VUV Photoabsorption of Thermally Processed Carbon Disulfide and Ammonia Ice Mixtures – Implications for Icy Objects in the Solar System

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Abstract

Many icy bodies in the solar system have been found to contain a rich mixture of simple molecules on their surfaces. Similarly, comets are now known to be reservoir of molecules ranging from water to amides. The processing of planetary/cometary ices leads to the synthesis of more complex molecules come of which may be the harbingers of life. Carbon disulphide (CS_2) and ammonia (NH_3) are known to be present on many icy satellites and comets. Reactions involving CS_2 and NH_3 may lead to the formation of larger molecules that are stable under space conditions. In this paper we present temperature dependent VUV spectra of pure CS_2 in the ice phase, and of CS_2 and NH_3 ices deposited as (i) layered, and (ii) mixed ices at 10 K and warmed to higher temperatures until their sublimation. Pure CS_2 ice is found to have a broad absorption in the VUV region, which is unique for a small molecule in the ice phase. In layered and mixed ices, the molecules tend to affect the phase change and sublimation temperature of each other and also leave behind a form of CS_2–NH_3 complex after thermal annealing. This study of CS_2-NH_3 ice system in layered and mixed configurations would hence support the detection of these species/complexes in mixed molecular ices analogous to that on planetary and cometary surfaces.

Introduction

Nitrogen is the fifth most abundant element and sulfur is the tenth most abundant element in the universe with several S-bearing and N-bearing molecules having been detected in astrophysical environments [1,2]. The ice phase chemistry of the ISM, comets, and several planetary bodies at various physical (temperature, pressure, etc.) conditions are well known [3,4]. The main objective of this work is to probe the influence of the reaction between S-bearing carbon disulfide (CS_2) and N-bearing ammonia (NH_3) molecules through their vacuum ultraviolet (VUV) absorption profiles.

Until the 1980s, the presence of CS_2 in interstellar environments was largely restricted due to observational constraints, as CS_2 lacks a permanent dipole moment. The presence of (CS_2) in the icy mantles of the ISM and other icy bodies has now been demonstrated [5,6]. The C–S bond was first identified in Comet West in 1980, which initiated the quest for the detection of CS_2 on comets [7]. The primary direct detection of CS_2 was made 15 years later, in 1995, by comparing the unidentified spectral lines of Comet 122P/de Vico in the UV-Visble region with the experimental spectra of supersonically cooled CS_2 [8]. In addition to comets, CS_2 has also been observed on planetary bodies such as the Jovian system [9,10], Earth's moon [11], etc.

NH_3 was first detected in the ISM in the 1960s [12]. The first identification of NH_3 in the solar system was made on Comet 1983d/IRAS-Araki-Alcock, where 6% of the gases sublimating from the comet were NH_3 [13]. NH_3 significantly contributes to the elemental composition of nitrogen on many comets including comet 1P/Halley [14,15]. It was also detected on comet 10P/Tempel 2 by the Herschel Observatory [16]. In addition to NH_3, its photodissociation product NH_2 (amidogen) has also been detected in the coma of comet C/2004 Q2 Machholz using the rovibrational lines in the 3 μm region [17]. NH_3 is also a main constituent of the mid and upper atmosphere of Titan, as revealed by the GCMS (Gas Chromatograph Mass Spectrometer) onboard the Huygens probe [18]. Furthermore, NH_3 has also been detected in the atmospheres of Jupiter and Saturn using the 6450 Å band [19]. NH_3 is also one of the prime surface components of Pluto's moon Charon [20].

The vacuum ultraviolet (VUV) spectra of small molecules such as CS_2, CH_4, OCS, NH_3, etc., have been extensively studied in the gas phase [21,22]. VUV experiments of such species using supersonic jet expansion methods have also been reported as the inhomogeneous broadening of lines can be eliminated by lowering the temperature, and both dynamical and structural information can be obtained using this method [23,24]. The absorption cross-section of CS_2 has been determined at elevated, cold and room temperatures of 383 K, 203 K and 295 K, respectively; and the temperature effects on the hot bands have been studied in the 180 – 230 nm region to aid the measurement of the abundance of CS_2 in the atmosphere of Jupiter and on comets [25]. The absorption spectrum of CS_2 has been recorded using synchrotron radiation in the 5.5 – 11.8 eV region and the valence and Rydberg transitions up to the first ionization potential have been determined [26]. In addition, there have been several experimental and theoretical studies in the gas phase that have recorded VUV spectra of CS_2 [1,27,28].

