



CLSI PROPOSAL SUBMISSION

GENERAL USER

Proposal #13-3048
02B1-1 (Far IR)

Date Submitted: 2010-08-19
Cycle 13 (January 2011 - June 2011)

Title of Proposal:	The far-infrared ro-vibrational spectrum of cyanogen isothiocyanate, NCNCS, and sulfur dicyanide, S(CN) ₂ , in the light of quantum monodromy
Type of Proposal:	General User
Proposal Duration:	4 cycles (24 months)
Subject of Research	Material and Chemical Sciences
Industrial Partners Involved?	No
Five Key Words	cyanogen iso-thiocyanate, NCNCS, high resolution, far-infrared, quantum monodromy
Funding Sources	NSERC, Max Planck Award Funds

RESEARCH TEAM						
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Spokesperson						
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Other Research Team Members						
Frank	De Lucia	Ohio State University	fcd@mps.ohio-state.edu	Physics	Faculty	Not Coming to CLS
Stephen	Ross	University of New Brunswick	sross@unb.ca	Physics	Faculty	Not Coming to CLS
Brenda	Winnewisser	The Ohio State University	winnebp@mps.ohio-state.edu	Department of Physics	Faculty	Not Coming to CLS
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BRIEF DESCRIPTION

Cyanogen iso-thiocyanate, NCNCS, (see Figure 1) is a particularly good example of a molecule exhibiting quantum monodromy. This is the topological property of the rotational-vibrational energy levels of chain molecules for which a two-dimensional bending potential energy function has the form of the bottom of a champagne bottle, with a hump or barrier at the linear conformation. NCNCS has been shown to clearly exhibit a distinctive monodromy-induced dislocation of the energy level patterns at the top of the potential energy hump [B. P. Winnewisser et al., Phys. Chem. Chem. Phys., 12, 8158-8189 (2010)]. The generalized semi-rigid bender (GSRB) Hamiltonian wave functions are used to show that the expectation values of any physical quantity which varies with the large amplitude bending coordinate will also exhibit monodromy-induced dislocations. This includes the rotational constant B and the electric dipole moment components μ_a and μ_b . The calculated expectation values of these latter quantities indicate sizable ro-vibrational transition moments that will make a far-infrared spectrum of NCNCS possible. This spectrum promises to have a highly anomalous but systematic form, qualitatively very different from that of either a linear or bent asymmetric rotor pattern. Since according to our knowledge there is no NCNCS infrared spectrum reported in the literature, except band centers from our ab-initio predictions [B. P. Winnewisser et al., Phys. Rev. Lett., 95, 243002 (2005)], we hope we can use the far-infrared spectrometer at the Canadian Light Source to study these spectra. This facility provides exceptionally high spectral resolution, and very intense far-infrared light from the synchrotron. A clean synthesis of NCNCS (see Figure 1) requires pyrolysis of S(CN)₂ (see Figure 2). The literature provides no gas phase far-infrared spectra of these species. Since we must identify possible impurities, the project must necessarily include the measurement of the FIR spectrum of S(CN)₂, which is known, from its pure rotational spectrum, to be a rather rigid molecule with a conventional small-amplitude vibrational spectrum. The project thus consists of measuring the FIR spectrum of these two related molecules in the gas-phase.

SCIENTIFIC MERIT

The concept of monodromy (Greek for "once around") in a champagne bottle potential function was introduced by the Canadian mathematician Larry Bates in 1991 [L. M. Bates, *Z. Angew. Math. Phys.*, 42, 837 (1991)]. He pointed out that the potential function is circularly symmetric with two conserved physical quantities: energy and angular momentum. At the energy of the top of the hump, called the monodromy point, the topology of the potential energy surface bifurcates according to Bates into two distinct spaces as indicated in Figure 1. This is a very fundamental and robust property of such two-dimensional potential surfaces with a singular point. The topology of such a system exists independently of what coordinates we might happen to choose to solve the Schroedinger equation. In quantum mechanics, classical monodromy translates into a dislocation or defect in the pattern of discrete energy levels around the monodromy point in the energy-momentum map. The change in topology involves the reclassification of one degree of freedom from rotational (below the barrier) to vibrational (above the barrier), a transition which is considerably more abrupt than was thought earlier.

Quantum monodromy is therefore a fundamental property of the ro-vibrational energy levels of chain molecules for which a two-dimensional bending potential energy function has the form of the bottom of a champagne bottle, with a hump or punt at the linear configuration. NCNCS is a particularly excellent example of such a molecule as shown already in an early study by Kroto and coworkers [M. A. King, H. W. Kroto, and B. M. Landsberg, *J. Mol. Spectrosc.* 113, 1 (1985)] and clearly exhibits a distinctive monodromy-induced dislocation of the energy level pattern at the top of the potential energy hump of the NCN bending mode (see Figure 1). Indeed, NCNCS [B. P. Winnewisser et al., *Phys. Rev. Lett.* 95, 243002 (2005)] and the water molecule [N. F. Zobov et al., *Chem. Phys. Lett.* 414, 193-197 (2005)] were the first two examples for which experimental confirmation of molecular quantum monodromy was obtained. We used the fast scan sub-millimeter spectroscopic technique (FASSST) at the Department of Physics of the Ohio State University to extend the measurements and spectral analysis to pure rotational transitions (end-over-end) in three bending vibrational states lying above the monodromy point [B. P. Winnewisser et al., *Phys. Chem. Chem. Phys.*, 12, 8158-8189 (2010)]. The analysis of 9204 lines assigned to 7 vibrational states showed that the topological properties of the bending potential function are mapped onto every aspect of the ro-vibrational energy levels involving excitation of the quasi-linear bending vibration. In order to model the large-amplitude dynamics of such a molecular system, and also to achieve some insight beyond satisfactory parameters for reproducing the spectrum, we used the generalized semi-rigid bender (GSRB) Hamiltonian.

The analysis was supplemented with information from ab initio calculations. In order to model the large amplitude dynamics of the NCNCS molecular system, we used the generalized semi-rigid bender (GSRB) Hamiltonian developed by Stephen C. Ross [see B. P. Winnewisser et al., *Phys. Chem. Chem. Phys.*, 12, 8158-8189 (2010)]. This Hamiltonian provides a good description of the energy levels over the seven bending states observed, coming close to experimental accuracy. High level ab initio calculations not only provided the molecular equilibrium structure of NCNCS, but also the electric dipole moment components μ_a and μ_b as functions of the large-amplitude bending coordinate. Calculated expectation values of these quantities for individual ro-vibrational levels show the now-recognizable monodromy pattern. Although the Hamiltonian is not new, the patterns exhibited by the data and reproduced by the model reveal forms that were unforeseen.

