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1,1-BI-2-NAPHTHOL SOLUTIONS UNDER UV-NEAR-RESONANCE RAMAN SCANNING

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ABSTRACTS

Measurements of the normal and UV near-resonance Raman spectra of BN in basic solution were made and analysed, and the results were published. Ground state geometry, vibrational frequencies, off-resonance Raman intensities and depolarization ratios of 1,1-bi-2-naphtholate dianion were studied using density functional theory (DFT) computations (BN2-). The observed Raman bands were allocated in detail based on the estimated and experimental findings of î, I, and F. UV resonance Raman spectra showed a substantial increase in the 1612 cm-1 Raman band of BN compared to the conventional Raman spectrum. According to depolarization ratios for the 1366 and 1612 cm-1 bands, it is clear that both transitions polarizabilities contribute to the 1366 cm-1 band, whereas onlytransitions polarizabilities contribute to 1612.

Introduction[=

Chemists and biochemists depend heavily on chiral compounds. Because of their very stable chiral conformation, chiral 1,1-binaphthyl compounds have become more popular. Asymmetric organic synthesis and catalytic processes have previously used them extensively as chiral inducers. 1,2 1,1-bi-2-naphthol (BN) and its derivatives, which are optically active, are particularly important C2-symmetric molecules. 1,1-bi-2-naphthol is widely used as a starting point for the production of chiral binaphthyl compounds, on the other hand. It has been frequently employed as ligands for asymmetric metal complexes and has proven excellent performance in chiral recognition with this particular type of chemical. 3-6 Using chiral binaphthol-derived titanium complexes, Ishii et al. studied asymmetric catalysis of the Friedel-Crafts process with fluoral. 5aThe steric and electronic characteristics of the chiral BN ligands influence the result of a specific asymmetric transformation. It has been extensively researched using several spectroscopic approaches, including as electronic absorption, IR, and Raman spectroscopies, to determine its structure and characteristics. The VCD spectra of BN were measured by Setnicka and coworkers, who then used density functional theory (DFT) computations to assign the observed VCD bands. 7 Calculations based on DFT were used to investigate the mechanism of BN isomerization. 8 BN adsorbed on silver colloids was examined by Nogueira and coworkers for the first time using surface-enhanced Raman (SER) spectroscopy, and empirical assignments for the observed Raman bands were provided. 9 Due of its near-UV absorption, the UVRR spectrum of BN in diverse solutions is likely to be observed and may give information on both the ground and excited states. But to our knowledge, the resonance Raman (RR) spectra of BN have not yet been reported in the literature.While this is the case, new spectroscopic methods for probing molecule chirality, sum-frequency generation (SFG) of chiral solution, are now under development as novel spectroscopic tools10-18. These tools were reviewed by Belkin and Shen17a and Fischer and Hache17b. The chiral sum-frequency spectroscopy of electron transitions,12,15 the chiral sum-frequency spectroscopy of vibrational transitions, and the doubly resonant SFG (DR-SFG) have all been used to investigate R(S)-BN solutions as a prototype for chiral compounds. The new chiral electrooptic effect: SFG from optical active BN liquids in the presence of a dc electric field,16 as well as second-harm Many aspects of the sum-frequency vibrational spectroscopy (SFVS) studies of chiral BN solution are shared by resonance Raman spectra of BN solution. To begin, the Placzek invariants 1 for vibrational peaks in RR spectra show that the intensity of the chiral vibrational peaks in infrared-visible sum-frequency vibrational spectra from isotropic chiral liquids is proportional to the square of the corresponding antisymmetric Raman tensor element14. 20 Using direct resonance Raman spectroscopy, it is possible to investigate the relationship between the SFG and the antisymmetric Raman

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tensors. As a second example, substantial resonance enhancement, thorough mode assignment, and the ability to deduce vibronic coupling for the modes are all benefits of using RR spectroscopy for sumfrequencies in the vibrational spectrum. 14,15.1,1-bi-2naphthol has been studied in a basic solution for its UV near-resonance Raman spectra. Intensity and depolarization ratio resonance enhancements,and the 1612 cm-1 and 1366 cm-1 antisymmetric Raman tensorsVibrational bands in RR spectra have been analysedqualitatively.Researchers have used DFT simulations to investigate the1,1-bi-2- ground state structures and vibrational spectraNapphol and 1,1-bis-2,naphtholate dianion, respectively (BN2-),because the two hydroxyl groups of BN may interact with one other in a basic solutiontake place, leading to the formation of BN2-.1,6assigning a number of molecular vibrational bandsBN spectra are shown here. in a succinct and reasonable mannerparticular tasks rather than a review of the literature7,9,18A search for vibrational spectra of Bn and Bn2 did not provide any results,9,14 Assignments of Raman bands for BN are discussed in this study.BN2 and BN3 have been addressed in further depth.Combiningpolarisation and DFT calculationsresults from experiments and BN2-Raman spectra compared withthe one of BN.

Experimental and Computational Methods

Without additional purification, 1,1-Bi-2-naphthol was acquired from Alfa Aesar and utilised in the experiment. Dissolving BN in 3 M NaOH aqueous yielded the BN2- and BN solutions.the concentration of acetone solvents, respectively,from 0.3 to 0.05 molars. The solutions that had been devised were permitted to3 days of equilibration before spectral measurements are recommendedLightpaths of 5 mm were used to collect UV-vis absorption spectra.utilising a Shimadu UV-C cell at ambient temperatureThe spectrometer 2401PC is used for this analysis. A Jobin-type instrument was used to capture the Raman spectra.Probe fitted with air-cooled cooling system: Labram HR 800 spectrometerScanner with 600 grooves/mm and a CCD detectora 2400 grooves/mm UV grating and a visible grating. AA 40 mm lens was utilised to capture the occurrence in its entirety.back-scattering of a laser beam to gather the scattered lightgeometry. The 325 nm and 514.5 nm lines of a He-Cd laserAnAr ion laser's nm line was employed as the excitation source for this experiment.The sample was powered at 3.5 mW and 1 mW.The CCD detector's data collecting duration ranged from 80 to 180 s.Spectra of the Raman effect. To limit the chance of the sample being harmed as a result of exposure.We found UV levels after continuous exposure to laser light.resonance A revolving cell is used to get the Raman spectra of a solution.Raman band depolarization ratios were analysed using theIdentical circumstances apply. The components that are perpendicular and parallel

samples of solution polarised Raman spectraparallel and perpendicular, polarizers were usedin accordance with the laser's incident polarisationbeam. Because the spectrometer does not have polarisationcapabilities,thepolarised scrambler avoids biases in polarisationdetectionBoth tetrachloromethane and cyclohexanes were studied for their Raman scattering propertiesthe depolarization ratios of the were checked and calibrated by measuringSpecies of interest.DFT computations were performed on BN and BN2- molecules.out of the three-parameter hybrid functional developed by Becke et al.(known as B3LYP),21 has been used for research purposes.BN systems' structures and characteristics.8,18 To cut backWe began our search for stable states with a low computational cost in mind.geometric optimization of the examined molecule's structure usingBasis sets of 6-31G, which do not have any symmetry,constraint. The final structures created from the collected data were thenUsing 6-31G* basis sets with the appropriate symmetry to optimiseA limitation on the (C2 point group). Calculations based on the analysis of frequency(with B3LYP/6-31G*) the final touches on the optimal structure had been completedin order to verify that the optimised structures are really energy-efficient.a theoretical vibrational spectrum may be obtained by combining these two methods. As a result ofindifference to anharmonicity and incomplete base setsVibrational frequencies are often underestimated when using DFT calculations.frequencies. Differences between the calculated and actual valuesThis may be scaled to adjust for both experimental and natural frequencies.