Gas phase photoabsorption spectra of NH_3 mixed with inert gases such as Xe and Kr have been recorded in the 105 – 225 nm region using synchrotron radiation and, in the case of the gaseous mixture of Xe and NH_3, the vibrational features in the <160 nm region were found to be enhanced, with 14 Rydberg states were identified in this experiment [29]. In addition, VUV cross-sections of the deuterated isotopologues of NH_3: NH_2D, NHD_2 and ND_3 have been experimentally measured in the 140 – 220 nm [30] and the 110 – 144 nm [31] regions at 298 K. It is to be noted that in gas phase: (i) the mean free path of the molecules is greater than the molecular dimensions, and (ii) the duration of photoabsorption event is smaller than the interval between the collisions; in contrast in solid ices: (i) the molecules have overlapping electron density, and (ii) the transition dipole in one molecule can resonate with neighbouring molecules that have possible transitions at comparable energies [32,33]. As a consequence, the absorption features of any given molecule in the ice phase can be broad and certain vibrational structures appear to be washed out from the spectra when compared to the gas phase data [34].

Hence, it is necessary to record the characteristic VUV absorptions of solid-phase molecules under astrophysical conditions to understand any deviation from the gas phase, to realise the interaction between the electronically excited states of the same or different molecules in ice phase, to probe the physico-chemical properties of molecules under extreme conditions, and to make their detection on icy solar system bodies feasible. VUV photoabsorption spectra of pure NH_3 ice, and of NH_3 dispersed in Ar under astrophysical conditions, are well known and have a maximum absorption at 122 nm and another broad absorption around 179 nm [4]. High-resolution VUV photoabsorption spectra of NH_3 were also acquired in 2019, in the 5.4 – 10.8 eV region, to determine its absolute photoabsorption cross-section and assign the electronic transitions from the ground state to the Rydberg states [35]. The VUV spectra of NH_3 in the ice phase from 25 K – 150 K revealed significant variations in the spectral signatures when compared to the gas phase spectrum; and an exciton feature was found to appear at 75 K at 194 nm [36,37,38]. However, the solid ice phase VUV photoabsorption spectrum of CS_2 is still not available and hence, in this work we are presenting the first VUV spectra of CS_2 ice in the 110 – 300 nm range under astrophysical conditions (i.e., at a lowest temperature of 10 K).

Recognising the importance of CS_2 and NH_3 and considering the ice phase chemistry that is possible on planetary bodies, it is essential to perform laboratory-based spectroscopic studies of these ice mixtures. In our previous work, the infrared spectra of CS_2 and NH_3 ice layers and mixtures were recorded upon thermal processing from 10 K to 340 K. When the ice mixtures of CS_2 and NH_3 were warmed to temperatures above 120 K, ammonium dithiocarbamate (NH_4NH_2CSS) was found to be synthesized which was a stable complex and was present on the substrate until 340 K [39]. Quantum chemical calculations of complex formation between CS_2 and NH_3 have revealed that these molecules interact through the chalcogen (S–N) bonds; and the Atoms in Molecule (AIM) analysis displayed the existence of a Bond Critical Point (BCP) between the S and N atoms [40]. In this work, we present the VUV photoabsorption spectra of CS_2 and NH_3 ice layers and mixtures, and their product formation upon thermal processing, for its identification on planetary and cometary surfaces.

Experiment

The present experiments were carried out at the National Synchrotron Radiation Research Center (NSRRC) in Taiwan. VUV light from the BL-03 beamline of the Taiwan Light Source (TLS) was dispersed with a cylindrical grating monochromator (focal length, f = 6 m) on a bending magnet beamline of the storage ring (1.5 GeV). The beam was then passed through a gold mesh having a transmission of about 90%. The photocurrent of the gold mesh was detected with an electrometer (Keithley 6512) to monitor and normalise the beam current during the experiments. The CS_2 and/or NH_3 molecules were deposited onto a lithium fluoride (LiF) VUV transparent window maintained at 10 K using a closed cycle helium refrigerator system. The VUV photoabsorption spectra were measured to the transmission limit of the optical components; i.e., over the 110 – 320 nm range for both CS_2 and NH_3 ices.

The VUV light from synchrotron was perpendicular to the solid samples and the transmitted light passed through a glass window coated with sodium salicylate to convert the incident UV light to visible light which was detected using a photomultiplier tube (Hamamatsu R943-02) operating in a photon-counting mode. The slit through which the VUV beam passes has a dimension of 250 x 250 µm before it falls on the substrate. The beam bandwidth is from 109 – 350 nm when passed through the LiF substrate. Detailed descriptions of the experimental setup, sample preparation methods, and spectral acquisition techniques are presented in an earlier publication [41]. Both the molecular samples were of high purity ($CS_2 \geq 99$ % pure, $NH_3 = 99$ % pure) and were purchased from Sigma Aldrich. A spectrum was recorded immediately after deposition, as well as at regular temperature intervals during warming of the sample to higher temperatures at a rate of 5 K min^{-1}.

Results and Discussion

Pure CS_2 ice

Pure CS_2 gas was deposited onto the substrate held at 10 K and a VUV photoabsorption spectrum was subsequently recorded. Three main absorption bands are observed in the VUV spectrum of a 10 K CS_2 ice, as shown in *Figure 1a*: the first band is centered at 118 nm, the second band ranges from 140 – 148 nm with a maximum intensity at 144 nm, and the third absorption feature is a broad band ranging from 164 – 259 nm with a maximum intensity at 237 nm. Such a broad absorption band of over a roughly 100 nm range is not observed for several other simple molecular ices, such as H_2O, NH_3, CH_4, O_2, N_2, etc., for which each VUV absorption band typically ranges over 10 – 60 nm. In fact, this band has a relatively higher absorption cross-section of 2 x 10^{-16} cm^2 in the gas phase [21]. This is important as such an extensive range of photoabsorption may overlap with and conceal the absorption features of many complex molecules.

