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Abstract

Glycine silver nitrate (GSN) and fully deuterated GSN (FDGSN) form two isotopic polymorphs. The effect of full deuteration brought about the isotopic polymorph of GSN. In order to study the effect of partial deuteration on isotopic polymorphs, crystals of C Deuterated GSN (CDGSN) and N deuterated GSN (NDGSN) were grown. The crystal structure of C-deuterated was similar to FDGSN forming 2 dimensional polymeric structures extended along the c-axis, In CDGSN, the silver ion is mononuclear similar to that in FDGSN with no Ag-Ag coordination. N deuterated had similar crystal structure to that of GSN. The nitrate ion, the silver ion and zwitterionic glycine form a three-dimensional network unlike the case in CDGSN. The silver ion is binuclear with Ag-Ag coordination similar to that in GSN. In both crystal structures the silver ion has an oxidation state of + 1. Hirshfeld surface analysis of all the above structures were carried out using the x-ray data. The globularity parameter is similar in all the strutures. For the entire complex it is observed that FDGSN and CDGSN has similar values, which is lower than that of GSN and NDSN. The asphericity for the entire complex in the case of NDGSN and GSN are close to 0 indicating the isotropic nature where as for FDGSN and CDGSN it is near 0.36 indicating oblate nature. NDGSN and GSN have higher Ag…O interactions compared to that of CDGSN and FDGSN. NDGSN and GSN have Ag…Ag interaction, which is totally absent in CDGSN and FDGSN. Raman measurements showed the partial deuteration of the compounds. The lattice modes of GSN and NDGSN are similar, and FDGSN and CDGSN are similar, further confirming the importance the C deuteration in forming the isotopic polymorph.

Introduction

Glycine is the only achiral amino acid. Being the most simplest amino acid, complexes of glycine have been studied from biological and as well from ferroelectricity point. There exists large number of complexes of amino acids which have shown ferroelectricity , like triglycine sulphate family of crystals [1], diglycine nitrate [2], glycine phosphate [3] and glycine silver nitrate [4]. The first organometallic crystal of glycine with silver and nitrate, which showed ferroelctricity was GSN [5]. It was observed that GSN undergoes displacive phase transition. It was concluded from the infrared study [6], the proton magnetic resonance study [7] and structural study using X-ray powder diffraction [8] that the displacive transition in GSN was due to the motion of the silver ions (Ag^{+}). Recrystallization of GSN from D_2O which leads to only deuteration of NH_3, raised the curie temperature to -43°C. This again showed that the in most probability the phase transition is due to the motion of the silver ions [9]. Deuteration in a molecule replaces H with D leads to minimum modification in a molecule. But it can bring in significant changes in the chemical and physical properties like kinetics, equilibrium constants etc. [10,11,12] because of the difference in atomic mass, volume and spin as compared to that of hydrogen. In general isotopic substitution doesn't bring about a structural change, but effects the molecular spectroscopy via the geometric effect[[13,14,15]. The perturbation resulting due to deuteration in molecular rearrangement has been extensively enumerated in the study by showed Klaus Merz and Anna Kupka[16]. The term isotopic polymorphism was coined to structures which exhibited structural changes on deuteration [17]. Many studies have been carried out to study the effect of deuteration on the structures and properties of the crystal [18,19]. Our

earlier study on fully deuterated GSN(FDGSN) showed that the crystal structure changes on full deuteration [20] showing isotopic polymorphism. In order to further understand the effect of deuteration, partially deuterated crystal of GSN were grown i.e CDGSN and NDGSN. Interestingly it was found that the CDGSN had crystal structure similar to that of FDGSN and NDGSN had structure similar to that of GSN. Incidentally this is the first instance where the C- deuteration alone is bringing about the change in crystal structure.

Crystallization

Colourless single crystals CDGSN were grown as three-dimensional crystals by mixing fully deuterated α glycine and silver nitrate in 1:1 ratio respectively in water. Colourless single crystals of NDGSN were grown as three-dimensional crystals by mixing α glycine and silver nitrate in 1:1 ratio respectively in deuterated water. For further improving the deuteration level of NDGSN, the crystal obtained during the first crystallization were again dissolved in deuterated water to obtain fresh crystals of NDGSN. Both the crystals were grown in dark.

Experimental

The room temperature data were collected on a Bruker-SMART Apex II 4K CCD diffractometer using Mo-Kα graphite-monochromated radiation (λ = 0.71073 Å).

For Raman measurements, a FT-Raman spectrometer (Bruker make MultiRAM) was used. The Raman scattered light from the sample, which was excited using 1064 nm Nd:YAG laser, was collected using a liquid nitrogen cooled Ge detector through an interferometer. The spectra were measured in the frequency region 60–3400 cm^{-1} in a single scan and a total of 100 scans were coadded at a resolution of 4 cm^{-1}. Lorentzian fit of the measured spectra was done to measure the spectral line positions.

Results and discussion

The structure of CDGSN at RT was determined using direct methods as implemented in SHELXS [21]. The atomic parameters so obtained were subjected to a series of isotropic and anisotropic full matrix least square refinements using SHELXL97[21]. All the reflections were used for refinement. In the initial stages of refinement, reflection weight (w) was taken to be 1/ $\sigma(F_o^2)$, which was derived using counting statistics. All the hydrogen atoms were located from the difference Fourier map and refined isotropically. Crystallographic and refinement details for CDGSN are summarized in Table 1. The asymmetric unit consists of glycine in the zwitter ionic form, a silver ion(Ag^+) and a nitrate ion(NO_3^-) [figure 1]. The bond distances in the C1gO2gO1g group (C1g-O1g = 1.262(2)Å & C1g-O2g = 1.248(3) Å) of glycine indicated that the group appears as a carboxylate, -COO..

It is important to mention here that GSN and NDGSN are more light and X-ray sensitive[5] as compared to that of FDGSN and CDGSN. The crystals when exposed to light and X-rays change in color form white

transparent to brown colour, hence the data quality of NDGSN is not that good as compared to that of CDGSN even though they have been collected under same conditions.

The structure of NDGSN at RT was determined using direct methods as implemented in SHELXS SHELXS97 and SHELXL97. University of GoÈ ttingen, Germany[21]. The atomic parameters so obtained were subjected to a series of isotropic and anisotropic full matrix least square refinements using SHELXL97 [21]. All the reflections were used for refinement. In the initial stages of refinement, reflection weight (w) was taken to be $1/\ \sigma(F_o^2)$, which was derived using counting statistics. Hydrogen atoms belonging to C and N of glycine molecule were refined using AFIX instruction as they could not be refined unlike the case of CDGSN Crystallographic and refinement details for NDGSN are summarized in Table 1. The asymmetric unit consists of glycine in the zwitter ionic form, a silver ion(Ag^+) and a nitrate ion(NO_3^-) [figure 2]. The bond distances in the C1gO2gO1g group (C1g-O1g = 1.27(1)Å & C1g-O2g = 1.22(1) Å) (Table 3a)of glycine indicated that the group appears as a carboxylate, -COO.

Crystallographic and refinement details for CDGSN and NDGSN are summarized in Table 1. .

Table 1
Crystallographic and Refinement details for CDGSN and NDGSN

	CDGSN	**NDGSN**
CCDC No.	2264620	2264621
Empirical formula	$C_2D_2H_3AgN_2O_5$	$C_2H_2D_3AgN_2O_5$
Formula weight	244.95	244.95
Temperature (K)	300K	300K
Wavelength (Å)	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic
Space group	P 2_1/c	P 2_1/c
Unit cell dimensions		
a (Å)	5.4603 (13)	5.5441 (9)
b (Å)	9.060 (2)	19.475 (3)
c (Å)	11.586 (3)	5.4468 (9)
β(°)	91.696 (10) °	99.947 (5)°
Volume (Å3)	572.9 (2)	579.25 (16)
Z	4	4
Calculated density (Mg m-3)	2.840	2.809
Absorption coefficient (mm-1)	3.48	3.44
θ range for data collection (°)	30.5°	30.6°
Limiting indices	-4 ≤ h ≤ 7 -12 ≤ k ≤ 12 -16 ≤ l ≤ 16	-4 ≤ h ≤ 7 -25 ≤ k ≤ 27 -7 ≤ l ≤ 6
Reflections collected/unique	10321/1729 Rint = 0.043	4237/1670 Rint = 0.025
θ max(°); Completeness to	30.5/0.992	30.5/0.941
Data/restraints/parameters	1729/112	1670/92
Goodness-of-fit on F^2	S = 1.09	S = 1.389

	CDGSN	NDGSN
Final R indices R[$F^2 > 2\sigma(F^2)$]	R1 = 0.025 wR(F2) = 0.062	R1 = 0. 0.083 wR(F2) = 0.215

Table 2
Comparison of cell parameters in GSN [5], NDGSN, FDGSN[20], CDGSN

	GSN[5]	NDGSN	FDGSN[20]	CDGSN
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	P $2_1/a$	P $2_1/c$	P $2_1/c$	P $2_1/c$
Unit cell dimensions				
a (Å)	5.451	5.5441 (9)	5.4372 (1)	5.4603 (13)
b (Å)	19.493	19.475 (3)	9.0488 (2)	9.060 (2)
c (Å)	5.541	5.4468 (9)	11.5456 (3)	11.586 (3)
β (°)	100.2	99.947 (5)°	91.926 (1)	91.696 (10)°
Volume ($Å^3$)	579.46	579.25 (16)	567.72 (2)	572.9 (2)

From Table – 2 it is observed that the structural parameters of GSN and NDGSN are similar and NDGSN crystallizes in $P2_1/c$ space group and that of FDGSN and CDGSN are similar. Between GSN and NDGSN, there is increase in lattice parameter a and decrease in c with very little change in the volume, whereas a comparison in FDGSN and CDGSN, there is increase in lattice parameters a, b and c and decrease in β in CDGSN compared to FDGSN, and there is appreciable increase in volume in CDGSN. A comparison of the bond distance and bond angles for FDGSN and CDGSN is given in Table 3a & Table 3b respectively.

