

# 3-Nitrobenzonitrile

sc-231879



The Power to Question

## Material Safety Data Sheet

Hazard Alert Code  
Key:

EXTREME

HIGH

MODERATE

LOW

### Section 1 - CHEMICAL PRODUCT AND COMPANY IDENTIFICATION

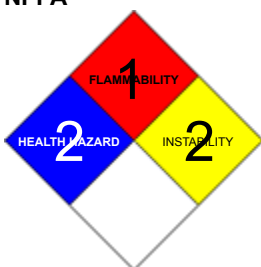
#### PRODUCT NAME

3-Nitrobenzonitrile

#### STATEMENT OF HAZARDOUS NATURE

CONSIDERED A HAZARDOUS SUBSTANCE ACCORDING TO OSHA 29 CFR 1910.1200.

#### NFPA



#### SUPPLIER

Santa Cruz Biotechnology, Inc.  
2145 Delaware Avenue  
Santa Cruz, California 95060  
800.457.3801 or 831.457.3800

#### EMERGENCY

ChemWatch  
Within the US & Canada: 877-715-9305  
Outside the US & Canada: +800 2436 2255  
(1-800-CHEMCALL) or call +613 9573 3112

#### SYNONYMS

C7-H4-N2-O2, CNC6H4NO2, "benzonitrile, m-nitro-", m-cyanonitrobenzene, m-nitrobenzonitrile

### Section 2 - HAZARDS IDENTIFICATION

#### CHEMWATCH HAZARD RATINGS

		Min	Max	
Flammability	1			
Toxicity	3			
Body Contact	2			
Reactivity	2			
Chronic	2			

Min/Nil=0  
Low=1  
Moderate=2  
High=3  
Extreme=4



#### CANADIAN WHMIS SYMBOLS



## **EMERGENCY OVERVIEW**

### **RISK**

Toxic if swallowed.

Contact with acids liberates very toxic gas.

May cause SENSITISATION by skin contact.

Harmful by inhalation and in contact with skin.

Irritating to eyes, respiratory system and skin.

### **POTENTIAL HEALTH EFFECTS**

#### **ACUTE HEALTH EFFECTS**

##### **SWALLOWED**

■ Toxic effects may result from the accidental ingestion of the material; animal experiments indicate that ingestion of less than 40 gram may be fatal or may produce serious damage to the health of the individual.

■ Aromatic nitriles, unlike aliphatic nitriles, do not appear to liberate cyanide within the body.

■ The substance and/or its metabolites may bind to haemoglobin inhibiting normal uptake of oxygen.

This condition, known as "methaemoglobinemia", is a form of oxygen starvation (anoxia).

■ Cyanide poisoning can cause increased saliva output, nausea without vomiting, anxiety, confusion, vertigo, dizziness, stiffness of the lower jaw, convulsions, spasm, paralysis, coma and irregular heartbeat, and stimulation of breathing followed by failure.

Often the skin becomes cyanosed (blue-grey), and this is often delayed.

##### **EYE**

■ This material can cause eye irritation and damage in some persons.

##### **SKIN**

■ Skin contact with the material may be harmful; systemic effects may result following absorption.

■ This material can cause inflammation of the skin on contact in some persons.

■ The material may accentuate any pre-existing dermatitis condition.

■ Open cuts, abraded or irritated skin should not be exposed to this material.

■ Entry into the blood-stream, through, for example, cuts, abrasions or lesions, may produce systemic injury with harmful effects.

Examine the skin prior to the use of the material and ensure that any external damage is suitably protected.

##### **INHALED**

■ Inhalation of dusts, generated by the material, during the course of normal handling, may be harmful.

■ The material can cause respiratory irritation in some persons.

The body's response to such irritation can cause further lung damage.

■ Persons with impaired respiratory function, airway diseases and conditions such as emphysema or chronic bronchitis, may incur further disability if excessive concentrations of particulate are inhaled.

If prior damage to the circulatory or nervous systems has occurred or if kidney damage has been sustained, proper screenings should be conducted on individuals who may be exposed to further risk if handling and use of the material result in excessive exposures.

#### **CHRONIC HEALTH EFFECTS**

■ Long-term exposure to respiratory irritants may result in disease of the airways involving difficult breathing and related systemic problems.