Figure 3 shows two monodromy plots for NCNCS. Panel a shows the experimental (connected by lines) and calculated quantum lattice of the effective rotational constants B_{eff} as a function of K_a and ν_b representing the end-over-end rotational contribution. The GSRB Hamiltonian allowed us to calculate the bending-rotation term values $E(K_a; \nu_b)$ with an uncertainty of approximately $\pm 1.5 \text{ cm}^{-1}$. In panel b of Figure 3 they are plotted for $J = K_a$ versus K_a yielding a two-dimensional energy-momentum map. This bending-energy-momentum map is the basis of our present proposal: the predicted bending vibrational energy eigenvalues, together with the electric dipole expectation values, provide us with excellent predictions of the FIR spectrum, both in wavenumber and intensity. An excerpt of the energy-momentum map is shown in Figure 4 which also indicates samples of the allowed a-type and b-type far-infrared transitions and their corresponding selection rules. In summary this will lead to a plethora of a-type and b-type ro-vibrational far-infrared bands extending from about 30 cm^{-1} to 250 cm^{-1} . The overlap of the various components of the band system is shown in Figure 5 with the overlaid signal/noise enhancements achievable with a synchrotron FIR source according to A. R. W. McKellar (*J. Mol. Spectrosc.* 262, 1-10 (2010)). The stick spectrum of NCNCS displayed in Figure 5 is presently limited to $J \leq 10$ (i.e., severely truncated) and $\nu_b \leq 6$. The observation of the FIR spectrum of NCNCS will without doubt advance our knowledge concerning the effects of monodromy on the spectra of quasi-linear molecules. In NCNCS the transition past the monodromy point can be followed with no interference of other vibrational modes, allowing us the study of the patterns that underly the spectra of other molecules including water. In contrast $\text{S}(\text{CN})_2$ will have a conventional, small-amplitude spectrum of an asymmetric rotor molecule.

EXPERIMENT PROCEDURE

The spectral region of interest is from 30 cm^{-1} to 250 cm^{-1} . In this spectral region the two molecules of interest have predicted far-infrared absorptions: 1) the precursor molecule sulfur dicyanide, $\text{S}(\text{CN})_2$, centered at 135 cm^{-1} as shown in Figure 2, and 2) NCNCS in the range from 30 cm^{-1} to 250 cm^{-1} shown in Figure 5. The chemical synthesis of $\text{S}(\text{CN})_2$ and NCNCS at the CLS facility will be the responsibility of Manfred Winnewisser. He has prepared both samples at OSU for the recent work on NCNCS. To 1: Sulfur dicyanide, $\text{S}(\text{CN})_2$, is synthesized by using 26.5 g of silver cyanide, AgCN , dispersed by vigorous stirring in 200 ml of carbon disulphide, CS_2 , in a three neck flask kept at a temperature of 30°C . Over a period of 30 min 10 ml of sulphur dichloride, SCI_2 , is added using a disposable syringe. After a reaction time of 10 min reflux of CS_2 was observed in the reflux condenser. The reaction is kept going for at least 10 more minutes after all SCI_2 is added. At this stage the solvent with the reaction product is simply transferred into a Schlenk tube. The lower part of this tube is cooled to dry ice temperature and the product $\text{S}(\text{CN})_2$ crystallizes out in beautiful colourless plate-like crystals. The bulk of the cold CS_2 solvent is then decanted off. The remaining CS_2 is removed by attaching the Schlenk tube to a vacuum line until the vapour pressure of the content [mainly $\text{S}(\text{CN})_2$ and un-reacted SCI_2] reaches less than 2 Torr. The sample is stored by keeping the Schlenk tube at dry ice temperature.

To 2: Cyanogen iso-thiocyanate, NCNCS, is prepared by the pyrolytic isomerization reaction of sulfur dicyanide, S(CN)₂. All NCNCS spectral measurements will be carried out in a flow regime with the Schlenk tube directly attached to the inlet port of the vacuum pyrolysis system, which in turn is connected to an inlet port of the absorption cell (2 m cold multi-reflection cell). In order to maintain sufficient S(CN)₂ vapor pressure in the pyrolysis tube for the isomerization reaction, the Schlenk tube will be kept at room temperature with a flow of dry argon as an entraining gas. The quartz pyrolysis tube will be heated to ca. 855C and the reaction zone, about 20 cm in length, is filled with crushed quartz chips which are secured on both sides with quartz wool. The hot reaction gases pass through a cold trap at -45C in order to remove the un-reacted S(CN)₂ before the gaseous reaction products enter the absorption cell. During the measurements a total pressure from 5 mTorr to 1 Torr can be maintained for the flow. From the FASSST spectra, which have a signal to noise of about 2000 : 1 for the strong NCNCS lines, only trace amounts of HCN and HNCS were identified. These are secondary reaction products of NCNCS and S(CN)₂. No S(CN)₂ lines could be identified. Thus, a very pure NCNCS gas sample can be expected.

All chemicals needed will be ordered from Sigma-Aldrich by the OSU team member Manfred Winnewisser and shipped directly to the CLS facility c/o Dr. Brant Billingham. The material safety data sheets will be provided by Sigma-Aldrich. Furthermore, the necessary chemical glassware and ancillary equipment will be provided by the OSU laboratory and shipped to CLS. The data collection will be the primary responsibility of Dennis Tokaryk and Manfred Winnewisser. The assignment and analysis of the spectra will be a joint effort by Dennis Tokaryk, Stephen Ross, Manfred Winnewisser and Brenda Winnewisser.

SUITABILITY

The spectrum of NCNCS presents two problems that make it necessary to use the far-infrared beamline at the CLS:

1. The spectrum of interest may well be entangled with that of the precursor molecule, S(CN)₂, which has an infrared band around 135 cm⁻¹. Therefore, the high resolution and high signal-to-noise ratio afforded by the synchrotron-based experiment is necessary to distinguish lines of NCNCS from those of S(CN)₂. Further, since the 135 cm⁻¹ band of the precursor is not yet known, we will measure it on its own, both to eliminate its signature from the NCNCS spectrum and because it is worthy of analysis and publication in its own right.

2. The NCNCS spectrum expected to be very dense in the 20-200 cm⁻¹ range (see Fig. 5) due to the presence of many overlapping hot bands, and we will only succeed in a convincing analysis if we obtain data at the maximum available resolution and with the highest signal-to-noise ratio possible. The far-infrared beamline at the CLS has proven itself capable of generating spectra that are highly competitive on both grounds, and its performance in the region of interest is expected to improve dramatically once the adaptive-optics system is put in place during Sept.-Oct. 2010.

The amount of beam-time requested is based on past experience by Dennis Tokaryk with the system, and gives realistic estimates of the time required necessary to set up the flow system, to properly calibrate the spectra, and to take background and data spectra, including optimizing the pyrolysis flow in real time. The synthesis of the precursor molecule will be carried out prior to the requested beamtime.

PAST PRODUCTIVITY - Shifts received in the past two years:

Access Mechanism	Cycle 10	Cycle 11	Cycle 12	Cycle 13
General User	34	0	38	42
Total Shifts	34	0	38	42

a) D. Tokaryk has had great success in obtaining gas-phase spectra of very high quality from stable 5-membered ring molecules (pyrrole, furan, thiophene, pyrazole, and imidazole), with 5 CLS publications so far on pyrrole, thiophene, and acrolein. Data on pyrazole in particular are particularly rich and complete; since upwards of 20 bands have been observed (and each band requires 3000-4000 lines to be assigned) finalizing the analysis is quite time-consuming. More recently, equally good spectra of the less stable species malonaldehyde, which required an on-site synthesis to create. These spectra are particularly challenging to analyze, involving systematic perturbations and a doubling of the spectrum due to a quantum-mechanical tunnelling effect. Significant progress has been made on most bands in this molecule, and time has been scheduled to complete the project by taking further data in Dec. 2010.