Table 3
a. Comparison of Bond Distances in FDGSN[20] and CDGSN

Atoms	**Bond distance (Å)**		**Atoms**	**Bond distance (Å)**	
	FDGSN[20]	CDGSN		FDGSN[20]	CDGSN
Ag1—O1g	2.2901 (9)	2.296 (2)	C1g—O1g	1.258 (1)	1.262 (2)
Ag1—O2gi	2.417 (1)	2.428 (2)	C1g—C2g	1.519 (1)	1.521 (3)
Ag1—O1n	2.534 (2)	2.539 (3)	C2g—N2g	1.468 (2)	1.469 (3)
Ag1-O3N	2.651				
Ag1-O2N	2.739				
Ag1-O1G	2.732				
N1—O1n	1.237 (2)	1.241 (3)	C2g—H4g	0.95 (2)	0.96(4)
N1—O3n	1.249 (2)	1.253 (3)	C2g—H5g	0.98 (2)	1.04(4)
N1—O2n	1.250 (1)	1.249 (3)	N2g—H1g	0.86 (3)	0.79(5)
C1g—O2g	1.250 (1)	1.248 (3)	N2g—H2g	0.91 (3)	1.03(5)
N2g—H3g	0.90 (3)	0.91(4)			

Table 3
b.. Comparison of Bond angles FDGSN[20] and CDGSN

Atoms	Bond angle (º)		Atoms	Bond angle(º)	
	FDGSN[20	CDGSN		FDGSN[20]	CDGSN
O1g—Ag1—O2g^{i}	117.60 (3)	117.70 (6)	C1g—C2g—H4g	110 (2)	111 (2)
O1g—Ag1—O1n	114.41 (4)	114.25 (7)	N2g—C2g—H5g	106 (1)	106 (2)
O2g^{i}—Ag1—O1n	127.90 (4)	127.96 (6)	C1g—C2g—H5g	114 (1)	114 (2)
O1n—N1—O3n	120.5 (1)	120.5 (2)	H4g—C2g—H5g	108 (2)	109 (3)
O1n—N1—O2n	120.6 (1)	120.5 (2)	C2g—N2g—H1g	114 (2)	118 (4)
O3n—N1—O2n	118.9 (1)	119.0 (2)	C2g—N2g—H2g	112 (2)	112 (3)
N1—O1n—Ag1	97.7 (1)	97.53 (17)	H1g—N2g—H2g	103 (2)	98 (4)
O2g—C1g—O1g	125.7 (1)	125.9 (2)	C2g—N2g—H3g	110 (2)	110 (3)
O2g—C1g—C2g	117.4 (1)	117.35 (18)	H1g—N2g—H3g	108 (3)	110 (4)
O1g—C1g—C2g	116.9 (1)	116.76 (19)	H2g—N2g—H3g	110 (3)	109 (4)
N2g—C2g—C1g	112.00 (9)	112.26 (17)	C1g—O1g—Ag1	113.60 (8)	113.64 (14)
N2g—C2g—H4g	107 (2)	105 (2)	C1g—O2g—Ag1^{ii}	121.53 (8)	121.61 (14)

Symmetry codes: (i) 1 + x, y, z (ii) -1 + x, y, z.

Equation of plane was calculated for the zwitter ionic glycine, the nitrate ion and the silver coordinated oxygens in FDGSN and CDGSN. It was observed that the nitrate ions are planar in both the structures. The zwitterionic glycine is nonplanar in both FDGSN and CDGSN, and the deviations[Table 4] are also same in both the structures. Similary the equation of plane Ag coordinated with oxygen in nonplanar, with similar deviations of atoms from the plane in both FDGSN and CDGSN

Table 4
Deviation of atoms form the plane in FDGSN[20] and CDGSN

atoms	Deviation of atoms from plane		atoms	Deviation of atoms from plane		atoms	Deviation of atoms from plane	
	Nitrate ion			Zwitterionic Glycine			Ag coordinated	
	FDGSN[20]	CDGSN		FDGSN[20]	CDGSN		FDGSN[20]	CDGSN
N1	0.0	0.0	N2G	0.132	0.132	AG1	0.012	0.013
O1N	0.0	0.0	C2G	0.164	0.164	O1G	0.028	0.027
O2N	0.0	0.0	C1G	0.018	0.018	O1N	0.067	0.066
O3N	0.0	0.0	O2G	0.103	0.103	O3N	0.073	0.072
			O1G	0.053	0.053	O2G	0.046	0.046

A comparison of the bond distance and bond angles for GSN and NDGSN is given in Table 5a & Table 5b respectively.

Table 5
a. Comparison of Bond Distances in GSN[5] & NDGSN

Atoms	Bond distance (Å)		Atoms	Bond distance (Å)	
	GSN[5]	NDGSN		GSN[5]	NDGSN
Ag1—Ag1i	2.877(6)	2.815 (2)	O1N—N1	1.28(3)	1.27 (1)
Ag1—O2G	2.25(2)	2.227(8)	O2N—N1	1.26(3)	1.24 (1)
Ag1—O1Gi	2.22(2)	2.282 (8)	O3N—N1	1.25(4)	1.25 (2)
Ag1—O1Gii	2.37(2)	2.412 (9)	N1G—H1G		0.8900
O1G—C1G	1.28(3)	1.27 (1)	N1G—H2G		0.8900
O2G—C1G	1.25(3)	1.23 (1)	N1G—H3G		0.8900
N1G—C2G	1.50(4)	1.49 (2)	C2G—H4G		0.9700
C1G—C2G	1.54(4)	1.53 (2)	C2G—H5G		0.9700

Symmetry codes: (i) 1, 1, 2; (ii) 1„ ; (iii) -1„ .

Table 5
b. Comparison of Bond Angles in GSN[5] & NDGSN

Atoms	Bond angle (º)		Atoms	Bond angle(º)	
	GSN[5]	NDGSN		GSN[5]	NDGSN
O2G—Ag1—O1Gi	163.1(7)	164.7 (3)	O2N—N1—O3N	123(2)	122.9(12)
O2G—Ag1—O1Gii	120.8(6)	120.3 (3)	O2N—N1—O1N	120(2)	118.4 (13)
O1Gi—Ag1—O1Gii	76.0(7)	75.0 (3)	O3N—N1—O1N	116(2)	118.6 (11)
O2G—Ag1—Ag1i	84.7(4)	86.9 (3)	C2G—N1G—H1G		109.5
O1Gi—Ag1—Ag1i	79.1(5)	78.2 (2)	C2G—N1G—H2G		109.5
O1Gii—Ag1—Ag1i	149.9(4)	148.3 (2)	H1G—N1G—H2G		109.5
C1G—O1G—Ag1i	130.0(17)	126.9 (8)	C2G—N1G—H3G		109.5
C1G—O1G—Ag1iii	123.8	125.8 (7)	H1G—N1G—H3G		109.5
Ag1i—O1G—Ag1iii	104.04	105.0 (3)	H2G—N1G—H3G		109.5
C1G—O2G—Ag1	120.8(15)	119.3 (7)	N1G—C2G—H4G		109.4
O2G—C1G—O1G	125(2)	127.3 (10)	C1G—C2G—H4G		109.4
O2G—C1G—C2G	119(2)	119.1(10)	N1G—C2G—H5G		109.4
O1G—C1G—C2G	116(3)	113.5 (10)	C1G—C2G—H5G		109.4
N1G—C2G—C1G	110(3)	111.1 (10)	H4G—C2G—H5G		108.0

Equation of plane was calculated for the zwitter ionic glycine, the nitrate ion and the silver coordinated oxygens in NDGSN and GSN. It was observed tht the nitrate ions are more planar NDGSN. The zwitterionic glycine is nonplanar in both NDGSN and GSN, and the deviations (Table 6) are also similar in both the strutures. Similary the equation of plane Ag coordinated with oxygen in nonplanar, with similar deviations of atoms from the plane in both NDGSN and GSN.

Table 6
Deviation of atoms form the plane in GSN[5] and CDGSN

atoms	Deviation of atoms from plane		atoms	Deviation of atoms from plane		atoms	Deviation of atoms from plane	
	Nitrate ion			Glycine ion			Ag coordinated	
	GSN[5]	NDGSN		GSN[5]	NDGSN		GSN[5]	NDGSN
N1	0.046	0.004	N2G	0.099	0.099	AG1	0.127	0.128
O1N	0.015	0.001	C2G	0.118	0.127	O1G	0.096	0.103
O2N	0.015	0.001	C1G	0.025	0.005	O2G	0.206	0.218
O3N	0.016	0.001	O2G	0.083	0.076	Ag1b	0.206	0.217
			O1G	0.038	0.043	O1B	0.225	0.232

Table 7 gives the comparison of torsion angle amongst the four complexes. It is observed that the conformation of glycine is similar in GSN & NDGSN. Similarly the conformation of DGSN and CDGSN are similar. But between the two there is difference in the conformation as shown in Fig. 3.