Skin contact with the material is more likely to cause a sensitisation reaction in some persons compared to the general population.

Substance accumulation, in the human body, may occur and may cause some concern following repeated or long-term occupational exposure.

Long term exposure to high dust concentrations may cause changes in lung function i.e. pneumoconiosis; caused by particles less than 0.5 micron penetrating and remaining in the lung. Prime symptom is breathlessness; lung shadows show on X-ray.

### Section 3 - COMPOSITION / INFORMATION ON INGREDIENTS

NAME	CAS RN	%
3-nitrobenzonitrile	619-24-9	>98

### Section 4 - FIRST AID MEASURES

#### SWALLOWED

- Give a slurry of activated charcoal in water to drink. NEVER GIVE AN UNCONSCIOUS PATIENT WATER TO DRINK.
- At least 3 tablespoons in a glass of water should be given.
- Although induction of vomiting may be recommended (IN CONSCIOUS PERSONS ONLY), such a first aid measure is dissuaded due to the risk of aspiration of stomach contents. (i) It is better to take the patient to a doctor who can decide on the necessity and method of emptying the stomach. (ii) Special circumstances may however exist; these include non-availability of charcoal and the ready availability of the doctor.

NOTE If vomiting is induced, lean patient forward or place on left side (head-down position, if possible) to maintain open airway and prevent aspiration.

#### EYE

If this product comes in contact with the eyes

- Immediately hold eyelids apart and flush the eye continuously with running water.
- Ensure complete irrigation of the eye by keeping eyelids apart and away from eye and moving the eyelids by occasionally lifting the upper and lower lids.
- Continue flushing until advised to stop by the Poisons Information Centre or a doctor, or for at least 15 minutes.
- Transport to hospital or doctor without delay.

#### SKIN

If skin contact occurs

- Immediately remove all contaminated clothing, including footwear.
- Flush skin and hair with running water (and soap if available).
- Seek medical attention in event of irritation.

#### INHALED

- If fumes or combustion products are inhaled remove from contaminated area.
- Lay patient down. Keep warm and rested.
- Prostheses such as false teeth, which may block airway, should be removed, where possible, prior to initiating first aid procedures.
- Apply artificial respiration if not breathing, preferably with a demand valve resuscitator, bag-valve mask device, or pocket mask as trained. Perform CPR if necessary.

#### NOTES TO PHYSICIAN

■ Symptoms of vasodilation and reflex tachycardia may present following organic nitrate overdose; most organic nitrates are extensively metabolised by hydrolysis to inorganic nitrites. Organic nitrates and nitrites are readily absorbed through the skin, lungs, mucosa and gastro-intestinal tract.

The toxicity of nitrates and nitrites result from their vasodilating properties and their propensity to form methaemoglobin.

- Most produce a peak effect within 30 minutes.
- Clinical signs of cyanosis appear before other symptoms because of the dark pigmentation of methaemoglobin.
- Initial attention should be directed towards improving oxygen delivery, with assisted ventilation, if necessary. Hyperbaric oxygen has not demonstrated conclusive benefits.
- Institute cardiac monitoring, especially in patients with coronary artery or pulmonary disease.

### Section 5 - FIRE FIGHTING MEASURES

Vapour Pressure (mmHG)	Negligible
------------------------	------------

Upper Explosive Limit (%)	Not available
Specific Gravity (water=1)	Not available
Lower Explosive Limit (%)	Not available

#### **EXTINGUISHING MEDIA**

- Foam.
- Dry chemical powder.
- BCF (where regulations permit).
- Carbon dioxide.

#### **FIRE FIGHTING**

- Alert Fire Brigade and tell them location and nature of hazard.
- Wear full body protective clothing with breathing apparatus.
- Prevent, by any means available, spillage from entering drains or water course.
- Use fire fighting procedures suitable for surrounding area.

When any large container (including road and rail tankers) is involved in a fire, consider evacuation by 800 metres in all directions.