A single factor was used to compute the frequencies.a study by 23 Oakes et al.it has been recommended that the standard value of 0.98 be usedThe porphyrins are an example of planar conjugate systems23 This element has a significant impact on the outcome.is used in this research. Assigning each person's vibrational frequencyChecking the Cartesian frequency was used for this purpose.movements in the regular mode of the relevant object All of the

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computations have been done.Gaussian 03 suite26 was used for the experiments.using a P4-3.0G processorWe use isolated single molecule calculations in this study.to anticipate the shape and frequency of solution-phase vibrations.If there are any mistakes or discrepancies, it may not be accurate.For a dianion, this is very important. However, at this point in time, the situation is rather different.literature on quantum mechanics tends to emphasise practise over theory.computations in chemistry. As an example, using a similar methodAccomplished ab initio computing was created by Markham et altreatment of the resonance effect of deuterium replacementImidazole, imidazolium, and their derivatives' Raman spectra,When the solvent impact is high, it's likely to be at least 22in contrast to what was found in this research. theoretical computations by Pasterny et al.showed that the computed results had not changed significantlyThe relationship between vibrational frequencies and medium polarity.

Results and DiscussionGround-State Geometries and Atomic Charges.

The ground-state geometric structure of BN2 was studied using DFT calculations. Calculations show that BN2- is the best candidate.Figure 1b shows that it possesses a trans-quinonoid-like structure.This is in line with the fundamental BN experiment's findingssolution.1,6 Table 1 shows the bond lengths, bond angles, and bond numbers.B3LYP/6-31G* was used to improve the dihedral angles of BN2. ForIn order to provide a point of reference, the BN structure was also estimated.outcomes were reported at the same theoretical levelResults from X-ray crystallography are shown in Table 1.Graph No. 27The BN structure drawing and atomic labelling utilised in Example 1a is shown in Figure 1a.this documentTable 1 shows the calculated bond lengths.According to the experimental results, the angles of BN are typically in accordCalculations using the B3LYP/6-31G* formula reveal thatThe BN molecule's two naphthol rings are almost parallel.They are in agreement with each other. There's a dihedral angle in the plane of92.7° is compatible with the naphthyl groups' planes.BN.27 Deprotonation's X-ray value (99.2°) is in line with this.leads to the formation of two naphthyl groups by hydroxyl radicalsbent in the direction of coplanarity, leading to riseA more pronounced dihedral angle (68.3°). Calculation of the DFT for BN2 viaalterations in the C-O and C-C bonds are clearly visible.near the hydroxyl groups. When compared to BN, the C1-the distances between BN2-C2, C2-C3, as well as C9-C10, are determined.while increasing by 0.067, 0.049, and 0.017The distance between C1 and C9 has been shown to decrease by 0.013 nm. Particularly,BN2-'s C-O bond length drops by 0.105 nmcomparing to BN's results based on the bond's calculationsBN2-'s dihedral angles and lengths suggest that it has a quinonoidlikestructure.Figure 1b illustrates the structure.This kind of analysis is called a natural population analysis (NPA).B3LYP/6-31G(d) for BN and BN2-ground states. Tableoxygen and carbon atoms are shown in figure 2 with their respective atomic charge distribution.Both BN and BN2-have ring carbon atoms. As you can see,C2 is the only carbon atom that does not have a negative charge.This one has a definite electric charge. Calculations based on the NPA show that UVRR Spectroscopic Study of 1,1□-Bi-2-napthol Solutions

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TABLE 1: Calculated Structural Parameters of BN and BN^{2-} and Experimental Values of BN

	BN^{2-} (calcd)[a]	BN (calcd)[a]	BN (exp)[b]
	bond distances (Å)		
C_1-C_2	1.454	1.387	1.382
C_2-C_3	1.467	1.418	1.410
C_3-C_4	1.367	1.373	1.351
C_4-C_{10}	1.423	1.418	1.418
C_5-C_{10}	1.414	1.420	1.426
C_5-C_6	1.383	1.376	1.353
C_6-C_7	1.420	1.416	1.393
C_7-C_8	1.377	1.377	1.369
C_8-C_9	1.437	1.423	1.411
C_9-C_{10}	1.452	1.435	1.423
C_9-C_1	1.417	1.430	1.424
C_2-O_{11}	1.263	1.368	1.370
$C_1-C_{1'}$	1.498	1.495	1.494
	bond angles (deg)		
$C_1-C_2-C_3$	115.4	121.3	121.1
$C_2-C_3-C_4$	124.0	120.4	120.2
$C_3-C_4-C_{10}$	120.8	120.8	121.6
$C_{10}-C_5-C_6$	122.1	121.0	121.0
$C_5-C_6-C_7$	118.3	119.7	120.5
$C_6-C_7-C_8$	121.2	120.8	120.3
$C_7-C_8-C_9$	122.5	121.1	121.6
$C_8-C_9-C_1$	122.6	122.1	122.4
$C_1-C_9-C_{10}$	121.8	119.9	119.7
$C_2-C_1-C_9$	120.2	118.8	119.1

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		dihedral angles (deg)	
$C_2-C_1-C_{1'}-C_{2'}$	111.1	86.5	
$C_2-C_1-C_{1'}-C_{9'}$	68.3	92.7	99.2

[a] DFT calculations using 6-31G* basis-sets. [b] X-ray results from ref 27.

TABLE 2: Calculated NPA Charges for BN and BN^{2-}

	BN	BN^{2-}
C1	−0.089	−0.145
C2	0.350	0.406
C3	−0.298	−0.298
C4	−0.190	−0.250
C5	−0.204	−0.229
C6	−0.245	−0.323
C7	−0.228	−0.274
C8	−0.214	−0.211
C9	−0.023	−0.028
C10	−0.074	−0.107
O11	−0.680	−0.731

UV-Visible Absorption Spectra.

Absorption spectra of 1,1-bi-2-naphthol dissolved in acetone and 3 M NaOH aqueous solution are shown in Figure 2 (left) and Figure (right). InThe absorption spectra of acetone show two peaks.324 nm and 336 nm are the best. BN is the primary solution for BNIt moves to 358 nm with an uneven absorption peak.a widened silhouetteIt should be noted that the excitonic splitting for BN and BN2- is different.because the anion's dihedral angle is no longer around 90 degrees, and

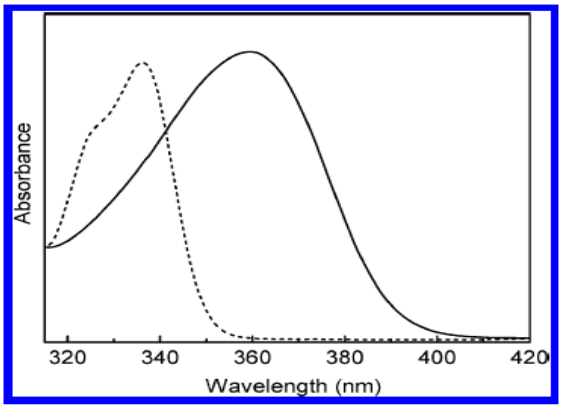

Figure 2. UV-visible absorption spectra of BN in a 3 M NaOHaqueous solution (solid line) and in an acetone solution (dot line).