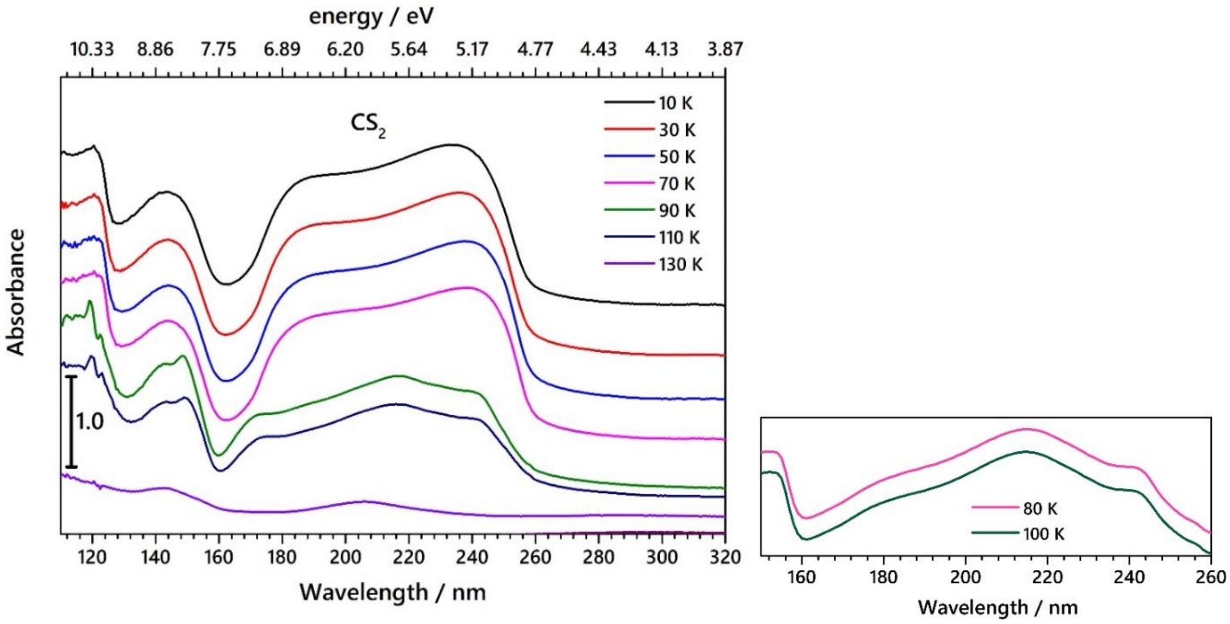

Figure 1a: *(Left) VUV photoabsorption spectra of pure CS_2 ice deposited at 10 K and subsequently warmed to higher temperatures; (Right) Another experiment: VUV photoabsorption spectra of pure CS_2 ice warmed to 80 K and 100 K showing signs of phase chage.*

Figure 1b displays a comparison of the VUV absorption spectra of CS_2 in the gas phase at 298 K with that in the ice phase at 10 K. It is evident from *figure 1b* that the Rydberg states present in the gas phase VUV spectrum do not appear in the ice phase since the electron densities overlap and quench the Rydberg states, as well as causing broadening of the absorption bands [5,7]. The maximum absorption appears to be redshifted in the ice phase compared to the gas phase spectrum. Such redshifts in VUV spectral signatures have been reported in a few astrochemical ices [42].