#### **GENERAL FIRE HAZARDS/HAZARDOUS COMBUSTIBLE PRODUCTS**

- Combustible solid which burns but propagates flame with difficulty; it is estimated that most organic dusts are combustible (circa 70%) - according to the circumstances under which the combustion process occurs, such materials may cause fires and / or dust explosions.
- Avoid generating dust, particularly clouds of dust in a confined or unventilated space as dusts may form an explosive mixture with air, and any source of ignition, i.e. flame or spark, will cause fire or explosion. Dust clouds generated by the fine grinding of the solid are a particular hazard; accumulations of fine dust (420 micron or less) may burn rapidly and fiercely if ignited - particles exceeding this limit will generally not form flammable dust clouds.; once initiated, however, larger particles up to 1400 microns diameter will contribute to the propagation of an explosion.
- In the same way as gases and vapours, dusts in the form of a cloud are only ignitable over a range of concentrations; in principle, the concepts of lower explosive limit (LEL) and upper explosive limit (UEL).are applicable to dust clouds but only the LEL is of practical use; - this is because of the inherent difficulty of achieving homogeneous dust clouds at high temperatures (for dusts the LEL is often called the "Minimum Explosible Concentration", MEC)
- A dust explosion may release of large quantities of gaseous products; this in turn creates a subsequent pressure rise of explosive force capable of damaging plant and buildings and injuring people.

Combustion products include carbon monoxide (CO), carbon dioxide (CO<sub>2</sub>), nitrogen oxides (NO<sub>x</sub>), other pyrolysis products typical of burning organic material.

May emit poisonous fumes.

#### **FIRE INCOMPATIBILITY**

- Avoid contamination with oxidising agents i.e. nitrates, oxidising acids, chlorine bleaches, pool chlorine etc. as ignition may result

### **Section 6 - ACCIDENTAL RELEASE MEASURES**

#### **MINOR SPILLS**

- Remove all ignition sources.
- Clean up all spills immediately.
- Avoid contact with skin and eyes.
- Control personal contact by using protective equipment.

#### **MAJOR SPILLS**

- Clear area of personnel and move upwind.
- Alert Fire Brigade and tell them location and nature of hazard.
- Wear full body protective clothing with breathing apparatus.
- Prevent, by any means available, spillage from entering drains or water course.

### **Section 7 - HANDLING AND STORAGE**

## PROCEDURE FOR HANDLING

- Avoid all personal contact, including inhalation.
- Wear protective clothing when risk of exposure occurs.
- Use in a well-ventilated area.
- Prevent concentration in hollows and sumps.

Empty containers may contain residual dust which has the potential to accumulate following settling. Such dusts may explode in the presence of an appropriate ignition source.

- Do NOT cut, drill, grind or weld such containers.
- In addition ensure such activity is not performed near full, partially empty or empty containers without appropriate workplace safety authorisation or permit.

## RECOMMENDED STORAGE METHODS

- Lined metal can, lined metal pail/ can.
- Plastic pail.
- Polyliner drum.
- Packing as recommended by manufacturer.

For low viscosity materials

- Drums and jerricans must be of the non-removable head type.
- Where a can is to be used as an inner package, the can must have a screwed enclosure.

<. All inner and sole packagings for substances that have been assigned to Packaging Groups I or II on the basis of inhalation toxicity criteria, must be hermetically sealed.

## STORAGE REQUIREMENTS

- Store in original containers.
- Keep containers securely sealed.
- Store in a cool, dry, well-ventilated area.
- Store away from incompatible materials and foodstuff containers.

## Section 8 - EXPOSURE CONTROLS / PERSONAL PROTECTION

### EXPOSURE CONTROLS

Source	Material	TWA ppm	TWA mg/m <sup>3</sup>	STEL ppm	STEL mg/m <sup>3</sup>	Peak ppm	Peak mg/m <sup>3</sup>	TWA F/CC	Notes
Canada - Ontario Occupational Exposure Limits	3-nitrobenzonitrile (Particles (Insoluble or Poorly Soluble) Not Otherwise)		10 (I)						
Canada - British Columbia Occupational Exposure Limits	3-nitrobenzonitrile (Particles (Insoluble or Poorly Soluble) Not Otherwise Classified (PNOC))		10 (N)						
Canada - Ontario Occupational Exposure Limits	3-nitrobenzonitrile (Specified (PNOS) / Particules (insolubles ou peu solubles) non précisées par ailleurs)		3 (R)						
US - Tennessee Occupational Exposure Limits - Limits For Air Contaminants	3-nitrobenzonitrile (Particulates not otherwise regulated Respirable fraction)		5						