Table 7
Comparison of torsion angle amongst GSN[5], FDGSN[20], CDGSN and NDGSN

atoms	Glycine			
	GSN[5]	FDGSN[20]	CDGSN	NDGSN
O2G-C1G-O1G	124.9	125.7	125.9 (2)	127.3 (10)
O1G-C1G-C2G	115.8	116.89	116.8 (2)	113.5 (10
O2G-C1G-C2G	119.2	117.4	117.4 (2)	119.2 (10)
C1G-C2G-N1G	109.8	112.00	112.3 (2)	111.1 (10)
O2G-C1G-C2G-N1G	-166.18	161.61	161.62	-166.7
O1-C1G-C2G-N1G	12.72	-19.57	-19.58	15.67
H3G-N1G-C1G-C2G		52.35	48.19	-41.76

Silver coordination:

The distances of the atoms less than 3 Å to the silver atom are shown in Fig. 4 and tabulated in Table 8. The oxidation state of silver ion is + 1. In FDGSN and CDGSN the silver ion is mononuclear and it is coordinated to four oxygen's, of which two are from the same nitrate ion forming a bidenate coordination, and the other two are oxygen's of the symmetry related glycine. All these four oxygens are in the same plane. There is also a hydrogen atom, H5g in this plane. Ag ion is also coordinated to O1G & O2N above

and below this plane. The coordination of the Ag-O bond distances in the axial plane are longer compared to that in the equatorial plane. The four oxygens in the plane form a distorted triangular coordination [23]. In CDGSN and FDGSN, only the Ag-O2g distance differ more than the standard deviations,.

The coordination of silver in NDGSN is similar to that of GSN. The silver ion is binuclear with oxidation state of + 1. The silver ion is coordinated to Ag and oxygens of zwitter ionic glycine. There is considerable change in the Ag-Ag coordination between NDGSN and GSN. Unlike FDGSN and CDGSN, here the Ag is coordinated to only oxygens of the zwitter ionic glycine in the equatorial plane, and is coordinated to only one of the nitrate oxygens in the axial plane. There is no coordination to the Hydrogen atom of zwitter ionic glycine in GSN and NDGSN. Incidentally the Hydrogen coordination to Ag in FDGSN and CDGSN is through the deuterated Hydrogen connected to C alpha carbon of glycine.

It is basically the coordination of Ag ion which brings about a change in the structure. It is also necessary to mention here that it is the fully deuterated DGSN and CDGSN which produces a new isotope polymorph of GSN, whereas partially deuterated GSN and NDGSN doesn't result in a new polymorph. Hence it can be said that it is the C-deuteration of glycine which brings about change in the structure.

Table 8
Silver coordination IN GSN, NDGSN, FDGSN and CDGSN

Atoms	**Bond distance (Å)**		**Atoms**	**Bond distance (Å)**	
	GSN	NDGSN		FDGSN	CDGSN
Ag1—Ag1i	2.877(6)	2.815 (2)	Ag1—O1g	2.2901 (9)	2.296 (2)
Ag1—O2G	2.25(2)	2.227 (8)	Ag1—O2gi	2.417 (1)	2.428 (2)
Ag1—O1Gi	2.22(2)	2.282 (8)	Ag1—O1n	2.534 (2)	2.539 (3)
Ag1—O1Gii	2.37(2)	2.412 (9)	Ag1—O3N	2.6506(1)	2.653(3)
Ag1—O1N	2.86(2)	2.857(9)	Ag1—O2N	2.7392(1)	2.748(2)
Ag—O2giii	2.85(2)	2.833(9)	Ag1-O1G	2.7318(1)	2.738(2)
			Ag1-H5G	2.81(2)	2.78(4)

Molecular interaction

i) CDGSN

Packing of the molecule is shown in Fig. 5. Like FDGSN in CDGSN too, the nitrate ion, the silver ion and the zwitter ionic glycine form a layered structure in the ab plane. and are stacked along the c-axis.. Two of the hydrogen H1G and H3G form N-H…O hydrogen bonds to the nitrate in the plane, the third hydrogen H2G forms N-H…O hydrogen bonds to nitrate ion as well as the zwitter ionic glycine to the plane above. There are C-H..O hydrogen bonds, C2G-H5G is hydrogen bonded to O1G of glycine in the plane, whereas C2G- H4G forms bifurcated hydrogen bonds with oxygen of the nitrate ion and zwitter ionic glycine to the

plane below. Two of the oxygens of the nitrate ion(O1N and O3N) are coordinated to the same silver ion. The total crystal structure is built up from these repeating units to give 2-dimensional polymeric structure extended along the c-axis. Figure 5 CDGSN looking down a-axis. A comparison of hydrogen bonding parameters between FDGSN and CDGSN is given in Table 9. It is observed that the D…A distances have increased in all the hydrogen bonds in CDGSN.

Table 9
Comparision of hhydrogen bonding papmeters between FDGSN[20] and CDGSN (Å, °)

	D—H	H…*A*	D…A	*D*—H…*A*
N2G—H1G...O3N^{i}(FDGSN)	0.86 (3)	2.19 (3)	3.046 (2)	174 (2)
CDGSN	0.79(5)	2.26(5)	3.054(3)	178(5)
N2G—H1G...O2N^{i}(FDGSN)	0.86 (3)	2.40 (3)	3.028 (2)	130 (2)
CDGSN	0.79(5)	2.49(5)	3.038(3)	127(4)
N2G—H1G...N1^{i}(FDGSN)	0.86 (3)	2.64 (3)	3.447 (2)	157 (2)
CDGSN	0.79(5)	2.73(5)	3.456(3)	154(4)
N2G—H2G...O3N^{ii}(FDGSN)	0.91 (3)	2.34 (3)	2.986 (2)	128 (2)
CDGSN	1.03(5)	2.29(5)	2.994(3)	124(4)
N2G—H2G...O2G^{iii}(FDGSN)	0.91 (3)	2.45 (3)	3.175 (2)	136 (2)
CDGSN	1.03(5)	2.38(5)	3.188(3)	134(4)
N2G—H2G...O1N^{iii}(FDGSN)	0.91 (3)	2.52 (3)	3.121 (2)	123 (2)
CDGSN	1.03(5)	2.45(5)	3.139(3)	124(4)
N2G—H3G...O2N^{iv}(FDGSN)	0.90 (3)	2.02 (3)	2.907(2)	166 (3)
CDGSN	0.91(4)	2.03(5)	2.921(3)	164(4)
C2G—H4G...O1N^{v}(FDGSN)	0.95 (2)	2.43 (2)	3.222 (2)	140 (2)
CDGSN	0.96(4)	2.45(4)	3.231(3)	138(3)
C2G—H4G...O2G^{v}(FDGSN)	0.95 (2)	2.63 (2)	3.388 (2)	137 (2)
CDGSN	0.96(4)	2.61(4)	3.401(3)	140(3)
C2G—H5G...O1G^{vi}(FDGSN)	0.98 (2)	2.55 (2)	3.457 (1)	155 (2)
CDGSN	1.04(4)	2.51(4)	3.474(3)	155(3)

Symmetry codes: (i) -1 + x, -1 + y, z; (ii) -x, -y, -z; (iii) -1-x, -y, -z; (iv) x, -1 + y, z; (v) -1-x, -1/2 + y, 1/2-z; (vi) -1 + x, y, z.

ii) NDGSN

Packing of the molecule is shown in Fig. 6. The Nitrate ion the silver ion and zwitterionic glycine form a three-dimensional network unlike the case in CDGSN. The N-H…O hydrogens bonds are all to the nitrate ions unlike the case in CDGSN where the hydrogen bonds are to nitrate as well as the zwitter ionic glycine. Two of the hydrogen's H1G and H2G form bifurcated hydrogen bond to nitrate, whereas H3G forms single N-H…O hydrogen bond to nitrate ion. The C-H…O hydrogen bonds are also to the nitrate ion, Both the oxygen's O1G and O2G are coordinated to the Silver ion, and hence do not participate in any hydrogen bond as acceptor unlike the case of CDGSN. A comparison of hydrogen bonding parameter between GSN and NDGSN is given in Table 10.

Table 10
Comparision of hydrogen bonding papmeters between NDGSN and GSN[5] (Å, °)

	D—H	H...A	D...A	D—H...A
N1G—H1G...O1Ni(NDGSN)	0.89	2.50	3.12 (2)	127.2
GSN			3.14	
N1G—H1G...O3Ni	0.89	2.05	2.94 (2)	176.4
			2.97(4)	
N1G—H1G...N1i	0.89	2.62	3.45 (2)	155.5
			3.40	
N1G—H2G...O2N	0.89	2.47	3.11 (1)	129.6
			3.12	
N1G—H2G...O2Nii	0.89	2.10	2.86 (1)	142.7
			2.88(3)	
N1G—H3G...O1Niii	0.89	2.19	2.97 (2)	145.7
			2.93(4)	
C2G—H4G...O3Niv	0.97	2.44	3.41 (12)	173.8
			3.06	
C2G—H5G...O1Ni	0.97	2.37	2.97 (1)	119.6
			2.95	

Hirshfeld surface Analysis

The size and shape of the Hirshfeld surface is ideal for use in comparing different structure having the same molecules [24, 25]. Crystal explorer [26, 27] was used to generate Hirshfeld surfaces and 2D finger plots using the cif files obtained using the single crystal X-ray diffraction data of the FDGSN[20], CDGSN and NDGSN determined by us, and for GSN the Cif file (REFCODE: GLYAGN [5], was obtained from CCDC Cambridge Structural Database [28] using ConQuest database.