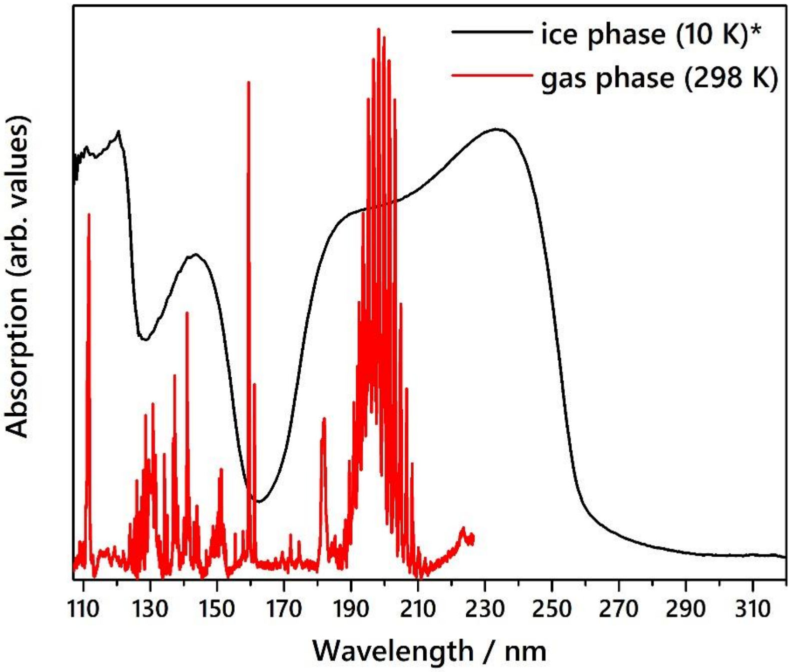

Figure 1b: *Comparison of the VUV photoabsorption spectrum of CS_2 in the ice phase (present work) with that in the gas phase by Sunanda et. al. (2015)* [15]. *******y-axis of the ice phase spectra at 10 K is scaled for better comparison of absorption profile with the gas phase spectra. So, the absorption cross-section of the ice and gas phases are not comparable.*

The absorption range and band intensities in the VUV spectra of CS_2 ice (*Figure 1a*) remained the same during warming to temperatures of up to 70 K. An evident decrease in absorption of the 164 – 259 nm band is noticed at 90 K which could be due to the phase change of CS_2 ice at 80 K (*Table 1*). This is evident from figure 1a (right), which is shows the VUV spectra of pure CS_2 at 80 K and 100 K recorded in the 150 nm – 260 nm region in a different experiment. The 80 K spectra shows clear signatures of phase change which is evident from the appearance of a new feature in the 210 nm region. At 80 K the band intensity maximum is at 215 nm. A similar change is noticed in the 140 – 148 nm region where the maximum intensity shifts to 141 nm and a split in the absorption band occurs. The sublimation of CS_2 starts at around 110 K and the ice fully desorbed once the substrate is warmed to 130 K. Throughout the course of thermal processing of the CS_2 ice, the wavelength range of absorption remains almost the same. It is important to note that the temperature of phase change can be precisely characterized only by IR spectroscopy through the sharpening of the vibrational modes. VUV spectroscopy gives only a rough estimate of the phase change temperature and hence a small deviation can be noticed when compared to our previous IR studies [37]. The sublimation temperature is usually found to be higher than that obtained in the IR studies, in both pure ices and ice mixtures, mainly because of the larger absorption cross-section in the VUV region compared to that in the IR.

NH_3 deposited above CS_2

The CS_2 gas was deposited on the substrate maintained at 10 K to form an icy layer on top of which NH_3 gas was deposited to form layered (1:1) ices. The VUV spectrum recorded at 10 K (*Figure 2*) shows the characteristic absorptions of CS_2 ice: 118 nm, 140 – 148 nm, and 164 – 259 nm, as discussed above. However, the band intensity is considerably lower in the 180 – 255 nm region compared to the VUV spectrum of pure CS_2 ice. The VUV spectrum of pure NH_3 ice is shown in *Figure 5* for comparison. The VUV absorption of NH_3 ice is observed at 120 – 145 nm with a maximum intensity at 141 nm and at 157 – 190 nm with a maximum intensity at 181 nm. It is interesting to note that the maximum absorption of CS_2 and NH_3 overlaps with that of H_2O ice (118 – 150 nm) which is abundant on many planetary surfaces. These icy layers were then warmed to higher temperatures and no significant changes were noticed till 60 K. The temperature-induced phase change for NH_3 ice from an amorphous phase to a crystalline state occurs at 65 K, and hence there is a blueshift of 4 nm in the 157 – 190 nm region where the maximum intensity shifts from 181 nm to 177 nm. It is to be noted that the photoabsorption spectrum of pure NH_3 exhibits a shift in the position of its maximum intensity from 176 nm to 168 nm (blueshift of 8 nm) due to its phase change at 65 K.

CS_2 is observed to start crystallising at 90 K; however, the crystallisation is complete only at 100 K. The phase change is evident through the decrease in intensity of the 160 – 190 nm region at 100 K with another indication being the spectral changes in the 194 – 275 nm region. The maximum intensity of this broad absorption band is redshifted by 6 nm from 215 nm to 221 nm compared to the pure crystalline CS_2 ice at 90 K. This increase in the temperature of the phase change of CS_2 from 90 K to 100 K could be due to the presence of crystalline NH_3 on top of CS_2 ice that slows the crystallisation of the latter. A similar change in the crystallization was also observed in our previous experiments with CS_2 and NH_3 ice layers probed by IR spectroscopy [39]. Such delayed crystallization was observed in the case of IR spectroscopy of Acetonitrile-water mixture [43]. In addition, a new band is observed to appear near 254 nm at 90 K, which then disappears at 110 K. This feature could be due to the crystalline CS_2 amidst crystalline NH_3. Both CS_2 and NH_3 start sublimating at 110 K, however, the absorbance at higher temperatures (120 – 140 K) could either be due to the crystalline CS_2 ice trapped beneath crystalline NH_3 ice that hampers the sublimation of CS_2 at 130 K, or due to the mixing of the ices at their interface which could possibly form complexes.