US - California Permissible Exposure Limits for Chemical Contaminants	3-nitrobenzonitrile (Particulates not otherwise regulated Respirable fraction)		5	(n)
US - Oregon Permissible Exposure Limits (Z-1)	3-nitrobenzonitrile (Particulates not otherwise regulated (PNOR) (f) Total Dust)	-	10	Bold print identifies substances for which the Oregon Permissible Exposure Limits (PELs) are different than the federal Limits. PNOR means "particles not otherwise regulated."
US - Michigan Exposure Limits for Air Contaminants	3-nitrobenzonitrile (Particulates not otherwise regulated, Respirable dust)		5	
US - Oregon Permissible Exposure Limits (Z-1)	3-nitrobenzonitrile (Particulates not otherwise regulated (PNOR) (f) Respirable Fraction)	-	5	Bold print identifies substances for which the Oregon Permissible Exposure Limits (PELs) are different than the federal Limits. PNOR means "particles not otherwise regulated."
US - Wyoming Toxic and Hazardous Substances Table Z1 Limits for Air Contaminants	3-nitrobenzonitrile (Particulates not otherwise regulated (PNOR)(f)- Respirable fraction)		5	

## PERSONAL PROTECTION



## RESPIRATOR

•Particulate. (AS/NZS 1716 & 1715, EN 1432000 & 1492001, ANSI Z88 or national equivalent)

## EYE

- Safety glasses with side shields.
- Chemical goggles.
- Contact lenses may pose a special hazard; soft contact lenses may absorb and concentrate irritants. A written policy document, describing the wearing of lens or restrictions on use, should be created for each workplace or task. This should include a review of lens absorption and adsorption for the class of chemicals in use and an

account of injury experience. Medical and first-aid personnel should be trained in their removal and suitable equipment should be readily available. In the event of chemical exposure, begin eye irrigation immediately and remove contact lens as soon as practicable. Lens should be removed at the first signs of eye redness or irritation - lens should be removed in a clean environment only after workers have washed hands thoroughly. [CDC NIOSH Current Intelligence Bulletin 59], [AS/NZS 1336 or national equivalent]

#### **HANDS/FEET**

- Wear chemical protective gloves, eg. PVC.
- Wear safety footwear or safety gumboots, eg. Rubber

#### **NOTE**

- The material may produce skin sensitisation in predisposed individuals. Care must be taken, when removing gloves and other protective equipment, to avoid all possible skin contact.
- Contaminated leather items, such as shoes, belts and watch-bands should be removed and destroyed.

Suitability and durability of glove type is dependent on usage. Important factors in the selection of gloves include

- frequency and duration of contact,
- chemical resistance of glove material,
- glove thickness and
- dexterity

#### **OTHER**

- Overalls.
- Eyewash unit.
- Barrier cream.
- Skin cleansing cream.

#### **ENGINEERING CONTROLS**

Engineering controls are used to remove a hazard or place a barrier between the worker and the hazard. Well-designed engineering controls can be highly effective in protecting workers and will typically be independent of worker interactions to provide this high level of protection.

The basic types of engineering controls are

Process controls which involve changing the way a job activity or process is done to reduce the risk.

Enclosure and/or isolation of emission source which keeps a selected hazard "physically" away from the worker and ventilation that strategically "adds" and "removes" air in the work environment.

### **Section 9 - PHYSICAL AND CHEMICAL PROPERTIES**

#### **PHYSICAL PROPERTIES**

Solid.

Does not mix with water.

Contact with acids liberates very toxic gas.

State	Divided solid	Molecular Weight	148.12
Melting Range (°F)	239- 243	Viscosity	Not Applicable
Boiling Range (°F)	Not available	Solubility in water (g/L)	Partly miscible
Flash Point (°F)	Not available	pH (1% solution)	Not applicable.
Decomposition Temp (°F)	Not Available	pH (as supplied)	Not applicable
Autoignition Temp (°F)	Not available	Vapour Pressure (mmHG)	Negligible
Upper Explosive Limit (%)	Not available	Specific Gravity (water=1)	Not available
Lower Explosive Limit (%)	Not available	Relative Vapour Density (air=1)	>1
Volatile Component (%vol)	Negligible	Evaporation Rate	Not applicable

#### **APPEARANCE**

Powder; does not mix well with water.