The following parameters were calculated using Crystal explorer [24] and are described below:

Globularity is a meaure of the degree to which the surface area differs from the value for a sphere of the same volume and is defined as

$$G = \frac{\left(36\pi V_H^2\right)^{1/3}}{S_H}$$

Where V_H and S_H denote molecular volume and surface area, and is 1.0 for a sphere and less than one as the molecular surface becomes more structured [24].

Globularity (Table 11) has been calcuated for nitrate and glyine molecule independently and also for the enitire comlex. The globularity for nitrate and glycine molecules when calculated independently follows the trend with maximum for GSN followed by NDGSN, CDGSN and FDGSN. It is also observed from structural data that the nitrate ions are planar in FDGSN and CDGSN, unlike the case with GSN and NDGSN reflecting more structured molecular surface of nitrate in FDGSN and CDGSN. In GSN [5] the hydrogen atoms have not been located and refined the volume and area reflects this, hence showing the lowest volume and area. The globularity parameter is similar in all the strutures. When the entire complex is considered, it is observed that FDGSN and CDGSN has similar values, which is lower than that of GSN and NDGSN.

Asphericity, Ω is measure of the anisotropy of an object and when applied to the atomic positions and is defined as

$$= \backslash\mathrm{raisebox}1ex\$1\$/\backslash\mathrm{raisebox}-1ex\$2\$\left(\sum_{i\neq j}\left(\ _i-\ _j\right)^2\right)\left(\sum_i\ _i\right)^{-2}$$

where λ_i are the three principal moments of inertia of the molecule. Ω has a value of zero for an isotropic object, 1.0 for a prolate object and 0.25 for an oblate object. [24]

Asphericity parameter ((Table 11))for nitrate molecule is similar in all the four strutures with a value close to zero showing the isotropic nature of nitrate molecule. In the case of glycine, NDGSN and GSN have similar values and FDGSN and CDGSN have similar values. When the entire molecule is considered it is observed that NDGSN and GSN are close to 0 indicating the isotropic natrure wheres as FDGSN and CDGSN indicae oblate nature .

Table 11
Comparsion of Hirshfeld parameters

Crystal structure		Volume ($Å^3$)	Area ($Å^2$)	Area/volume ($Å^{-1}$)	Globularity	Asphericity
CDGSN	nitrate	40.32	63.19	1.567	0.900	0.040
NDGSN	nitrate	43.45	65.93	1.517	0.907	0.035
FDGSN	nitrate	39.97	62.92	1.574	0.898	0.038
GSN	nitrate	49.57	71.55	1.443	0.912	0.038
CDGSN	glycine	69.55	92.04	1.323	0.889	0.071
NDGSN	glycine	69.82	92.02	1.318	0.891	0.048
FDGSN	glycine	68.95	91.50	1.327	0.889	0.071
GSN	glycine	61.55	84.01	1.364	0.897	0.063
CDGSN	Entire crystal	137.27	167.85	1.222	0.767	0.366
NDGSN	Entire crystal	138.86	157.43	1.134	0.824	0.044
FDGSN	Entire crystal	135.99	166.92	1.227	0.766	0.366
GSN	Entire crystal	138.56	155.41	1.122	0.833	0.038

Hirshfeld surfaces are mapped using the normalized contact distance (dnorm), which is defined as:

$$d_{norm=}\frac{d_i - r_i^{vdw}}{r_i^{vdw}} + \frac{d_e - r_e^{vdw}}{r_e^{vdw}}$$

The various parameters given are d_{norm}, which is a ratio encompassing the distances of any surface point to the nearest interior (d_i) and exterior (d_e) atom and the van der Waals radii of the atoms [24,25,29,30]. The negative d_{norm} visualized by red colour in the Hirshfeld surfaces indicates the sum of di and de is shorter than the sum of the relevant Van der Waals radii considered as the closest contact. The d_{norm} equal to zero visualized by white colour denotes intermolecular distances close to Van der Waals whereas contacts longer than the sum of Van der Waals radii with positive d_{norm} values are colored with blue. The surfaces are shown as transparent to allow visualization of the different moieties. The d_{norm} values when compared for nitrate molecules(Table 12 Fig. 7) in all the four structures shows that, FDGSN and CDGSN has more red spots compared to that in the case of NDGSN and GSN indicating more intermolecular interactions in CDGSN and FDGSN. The same when compared for glycine molecule(Table 13 Fig. 8), it is

observed that in NDGSN and GSN has more red spots compared to that in FDGSN and CDGSN. When the entire complex is considered, it is observed that mean d_{norm} (Table 14 and Fig. 9) value of CDGSN is more than that of FDGSN. The number of red spots are also more in CDGSN indicating more numbar of intermolecular interactions in CDGSN. Comparing GSN and NDGSN shows more red spots in NDGSN.

Shape index S is a dimensionless measure of shape and is s defined as

$$\mathrm{S} = \frac{2}{\pi}\arctan\left(\frac{_1 + _2}{_1 - _2}\right)$$

where principal curvatures are $_1$ and $_2$. Mapping is in the range-1.0 (concave) through 0.0 (minimal surface) to + 1.0 (convex)[24, 25]

The shape index is extremely sensitive to the change in surface shape giving a visual identification of the regions using complementary pairs of red and blue colored schemes. The concave red-colored region on the shape index represents the cluster of the surface around the acceptor atoms and the blue-colored bumps represent the cluster of the surface around the donor atoms. In the case of nitrate molecule (Table 12, Fig. 7) it can be seen that the concave red coloured regions are more in GSN and NDGSN compared to that of FDGSN and CDGSN, this is basically because the two of the nitrate oxygens are coordinated to the Ag ion in FDSN and CDGSN. In the case of glycine molecule(Table 13, Fig. 8), it is observed that GSN and NDGSN has more red coloured regions. The mean value of shape index is minimum in NDGSN, compared to other three structures and shows more number of red and blue spots.

Curvedness, C is defined,

$$\mathrm{S} = \frac{2}{\pi}\ln\sqrt{\frac{_1{}^2 + _2{}^2}{2}}$$

where principal curvatures are $_1$ and $_1$. Mapping is in the range − 4.0 (flat) through 0.0 (unit sphere) to + 0.4(singular) [24, 25]

The curvedness is a measure of the shape of the surface area of the molecule.The flat areas of the surface correspond to low values of curvedness, whereas sharp curvature areas correspond to high values of curvedness and usually tend to divide the surface into patches, indicating interactions between neighbouring molecules. The curvedness map displays large regions of green (relatively flat) separated by dark blue boundaries (large positive curvatures),. In the case of nitrate molecule(Table 12 Fig. 7) NDGSN shows more sharp curvatures followed by CDGSN. In the case of glycine molecule(Table 13 Fig. 8) and the entrire complex(Table 14 Fig. 9) NDGSN and GSN shows more sharp curvatures followed by CDGSN.

A plot of d_i versus d_e is a 2D fingerprint plot which recognizes the existence of different types of intermolecular interactions. Figure 10 shows the 2D Finger plots of C..H, N..H, O..H, H..H, Ag…o and Ag…Ag interactions. The Table 15 gives the percentage of different contacts. It can be from the Table 10 that C… H. N…H and O… H interactions are higher in CDGSN and FDGSN as compared to NDGSN. The H…H

interactions are higher in NDGSN. NDGSN and GSN have higher Ag…O interactions compared to that of CDGSN and FDGSN. NDGSN and GSN have Ag…Ag interaction, which is totally absent in CDGSN and FDGSN.

Table 15
percentages of different contacts in CDGSN, NDGSN, FDGSN and GSN

Refcode	N…H	C…H	O…H	H…H	Ag-O	Ag-Ag
CDGSN	0.2	0.3	65	1.1	14.0	0.0
NDGSN	0.1	1.1	61.3	2.3	17.7	2.0
FDGSN	0.2	0.3	65.3	0.9	13.9	0.0
GSN					24.8	2.1

Spectroscopic results

Since the x-ray doesn't directly show the deuteration in the compound, Raman scattering experiments were carried out for NDGSN and CDGSN. Lattice modes of GSN and FDGSN were also recorded (Fig. 11). Modes below 200 corresponds to vibrational modes of lattice modes, as observed form the Table 16a, it can be seen that GSN and NDSN have similar modes and FDGSN and CDGSN have similar modes confirming the similarity of structure as obtained from single crystal X-ray diffraction studies.