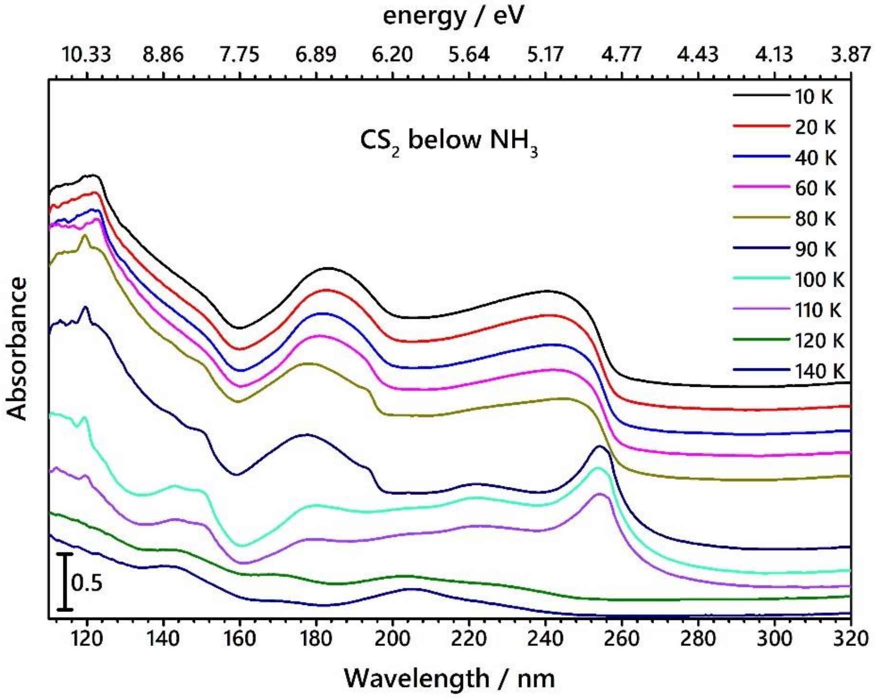

Figure 2: *VUV photoabsorption spectra of CS_2 below NH_3 ice deposited at 10 K and subsequently warmed to higher temperatures.*

CS_2 deposited above NH_3

NH_3 gas was deposited on the substrate maintained at 10 K to form an icy layer and then the CS_2 gas was deposited on top of the NH_3 ice to form layered (1:1) ices. The deposition conditions were the same as in the case of CS_2 below NH_3, so as to obtain the same ice thickness in each experiment. This was ensured by measuring the pressure of the gas inlet into the deposition line from the sample compartment. The recorded VUV spectrum at 10 K displays all the absorption features of NH_3 and CS_2, as shown in *Figure 3*. Similar to the previous case of CS_2 below NH_3, the band intensity is lower in the 180 – 255 nm region when compared to the VUV spectrum of pure CS_2 ice. In addition to the absorption peaks observed in the case of CS_2 below NH_3 ices, there are vibronic features observed in the 128 – 144 mm range. When the icy layers are warmed to 20 K there is an increase in the intensity of the vibronic peaks. As the phase change of NH_3 occurs at 65 K, there is a significant blueshift of 7 nm in the 157 – 190 nm region where the maximum absorption shifts from 182 nm to 175 nm at 70 K; and further blueshifts to 171 nm at 90 K.

The phase change of CS_2 ice is observed at 90 K through a decrease in the intensity of the 194 – 254 nm region. Although the NH_3 ice reaches its sublimation temperature at 90 K, intense absorption features of NH_3 are observed to persist until 120 K. NH_3 fully desorbs only after 140 K, due to the fact that the crystalline CS_2 ice above prevents the crystalline NH_3 ice from sublimating.