No other member of the research team has previous experience working at the CLS, or at any other synchrotron facility with a far-IR beamline.

b) The spokesperson of the research team, Dennis Tokaryk, has extensive experience with running experiments of this type at the CLS. He has been involved in collecting and analyzing data on acrolein, pyrrole, pyrazole, furan, and thiophene. Stephen Ross developed the GSRB Hamiltonian that was used in the predictions of the far-infrared spectrum of NCNCS and which is displayed in Figure 5. His expertise will be essential during the analysis of the expected far-infrared data to be obtained at the CLS. Manfred Winnewisser has extensive experience in the chemical synthesis of unstable molecular species, and he and Brenda P Winnewisser both have credentials in high-resolution millimeter wave and Fourier transform spectroscopy of unstable species. The Winnewissers had in the past an intensive collaboration with Bruker Optics to develop and build Bruker's first high resolution and performance Fourier transform spectrometer, the HR120FTS. [A. Keens, J. Mol. Structure 695-696, 379-384 (2004)]. The CLS Bruker spectrometer, IFS125HR, is the latest model of this early development. Frank DeLucia designed and built with his research group

the fast scan sub-millimeter spectroscopic technique (FASSST) spectrometer, which allowed us to obtain superb NCNCS rotational spectra, that provided the basis for this application. The microwave laboratory at OSU has broad expertise with data reduction and assignment procedures. The computer-aided assignment of asymmetric rotor spectra (CAAARS) provides an integrated suite of computer programs to simplify and speed up the spectral analysis [I. R. Medvedev et al., J. Mol. Structure 742 229-236 (2005)]. The rotational spectrum of S(CN)₂ was measured in the OSU laboratory prior to the NCNCS measurements.

BEAMLINE REQUIREMENTS

Beamline:	02B1-1 (Far IR)
CLS Staff Contacted:	Brant Billingham
Endstation:	
Technique:	High Resolution Gas-phase spectroscopy
Wavelength / Energy Range:	30-250 cm ⁻¹ Angstrom
Spotsize on Sample:	1-1.5 mm
Energy Resolution:	deltaE/E

SCHEDULING REQUIREMENTS

Total # shifts for entire proposal:

21

Anticipated Timeline

of 8-hour shifts requested

Cycle

Cycle 13 - January - June, 2011

21

Cycle 14 - July - December, 2011

0

Cycle 15 - January - June, 2012

0

Cycle 16 - July - December, 2012

0

Specific scheduling requirements:

Some shifts (~6) are required for setting up the pyrolysis apparatus and adjusting conditions to create NCNCS

Preferred dates (current cycle)

2011-04-24 to 2011-06-30

Unacceptable dates (current cycle)

SAFETY AND MATERIALS

Chemical Information

Are you bringing any hazardous chemical materials to the CLS? Yes

Chemical Materials

Name	CAS/UN #	State	Quantity	Units	Known Hazards
AgCN	506-64-9	solid	100	g	Toxic
CS2	75-15-0	liquid	500	g	Flammable, Toxic
SCI2	10545-99-0	liquid	50	g	Dangerous Reactive Material, Flammable, Toxic

Will any sample preparation be done while at the CLS? No

Will any chemical waste be generated while at the CLS? No

Biological Information

Are you bringing any biological materials to the CLS? No

Does this research involve human tissue and/or biological fluids? No

Does this research involve the study of aboriginal people's culture? No

Does this research involve:

Live animals? No

Animal tissue and/or biological fluids from live animals? No

Does your work involve Genetically Modified Organisms, Genetically Modified Microorganisms or Transgenic Organisms? No

Radioactive Material Information

Are you bringing anything radioactive? No

Nano Material Information

Are you bringing any nanomaterials to the CLS? No

Pesticide Information

Are you bringing pesticides to the CLS? No

EQUIPMENT

Are you bringing any equipment to the CLS to assist you with this experiment? Yes

Name	Commercial Product	Precautions	Make	Model	Manufacturer
Pyrolysis furnace	N				

ANCILLARY FACILITIES REQUESTED

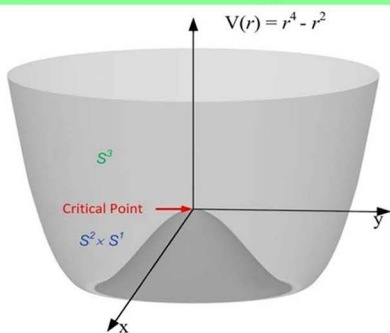
Fume Hood

Wet Lab

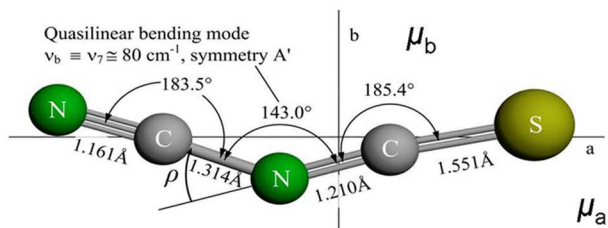
Person(s) Preparing Samples

Manfred Winnewisser - Wet Lab, Fume Hood

Large amplitude bending potential function



Ab initio equilibrium structure of NCNCS
CCSD(T)/cc-pV5Z level of theory



Winnewisser et al.
PRL **95**, 243002 (2005)

PHYSICAL REVIEW LETTERS

week ending
9 DECEMBER 2005

TABLE I. *Ab initio* predicted harmonic and anharmonic fundamental vibrational modes for NCNCS (Symmetry C_s).

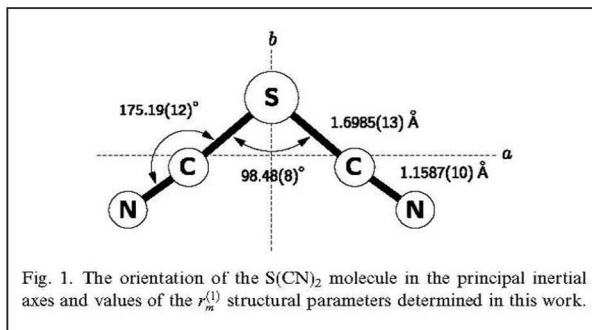
ν	Γ	ω^a	ν^a	Harmonic potential energy distribution
				[N(1)C(2)N(3)C(4)S(5)]
ν_1	A'	2302	2258	73% 1-2 s ^b , 22% 2-3 s
ν_2	A'	2058	2024	74% 3-4 s, 15% 4-5 s, 10% 1-2 s
ν_3	A'	1188	1178	47% 2-3 s, 41% 4-5 s, 13% 1-2 s
ν_4	A'	688	662	39% 4-5 s, 31% 2-3 s, 25% 3-4 s
ν_5	A'	483	472	68% 3-4-5 b, 19% 1-2-3 b, 11% 2-3-4 b
ν_8	A''	452	454	65% 2-3-4-5 t, 35% 1-2-3-4 t
ν_6	A'	444	447	74% 1-2-3 b, 25% 3-4-5 b
ν_9	A''	430	429	65% 1-2-3-4 t, 35% 2-3-4-5 t
ν_7	A'	89	80	94% 2-3-4 large amplitude bend

^a ω stands for harmonic wave number in cm^{-1} , ν for anharmonic wave number in cm^{-1} .
^bs stands for stretching, b for bending, t for torsional vibration.