Table 16
a: Raman modes in NDGSN & CDGSN in the lattice region

Raman modes	GSN (cm^{-1}) [8]	NDGSN (cm^{-1})	FDGSN (cm^{-1}) [20]	CDGSN (cm^{-1})
Lattice modes	83	83	94	87
	107	106		
	118	119	120	121
	144	145		
	193	188		

Raman spectra corresponding to the internal modes of NDGSN and CDGSN is shown in Fig. 12 and Fig. 13 respectively. The assignment of the internal modes for NDGSN and CDGSN was achieved by comparing the Raman frequencies of the parent molecules i.e.N-deuterated glycine 31, 32,33,34], C deuterated glycine[[32, 33, 35] silver nitrate[36, 37, 38], GSN [8] and FDGSN [20] reported earlier as one expects close correspondence between the internal frequencies of these molecules. The vibrations corresponding to nitrate ions could be identified by comparing with the Raman spectra of $AGNO_3$ and also with that in GSN and FDGSN and have been listed in Table 16b. The internal vibrations of the zwitter ionic glycine can be considered as vibrations belonging to NH^{3+}, CH_2 and COO^- groups. For identifying the

Raman modes due to glycine in NDGSN and CDGSN, the Raman modes in N deutertaed glycine[31, 32, 33, 34] and C deuterated glycine[33, 34, 35] was used respectively. The modes corresponding to backbone N-C-COO, ND_3 and CH_2 for NDGSN are enumerated in Table 16c. The appearance of various modes associated with ND_3 and CH_2 group in Table 16c confirms the N deuteration in NDGSN. The modes corresponding to ND stretch were identified using the modes of ND stretch in FDGSN[20], since the same were not recorded in NDGLY in the References 31, 32, 33, 34. The modes corresponding to backbone N-C-COO, NH_3 and CD_2 for CDGSN are enumerated in Table 16d., similarly the various modes associated with CD_2 and NH_3 group in Table 16d confirms the C-deuteration in CDGSN. It can be observed from the Raman spectra in the region between 1900 to 3500 cm^{-1}, there are also modes corresponding to ND_3, showing there is partial deuteration of hydrogens attached to Nitrogen of glycine. This again shows that the importance of C-deuteration alone is important in bringing about isotopic polymorphism.

Table 16
b Raman Modes corresponding to nitrate molecule in CDGSN and NDSN

Raman modes	**$AGNO_3$ (cm^{-1})** **[36, 37,38]**	**GSN(cm^{-1})** **[8]**	**NDGSN(cm^{-1})**	**FDGSN(cm^{-1}) [20]**	**CDGSN(cm^{-1})**
v_4 NO_3^- ion	711	706	706	715	714
v_4 NO_3^- ion	731	721	720	725	725
v_2 NO_3^- ion	807	825	822	825	825
v_1 NO_3^- ion	1047	1050	1050	1046	1046
v_3 NO_3^- ion	1305	1329	1319	1336	1331
v_3 NO_3^- ion	1350	1354	1359	1362	1361

Table 16
c: Raman modes in NDGSN due to Zwitter ionic glycine

Raman modes	NDGLY (cm^{-1}) [31, 32, 33, 34]	NDGSN(cm^{-1})
Internal vibrations of the zwitter ionic glycine		
δ NCC (CCN bend)	330	336
CO_2 rock (r(COO))	493	525
CO_2 wag (γ(COO))	595	589
CO_2 bend (δ(COO)	666	654
C-C stretch	1001	998
C-N stretch	1017	1020
v_s COO (symm str)	1403	1416
va_s COO(symm str)	1592	1571
Raman modes corresponding to ND^{3+} vibrations		
ND_3 rock	763	749
	823	835
ND_3 symm defor	1166	1146
	1176	1167
ND_3 Asymm defor	1187	1180
ND_3 v(S)		2205
		2220
ND_3 va(S) sym. str.		2367
Raman modes corresponding to CH_2 vibration		
CH_2 ρ rock	964	971
CH_2 torsion	1269	1280
CH_2 wag ω	1323	Merged with NO_3
CH_2 bend δ	1441	1448
CH_2 v(S) sym. str	2972	2972

Raman modes	NDGLY (cm^{-1}) [31, 32, 33, 34]	NDGSN(cm^{-1})
CH_2 v(A) sym str	3007	3011

Table 16
d: Raman modes in CDGSN due to Zwitter ionic glycine

Raman modes	CDGLY(cm^{-1}) [33, 34, 35]	CDGSN(cm^{-1})
Internal vibrations of the zwitter ionic glycine		
δ NCC (CCN bend)	355	329
CO2 wag	539	532
CO_2 bend	668	667
C-C stretch	914	903
C-N stretch	1187	1186
v_s COO (symm str)	1396	1395
	1413	1413
va_s COO(asymm str)	1568	1556
Raman modes corresponding to NH^{3+} vibrations		
NH_3 tor	462	476
NH_3 rock	1111	1095
NH_3 symm defor	1498	1495
NH_3 Asymm deformation	1629	1611
	1663	1650
NH_3 v(S) sym. str		3069
NH_3 v(S) sym. str		3105
Raman modes corresponding to CD_2 vibrations		
CD_2 ρ rock	809	798
CD_2 wag ω	867	873
CD_2 torsion	941	933
CD_2 bend δ	1039	1030
CD_2 v(S) sym. str	2160	2158

Raman modes	CDGLY(cm^{-1}) [33, 34, 35]	CDGSN(cm^{-1})
CD_2 v(A) sym str..	2255	2267

Conclusion

In order to study the effect of partial deuteration on isotopic polymorphs, crystals of C Deuterated GSN (CDGSN) and N deuterated GSN (NDGSN) were grown. Single crystal x-ray diffraction showed CDGSN and NDGSN, both crystallize in P $2_1/c$ space group. In the crystal structure of CDGSN, there are 2 dimensional polymorphic structures extended along the c-axis, similar to that of FDGSN. In CDGSN, the silver ion is mononuclear similar to that in FDGSN with no Ag-Ag coordination. In NDGSN the nitrate ion the silver ion and zwitterionic glycine form a three-dimensional network similar to that of GSN. The silver ion is binuclear with Ag-Ag coordination similar to that in GSN. In both crystal structures the silver ion has an oxidation state of + 1. The globularity parameter is similar in all the strutures. For the entire complex the globularity parameter has similar values for FDGSN and CDGSN, which is lower than that of GSN and NDSN. The asphericity for the entire complex in the case of NDGSN and GSN are close to 0 indicating the isotropic natrure whereas for FDGSN and CDGSN it is near 0.36 indiacting oblate nature. NDGSN and GSN have higher Ag…O interactions compared to that of CDGSN and FDGSN. NDGSN and GSN have Ag…Ag interaction, which is totally absent in CDGSN and FDGSN. Raman measurements showed the partial deuteration of the compounds. The lattice modes of GSN and NDGSN are similar, and FDGSN and CDGSN are similar but different from that of GSN and NDGSN. Hence it is observed that CDGSN and FDGSN form similar isotopic polymorph, but différent from GSN and NDGSN which form similar isotopic polymorph, further confirming the importance the C deuteration in forming the isotopic polymorph.

Declarations

Ethical Approval

Not Applicable

Competing interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Authors' contributions

R.C.: Preparation ,characterization, analysis , Hirshfeld surfaces analysis Writing- Reviewing and Editing. R.R.C.: Analysis, Reviewing and Editing. F.C.: Data Collection- Reviewing and Editing. P. R. Data Collection- Reviewing and Editing, H.B.: Raman Experiment, Reviewing and Editing

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Availability of data and materials

The cif files describing the structure have been deposited in the CCDC database and the ccdc number is given in the manuscript

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Combined Figures and Tables

Figure 7/Table 12, Figure 8/Table 13, and Figure 9/Table 14 are available in the Supplementary Files section

Figures

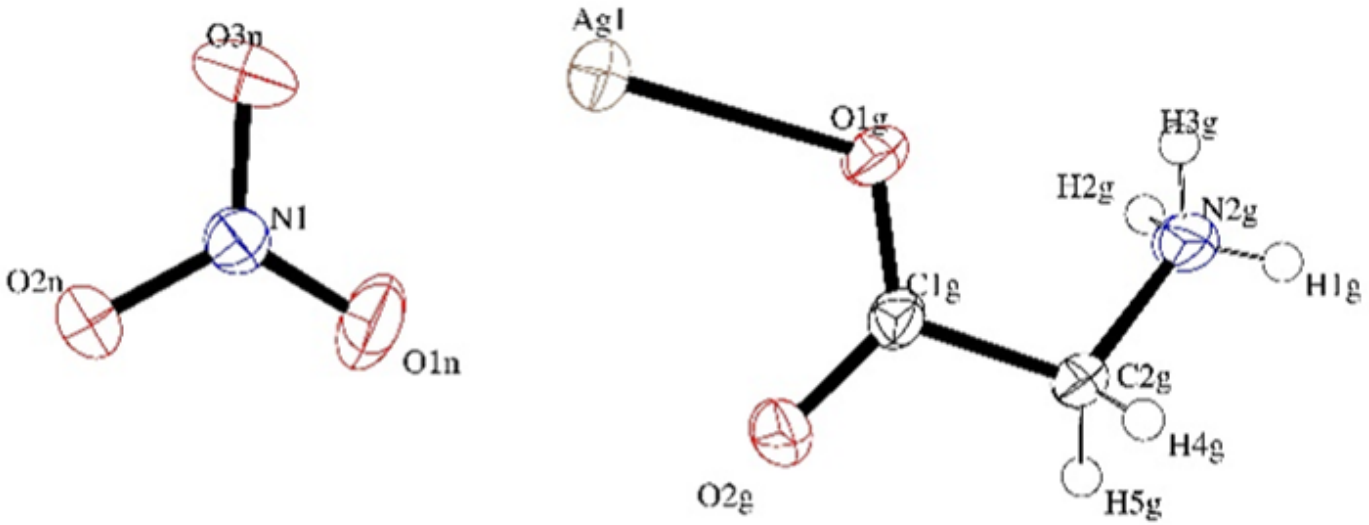

Figure 1

Ortep [L. J. Farrugia , 1997 [22] picture of asymmetric unit of CDGSN with 50% ellipsoidal probability