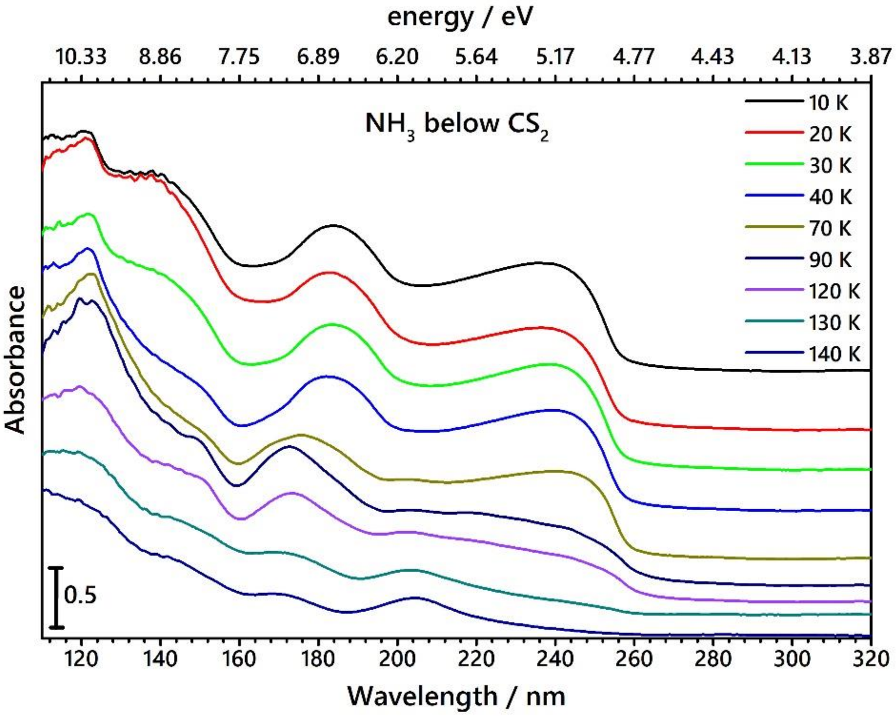

Figure 3: *VUV photoabsorption spectra of NH_3 below CS_2 ice deposited at 10 K and subsequently warmed to higher temperatures.*

CS_2 and NH_3 ice mixtures

CS_2 and NH_3 gases were mixed in the gas line in a 1:1 ratio and deposited on the LiF substrate maintained at 10 K. The VUV spectrum obtained at 10 K (*Figure 4*) shows characteristic absorptions of both CS_2 and NH_3. The broad characteristic feature of CS_2 ice in the 160 – 255 nm region closely resembles that of pure CS_2, unlike that of the layered ices (*Table 1*).

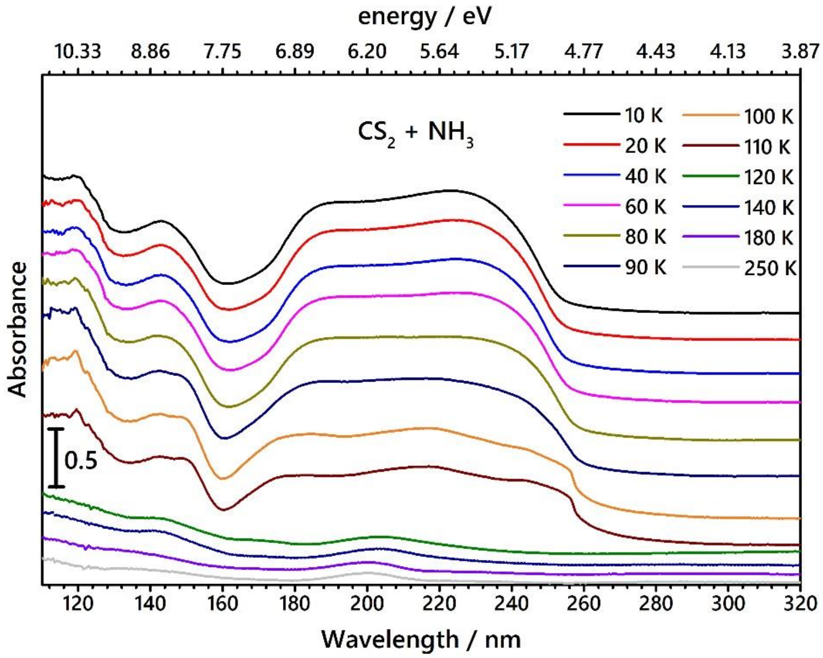

Figure 4: *VUV photoabsorption spectra of CS_2 + NH_3 ice mixture deposited at 10 K and subsequently warmed to higher temperatures.*

As the ice mixtures are warmed to higher temperatures there is a negligible decrease in the absorption intensity at each temperature. The phase change of CS_2 (originally at 80 K for pure CS_2 ice according to IR studies) initiates at 90 K, but the ice fully turns crystalline only at 100 K. This is because the NH_3 molecules mixed with CS_2 deter the CS_2 crystallisation process. The VUV spectrum at 100 K develops a shoulder at 254 nm which is similar to the additional feature noticed in the case of CS_2 below NH_3, where a distinct peak appears at 254 nm from 90 K to 110 K (*Figure 4*). Both the CS_2 and NH_3 ices sublimate beyond 110 K. However, there is still an absorbance noticed around 120 K which remains up to 250 K. This indicates that a new molecular species is formed upon thermal processing of the ice mixtures. The VUV spectra at 250 K is distinct with a feature centered at 200 nm. This is likely to be a residue/complex formed by CS_2 and NH_3, which is speculated to be ammonium dithiocarbamate (NH_4NH_2CSS) as observed in the case of the IR studies [37]. The complex obtained as a product of thermal processing of these ices in our previous experiments probed by IR spectroscopy was identified to be ammonium dithiocarbamate (NH_4NH_2CSS) using the intense vibrational bands at 1220 and 1110 cm^{-1}. However, such an unambiguous identification of the product is not possible using VUV investigations. Further experiments with mass spectroscopic data would be necessary for the unique identification of such products.