Larger splits may be induced by this method. There are a number of possible explanations for the wider peak width shown in BN2. The Franck-Condon trend is also a significant contributor to peak width.in the spectrum of absorption. The most compelling proof thatThe doublet's Franck-Condon progression wasthe electronic spectrum, as recently by Fischer et al.15,2HN and BN are certainly chemically similar.owns up to its own doublet. The solvent impact is also a factor.is also critical in creating a more rounded silhouette. The colour change from red toBasic solution BN's UV absorbance is higher than that of its solution in water.This may be ascribed to the improved electrical properties of acetoneon the excited states of BN2, which had been well-knownconjugate anionic bases of hydroxyaryls.

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Raman Spectra.

BN2- dianion contains 34 atoms and 96 \smodes of vibration, which, according to the C2 symmetry, can\sbe categorized as ¡) 49A + 47B. The vibrations of BN molecule,which having two extra hydrogen atoms, may be classedas ¡) 52A + 50B. According to the vibrational selection criteria,all of these modes are active for both IR and Raman transitions.For regular nonresonance Raman, depolarization ratios generallyhave a value between 0 and 0.75. The depolarization ratio isless than 0.75 for a completely symmetric mode, while it equals0.75 for a nontotally symmetric mode. As such, polarized Ramanmeasures may be used to estimate the symmetry of aparticularmode.Nogueira et al. examined the SERS of BN with 1064 nmexcitation and recommended preliminary designations for numerous strongRaman bands.9 In this article, the UV resonance Raman spectraand normal Raman spectra of BN in the basic solution wererecorded. More full assignments and some reassignmentsof Raman bands have been created on the basis of DFTcomputations, polarization measurements, and comparison ofRaman spectra of BN2- with those of BN. Figure 3 depicts thetypical Raman spectra of BN in an acetone solution or as solidpowder with 514.5 nm excitation, normal (ìex) 514.5 nm) andnear-resonance (ìex) 325 nm) Raman scattering of BN inaqueous NaOH solution, where the Raman emissions owing to thesolvent (acetone) are designated as “S”. Tables 3 and 4 list theexperimentally observed and DFT-calculated frequencies, intensities,depolarization ratios, and assignments of Raman bandsof BN and BN2-. The tasks will be addressed in depthin the following section 3.3.1. Because of the steric hindranceUtilizing OH group and hydrogen bonding in BN solutions,7 wetreat BN and BN2- as hard molecules and do not construct theaverage for the dihedral angle between two aromatic planes fordependant qualities. Although a similar method was utilized incertain similar references,7,18 additional extensive research arerequired. A recent work relevant to this has been undertaken byDevlin et al., who thoroughly explored

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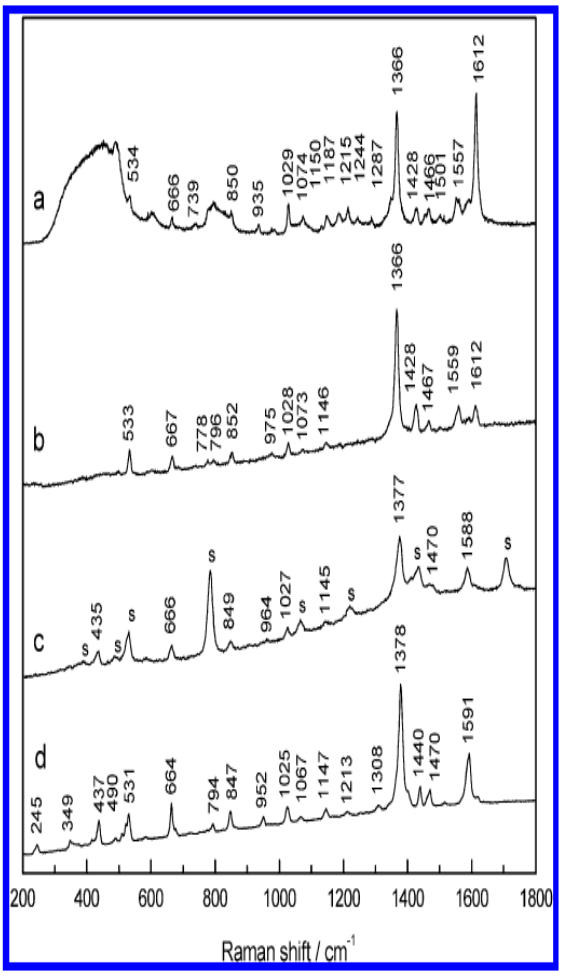

Figure 3. Raman spectrum of BN (a) in a 3 M NaOH aqueous solution,ìex) 325 nm; (b) in a 3 M NaOH aqueous solution, ìex) 514.5 nm;(c) in an acetone solution, ìex) 514.5 nm; (d) as a solid powder, ìex)514.5 nm.conformational analysis of some chiral molecules using IRand VCD spectroscopies and ab initio density functionaltheory.

Raman Spectra Excited at 514.5 nm.

Raman spectra of the BN in 3 M NaOH aqueous solution as well as in acetone stimulated at 514.5 nm are shown in Figure 4. Fig. 5 illustrates.Raman spectra's Cartesian displacements fromBased on B3LYP/6-31G*, we've arrived at BN2. Raman spectroscopy revealsBN2- (Figure 4b), a significant Raman band was seen533, 667, 852, 975, 1028, 1366, 1428, 1467, 1559, and 1592A density of 1612 cm-1. These bands are seen as a good match forvibrations that are completely symmetrical due to the depolarization ratios that they exhibitless than 0.75. The BN2-band's strongest band could be seen.It seems that the 1377 cm-1 matches to the 1366 cm-1.as seen in Figure 4a) because of the presence of theirSimilar levels of depolarization and intensity. 1064 nm is the wavelength in question.This band was also noticed with an exuberant BN SERS.the C-O stretching was assigned with high severitymode.9 Our DFT calculation, on the other hand, fails to uncover a sufficientin the area, a possible candidate for C-O stretching contrary toWhen using the B3LYP/6-31G* formula, an extremely powerfulDue to the C9C10/C9C1 stretching mode, Raman is seen at 1357 cm-1.to the naphthalene î5 structural mode, as perScherer30). As a result, we assign the 1366 cm-1 band toVibrational BN2- to the A-symmetry C9C10/A9C1 stretching vibration.A similar way of operation was observed for the neutral BN molecular molecule.A notable Raman intensity was found at 1387 cm-