### **Section 10 - CHEMICAL STABILITY**

## CONDITIONS CONTRIBUTING TO INSTABILITY

- Presence of incompatible materials.
- Product is considered stable.
- Hazardous polymerisation will not occur.

## STORAGE INCOMPATIBILITY

- Avoid strong acids, acid chlorides, acid anhydrides and chloroformates.
- Nitriles may polymerise in the presence of metals and some metal compounds.
- They are incompatible with acids; mixing nitriles with strong oxidising acids can lead to extremely violent reactions.
- Nitriles are generally incompatible with other oxidising agents such as peroxides and epoxides.
- The combination of bases and nitriles can produce hydrogen cyanide. Nitriles are hydrolysed exothermally in both aqueous acid and base to give carboxylic acids (or salts of carboxylic acids).
- The covalent cyano group is endothermic and many organic nitriles are reactive under certain conditions; N-cyano derivatives are reactive or unstable.
- The majority of endothermic compounds are thermodynamically unstable and may decompose explosively under various circumstances of initiation.
- Many but not all endothermic compounds have been involved in decompositions, reactions and explosions and, in general, compounds with significantly positive values of standard heats of formation, may be considered suspect on stability grounds.

BRETHERRICK L. Handbook of Reactive Chemical Hazards.

- Nitroaromatic and in particular polynitroaromatic compounds may present a severe explosion risk if subjected to shock or heated rapidly and uncontrollably as in fire situations.
- In addition, when such compounds are heated more moderately with caustic alkalies, even when water or organic solvents are present, there is also a risk of violent decomposition or explosion - several industrial accidents, which probably were due to such interactions, have occurred; this potential hazard often remains unacknowledged.
- Aromatic nitro compounds range from slight to strong oxidizing agents. If mixed with reducing agents, including hydrides, sulfides and nitrides, they may begin a vigorous reaction that culminates in a detonation. The explosive tendencies of aromatic nitro compounds are increased by the presence of multiple nitro groups.
- A range of exothermic decomposition energies for nitro compounds is given as 220-410 kJ/mol. The relationship between energy of decomposition and processing hazards has been the subject of discussion; it is suggested that values of energy released per unit of mass, rather than on a molar basis (J/g) be used in the assessment. For example, in "open vessel processes" (with man-hole size openings, in an industrial setting), substances with exothermic decomposition energies below 500 J/g are unlikely to present a danger, whilst those in "closed vessel processes" (opening is a safety valve or bursting disk) present some danger where the decomposition energy exceeds 150 J/g.
- Avoid reaction with oxidising agents, bases and strong reducing agents.

For incompatible materials - refer to Section 7 - Handling and Storage.

## Section 11 - TOXICOLOGICAL INFORMATION

3-nitrobenzonitrile

### TOXICITY AND IRRITATION

■ unless otherwise specified data extracted from RTECS - Register of Toxic Effects of Chemical Substances.

■ Contact allergies quickly manifest themselves as contact eczema, more rarely as urticaria or Quincke's oedema. The pathogenesis of contact eczema involves a cell-mediated (T lymphocytes) immune reaction of the delayed type. Other allergic skin reactions, e.g. contact urticaria, involve antibody-mediated immune reactions. The significance of the contact allergen is not simply determined by its sensitisation potential the distribution of the substance and the opportunities for contact with it are equally important. A weakly sensitising substance which is widely distributed can be a more important allergen than one with stronger sensitising potential with which few individuals come into contact. From a clinical point of view, substances are noteworthy if they produce an allergic test reaction in more than 1% of the persons tested.

Asthma-like symptoms may continue for months or even years after exposure to the material ceases. This may be due to a non-allergenic condition known as reactive airways dysfunction syndrome (RADS) which can occur



following exposure to high levels of highly irritating compound.  
No significant acute toxicological data identified in literature search.

## Section 12 - ECOLOGICAL INFORMATION

This material and its container must be disposed of as hazardous waste.

## Section 13 - DISPOSAL CONSIDERATIONS

### US EPA Waste Number & Descriptions

#### A. General Product Information

Reactivity characteristic: use EPA hazardous waste number D003 (waste code R).

#### Disposal Instructions

All waste must be handled in accordance with local, state and federal regulations.

- Containers may still present a chemical hazard/ danger when empty.
- Return to supplier for reuse/ recycling if possible.