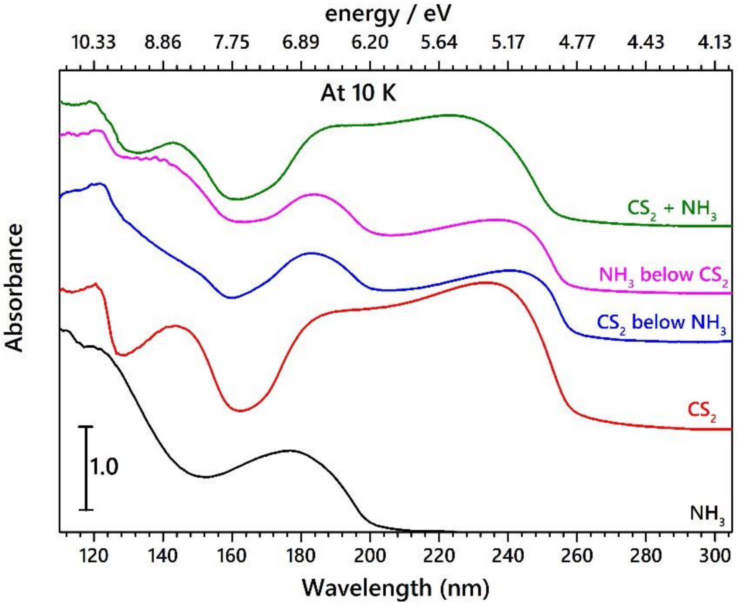

Figure 5: *Comparison of the VUV photoabsorption spectra of pure CS_2 ice, pure NH_3 ice, CS_2 below NH_3, NH_3 below CS_2, and the CS_2 + NH_3 ice mixture deposited at 10 K.*

The unique VUV spectral signatures at 10 K of the pure CS_2 and NH_3 ices, along with the layered and mixed ices spectra, are presented in *Figure 5*. It is evident that the presence of molecules above or beneath another molecular species alters the relative absorption of the regions of interest in the VUV spectra. However, the wavelength range of the major absorption bands remains almost the same with a negligible shift of only a few nanometers. A notable difference is observed in the 130 – 150 nm region of NH_3 below CS_2, where the absorption of CS_2 is not distinct as in the case of CS_2 below NH_3. This is due to the presence of NH_3 ice on top in the 130 – 140 nm region which overlaps the CS_2 absorption band and washes off the feeble features of Rydberg states that is visible in the NH_3 below CS_2 configuration (*Figure 3*). The VUV photoabsorption spectra of the layered and mixed ices at 130 K are presented in *Figure 6*. There are significant absorptions present at 130 K; a temperature which is beyond the sublimation point of CS_2 and NH_3. These absorptions could be complexes of CS_2–NH_3 that are produced due to thermal processing of these ices. It is to be noted that the VUV absorptions of the complexes in the case of the layered ices are observed to be present only up to 140 K, while in the mixed ices they are present up to 250 K. This could be because of the higher abundance of CS_2–NH_3 complexes in the experiment with mixed ices compared to the layered ice experiments where the porous amorphous CS_2 and NH_3 ices can mix only at their interface.

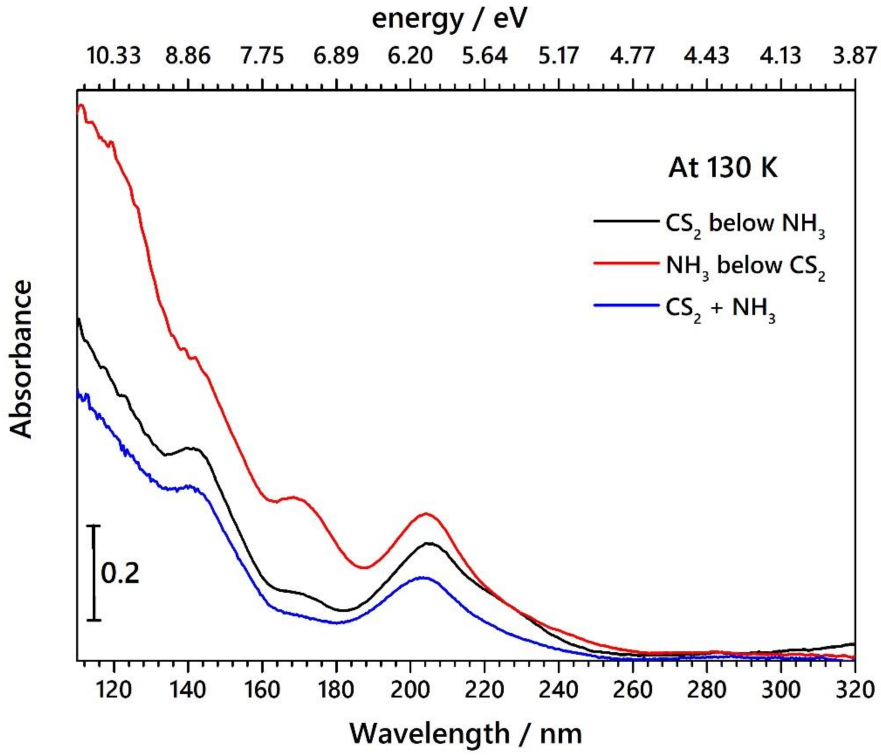

Figure 6: *Comparison of the VUV photoabsorption spectra of CS_2 below NH_3, NH_3 below CS_2, and $CS_2 + NH_3$ ice mixture after warming to 130 K.*