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1.This is quite close to the actual figure that was measured (1377 cm-1). The B3LYP /However, BN's 6-31G* computation shows that this mode is present.Because of the C9C10/C9C1 stretches, the O11-H18 bondsThis mode also involves in-plane bending. Because of this,predicted that the -OH group deprotonation would lead toan obvious impact on the frequency of the signal. Predicted results of DFT calculationsDeprotonation causes a 30 cm-1 shift in this phase.Experiments revealed an 11 cm-1 decrease in theBN2 has a 1366 cm-1 band, compared to BN, which has a 990 cm-1 band.but still substantially different from the calculated valueThe theoretical forecast was correct.Threepolarised Raman bands may be seen between 1550 and 1650 cm-1.detected at a wavelength of 1559, 1592, and 1612 cm-1the dianion BN2. Bands 1559 and 1612 cm-1 of BN2- may be seen asA lot more powerful than the 1592 cm-1 range. According to Nogueira et al.,The C-C stretching of these bands has been scientifically linked to them.Rings of naphthyl According to our density functional theory (DFT) calculations for the BN2-dianion,notwithstanding the fact that the weak 1592 cm-1 band might be blamed onring stretching of the naphthyl's C7, 8, 3, 4, and C10, 5 bondsBoth the C2O11 and the powerful 1559 and 1612 cm-1 bands are involved.both stretching and the C3C4/C5C6 stretching of naphthyl are used The BN'ssolid, with a strong 1591 cm-1 band and a weak 1619 cm-1 band.In this area, cm-1 were detected. We believe they're the result ofThe B3LYP/6- model predicts vibrations of 1606 and 1630 cm-1.Calculation results from the 31G* show that these two modes are linked.mostly by the stretching and bending of naphthyl CC and O11H18,as well as an important contribution from the 1630 cm-1 modefrom the stretching of C2O11. Because they both rely on vibrations,The deprotonation of -OH groups is a process thatsubstantial frequency shifts are likely to occur in these two cases.modes. This seems to be the explanation for the apparent disparity between theThe 1550-1650 cm-1 range in the BN and BN2-Raman spectra.Most BN and BN2-related vibrations occur between 900 and 1500 Hz.Naphthyl in-plane CC stretching and CC stretchingCH is buckling under the strain. At 1467 nm, we found two distinct Raman bands.as well as 1428 cm-1 for BN2 (Figure 3b). In this case, the matching bandsFor the BN solid, 1470 and 1440 cm-1 were observedA band at 1440 cm-1 is overlapping with BN in acetone solution.It's a solvent band Our DFT calculations reveal the followingthe CC stretching of naphthyl has been divided into two bands.in-plane bending connected to the C-H through the î29Naphthalene may exist in four different forms, according to Scherer's notation30.Downshifts of 1 cm-1 and 35 cm-1 are predicted by DFT calculations.BN2's two modes of operation, as opposed to BN1The BN. In our experiments, we saw a 3 cm-1 decrease inwith a downshift of 12 cm-1 for the 1428 cm-1With comparison to their BN2 cousins, the band of BN2 isqualitatively identical to what was predicted.At 1146 and 1028 nanometers, we see the Raman bands of BN2-with an in-plane vibration frequency of 975 cm-1 for the naphthyl groupsIt'll look something like this: at the plane of Scherer's î6, bending of the C6/C7Hstretch of the C6C7 bond, and in-plane deformation, both at î24 and î32of the naphthyl ring kind). According to the B3LYP/6-31G* calculations,for each of these modes was 1143 cm-1, 1024 cm-1, and 975 cm-1.A similar pattern was seen for BN molecules.It was determined that the wavelengths were at 1145, 1027 cm-1, and 964 cm-1.similarity between the frequencies and intensities of and 957 cm-1BN and BN2-bands show that deprotonation has occurredThe CH and CC are only slightly affected by -OH groups.A moderate effect is produced by a short distal benzoring limb stretch.The naphthyl ring's in-plane deformation.As shown by our DFT results, the vibration of BN andThis area of 700-850 cm-1 is mostly attributable to the inplane.Napthyl ring deformations. We add meaning to what we see.Bands 852 cm-1 and 849 cm-1 of BN2 to the 852 cm-1 of BNchanges in the shape of the distal benzo ringis mostly attributable to the C3C4C10 expanding out of phase andIn other words, the bond angles of C6C7C8. Calculations based on DFT suggest that this band will@ 835 cm-1 for BN2 and 848 cm-1 for BN,having Raman intensities that are not excessive. In spite of the DFT,The estimated recurrence interval matches the measured value ofBecause of this, I was surprised to find out how common this mode is in BN2.with the use of DFTs.

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TABLE 3: Calculated and Observed Frequencies (ν, in cm^{-1}), Raman Intensities (I), and Depolarization Ratios (ρ) of BN

	calcd			obsd			
symmetry	ν^a	I^a	ρ^a	ν^b	ν^c	ρ^c	assignment[d]
B	1630	1.3	0.75	1619			νC_1-C_2, νC_2-O_{11}, νC_3-C_4, νC_5-C_6, νC_7-C_8, $\delta O-H$
A	1606	211	0.48	1591	1588	0.47	$\nu C_1-C_{1'}$, νC_2-C_3, νC_6-C_7, νC_9-C_{10}, $\delta O-H$
A	1498	38	0.05	1517			$\nu\ C_2-O_{11}$, δC_3-H, δC_7-H
A	1454	48	0.37	1470	1470	~0.20	νC_7-C_8, νC_1-C_9, $\nu C_{10}-C_5$
B	1451	34	0.75	1440			νC_7-C_8, νC_1-C_9, $\nu C_{10}-C_5$
A	1387	199	0.03	1378	1377	0.15	νC_9-C_{10}, $\delta O-H$, $\nu\ C_2-O_{11}$
A	1305	40	0.01	1308			$\nu C_1-C_{1'}$, $\delta O_{11}-H$
A	1287	5.5	0.745	1274	1282	~0.40	$\nu C-O$, νC_8-C_9, δC_5-H, δC_7-H, δC_8-H
B	1254	2.3	0.75	1255			δC_5-H, δC_8-H
B	1214	5.6	0.75	1213			$\delta O_{11}-H$
A	1158	12	0.69	1147	1145	~0.50	δC_6-H, δC_5-H, δC_4-H, δC_7-H
A	1076	7.4	0.02	1067	1067		$\nu C_1-C_{1'}$, $\delta C_7-C_8-C_9$, $\delta C_{10}-C_5-C_6$, δC_4-H
A	1037	24	0.04	1025	1027	0.17	νC_6-C_7, $\delta C_6-C_7-C_8$, $\delta C_5-C_6-C_7$, δC_5-H, δC_6-H, δC_7-H, δC_8-H
A	957	9.1	0.18	952	964	0.11	$\delta C_1-C_2-C_3$, $\delta C_{10}-C_5-C_6$, $\delta C_6-C_7-C_8$, $\delta C_8-C_9-C_{10}$
A	848	23	0.05	847	849	0.05	$\delta C_3-C_4-C_{10}$, $\delta C_6-C_7-C_8$
B	790	12	0.75	794			γC_8-H, γC_3-H, γC_4-H, γC_5-H
A	668	27	0.07	664	666	0.06	$\delta C_7-C_8-C_9$, $\delta C_{10}-C_5-C_6$
A	581	5.2	0.13	582	584	0.10	τC_1, τC_2, τC_4, τC_{10}, τC_3, γC_3-H, γC_4-H, γC_6-H, γC_8-H, γC_5-H
A	533	12	0.12	531	531		$\delta C_6-C_7-C_8$, $\delta C_9-C_{10}-C_5$, $\delta C_2-C_3-C_4$
B	523	9.4	0.75	522			$\delta C_6-C_7-C_8$, $\delta C_9-C_{10}-C_5$, $\delta C_2-C_3-C_4$
A	508	5.4	0.16	509			τC_9, τC_{10}, τC_1, τC_4, γC_4-H, γC_5-H, γC_8-H, $\delta O_{11}H$
B	485	3.5	0.75	490			τC_9, τC_{10}, τC_5, τC_8, γC_5-H, γC_8-H, γC_4-H
B	523	9.4	0.75	522			$\delta C_6-C_7-C_8$, $\delta C_9-C_{10}-C_5$, $\delta C_2-C_3-C_4$
A	508	5.4	0.16	509			τC_9, τC_{10}, τC_1, τC_4, γC_4-H, γC_5-H, γC_8-H, $\delta O_{11}H$
B	485	3.5	0.75	490			τC_9, τC_{10}, τC_5, τC_8, γC_5-H, γC_8-H, γC_4-H
A	434	10	0.10	437	435	0.32	τC_9, τC_{10}, τC_5, τC_8, γC_5-H, γC_8-H
A	423	5.0	0.57	416			τC_5, τC_8, τC_3, γC_5-H, γC_8-H, γC_3-H
A	364	3.4	0.71	374			τC_4, τC_1, τC_2, τC_3, τC_9, γC_4-H, γC_7-H, $\gamma O_{11}H$
A	346	4.3	0.64	349			$\gamma O-H$
A	232	1.5	0.66	245			τ_{butt}