FIG. 1:

The volume defined by the champagne bottle potential function for the CNC two-dimensional bending mode of NCNCS bifurcates into two separate spaces with separate topologies at the critical point. The molecular structure, the IR band centers and the electric dipole moment components μ_a and μ_b as a function of the bending coordinate ρ were obtained by *ab-initio* calculations.

Molecular structure of $\text{S}(\text{CN})_2$ and lowest vibrational term values
 Z. Kisiel et al., J. Mol. Spectrosc. **246**, 39 – 56, (2007)



Lowest normal mode ν_4 at 135 cm^{-1} , Symmetry species A_1 , $\angle\text{CSC}$ bend. IR spectrum was taken in dilute samples of $\text{S}(\text{CN})_2$ in KBr.
 L. Pierce et al., J. Chem. Phys. **43**, 3423 (1965)

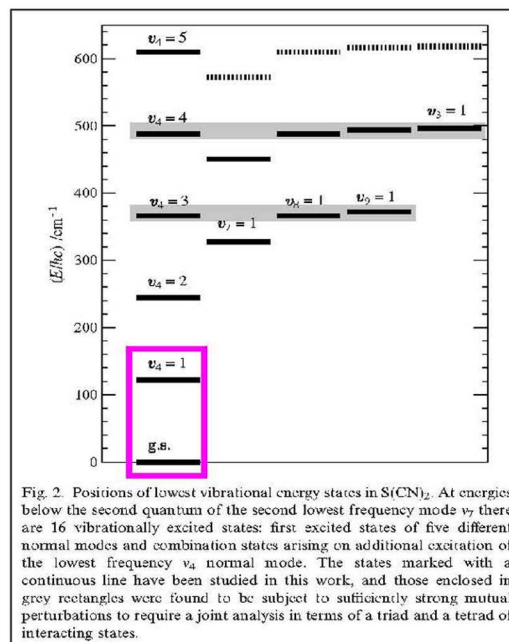


FIG. 2:

To our knowledge there do not exist any gas phase infrared spectra for $\text{S}(\text{CN})_2$ in the literature. Therefore the lowest energy bending mode ν_4 around 135 cm^{-1} must be measured during the planned campaign at the CLS.

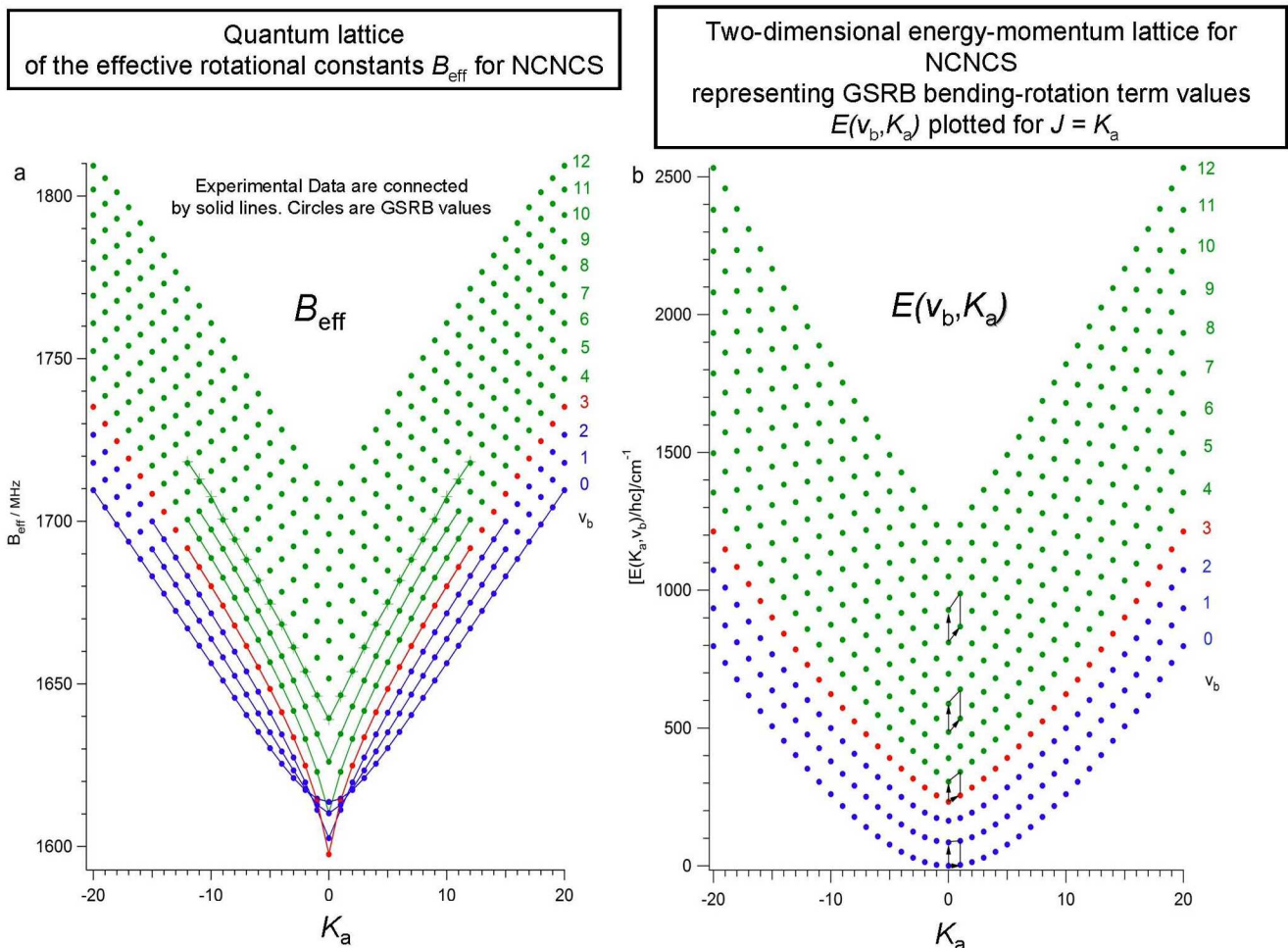


FIG. 3:

Monodromy plots for NCNCS. Panel **a** shows the experimental and calculated quantum lattice of the effective rotational constants B_{eff} as a function of K_a and v_b , representing the end-over-end rotational energy contribution. Panel **b** displays the corresponding two-dimensional bending-rotation energy-momentum map for NCNCS calculated by the GSRB. This map is the GSRB calculated basis for the far-infrared spectrum to be observed at the CLS facility.