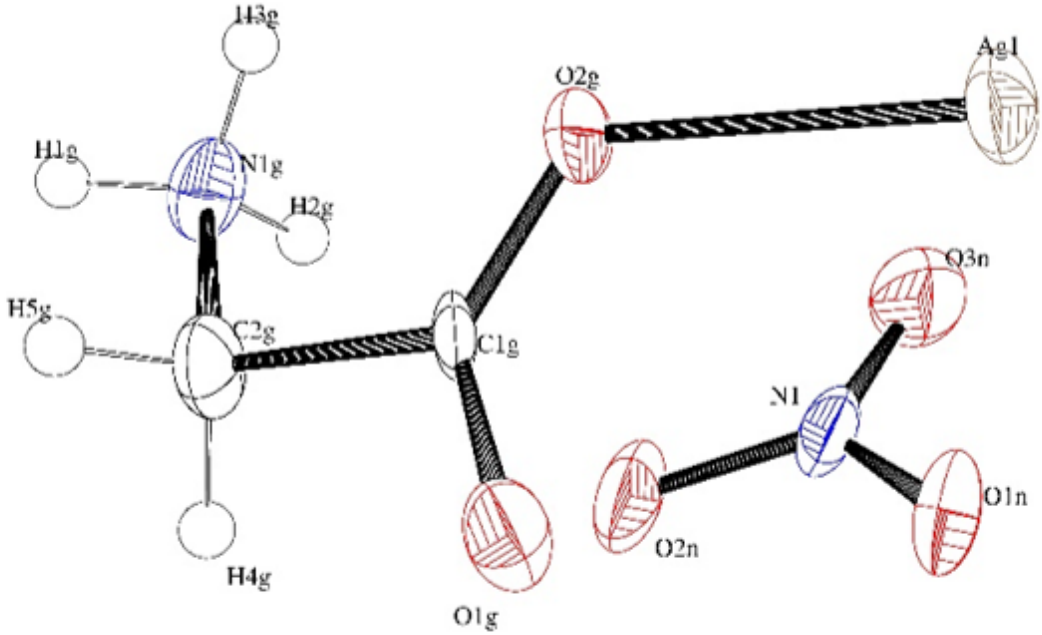

Figure 2

Ortep [22] picture of asymmetric unit of NDGSN with 50% ellipsoidal

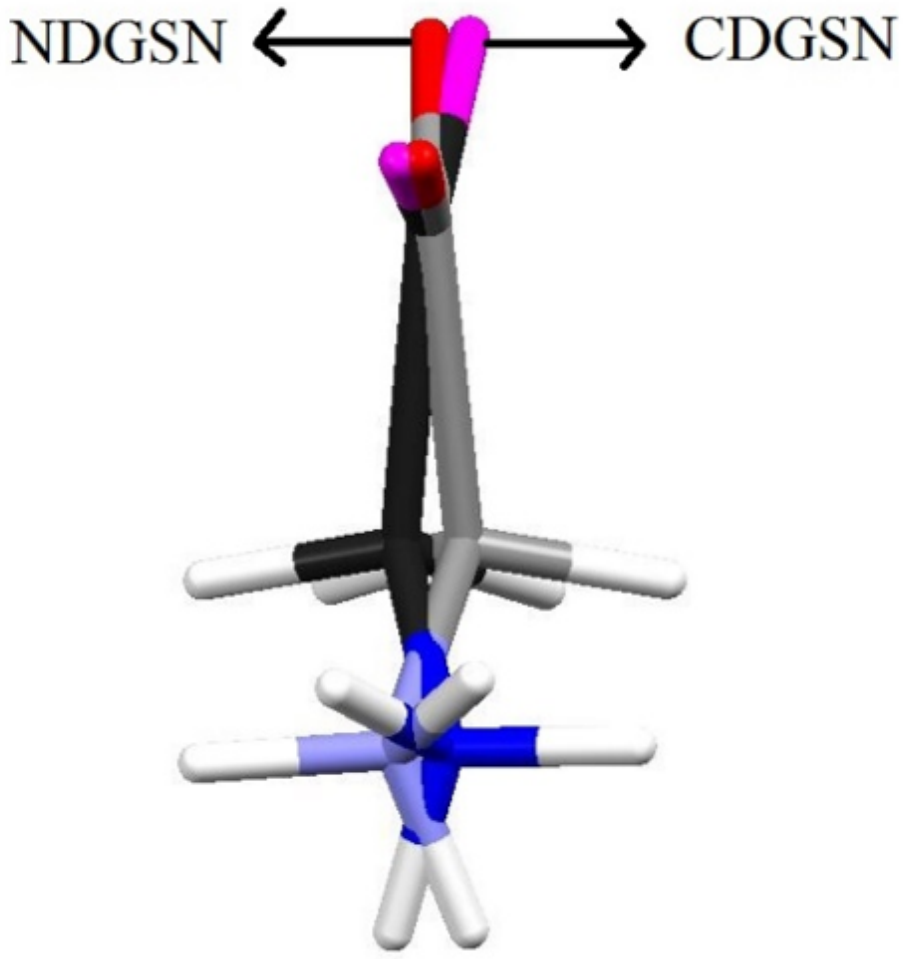

Figure 3

Conformation of Glycine molecule in NDGSN and CDGSN

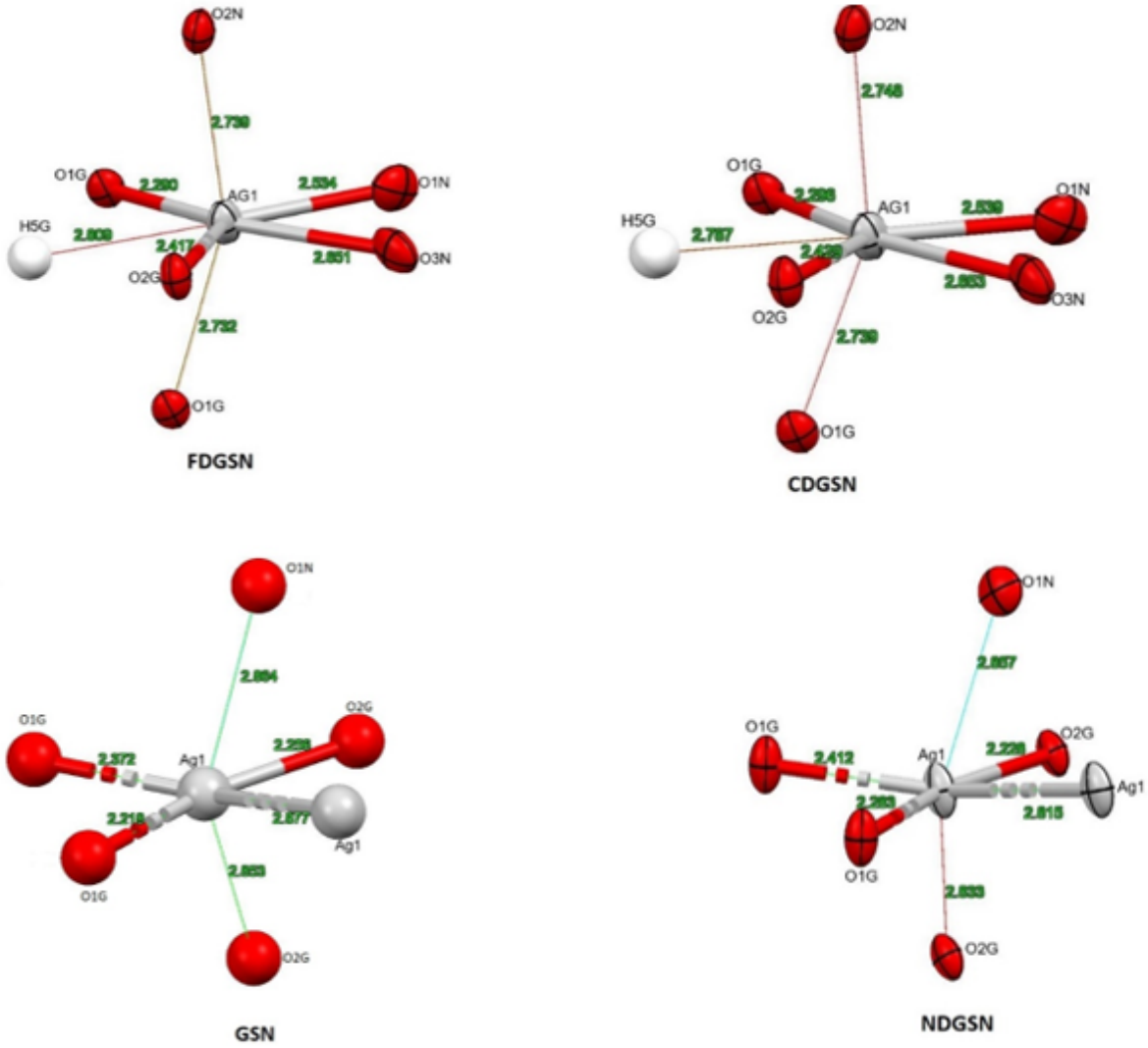

Figure 4

a and 4b gives the coordination distances of silver in GSN and NDGSN respectively