a Calculated with B3LYP/6-31G*; frequency scaling factor) 0.98. *b* From solid Raman spectra excited at 514.5 nm. *c* From solution Ramanspectra (in acetone) excited at 514.5 nm. *d* Mode assignments: *î*, bond stretching; *ä*, in-plane (naphthyl) bond bending; *ç*, out-of-plane (naphthyl) wagging of hydrogen atoms; *ô*, out-of-plane (naphthyl) torsion of carbon atoms; *ô*butt, butterly torsion between two naphthyl rings.

TABLE 4: Calculated and Observed Frequencies (ν, in cm^{-1}), Raman Intensities (I), and Depolarization Ratios (ρ) of BN^{2-}

	calcd			obsd			
symmetry	ν^a	I^a	ρ^a	ν^b	ν^c	ρ^b	assignment[d]
A	1623	57	0.14	1612	1612	0.57	νC_2-O_{11}, νC_3-C_4, νC_5-C_6, νC_7-C_8
A	1611	181	0.70	1592	1590	0.55	νC_7-C_8, νC_3-C_4, $\nu C_{10}-C_5$
A	1558	90	0.34	1559	1557	0.37	$\nu\ C_2-O_{11}$, νC_5-C_6, νC_3-C_4
A	1525	27	0.43	1549		0.52	νC_6-C_7, νC_4-C_{10}, δC_7-H
A	1500	163	0.18		1502		νC_8-C_9, $\nu C_{10}-C_5$, δC_8-H, δC_5-H,
A	1453	102	0.63	1467	1466	0.34	νC_1-C_9, νC_3-C_4, δC_6-H, δC_7-H, δC_8-H
B	1444	9.0	0.75		1455		νC_1-C_9, νC_3-C_4, δC_6-H, δC_7-H, δC_8-H
A	1416	117	0.71	1428	1428	0.40	νC_1-C_3, νC_3-C_4, νC_5-C_6, δC_3-H, δC_4-H
A	1357	135	0.14	1366	1366	0.15	νC_9-C_{10}, νC_1-C_9, νC_5-C_{10}
A	1297	96	0.08		1287		$\nu C_1-C_{1'}$, νC_1-C_2
A	1234	69	0.23		1244		νC_1-C_3, $\nu C_{10}-C_5$, δC_7-H, δC_8-H
A	1218	26	0.47		1215		$\nu C_{10}-C_4$, νC_8-C_9, δC_4-H, δC_8-H
A	1156	12	0.48		1187		$\nu C_1-C_{1'}$, δC_7-H, δC_7-H
A	1143	30	0.69	1146	1150	~0.50	δC_6-H, δC_7-H
A	1128	11	0.27		1132		δC_3-H, δC_6-H, δC_7-H
A	1049	51	0.16	1073	1074	~0.25	$\nu C_1-C_{1'}$, δC_4-H, $\delta C_7-C_3-C_4$
A	1024	48	0.26	1028	1029	0.18	νC_6-C_7, $\delta C_6-C_7-C_8$, $\delta C_5-C_6-C_7$, δC_5-H, δC_6-H, δC_7-H
A	975	5.4	0.09	975	980	0.30	$\delta C_8-C_9-C_{10}$, $\delta C_6-C_7-C_8$, $\delta C_1-C_1-C_2$
B	949	0.8	0.75		935		$\delta C_1-C_2-C_3$, δC_4-H
A	1049	51	0.16	1073	1074	~0.25	$\nu C_1-C_{1'}$, δC_4-H, $\delta C_7-C_3-C_4$
A	1024	48	0.26	1028	1029	0.18	νC_6-C_7, $\delta C_6-C_7-C_8$, $\delta C_5-C_6-C_7$, δC_5-H, δC_6-H, δC_7-H
A	975	5.4	0.09	975	980	0.30	$\delta C_8-C_9-C_{10}$, $\delta C_6-C_7-C_8$, $\delta C_1-C_1-C_2$
B	949	0.8	0.75		935		$\delta C_1-C_2-C_3$, δC_4-H
A	835	25	0.05	852	850	0.06	$\delta C_3-C_4-C_{10}$, $\delta C_6-C_7-C_8$, $\delta C_5-C_6-C_7$
B	805	2.6	0.75	796		0.75	γC_7-H, γC_4-H, γC_3-H, τC_9, τC_2
B	760	14	0.75	778		0.75	νC_9-C_{10}, γC_7-H, γC_8-H, γC_3-H, γC_4-H
A	730	9.2	0.73	737	739	~0.67	δC_3-C_4, $\delta C_5-C_6-C_7$
A	659	41	0.18	667	666	0.19	τC_3, τC_6, γC_3-H, γC_4-H, γC_5-H
A	522	32	0.10	533	534	0.16	$\delta C_6-C_7-C_8$, $\delta C_9-C_{10}-C_5$, $\delta C_2-C_3-C_4$

a Calculated with B3LYP/6-31G*; frequency scaling factor)0.98. *b* From solution Raman spectrum (in 3 M NaOH) excited at 514.5 nm.*c*From solution Raman spectra (in 3 M NaOH) excited at 325 nm. *d* Mode assignments: *î*, bond

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stretching; *ä*, in-plane (naphthyl) bond bending; *ç*, out-of-plane (naphthyl) wagging of hydrogen atoms; *ô*, out-of-plane (naphthyl) torsion of carbon atoms.The two weak Raman bands at 796 and 778 cm-1 of BN2- \shave the depolarization ratios approximately 0.75 and are consequently considered\sas belonging to the asymmetry vibrations. On the basis of theagreement of estimated and observed frequencies and depolarizationratios, we provisionally allocate these two bands to the computedvibrations of BN2- at 805 and 760 cm-1. According to the DFTcalculations, the vibration estimated at 760 cm-1 is due to thein-plane breathing mode of naphthyl ring (Scherer's î8 modefor naphthalene), while the one at 805 cm-1 is attributable tothe C-H out-of-plane wiggling mode of naphthyl ring.