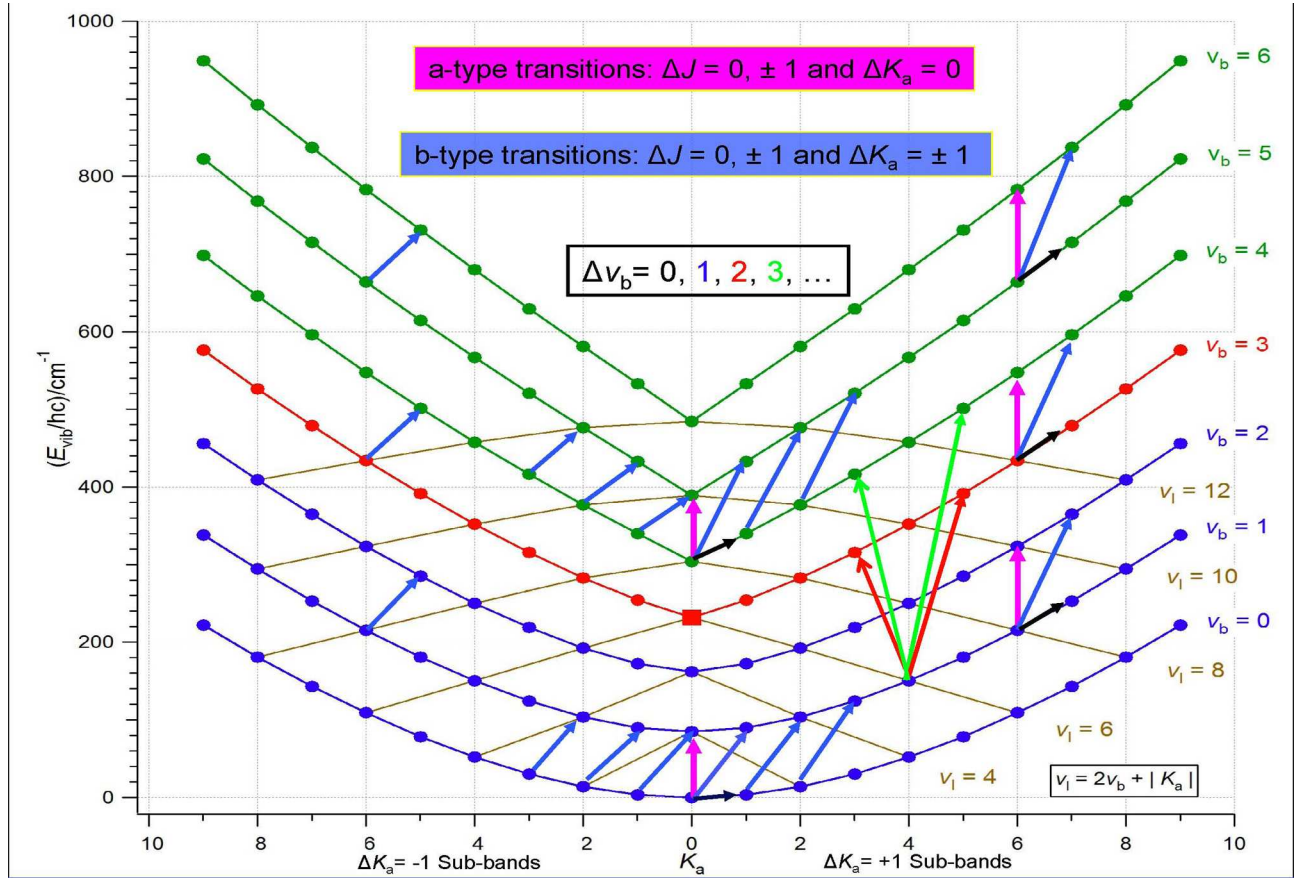


FIG. 4:

Excerpt of the energy-momentum map which indicates samples of the allowed a-type and b-type ro-vibrational far-infrared transitions. The selection rules lead to a plethora of ro-vibrational far-infrared bands extending from about 30 cm^{-1} to 250 cm^{-1} . Please note: the red square in the middle of energy-momentum plot indicates the energy level closest to the classical monodromy point which is the singular point in the potential energy surface.

Pyrolytic isomerization reaction of sulfur dicyanide, $S(CN)_2$ yields pure cyanogen iso-thiocyanate, NCNCS

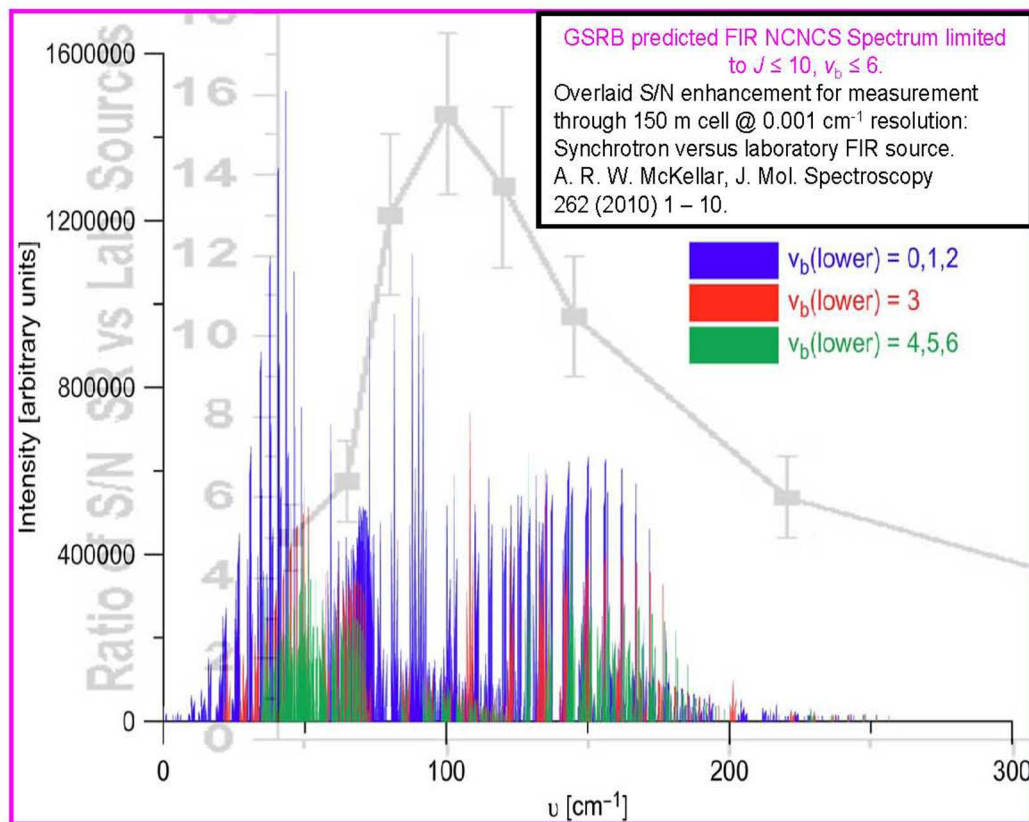


FIG. 5:

The overlap of the various components of the far-infrared sub-bands indicated in **Figure 4** will lead to a rather complex but systematic band system for NCNCS. The stick spectrum of NCNCS was predicted from calculations with the GSRB Hamiltonian. The present display is severely truncated to $J \leq 10$ and $\nu_b \leq 6$. The overlaid Signal/Noise enhancements achievable with the Synchrotron FIR source should allow us to observe a very interesting and so far unique spectrum.

