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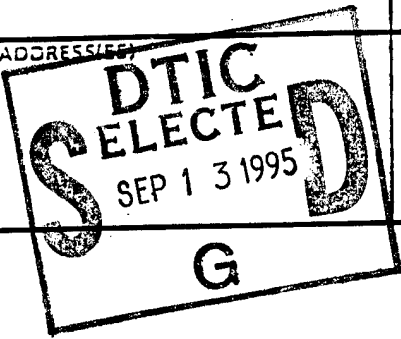
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A. V. Fedorov and D. L. Snavely

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## Vibrational overtone spectrum of cycloheptatriene

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### Abstract

The spectrum of the first through fifth vibrational overtone absorptions of cycloheptatriene are reported. The spectrum for the first and second overtones were recorded using a liquid sample while the third, fourth and fifth overtones were recorded for the gaseous samples. Four progressions belonging to the olefinic and methylenic C-H bond stretches are identified by combining both the gaseous and liquid data. Weak progressions lying in between these strong stretching absorptions belong to the C-H bend and stretch combinations.

### Introduction

The role of vibrational excitation and internal vibrational redistribution (IVR) in chemical reactions can be determined through spectroscopic study of vibrational overtones. The analysis of overtone spectra can provide information about pathways of chemical reactions. Small polyatomic molecules and open chain hydrocarbons have been studied.<sup>1</sup> The overtone spectra of large cyclic molecules, of which little is known, could be used as models for the vibrational behavior of polymers, proteins and other macromolecules.

The overtone spectra of liquid five, six, seven and eight member cyclic alkanes and the corresponding alkenes (except for the C<sub>8</sub> alkene) have been recorded.<sup>2</sup> For cyclopentane and cyclohexane the progression of methylenic transitions was observed. Each overtone of this progression contained two peaks. These peaks were assigned to the distinct axial and equatorial C-H bond stretches.<sup>3</sup> For seven and eight member cyclic alkanes only one methylenic progression was observed. For cyclopentene, cyclohexene and cycloheptene

both the methylenic and the olefinic progressions were identified and assigned. Later Henry and coworkers<sup>4</sup> studied the overtone gas-phase spectrum of methyl substituted cyclohexane. In gaseous trimethylcyclohexane it was possible to distinguish between axial and equatorial C-H oscillators using overtone spectroscopy.<sup>4</sup> In addition to the typical pattern in bond length ordering in saturated hydrocarbons<sup>5</sup> ( $r_{\text{CH}}(\text{methyl}) > r_{\text{CH}}(\text{methylene}) > r_{\text{CH}}(\text{methyne})$ ) the pattern for axial and equatorial bond length ( $r_{\text{CH}}(\text{eq}) > r_{\text{CH}}(\text{ax})$ ) was reported. The anharmonicities in this case were  $-60.4 \text{ cm}^{-1}$  for equatorial and  $-59.6 \text{ cm}^{-1}$  for axial C-H bonds.

Lespade and colleagues studied the overtone spectra of cyclohexene-3,3,6,6-d<sub>4</sub><sup>6</sup> and cyclopentene-3-h<sub>1</sub><sup>7</sup>. They proposed two ways of delocalization of the molecular wavefunction of high energy vibrational transitions: Fermi resonance coupling with combination states involving CH<sub>2</sub> and CCH deformation modes and coupling with the large amplitude motions. Only Fermi resonance coupling was observed in cyclohexene; however, both mechanisms occurred for cyclopentene. Wong and coworkers<sup>8</sup> also studied the overtone spectra of some cycloalkanes and cycloalkenes. They resolved the axial and equatorial C-H bond stretching absorptions for cyclobutane, cyclopentane, cyclopentene and cyclohexane. The equatorial bands were consistently more intense than the axial ones. Manzanares et al.<sup>9</sup> recorded the second and third overtone spectra of all cis-1,4-polybutadiene solution in CCl<sub>4</sub>. Although the carbon chain in polymers is not cyclic, methylenic C-H oscillators are in a semi-rigid frame inside the polymer. This makes the properties of the polymeric C-H oscillators similar to those of cyclic hydrocarbons so that it was possible to resolve the axial and equatorial methylenic oscillators. The vibrational overtone spectrum of gaseous cyclopentadiene was recorded from 6,400 to 17,000  $\text{cm}^{-1}$  with three dark regions around 10,000, 12,500 and 14,800  $\text{cm}^{-1}$ .<sup>10</sup> The aliphatic (methylenic) and olefinic progressions were identified. Methylenic absorptions were not well resolved and no distinction between C-H<sub>ax</sub> and C-H<sub>eq</sub> was made.

Benzene is also a cyclic hydrocarbon. The local mode picture of benzene<sup>11</sup> is simple, because all C-H oscillators are equivalent and only one peak appears in the high overtone spectrum. Low overtones of benzene are more complicated to analyze because of the Fermi resonance but several theories have already been developed<sup>11</sup> to explain this phenomenon.