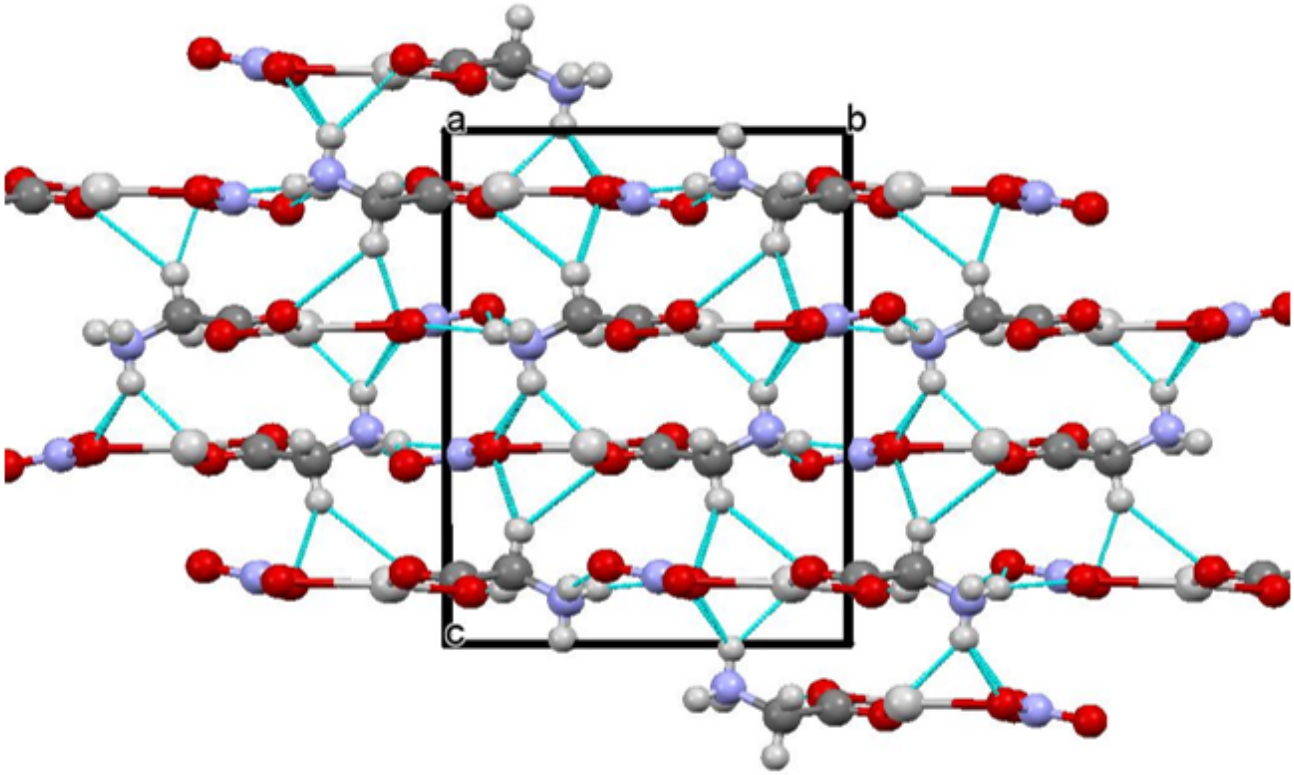

Figure 5

packing diagram of CDGSN looking down a-axis.

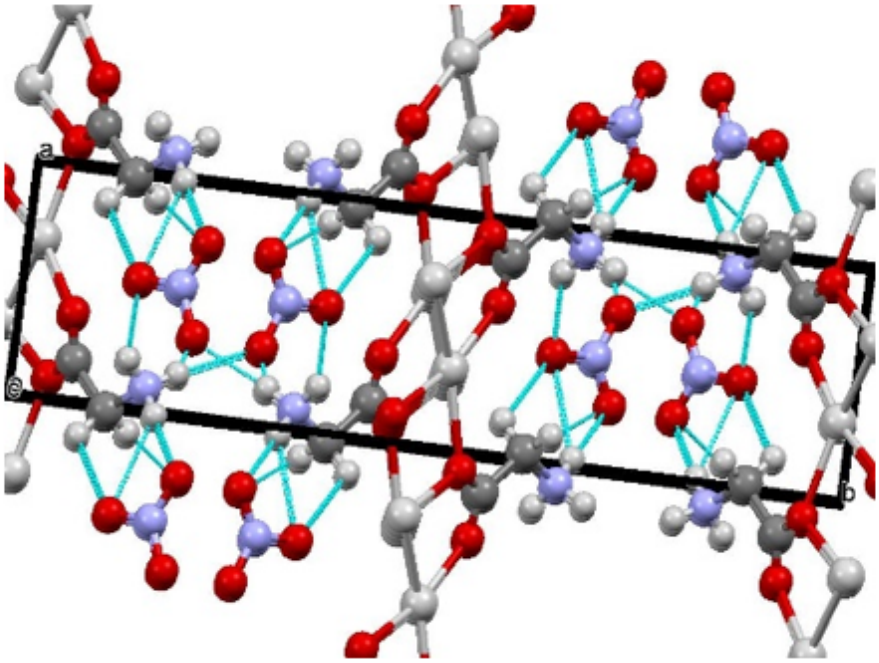

Figure 6

packing diagram of NDGSN looking down a-axis.

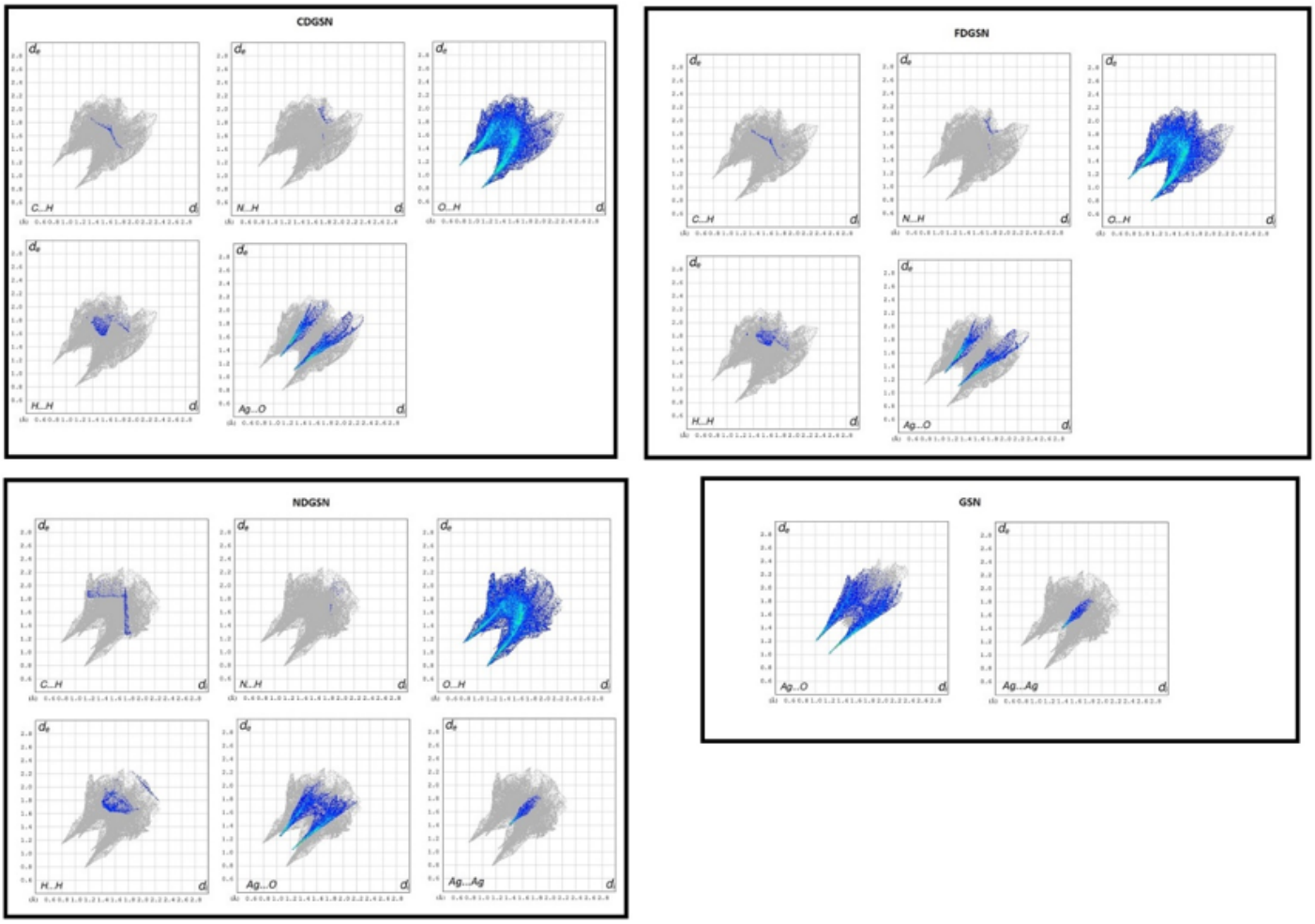

Figure 7

Figure 10. 2D fingerprint plot which recognizes the existence of different types of intermolecular interactions