1. PRODUCT AND COMPANY IDENTIFICATION

Product name : Silver cyanide

Product Number : 184535
Brand : Aldrich

Company : Sigma-Aldrich Canada, Ltd
2149 Winston Park Drive
OAKVILLE ON L6H 6J8
CANADA

Telephone : +19058299500
Fax : +19058299292
Emergency Phone # : 1-800-424-9300

2. HAZARDS IDENTIFICATION

Emergency Overview

Target Organs

Nerves., Blood, Liver, Eyes

WHMIS Classification

D1A	Very Toxic Material Causing Immediate and	Highly Toxic
D2B	Serious Toxic Effects	Moderate eye irritant

GHS Label elements, including precautionary statements

Pictogram



Signal word : Danger

Hazard statement(s)

H302	Harmful if swallowed.
H316	Causes mild skin irritation.
H318	Causes serious eye damage.

Precautionary statement(s)

P280	Wear protective gloves/eye protection/face protection.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

HMIS Classification

Health hazard:	2
Chronic Health Hazard:	*
Flammability:	0
Physical hazards:	0

Potential Health Effects

Inhalation	May be harmful if inhaled. Causes respiratory tract irritation.
Skin	May be harmful if absorbed through skin. Causes skin irritation. May be fatal if absorbed through skin.
Eyes	Causes eye irritation.
Ingestion	Toxic if swallowed.

3. COMPOSITION/INFORMATION ON INGREDIENTS

Formula : CAgN
Molecular Weight : 133.89 g/mol

CAS-No.	EC-No.	Index-No.	Concentration
Silver cyanide			
506-64-9	208-048-6	006-007-00-5	-

4. FIRST AID MEASURES

General advice

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

If inhaled

If breathed in, move person into fresh air. If not breathing give artificial respiration. Consult a physician.

In case of skin contact

Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

5. FIRE-FIGHTING MEASURES

Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

Special protective equipment for fire-fighters

Wear self contained breathing apparatus for fire fighting if necessary.

6. ACCIDENTAL RELEASE MEASURES

Personal precautions

Wear respiratory protection. Avoid dust formation. Avoid breathing dust. Ensure adequate ventilation. Evacuate personnel to safe areas.

Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

Methods and materials for containment and cleaning up

Pick up and arrange disposal without creating dust. Keep in suitable, closed containers for disposal.

7. HANDLING AND STORAGE

Precautions for safe handling

Avoid contact with skin and eyes. Avoid formation of dust and aerosols.

Provide appropriate exhaust ventilation at places where dust is formed. Normal measures for preventive fire protection.

Conditions for safe storage

Keep container tightly closed in a dry and well-ventilated place.

Do not store near acids.

Light sensitive. Keep in a dry place.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Personal protective equipment

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face particle respirator type N100 (US) or type P3 (EN 143) 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).

Hand protection

Handle with gloves.

Eye protection

Face shield and safety glasses

Skin and body protection

Choose body protection according to the amount and concentration of the dangerous substance at the work place.

Hygiene measures

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance

Form	powder
Colour	beige

Safety data

pH	no data available
Melting point	no data available
Boiling point	no data available
Flash point	no data available
Ignition temperature	no data available
Lower explosion limit	no data available
Upper explosion limit	no data available
Water solubility	insoluble

10. STABILITY AND REACTIVITY

Chemical stability

Stable under recommended storage conditions.

Conditions to avoid

Contact with acids liberates very toxic gas.

Materials to avoid

acids, Aluminum

Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, nitrogen oxides (NOx), Silver/silver oxides

11. TOXICOLOGICAL INFORMATION

Acute toxicity

Skin corrosion/irritation

Skin - rabbit - Mild skin irritation - 24 h

Serious eye damage/eye irritation

Eyes - rabbit - Severe eye irritation - 24 h

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

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.

Reproductive toxicity

no data available

Specific target organ toxicity - single exposure (GHS)

no data available

Specific target organ toxicity - repeated exposure (GHS)

no data available

Aspiration hazard

no data available

Potential health effects

Inhalation	May be harmful if inhaled. Causes respiratory tract irritation.
Ingestion	Toxic if swallowed.
Skin	May be harmful if absorbed through skin. Causes skin irritation. May be fatal if absorbed through skin.
Eyes	Causes eye irritation.

Additional Information

RTECS: VW3850000

12. ECOLOGICAL INFORMATION

Toxicity

no data available

Persistence and degradability

Bioaccumulative potential

Bioaccumulation	Cyprinus carpio (Carp) - 41 d Bioconcentration factor (BCF): 866
-----------------	---

Mobility in soil

no data available

PBT and vPvB assessment

no data available

Other adverse effects

Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

13. DISPOSAL CONSIDERATIONS

Product

Observe all federal, state, and local environmental regulations. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

Contaminated packaging

Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)

UN-Number: 1684 Class: 6.1 Packing group: II
Proper shipping name: Silver cyanide
Reportable Quantity (RQ): 1 lbs
Marine pollutant: No
Poison Inhalation Hazard: No

IMDG

UN-Number: 1684 Class: 6.1 Packing group: II EMS-No: F-A, S-A
Proper shipping name: SILVER CYANIDE
Marine pollutant: Marine pollutant

IATA

UN-Number: 1684 Class: 6.1 Packing group: II
Proper shipping name: Silver cyanide

15. REGULATORY INFORMATION

DSL Status

All components of this product are on the Canadian DSL list.

WHMIS Classification

D1A	Very Toxic Material Causing Immediate and	Highly Toxic
D2B	Serious Toxic Effects	Moderate eye irritant

16. OTHER INFORMATION

Further information

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1. PRODUCT AND COMPANY IDENTIFICATION

Product name : Carbon disulfide

Product Number : 180173
Brand : Sigma-Aldrich

Company : Sigma-Aldrich Canada, Ltd
2149 Winston Park Drive
OAKVILLE ON L6H 6J8
CANADA

Telephone : +19058299500
Fax : +19058299292
Emergency Phone # : 1-800-424-9300

2. HAZARDS IDENTIFICATION

Emergency Overview

Target Organs

Eyes, Nerves., Liver, Kidney, Heart, Cardiovascular system., Male reproductive system., Female reproductive system.

WHMIS Classification

B2	Flammable liquid	Flammable liquid
D2A		Reproductive hazard
D2B		Moderate skin irritant
		Moderate eye irritant
		Mutagen

GHS Label elements, including precautionary statements

Pictogram



Signal word : Danger

Hazard statement(s)

H225	Highly flammable liquid and vapour.
H302	Harmful if swallowed.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H361	Suspected of damaging fertility or the unborn child.
H372	Causes damage to organs through prolonged or repeated exposure if inhaled.
H402	Harmful to aquatic life.

Precautionary statement(s)

P210	Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
P281	Use personal protective equipment as required.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P314	Get medical advice/attention if you feel unwell.

HMIS Classification

Health hazard:	2
Chronic Health Hazard:	*
Flammability:	3
Physical hazards:	0

Potential Health Effects

Inhalation	May be harmful if inhaled. Causes respiratory tract irritation.
Skin	May be harmful if absorbed through skin. Causes skin irritation.
Eyes	Causes eye irritation.
Ingestion	May be harmful if swallowed.

3. COMPOSITION/INFORMATION ON INGREDIENTS

Formula	: CS ₂
Molecular Weight	: 76.14 g/mol

CAS-No.	EC-No.	Index-No.	Concentration
Carbon disulphide			
75-15-0	200-843-6	006-003-00-3	-

4. FIRST AID MEASURES

General advice

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

If inhaled

If breathed in, move person into fresh air. If not breathing give artificial respiration. Consult a physician.

