Keep away from sources of ignition - No smoking. Take precautionary measures against static discharges. Vapours can form explosive mixtures with air. Usual measures for fire prevention. Remove all sources of ignition. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

**Advice on general occupational hygiene**

Remove contaminated, saturated clothing immediately. Draw up and observe skin protection programme. Wash hands and face before breaks and after work and take a shower if necessary. When using do not eat, drink, smoke, sniff. Avoid contact with skin, eyes and clothes. Provide adequate ventilation. Wash hands and face before breaks and after work and take a shower if necessary.

**7.2. Conditions for safe storage, including any incompatibilities**

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**Requirements for storage rooms and vessels**

Keep container tightly closed. Keep locked up. Store in a place accessible by authorized persons only. Provide adequate ventilation as well as local exhaust at critical locations. Keep in a cool, well-ventilated place. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Keep container tightly closed in a cool, well-ventilated place.  
Handle and store contents under inert gas. Protect from moisture.  
storage temperature: +2°C - +8°C

**Hints on joint storage**

Do not store together with: Oxidizing agent. Pyrophoric or self-heating substances. Keep container tightly closed. Store in a cool dry place. Keep away from incompatible materials like finely powdered metals. Protect from heat. Keep away from food, feed and beverages.

**Further information on storage conditions**

Keep away from sources of ignition - No smoking.  
To follow: National regulations!

**SECTION 8: Exposure controls/personal protection****8.1. Control parameters****Additional advice on limit values**

To date, no national critical limit values exist.

**8.2. Exposure controls****Appropriate engineering controls**

If handled uncovered, arrangements with local exhaust ventilation have to be used. Do not breathe dust. The receiver of our product is singularly responsible for adhering to existing laws and regulations.

**Individual protection measures, such as personal protective equipment****Eye/face protection**

Suitable eye protection: goggles.  
Tightly fitting safety goggles. Face shield (8-inch minimum). Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

**Hand protection**

When handling with chemical substances, protective gloves must be worn with the CE-label including the four control digits. The quality of the protective gloves resistant to chemicals must be chosen as a function of the specific working place concentration and quantity of hazardous substances. For special purposes, it is recommended to check the resistance to chemicals of the protective gloves mentioned above together with the supplier of these gloves. Wear suitable gloves.

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands. The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

**Skin protection**

Use of protective clothing.

**Respiratory protection**

In case of inadequate ventilation wear respiratory protection. If technical exhaust or ventilation measures are not possible or insufficient, respiratory protection must be worn.

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Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

**Environmental exposure controls**

Discharge into the environment must be avoided.

**SECTION 9: Physical and chemical properties**
**9.1. Information on basic physical and chemical properties**

Physical state:	solid
Colour:	white/ whitish
Odour:	No data available
Odour threshold:	not determined

**Test method**
**Changes in the physical state**

Melting point/freezing point:	136 - 140 °C	decomposition
Boiling point or initial boiling point and boiling range:	not determined	
Sublimation point:	not determined	
Softening point:	not determined	
Flash point:	No data available	

**Flammability**

Solid/liquid:	Flammable solid. (H228) Category 1 °C
Gas:	not applicable

**Explosive properties**

Risk of explosion if heated under confinement.

Lower explosion limits:	not determined
Upper explosion limits:	not determined
Auto-ignition temperature:	not determined
Decomposition temperature:	not determined
pH-Value:	No data available
Viscosity / dynamic:	not applicable
Viscosity / kinematic:	not applicable
Flow time:	not applicable
Water solubility:	No data available

**Solubility in other solvents**

Soluble in: Tetrahydrofurane (THF), Dichloromethane (DCM), Acetone, Dimethylformamide (DMF), Dimethylsulfoxide (DMSO), N-Methylpyrrolidone (MNP)

Dissolution rate:	not determined
Partition coefficient n-octanol/water:	No data available
Vapour pressure:	No data available
Density:	No data available
Bulk density:	No data available
Relative vapour density:	No data available

**9.2. Other information**

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**Information with regard to physical hazard classes**

Sustaining combustion: No data available  
Oxidizing properties  
No data available

**Other safety characteristics**

Solvent separation test: No data available  
Solid content: not determined  
Evaporation rate: not determined

**Further Information****SECTION 10: Stability and reactivity****10.1. Reactivity**

Flammable. Risk of explosion if heated under confinement.  
Danger of dust explosion.

**10.2. Chemical stability**

Stable under recommended storage conditions.  
Moisture-sensitive.  
Photosensitive.