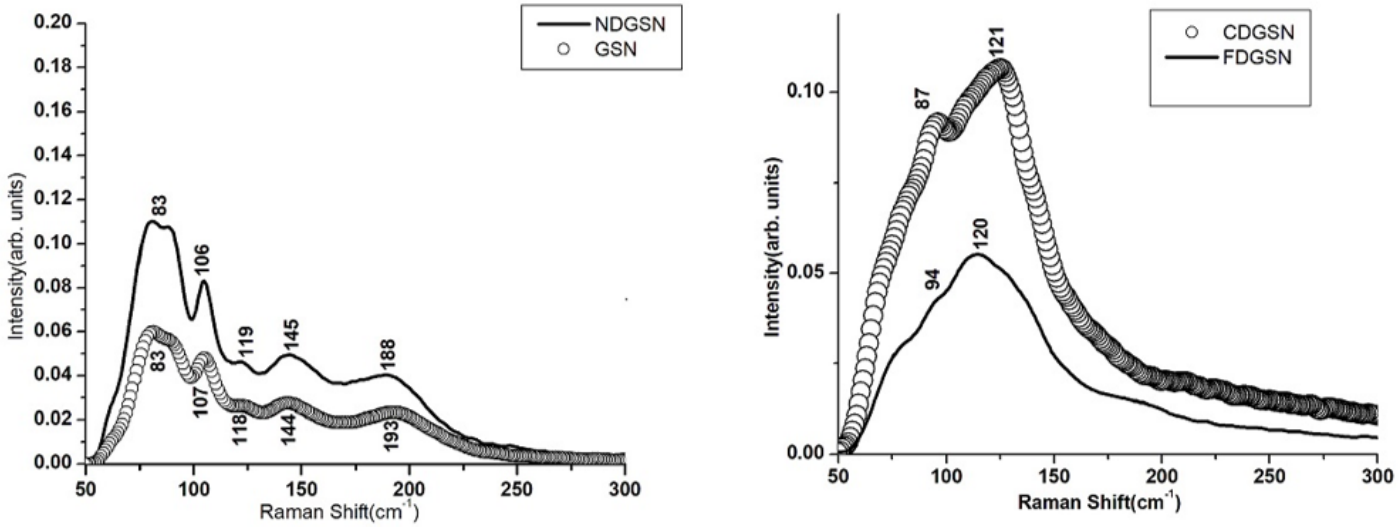

Figure 8

Figure 11 Raman Spectra of GSN, NDGSN, FDGSN and CDGSN in the lattice mode region

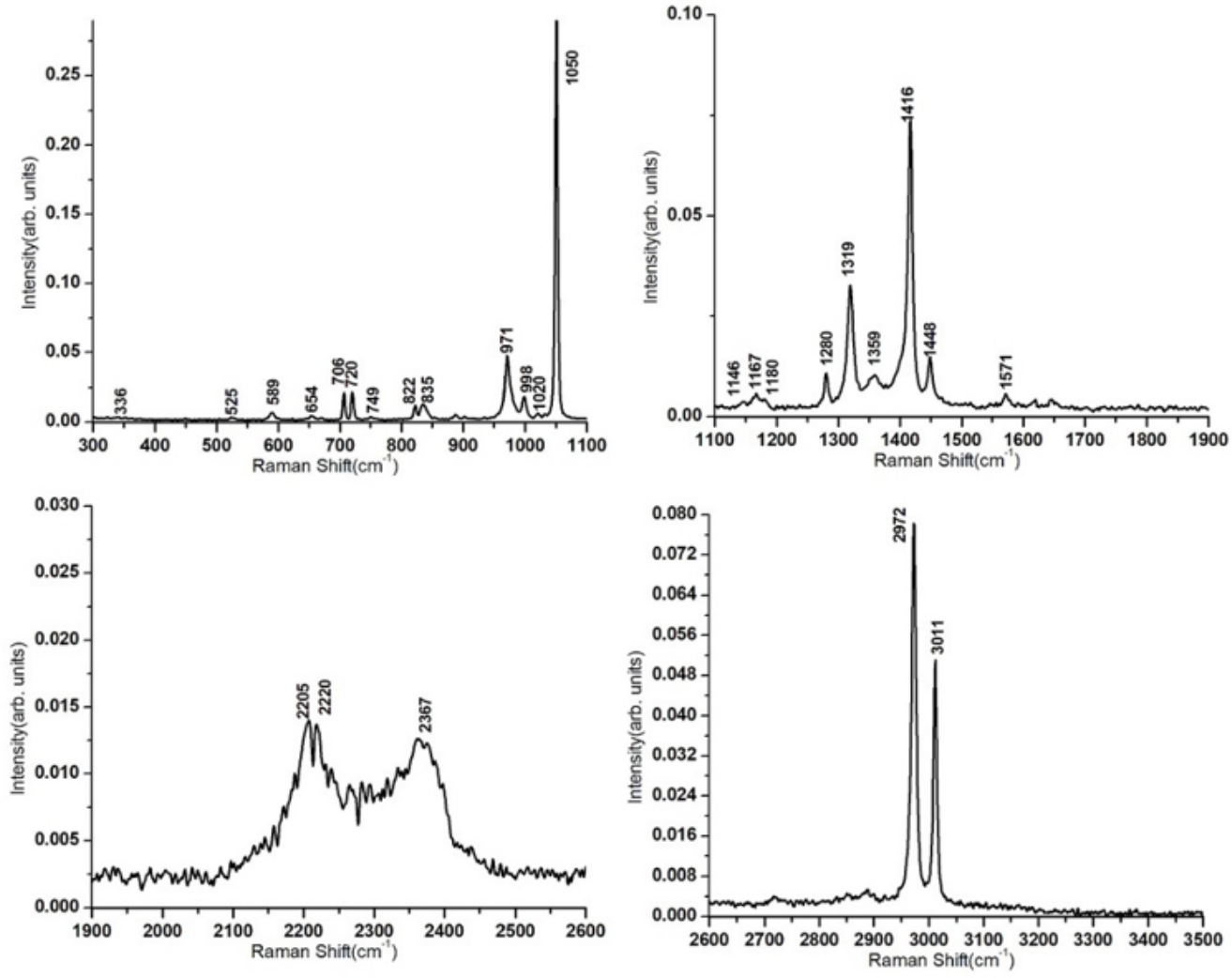

Figure 9

Figure. 12 Raman Spectra of NDGSN showing internal vibrations

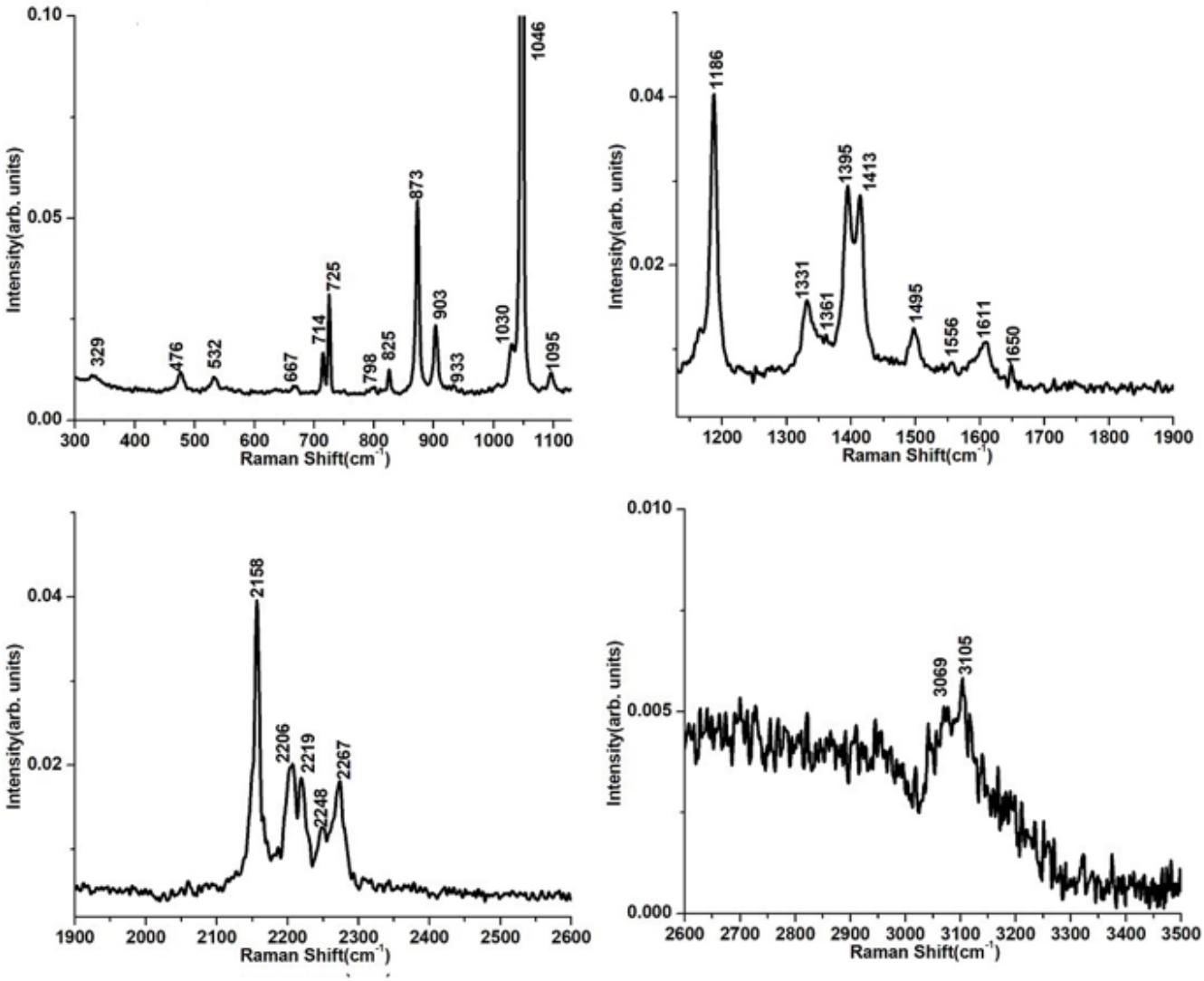

Figure 10

Figure. 13 Raman Spectra of CDGSN showing internal vibrations

Supplementary Files

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- combinedtableandfigure.docx