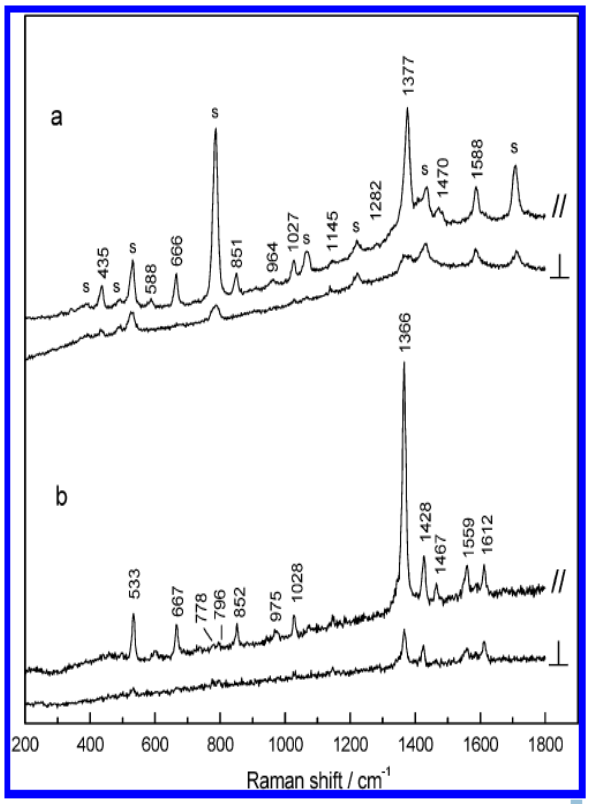
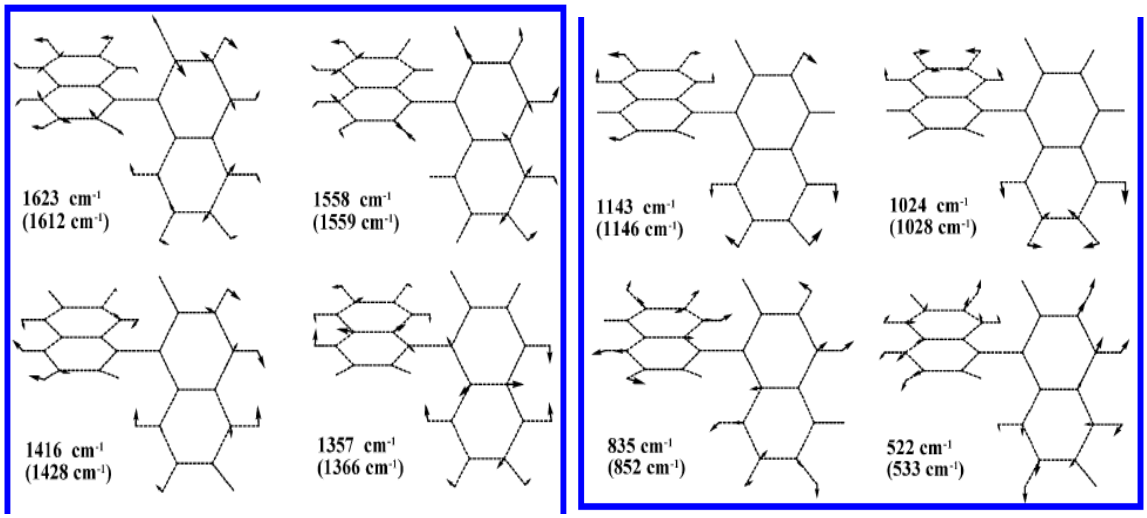


Figure 4. Polarized Raman spectra of BN (a) in an acetone solution;(b) in a 3 M NaOH solution with the excitation wavelength *ì*ex) 514.5nm.



Figure

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5. Schematic diagram showing the Cartesian displacementsof selected Raman active modes of BN2- calculated with B3LYP/6-31G*.

The calculated (plain text) and the measured (in parenthesis)frequencies have been shown for each mode.A strong Raman band with A symmetry is predicted by DFT calculations for BN2 at 659 cm-1. This mode is assigned to the 667 cm-1 strong band of BN2. The Cartesian atomic numberThis mode's displacements point to the C-H out-of-plane.wagging. This experiment's depolarization ratio was found to be 19.According to the estimated value, modes are in agreement (0.18). Its oppositeConsistent with this finding, BN was seen at 666 cm-1.by doing a DFT calculationThere was a prominent Raman band in the low-frequency area of the spectrum.BN2- (in a 3 M NaOH solution) was detected at 533 cm-1 andwith respect to the BN solid, at 531 cm-1. The BN Raman spectrumRaman spectroscopy, this band is overlapped by an acetone solution.of acetone We attribute it to the naphthyl deformation that occurs in-plane.Scheler's naphthalene î33 mode, which came up with a value of 522.cm-1 for BN2-, and 533 cm-1 for BN. ' Experimentation's worthThis mode's depolarization ratio in BN2 is 0.16, which is compatible within accordance with the estimated value (0.10).In the solid state, there existed a 435 cm-1 Raman band for BN.both in their natural condition and in an acetone solution. In the blink of an eye, this band had entirely disbandedin the neighbourhood of BN2. We believe it to be an O-H out-of-plane anomaly.a swaying motion. DFT calculations indicate a very skewed result.O-H rocking vibrations at a lower, more manageable frequencyAt a distance of 346 cm-1, Calculation versus experimentation is the difference.believes that this is because hydrogen bonding has been overlooked.that is predicted to occur in the calculating modelin order to have a major impact on O-H rocking out of plane.modes of BN moleculeDFT computing has been used in the preceding investigations to provide semiquantitative results.forecasts of the change in vibrational frequencyDeprotonation of hydroxyls in BN causes bands. TheThe effects of deprotonation on intensity and depolarization are also readily apparent.Figures show the ratios and other features of Raman bandsThere are three and four of them). This is something that has not been addressed in this work, and it should be.because of the deprotonation phenomenon, should be examined furtherare crucial to the success of a project.

UV Near-Resonance Raman Spectra (UVRRS) Excited at 325 nm.