In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

5. FIRE-FIGHTING MEASURES

Suitable extinguishing media

For small (incipient) fires, use media such as "alcohol" foam, dry chemical, or carbon dioxide. For large fires, apply water from as far as possible. Use very large quantities (flooding) of water applied as a mist or spray; solid streams of water may be ineffective. Cool all affected containers with flooding quantities of water.

Specific hazards arising from the chemical

Flash back possible over considerable distance. Container explosion may occur under fire conditions. Vapours may form explosive mixture with air. May explode when heated.

Special protective equipment for fire-fighters

Wear self contained breathing apparatus for fire fighting if necessary.

Further information

Use water spray to cool unopened containers.

6. ACCIDENTAL RELEASE MEASURES

Personal precautions

Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.

Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

Methods and materials for containment and cleaning up

Contain spillage, and then collect with non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and place in container for disposal according to local / national regulations (see section 13).

7. HANDLING AND STORAGE

Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.

Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

Conditions for safe storage

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage. Store in cool place.

Refrigerate before opening.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Components with workplace control parameters

Components	CAS-No.	Value	Control parameters	Update	Basis
Carbon disulphide	75-15-0	TWA	4 ppm	2006-11-29	Canada. British Columbia OEL
Remarks	Contributes significantly to the overall exposure by the skin route.				
		STEL	12 ppm	2006-11-29	Canada. British Columbia OEL
	Contributes significantly to the overall exposure by the skin route.				
		TWAE V	1 ppm	2007-12-31	Canada. Ontario OELs
	Skin				
		TWA	1 ppm 3.1 mg/m ³	2009-04-30	Canada. Alberta, Occupational Health and Safety Code (table 2: OEL)
	Substance may be readily absorbed through intact skin				
		TWAE V	4 ppm 12 mg/m ³	2006-12-29	Canada. Quebec OELs
	Skin (percutaneous)				
		STEV	12 ppm 36 mg/m ³	2006-12-29	Canada. Quebec OELs
	Skin (percutaneous)				

Personal protective equipment

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type AXBEK (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).

Hand protection

Handle with gloves.

Eye protection

Face shield and safety glasses

Skin and body protection

Choose body protection according to the amount and concentration of the dangerous substance at the work place.

Hygiene measures

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance

Form	liquid
Colour	colourless
Odour	Stench.

Safety data

pH	no data available
Melting point	112 °C (234 °F) - lit.
Boiling point	46 °C (115 °F) - lit.
Flash point	-30 °C (-22 °F) - closed cup
Ignition temperature	100 °C (212 °F)
Lower explosion limit	1.3 %(V)
Upper explosion limit	50 %(V)
Vapour pressure	394.956 hPa (296.241 mmHg) at 20 °C (68 °F) 1,342.711 hPa (1,007.116 mmHg) at 55 °C (131 °F)
Density	1.266 g/mL at 25 °C (77 °F)
Water solubility	no data available
Partition coefficient: n-octanol/water	log Pow: 2.16
Relative vapour density	2.63 - (Air = 1.0)

10. STABILITY AND REACTIVITY

Chemical stability

Stable under recommended storage conditions.

Possibility of hazardous reactions

Vapours may form explosive mixture with air.

Conditions to avoid

Heat, flames and sparks.

Materials to avoid

Alkali metals, Zinc, Amines, Azides, Oxidizing agents

Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Sulphur oxides

11. TOXICOLOGICAL INFORMATION

Acute toxicity

LD50 Oral - rat - 1,200 mg/kg

LC50 Inhalation - rat - 2 h - 25 mg/l

Skin corrosion/irritation

no data available

Serious eye damage/eye irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

Laboratory experiments have shown mutagenic effects.

Genotoxicity in vivo - Human
Sister chromatid exchange

Carcinogenicity

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.

Reproductive toxicity

Suspected human reproductive toxicant
May cause reproductive disorders.

Specific target organ toxicity - single exposure (GHS)

no data available

Specific target organ toxicity - repeated exposure (GHS)

Inhalation - Causes damage to organs through prolonged or repeated exposure.

Aspiration hazard

no data available

Potential health effects

Inhalation	May be harmful if inhaled. Causes respiratory tract irritation.
Ingestion	May be harmful if swallowed.
Skin	May be harmful if absorbed through skin. Causes skin irritation.
Eyes	Causes eye irritation.

Signs and Symptoms of Exposure

May cause convulsions.

Additional Information

RTECS: FF6650000

12. ECOLOGICAL INFORMATION**Toxicity**

Toxicity to fish	LC50 - other fish - 162 mg/l - 96 h
Toxicity to algae	Growth inhibition EC50 - Chlorella pyrenoidosa - 21 mg/l - 96 h

Persistence and degradability

no data available

Bioaccumulative potential

no data available

Mobility in soil

no data available

PBT and vPvB assessment

no data available

Other adverse effects

no data available

13. DISPOSAL CONSIDERATIONS**Product**

Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Observe all federal, state, and local environmental regulations. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging

Dispose of as unused product.

14. TRANSPORT INFORMATION**DOT (US)**

UN-Number: 1131 Class: 3 (6.1) Packing group: I
Proper shipping name: Carbon disulfide
Reportable Quantity (RQ): 100 lbs
Marine pollutant: No
Poison Inhalation Hazard: No

IMDG

UN-Number: 1131 Class: 3 (6.1) Packing group: I EMS-No: F-E, S-D
Proper shipping name: CARBON DISULPHIDE
Marine pollutant: No

IATA

UN-Number: 1131 Class: 3 (6.1)
Proper shipping name: Carbon disulphide
IATA Passenger: Not permitted for transport
IATA Cargo: Not permitted for transport

15. REGULATORY INFORMATION**DSL Status**

All components of this product are on the Canadian DSL list.

WHMIS Classification

B2	Flammable liquid	Flammable liquid
D2A		Reproductive hazard
D2B		Moderate skin irritant
		Moderate eye irritant
		Mutagen

16. OTHER INFORMATION**Further information**

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The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Co., shall not be held liable for any damage resulting from handling or from contact with the above product. See reverse side of invoice or packing slip for additional terms and conditions of sale.



255 Norman.
Lachine (Montreal), Que
H8R 1A3

Material Safety Data Sheet

EMERGENCY NUMBERS:

(USA) CHEMTREC : 1(800) 424-9300 (24hrs)
(CAN) CANUTEC : 1(613) 996-6666 (24hrs)
(USA) Anachemia : 1(518) 297-4444
(CAN) Anachemia : 1(514) 489-5711

WHMIS	Protective Clothing	TDG Road/Rail
WHMIS Class: E D-1A F		TDG CLASS: 8 PG: UN1828 PIN: I

Section I. Product Identification and Uses

Product name	SULFUR DICHLORIDE	CI#	Not available.
Chemical formula	SCl ₂	CAS#	10545-99-0
Synonyms	Chlorine sulfide, Dichlorosulfane, Monosulfur dichloride, Sulfur chloride, AC-8745T, 88274	Code	AC-8745T
Supplier	Anachemia Science. 500 - 2nd Ave. Ville St. Pierre (Montreal), Que H8R 1M3	Formula weight	102.97
Material uses	For laboratory use only.		
		Supersedes	

Section II. Ingredients

Name	CAS #	%	TLV
1) SULFUR DICHLORIDE	10545-99-0	80	Not established by ACGIH Exposure limits: ACGIH Ceiling 1 ppm (6 mg/m ³)
2) SULFUR MONOCHLORIDE	10025-67-9	0-20	

Toxicity values of the hazardous ingredients

SULFUR DICHLORIDE:
LD50: Not available.
LC50: Not available.
SULFUR MONOCHLORIDE:
ORAL (LD50): Acute: 132 mg/kg (Rat).
VAPOR (LC50): Acute: 150 ppm (Mouse). 2500 mg/m³ (Rat) (4 hour(s)).