**10.3. Possibility of hazardous reactions**

No data available

**10.4. Conditions to avoid**

Keep away from sources of heat (e.g. hot surfaces), sparks and open flames. Explosion risk. Protect from moisture.  
Keep away from heat.  
Keep away from heat/sparks/open flames/hot surfaces. - No smoking.  
Sensitivity to light.

**10.5. Incompatible materials**

Oxidizing agents, strong.

**10.6. Hazardous decomposition products**

Thermal decomposition can lead to the escape of irritating gases and vapours.  
In case of fire may be liberated: Carbon dioxide (CO<sub>2</sub>). Carbon monoxide (CO). Nitrogen oxides (NO<sub>x</sub>).  
Phosphorus oxides. Fluorhydric acid.

**Further information**

In case of fire: See chapter 5.

**SECTION 11: Toxicological information****11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008****Toxicokinetics, metabolism and distribution**

No data available

**Acute toxicity**

Based on available data, the classification criteria are not met.  
Symptoms: Mucosal irritations. Coughing. shortage of breath.  
Possible effects: Damage of respiratory tract.

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CAS No	Chemical name				
	Exposure route	Dose	Species	Source	Method
56602-33-6	(Benzotriazol-1-yloxy)tris(dimethylamino)phosphonium hexafluorophosphate (BOP)				
	oral	Data lacking			
	dermal	Data lacking			
	inhalation	Data lacking			

**Irritation and corrosivity**

Causes skin irritation.

Causes serious eye irritation.

**Sensitising effects**

Based on available data, the classification criteria are not met.

**Carcinogenic/mutagenic/toxic effects for reproduction**

Based on available data, the classification criteria are not met.

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

In vitro mutagenicity/genotoxicity:

Ames test negative.

Data sources: literature value

**STOT-single exposure**

May cause respiratory irritation. ((Benzotriazol-1-yloxy)tris(dimethylamino)phosphonium hexafluorophosphate (BOP))

**STOT-repeated exposure**

Based on available data, the classification criteria are not met.

**Aspiration hazard**

Based on available data, the classification criteria are not met.

**Specific effects in experiment on an animal**

No data available

**Additional information on tests**

No data available

**Practical experience**

No data available

**11.2. Information on other hazards****Other information**

No data available

**Further information**

This substance is classified as hazardous according to Regulation (EC) No 1272 (2008).

RTECS: No data available

Fluoride ion can reduce serum calcium levels possibly causing fatal hypocalcemia.

Warning - substance not yet tested completely.

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

**SECTION 12: Ecological information****12.1. Toxicity**

No data available



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CAS No	Chemical name					
	Aquatic toxicity	Dose	[h]   [d]	Species	Source	Method
56602-33-6	(Benzotriazol-1-yloxy)tris(dimethylamino)phosphonium hexafluorophosphate (BOP)					
	Aquatic toxicity	Data lacking				

**12.2. Persistence and degradability**

No data available

**12.3. Bioaccumulative potential**

No data available

**12.4. Mobility in soil**

No data available

**12.5. Results of PBT and vPvB assessment**

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

**12.6. Endocrine disrupting properties**

No data available

**12.7. Other adverse effects**

Warning - substance not yet tested completely.

**Further information**

Do not allow to enter into surface water or drains. Do not allow to enter into soil/subsoil.

Discharge into the environment must be avoided.

**SECTION 13: Disposal considerations**
**13.1. Waste treatment methods**
**Disposal recommendations**

Do not allow to enter into surface water or drains. Do not allow to enter into soil/subsoil. Dispose of waste according to applicable legislation. Dispose of waste according to applicable legislation.

Consult the appropriate local waste disposal expert about waste disposal.

**Contaminated packaging**

Non-contaminated packages may be recycled.

Handle contaminated packages in the same way as the substance itself.

**SECTION 14: Transport information**
**Land transport (ADR/RID)**
**14.1. UN number or ID number:**

UN 1325

**14.2. UN proper shipping name:**

 FLAMMABLE SOLID, ORGANIC, N.O.S.  
 (Tri(dimethylamino)benzotriazol-1-yloxyphosphonium  
 hexafluorophosphate)

**14.3. Transport hazard class(es):**

4.1

**14.4. Packing group:**

II

Hazard label:

4.1



Classification code:

F1

Special Provisions:

274

Limited quantity:

1 kg

Excepted quantity:

E2

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Transport category: 2  
Hazard No: 40  
Tunnel restriction code: E

**Inland waterways transport (ADN)**

**14.1. UN number or ID number:** UN 1325  
**14.2. UN proper shipping name:** FLAMMABLE SOLID, ORGANIC, N.O.S.  
(Tri(dimethylamino)benzotriazol-1-yloxyphosphonium  
hexafluorophosphate)  
**14.3. Transport hazard class(es):** 4.1  
**14.4. Packing group:** II  
Hazard label: 4.1