Otherwise:

- If container can not be cleaned sufficiently well to ensure that residuals do not remain or if the container cannot be used to store the same product, then puncture containers, to prevent re-use, and bury at an authorised landfill.
- Where possible retain label warnings and MSDS and observe all notices pertaining to the product.

Legislation addressing waste disposal requirements may differ by country, state and/ or territory. Each user must refer to laws operating in their area. In some areas, certain wastes must be tracked.

A Hierarchy of Controls seems to be common - the user should investigate:

- Reduction
- Reuse
- Recycling
- Disposal (if all else fails)

This material may be recycled if unused, or if it has not been contaminated so as to make it unsuitable for its intended use. Shelf life considerations should also be applied in making decisions of this type. Note that properties of a material may change in use, and recycling or reuse may not always be appropriate. In most instances the supplier of the material should be consulted.

- DO NOT allow wash water from cleaning or process equipment to enter drains.
- It may be necessary to collect all wash water for treatment before disposal.
- In all cases disposal to sewer may be subject to local laws and regulations and these should be considered first.
- Where in doubt contact the responsible authority.
- Recycle wherever possible.
- Consult manufacturer for recycling options or consult local or regional waste management authority for disposal if no suitable treatment or disposal facility can be identified.
- Dispose of by: burial in a land-fill specifically licenced to accept chemical and / or pharmaceutical wastes or Incineration in a licenced apparatus (after admixture with suitable combustible material)
- Decontaminate empty containers. Observe all label safeguards until containers are cleaned and destroyed.

## Section 14 - TRANSPORTATION INFORMATION

DOT:

Symbols:	None	Hazard class or Division:	6.1
Identification Numbers:	UN2811	PG:	II
Label Codes:	6.1	Special provisions:	IB8, IP2, IP4, T3, TP33
Packaging: Exceptions:	153	Packaging: Non-bulk:	212
Packaging: Exceptions:	153	Quantity limitations: Passenger aircraft/rail:	25 kg

Quantity Limitations: Cargo 100 kg  
aircraft only:

Vessel stowage: Location: B

Vessel stowage: Other: None

Hazardous materials descriptions and proper shipping names:

Toxic solids, organic, n.o.s.

**Air Transport IATA:**

ICAO/IATA Class:	6.1	ICAO/IATA Subrisk:	None
UN/ID Number:	2811	Packing Group:	II
Special provisions:	A3		
Cargo Only			
Packing Instructions:	676	Maximum Qty/Pack:	100 kg
Passenger and Cargo		Passenger and Cargo	
Packing Instructions:	669	Maximum Qty/Pack:	25 kg
Passenger and Cargo Limited Quantity		Passenger and Cargo Limited Quantity	
Packing Instructions:	Y644	Maximum Qty/Pack:	1 kg

Shipping name: TOXIC SOLID, ORGANIC, N.O.S. (contains 3-nitrobenzonitrile)

**Maritime Transport IMDG:**

IMDG Class:	6.1	IMDG Subrisk:	None
UN Number:	2811	Packing Group:	II
EMS Number:	F-A, S-A	Special provisions:	274
Limited Quantities:	500 g		

Shipping name: TOXIC SOLID, ORGANIC, N.O.S. (contains 3-nitrobenzonitrile)

## Section 15 - REGULATORY INFORMATION

**3-nitrobenzonitrile (CAS: 619-24-9) is found on the following regulatory lists;**

"Canada Non-Domestic Substances List (NDSL)", "US Toxic Substances Control Act (TSCA) - Chemical Substance Inventory"

## Section 16 - OTHER INFORMATION

### LIMITED EVIDENCE

■ Cumulative effects may result following exposure\*.

\* (limited evidence).

### Denmark Advisory list for selfclassification of dangerous substances

Substance	CAS	Suggested codes
3- nitrobenzonitrile	619- 24- 9	R43 N; R50

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■ Classification of the preparation and its individual components has drawn on official and authoritative sources as well as independent review by the Chemwatch Classification committee using available literature references.

A list of reference resources used to assist the committee may be found at:  
[www.chemwatch.net/references](http://www.chemwatch.net/references).

■ The (M)SDS is a Hazard Communication tool and should be used to assist in the Risk Assessment. Many factors determine whether the reported Hazards are Risks in the workplace or other settings.

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