Section III. Physical Data

Physical state and appearance / Odor	Red liquid. Unpleasant odor.
pH (1% soln/water)	Not applicable.
Odor threshold	Not available.
Percent volatile	Not available.
Freezing point	Not available.
Boiling point	Not available.
Specific gravity	Not available.
Vapor density	3.55 (Air = 1)
Vapor pressure	170 mm of Hg (@ 20°C)
Water/oil dist. coeff.	Not available.
Evaporation rate	Not available.
Solubility	Decomposes in water.

Section IV. Fire and Explosion Data

Flash point	Not available.
Flammable limits	Not available.
Auto-ignition temperature	Not available.
Fire degradation products	Hydrogen chloride. Hydrogen sulfide. Oxides of sulfur (SO ₂ , SO ₃ ...).
Fire extinguishing procedures	Use dry chemical powder. DO NOT use water. Wear adequate personal protection to prevent contact with material or its combustion products. Self contained breathing apparatus with a full facepiece operated in a pressure demand or other positive pressure mode.
Fire and Explosion Hazards	Flammable/explosive hydrogen gas may be formed upon contact of this product with metals in the presence of moisture. Container explosion may occur under fire conditions or when heated. Reacts violently with water. The sensitivity to impact is not available. Emits toxic fumes under fire conditions.

Section V. Toxicological Properties

Routes of entry	Ingestion and inhalation. Eye contact. Skin contact.
Effects of Acute Exposure	May be fatal by ingestion, inhalation, or by skin absorption. Severe lachrymator. Target organs: eyes, skin, respiratory system, lungs. 5 ppm (SULFUR MONOCHLORIDE) is immediately dangerous to life or health.
Eye	Causes severe burns and loss of vision. May cause permanent damage.
Skin	Causes severe burns.
Inhalation	Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract. Inhalation may be fatal as a result of spasm, inflammation and edema of the larynx and bronchi, chemical pneumonitis and pulmonary edema. Symptoms of exposure may include burning sensation, coughing, laryngitis, dyspnea, headache, nausea, and vomiting.
Ingestion	Burns in mouth, pharynx and gastrointestinal tract. See inhalation.

Section V. Toxicological Properties

Effects of Chronic Overexposure Repeated inhalation can produce varying degree of respiratory irritation or lung damage. To the best of our knowledge, the chemical, physical, and toxicity of this substance has not been fully investigated. Carcinogenic effects: Not available. Mutagenic effects: Not available. Teratogenic effects: Not available. Toxicity of the product to the reproductive system: Not available.

Section VI. First Aid Measures

Eye contact IMMEDIATELY flush eyes with copious quantities of water for at least 15 minutes holding lids apart to ensure flushing of the entire surface. Seek immediate medical attention.

Skin contact Immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Seek immediate medical attention. Wash contaminated clothing before reusing. Discard contaminated leather articles such as shoes and belt.

Inhalation Remove patient to fresh air. Administer approved oxygen supply if breathing is difficult. Administer artificial respiration or CPR if breathing has ceased. Seek immediate medical attention.

Ingestion If conscious, wash out mouth with water. Seek immediate medical attention. Never give anything by mouth to an unconscious or convulsing person.

Section VII. Reactivity Data

Stability Stable. Conditions to avoid: High temperatures, sparks, open flames and all other sources of ignition, contamination.

Hazardous decomp. products Hydrogen chloride, sulfur oxides (SO₂, SO₃...), hydrogen sulfide. Readily hydrolyzed by moisture.

Incompatibility Reacts violently with water, acids, alcohols, bases, peroxides, amines, antimony, antimony sulfide, arsenic sulfide, chromyl chloride, sodium peroxide, phosphorus oxides, alkenes, terpenes, unsaturated glycerides, mercury oxide, acetone, aluminum, dimethylsulfoxide, tin, dimethylformamide, sodium, potassium, ammonia, dinitrogen pentoxide, nitric acid, perchloryl fluoride, lithium hexafluoroisopropylidene amide, oxidizing agents. Organic materials, metals, plastics. Iron or ferric chloride plus toluene.

Reaction Products Reacts with water and steam to produce toxic and corrosive fumes. Hazardous polymerization will not occur.

Section VIII. Preventive Measures

SULFUR DICHLORIDE

page 4/4

Protective Clothing in case of spill and leak Wear self-contained breathing apparatus, rubber boots and heavy rubber gloves. Full suit.

Spill and leak Evacuate the area. Absorb on sand or vermiculite and place in a closed container for disposal. Ventilate area and wash spill site after material pick up is complete. DO NOT empty into drains. DO NOT touch spilled material.

Waste disposal According to all applicable regulations.

Storage and Handling Store in a cool place away from heated areas, sparks, and flame. Store in a well ventilated area. Store away from incompatible materials. Do not add any other material to the container. Do not wash down the drain. Do not breathe gas/fumes/vapor/spray. In case of insufficient ventilation, wear suitable respiratory equipment. Keep away from direct sunlight or strong incandescent light. Keep container tightly closed and dry. Keep under inert atmosphere. Store under nitrogen. Manipulate under an adequate fume hood. Empty containers may contain a hazardous residue. Handle and open container with care. Take off immediately all contaminated clothing. Never add water to this product. This product must be manipulated by qualified personnel. Do not get in eyes, on skin, or on clothing. Wash well after use. In accordance with good storage and handling practices. Do not allow smoking and food consumption while handling. After handling, always wash hands thoroughly with soap and water. Do not allow water to get inside container because of violent reaction.

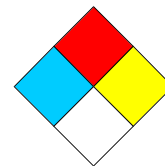
Section IX. Protective Measures

Protective clothing Face shield and splash goggles. Impervious gloves, apron, coveralls, and/or other resistant protective clothing. Sufficient to protect skin. A OSHA/MSHA jointly approved respirator is advised in the absence of proper environmental controls. If more than TLV, do not breathe vapor. Wear self-contained breathing apparatus. Do not wear contact lenses. Make eye bath and emergency shower available.

Engineering controls Use in a chemical fume hood to keep airborne levels below recommended exposure limits. Do not use in unventilated spaces.

Section X. Other Information

Special Precautions or comments Corrosive! Highly toxic! Dangerously reactive material! Lachrymator. Causes severe burns! Do not breathe vapor. Avoid all contact with the product. Avoid prolonged or repeated exposure. Use in a chemical fume hood. Handle and open container with care. Never add water to this product. Reacts violently with water.
RTECS NO: WS4300000 (Sulfur monochloride).
RTECS NO: WS4510000 (Sulfur dichloride).



NFPA

Prepared by MSDS Department/Département de F.S..

Validated 13-Jan-2010

Telephone# (514) 489-5711

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