Classification code: F1  
Special Provisions: 274  
Limited quantity: 1 kg  
Excepted quantity: E2

**Marine transport (IMDG)**

**14.1. UN number or ID number:** UN 1325  
**14.2. UN proper shipping name:** FLAMMABLE SOLID, ORGANIC, N.O.S.  
(Tri(dimethylamino)benzotriazol-1-yloxyphosphonium  
hexafluorophosphate)  
**14.3. Transport hazard class(es):** 4.1  
**14.4. Packing group:** II  
Hazard label: 4.1



Special Provisions: 274  
Limited quantity: 1 kg  
Excepted quantity: E2  
EmS: F-A, S-G

**Air transport (ICAO-TI/IATA-DGR)**

**14.1. UN number or ID number:** UN 1325  
**14.2. UN proper shipping name:** FLAMMABLE SOLID, ORGANIC, N.O.S.  
(Tri(dimethylamino)benzotriazol-1-yloxyphosphonium  
hexafluorophosphate)  
**14.3. Transport hazard class(es):** 4.1  
**14.4. Packing group:** II  
Hazard label: 4.1



Special Provisions: A3 A803  
Limited quantity Passenger: 5 kg  
Passenger LQ: Y441  
Excepted quantity: E2

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IATA-packing instructions - Passenger:	445
IATA-max. quantity - Passenger:	15 kg
IATA-packing instructions - Cargo:	448
IATA-max. quantity - Cargo:	50 kg

**14.5. Environmental hazards**

ENVIRONMENTALLY HAZARDOUS: No

**14.6. Special precautions for user**

Warning: flammable solids.

**14.7. Maritime transport in bulk according to IMO instruments**

not applicable

**SECTION 15: Regulatory information****15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture****EU regulatory information**

Restrictions on use (REACH, annex XVII):

Entry 40

Information according to 2012/18/EU Not subject to 2012/18/EU (SEVESO III)  
(SEVESO III):**Additional information**

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**National regulatory information**

Employment restrictions:	Observe restrictions to employment for juveniles according to the 'juvenile work protection guideline' (94/33/EC).
Water hazard class (D):	3 - highly hazardous to water
Skin resorption/Sensitization:	Causes allergic hypersensitivity reactions.

**15.2. Chemical safety assessment**

For this substance a chemical safety assessment has not been carried out.

**SECTION 16: Other information****Abbreviations and acronyms**

CLP: Classification, labelling and Packaging  
REACH: Registration, Evaluation and Authorization of Chemicals  
GHS: Globally Harmonised System of Classification, Labelling and Packaging of Chemicals  
UN: United Nations  
CAS: Chemical Abstracts Service  
DNEL: Derived No Effect Level  
DMEL: Derived Minimal Effect Level  
PNEC: Predicted No Effect Concentration  
ATE: Acute toxicity estimate  
LC50: Lethal concentration, 50%  
LD50: Lethal dose, 50%  
LL50: Lethal loading, 50%  
EL50: Effect loading, 50%  
EC50: Effective Concentration 50%  
ErC50: Effective Concentration 50%, growth rate  
NOEC: No Observed Effect Concentration  
BCF: Bio-concentration factor  
PBT: persistent, bioaccumulative, toxic  
vPvB: very persistent, very bioaccumulative  
ADR: Accord européen sur le transport des marchandises dangereuses par Route

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(European Agreement concerning the International Carriage of Dangerous Goods by Road)  
RID: Regulations concerning the international carriage of dangerous goods by rail  
ADN: European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways  
(Accord européen relatif au transport international des marchandises dangereuses par voies de navigation intérieures)  
IMDG: International Maritime Code for Dangerous Goods  
EmS: Emergency Schedules  
MFAG: Medical First Aid Guide  
IATA: International Air Transport Association  
ICAO: International Civil Aviation Organization  
MARPOL: International Convention for the Prevention of Marine Pollution from Ships  
IBC: Intermediate Bulk Container  
SVHC: Substance of Very High Concern  
For abbreviations and acronyms, see table at <http://abbrev.esdscom.eu>

**Relevant H and EUH statements (number and full text)**

H228	Flammable solid.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.
EUH044	Risk of explosion if heated under confinement.

**Further Information**

The information is based on the present level of our knowledge. It does not, however, give assurance of product properties and establishes no contract legal rights. The receiver of our product is singularly responsible for adhering to existing laws and regulations.