The 900-1620 cm-1 area of the 325 nm excited resonance Raman spectra of BN in basic solution revealed numerous peculiarities (Figure 3a). Figure 3a illustrates this.the BN Raman band at 1612 cm-1 in basic solutionamazing improvement, much more powerful than the 1366 bandcm-1. This significant increase in resonance might be the consequence ofRaman scattering and the approximate double resonanceTsuboi's law of near-resonance enhancingmentioned in the following paragraphs.For starters, the double resonance is defined32.shows an increase in the scattered photon's intensitywhere I the energy of the photons, pö1both the incident and scattering photons' pö2 are in agreement.as well as (ii) the two excitation energy levelsVibrational frequency differences are equivalent to the difference between p(ö1-oe2)of a single molecule. Using third-order timedependent models, Peticolas et al.33,

The Raman transition may be calculated using perturbation theory.

$$\alpha_{gf,gi}^{\rho\sigma} = -\sum_{e,s}\left\{\frac{M_{ge}^{\rho}h_{es}M_{sg}^{\sigma}\langle f|Q|i\rangle}{[E_e^0 - E_g^0 + (f-i)\hbar\Omega - \hbar\omega_L][E_s^0 - E_g^0 - \hbar\omega_L]} + \text{c.c.}\right\} \quad (1)$$

where *M*geF _ □_g 0 j*i*Fj_e 0□, *h*es_ □_e 0j@*HE/@Q*j_s0□, _g , _e0, and _s 0are the electronic ground and excited states at *Q*) *Q*0respectively, *Q* is the normal vibration coordinate, and j*i*□□andj*f*□□are initial and final vibration states in the ground electronicstate. Because the sum over vibrational levels does not appearin eq 1, this expression also contains

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$$A_{gf,gi}^{\rho\sigma} = -\sum_{e}\left\{\frac{M_{ge}^{\rho}h_{ee}M_{eg}^{\sigma}\langle f|Q|i\rangle}{[E_e^0 - E_g^0 - (\hbar\omega_L - (f-i)\hbar\Omega)][E_e^0 - E_g^0 - \hbar\omega_L]} + \text{c.c.}\right\} \quad (2)$$

a “trace” (e) s) B typeterm This term may be nonzero only for completely symmetric modes.From UV absorption spectra of BN in a 3 M NaOH aqueous\ssolution (Figure 2), the incoming photon energy pöL (ìex) 325nm) is virtually resonant to the longest-wavelength absorption peakabout 358 nm, and the scattered photon energy (pöL - (f -i)p¿) for the ¿) 1612 cm-1 mode is more close to theabsorption peak, so, on the basis of eq 2, Agf,giFó is approximatedouble-resonance enhancement. Also, eq 2suggests that the 1612 cm-1 band is more favourablyimprovedthan that at 1366 cm-1, because the scattering photon energyfor the 1612 cm-1 band is near the absorption peak. We cancan use eq 1 to make comparable and qualitative talks onother B terms, since two excitation energy levels Ee0 and Es0of BN in an acetone solution come from the excitonic splittingof two degenerate levels and p(ö1 - ö2)) jEs0 - Ee0j) 0.22eV (1775 cm-1),14,19 which is nearly comparable to thefrequency of the 1612 cm-1 band and meets the abovecondition (ii) (ii). Here, we have assumed that for BN in basicsolution jEs0 - Ee0j 0.22 eV. The foregoing doubly resonantfeature is worth examining further, since strong resonanceimprovement, better assignment of modes by their selectedresonance enhancement, and potential deduction of vibronicconnections for the modes are known to be the benefits ofdoubly resonant Raman spectroscopy.14,32Second, on the basis of actual findings of variousmolecules, Hirakawa and Tsuboi35 developed the termed Tsuboi’srule: “If a Raman line grows stronger as the excitementline is moved closer to the frequency of an electronic band Ar X, then the equilibrium conformation of the molecule iswarped along the normal coordinate for the Raman line in thetransition from the ground state (X) to the excited state (A).”On the basis of a similar approach, Markham et al. made ab initiocalculation of the dimensionless displacement parametersIt described convincingly the impact of deuterium substitutionon RR spectra of imidazole and imidazolium.22

The relatedelectromagnetic spectrum of BN arises from the conjugated ð f ð*transition of naphthol chromophore.18,19 According to theforegoing theoretical explorations of the conjugate anionicbases of hydroxyaryls, the S0 f S1 excitation of naphtholateand phenolate induces large immigration of electronfrom the oxygen atom to the distal rings. This is predicted toresult in large alterations for the distances of the C2-O11bond. Our DFT computation indicates that the 1612 cm-1mode involves a strong contribution from the stretching ofC2-O11 bonds, so according to Tsuboi rule, the 1612 cm-1band is favourably resonant increased at the excitation ìex)325 nm.For further work, quantitative calculations of RR intensityare needed to account for the resonance enhancement withoutimmediately resorting to the idea of double resonance enhancement.Resonance Raman intensities have been well-formulatedeither in a tranditional sum-over-state picture39,34 or equivalentlyin the time-dependent resonance Raman formulas.40,41 Althoughthey are theoretically equivalent with each other, the

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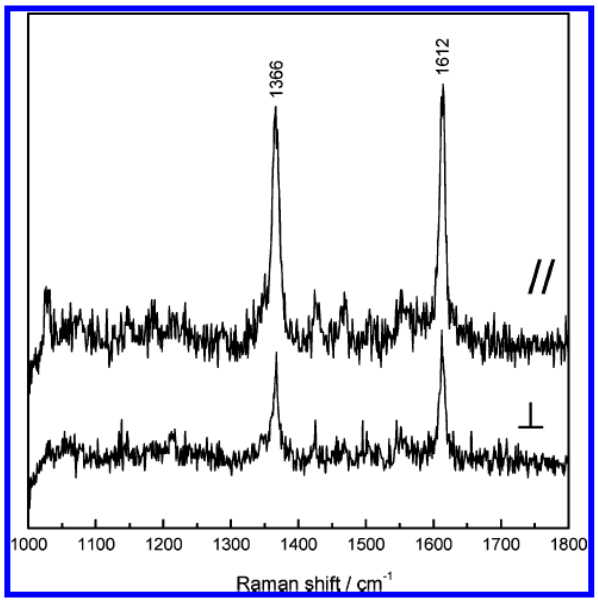

timedependent **Figure 6.** Polarized Raman spectrum of BN in a 3 M NaOH aqueoussolution with the excitation wavelength ìex) 325 nm.