Table 1: *Characteristic VUV absorptions of CS_2 and NH_3 ices at 10 K, observed phase change temperatures and sublimation temperatures of CS_2 and NH_3 ices in pure, layered, and mixed forms.*

Experiments	**Observed VUV absorptions**		**Phase change**		**Sublimation**	
	CS_2	**NH_3**	**CS_2**	**NH_3**	**CS_2**	**NH_3**
Pure CS_2	110-118 nm, 140-180 nm, 164-259 nm*#	-	80 K (80 K)&	-	130 K	-
Pure NH_3	-	110-145 nm, 155-200 nm*	-	80 K (65 K)&	-	95 K
CS_2 below NH_3	110-118 nm, 157-190 nm*#, 200-260 nm	118-145 nm, 160-178 nm@	100 K	80 K	140 K	110 K
NH_3 below CS_2	110-118 nm, 157-190 nm#, 200-260 nm	128-144 nm* 155-185 nm@	90 K	90 K	140 K	140 K
$CS_2 + NH_3$	110-118 nm, 140-180 nm, 164-250 nm*#	118-145 nm	100 K	90 K	130 K	110 K

* Intense absorption features

\# Broad features

@ Overlapping bands, not significant due to lower absorption cross section of NH_3 compared to CS_2

& Actual values of phase change obtained by IR investigations in Ref 39.

Astrophysical Implications

It is well known from the observations carried out by various observatories and spacecrafts that the molecules present on planets or comets are heterogeneously distributed across the surface. It is evident from this study that the ice configuration of even the simple molecules like CS_2 and NH_3 can significantly affect the VUV absorption signatures of these ices. The experiments in this work performed at astrophysical conditions to record the VUV photoabsorption of CS_2–NH_3 ices system in both layered and mixed configurations can provide laboratory evidence for the detection of these species/complexes on a planetary or cometary surface. This work also stresses upon the fact that the thermal processing of planetary ices is one of the important stimulant for the synthesis of complex molecules in space. *Table 1* explains the variations in the phase change and sublimation temperatures of these simple molecules as an effect of its configuration i.e., in an actual planetary scenario, if the molecule is present on the surface of the ice or beneath the surface plays a major role in its physical properties and the spectral features when probed using VUV spectroscopy.

Conclusion

The VUV photoabsorption spectra of pure CS_2, layered CS_2 + NH_3, and mixed CS_2 + NH_3 ices were recorded between 10 K and 150 K. The ices were thermally processed and VUV spectra were recorded at various temperatures. The observed VUV absorptions, phase changes and sublimation temperatures of these ices are summarized in *Table 1*. The VUV spectrum of pure CS_2 ice exhibits a broad and intense feature in the 164 – 259 nm range as well as signatures of a phase change at 90 K. The broad absorption range of CS_2 in the VUV region is very distinctive and this is, to the best of our knowledge, the only small molecule known to display such broad absorption in the ice phase. This implies that the photoabsorption of CS_2 on an icy solar system body could very well interfere with that of many large or complex molecules, and thus caution must be taken when assigning a molecule unambiguously using a VUV absorption signature when CS_2 may be present. The NH_3 ices have their main absorption features in the 110-145 nm and 155-200 nm regions and undergo a phase change at 65 K which is also known from previous experimental investigations.

When NH_3 is deposited above CS_2, the 157-190 nm region has an intense absorption as the individual absorptions of CS_2 and NH_3 overlap in this region. The phase change of CS_2 occurs at 100 K as the crystalline NH_3 on top hinders the crystallisation process of CS_2. An additional feature is observed around 254 nm which we attribute to the formation of complexes between crystalline NH_3 and amorphous CS_2. When CS_2 is deposited above NH_3, the VUV absorption maximum is in the 128-144 nm region. The phase change of both CS_2 and NH_3 takes place at 90 K. In the case of mixed CS_2 + NH_3 (1:1) ices the VUV spectra closely resemble that of the pure CS_2 ices. This is due to the low absorption cross-section of NH_3 ice compared to CS_2 ice. The phase change temperature of both CS_2 and NH_3 is raised by 20 K because the presence of one molecule hampers the crystallisation of the other. Thermal processing of mixed ices is likely to leave behind some residue that is present even after 130 K and remains on the substrate up to 250 K. Based on past IR studies of this thermal reaction, we cautiously suggest that this residue could be ammonium dithiocarbamate (NH_4NH_2CSS).

The data presented in this work is important for the detection of simple and complex species on cometary and planetary surfaces. The laboratory thermal processing of many more molecules, as well as their molecular mixtures, are essential to better understand the chemistry of planetary bodies and on cometary surfaces during their thermal processing. Such studies also help in the detection of simple to complex molecules that could be produced as a result of the thermal processing of such astrochemical ices.

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