For systems with a large number of vibrational modes, the timedependent technique has been shown to be more efficient in computing. ForOne enthusiastic person is involved in the near-resonance scenario discussed in this study.they've contributed to the RR intensity by being in an intermediate statenot yet been properly recognised. Thus, making a decision is challenging.employing a time-dependent approach for direct quantitative computingof the RR scattering.40, 42; departures from the normalbands such as 1612 cm-1 have a distinct intensity patternBN2-band following RR spectra modelling utilising time-dependentAdditional resonance enhancement using the RR techniqueThe mechanisms may need thorough examination.The energy denominator in RR formulas42 features such as this one.This part is finished.Polarization is a key component of this section. UVRR Spectra's properties. The loss of polarityin resonance, the ratio of the 1366 and 1612 cm-1 bandsBN2-Raman spectra at 325 nm (ex) were found to be 0.420.15 and 0.57, respectively, in conventional Raman spectroscopyAt 514.5 nm, as shown in Figure 4b, respectively, we can discern spectra.Thepolarisation qualities are described by the depolarization F.expresses itself

$$\rho = \frac{5\sum^1 + 3\sum^2}{10\sum^0 + 4\sum^2} = \frac{5(\sum^1/\sum^2) + 3}{10(\sum^0/\sum^2) + 4} \qquad (3)$$

in the form of20 where Placzek invariants □0, □2, and □1describe the isotropic,symmetric anisotropy, and antisymmetric part of the Ramantensors, respectively

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$$\sum^0 = \frac{1}{3}|\alpha_{xx} + \alpha_{yy} + \alpha_{zz}|^2$$

$$\sum^1 = \frac{1}{2}\{|\alpha_{xy} - \alpha_{yx}|^2 + |\alpha_{xz} - \alpha_{zx}|^2 + |\alpha_{yz} - \alpha_{zy}|^2\}$$

$$\sum^2 = \frac{1}{2}\{|\alpha_{xy} + \alpha_{yx}|^2 + |\alpha_{xz} + \alpha_{zx}|^2 + |\alpha_{yz} + \alpha_{zy}|^2\} + \frac{1}{3}\{|\alpha_{xx} - \alpha_{yy}|^2 + |\alpha_{xx} - \alpha_{zz}|^2 + |\alpha_{yy} - \alpha_{zz}|^2\} \quad (4)$$

It is known20 that in normal Raman spectra, antisymmetrictransition polarizability or □1 is zero, but in resonance Raman scattering, □1 can be nonzero. Thus, for the normal Ramanspectra, the depolarization ratio F' is and in resonance cases.

$$\rho' = \frac{3}{4 + 10(\sum^0/\sum^2)} \quad (5) \qquad \rho = \rho' + \frac{5(\sum^1/\sum^2)}{4 + 10(\sum^0/\sum^2)} \quad (3')$$

F)0.42 > F□□) 0.15 for the 1366 cm-1 band of BN2- and F) 0.47 _ F□□) 0.57 for the 1612 cm-1 band. Therefore, for the1366 cm-1 band of BN2-, not only the symmetric partcontributes to this band but also the antisymmetric part;however, the 1612 cm-1 band does not include an antisymmetricRaman scattering contribution. The result for the 1366 cm-1band of BN2- agree with DR-SFV spectra of BN,14,18 in whichthe 1377 cm-1 band of BN (corresponding to 1366 cm-1 ofBN2-) is most intensive and the strength of DR-SFVS fromisotropic chiral liquids is proportional to the square of thecorresponding antisymmetric Raman scattering tensor. But the1612 cm-1 band is beyond the measured frequency region ofDR-SFVS in ref 14 and needs to be further investigated by theDR-SFVS method.For the 1366 cm-1 band of BN2- in the normal Ramanspectra, F□□) 0.15, and so by use of eq 5

$$\sum^0/\sum^2 = 1.6 \quad (6)$$

Since in resonance cases F) 0.42, using eqs 3□, 6 and 5, weGet.

$$\sum^1/\sum^2 = 1.08 \quad (7)$$

From eqs 4 and 7, we can estimate the order of magnitude forthe ratio *K* between antisymmetric (Ranti) and symmetrictransition polarizabilities (Rsym)

$$K = \frac{\alpha_{anti}}{\alpha_{sym}} \approx (\sum^1/\sum^2)^{(1/2)} = 1.04 \quad (8)$$

On the basis of the nonadiabatic correction terms of antisymmetrictransition polarizability, Buckingham and Liu36,37 gavethe following formula of the order of magnitude of Ranti/Rsym

$$K' = \frac{\alpha_{anti}}{\alpha_{sym}} \approx \frac{\hbar\Omega}{E_e^0 - E_s^0} \quad (9)$$

where *E*e0 and *E*s0 are the energies of the excitation electronicstates coupled by the mode p¿, and ¿ is the frequency of thevibration band. Here, for the

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1366 cm-1 band, from theabsorption spectra of BN in acetone solution,19,14 the two peaksin the absorption spectrum come from transitions to the twoexciton states separated by 0.22 eV, which corresponds to (*E*e0- *E*s 0) in

$$K' \approx \frac{1366}{0.22 \times 8065.7} = 0.77 \qquad (10)$$

the above equation,14 thus Eqs. 8 and 10 reveal that the near-degeneracy of the excited-state levels (excitonic splittings) is critical for the experiment and theory to accord qualitatively.BN.37's transition polarizability is antisymmetric The nonresonanceSimilar to K, Raman scattering of tetrahydrofuran occurs in the large-amplitude vibration modes of the î16.an additional î17 groups.BN2- has 38 more bands, including 935, 1074, 1150, 1187, and 1187.Resonance is also seen at 1215 cm-1, 1244 cm-1, and 1287 cm-1.but cannot be quantified with certainty in the near-resonancewater solution with 3M NaOH and polarised Raman spectra of bismuth (BN)Figure 6 shows the answer.Antisymmetric Raman scattering is currently being investigated in this topic.Qualitative and preliminaries. To discuss the antisymmetricalrolePolarizability in an SFG with two double-resonant modesWe need to do further research before conducting a direct Raman spectroscopic analysis.both in terms of actual measures and theoretically derived ones. Inbroad experimental considerations I in general, when isotropic, symmetric, and homogeneousA given Raman band is formed through antisymmetric scattering.Circular measurement of the reversal coefficient is required.dispersion of polarised light at an angle of 180 degrees to directly andii) RR excitation, quantitatively distinguish 0, 2, and 1.20to plot profiles and dispersion curves for a certain RamanHistorically, bands have played a significant role in both theoretical and experimentalinvestigation-crucial work done by the RR spectrum group 20due to the lack of resonance in antisymmetric Raman scatteringThe slope of the antisymmetric Raman tensors is substantially steeper than that of theones that are symmetrical due to the time-reversal symmetry arguments37or the effects of interference from various vibronictransitions.20 Quantitative analysis may be found in RR spectra theory.calculations of RR intensity, depolarization ratios, and theirin order to take into consideration the frequency dependency of the excitation frequenciesfor a better sound quality. Then, there's the addition of BN.Dr-SFVS and RRR spectrums should be used to look at systems in depth.

Conclusions

For the first time, we have analysed the normal and UV near-resonance Raman (UVRR) spectra of 1,1-bi-2-naphthol (BN).Raman scattering of acetone-based BN in the presence of polarisedBNWe also looked at the effects of BN and B in a 3 M NaOH aqueous solution.Calculations were made using density functional theory.to investigate the vibrational frequencies and the condition of the matterstructure of BN2- The Raman band assignments noticedare based on measurements and calculations, and as a result,intensities and depolarization ratios. Analyzed by us1612 and 1612 BN basic solution depolarization ratiosNormal and UV resonance Raman spectra show 1366 cm-1.suggesting that symmetry and antisymmetry were both possibleThe 1366 cm-1 band is mostly made up of Raman tensor contributions, howeverThe 1612 cm-1 band is made up entirely of the symmetrical portion of this signal.

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