Cycloheptatriene is a special molecule among cyclic hydrocarbons. Being a cyclic polyene (containing three conjugated double bonds) cycloheptatriene also has a methylenic group. It was calculated<sup>12</sup> that the most stable conformation of cycloheptatriene is the so-called "perturbed boat" conformation which is the linear combination of particular amount of boat (77%) and chair (23%) forms of a seven-member ring (Figure 1). The degree of interaction of the methylenic hydrogens with the conjugated  $\pi$ -systems is different and, therefore, these hydrogens can be referred to the pseudo-axial and pseudo-equatorial C-H oscillators. In addition to that two different olefinic C-H oscillators may exist in this conformation. The IR and Raman spectra of cycloheptatriene were recorded by Paulick and colleagues<sup>13</sup>. Three transitions (3060, 3027 and 3015  $\text{cm}^{-1}$ ) were reported in the C-H stretch fundamental region. A normal coordinate analysis has been done<sup>13</sup> and transitions from 200 to 3060  $\text{cm}^{-1}$  were assigned to the different motions of the cycloheptatriene.

The purpose of this work is to discover and interpret the overtone spectrum of cycloheptatriene and understand the processes occurring at high vibrational energies in this molecule.

## Experiment

The first and second overtone of cycloheptatriene were recorded at 4  $\text{cm}^{-1}$  resolution on a Mattson FT near-IR spectrometer with a tungsten lamp and quartz beam splitter. A Pd-Se detector was used to record the spectra in the 4000-9000  $\text{cm}^{-1}$  region. The first overtone spectrum was recorded for solution of cycloheptatriene in  $\text{CCl}_4$  (1:5  $\text{C}_7\text{H}_8:\text{CCl}_4$  ratio). The second overtone spectrum was recorded for neat liquid cycloheptatriene.

The third, fourth and fifth overtone spectra of gaseous cycloheptatriene were obtained by using intracavity laser photoacoustic spectroscopy. The sample was vacuum-

transferred into a 20 by 1.5 cm photoacoustic cell equipped with a 1751XA<sup>II</sup> Qualitone microphone and Brewster's angle quartz windows. To increase the signal-to-noise ratio, argon was added to the photoacoustic cell to obtain a total pressure of approximately 500 torr.

The excitation source was a Spectra-Physics series 2000 argon ion laser which pumped Spectra-Physics Model 3900S CW Ti:Sapphire laser or dye laser with the three-plate birefringent filter ( $2\text{ cm}^{-1}$  bandwidth). Two regions of the Ti:Sapphire laser ( $10,000\text{--}11,765\text{ cm}^{-1}$  and  $11,765\text{--}14,286\text{ cm}^{-1}$ ) were used to record the third and fourth overtone spectra. A Rhodamine 6G dye ( $16,000\text{--}17,500\text{ cm}^{-1}$ ) was used to record the fifth overtone spectrum of cycloheptatriene. An Oriel Motor Mike with the 18007 control unit controlled the birefringent filter rotation. A McPherson Model 270 0.35 meter scanning monochromator with McPherson Model 789A scan control unit was used to measure the initial and final wavelengths of the scanning region. Because the resolution of the monochromator was  $0.3\text{ cm}^{-1}$  the measurements were limited by the  $2\text{ cm}^{-1}$  resolution of the birefringent filter.

The PTI Model 03-OC4000 optical chopper chopped the argon laser beam at 250 Hz, providing the reference signal for an EG&G Brookdeal Electronics Model 5207 lock-in amplifier. An IBM computer was connected with both the lock-in amplifier and Oriel Motor Mike and recorded the photoacoustic signal controlling the wavelength scan.

The positions of the peaks were corrected using a calibration procedure. The mechanical scan of the motor mike does not have a linear dependence on the wavelength. Therefore, the real wavelength values measured after each  $500\text{ }\mu\text{m}$  of the micrometer scan were used to correct the spectra.

## Results and discussion

The first and second vibrational overtone spectrum of liquid cycloheptatriene and a combination band region between the overtones are shown in Figure 2. The third, fourth and fifth overtones of the spectrum of gaseous cycloheptatriene is shown in Figure 3. The peak

positions and vibrational assignments are listed in Table 1. Several Birge-Sponer plots<sup>14</sup> for the vibrational progressions are shown in Figure 4. The vibrational parameters for these progressions are given in Table 2. Because cycloheptatriene is not a polar molecule interactions in the liquid phase are not significant. Therefore, it was possible to compare the overtone data for liquid and gaseous cycloheptatriene and fit these data into one Birge-Sponer plot.

Methylenic C-H The two methylenic hydrogens of cycloheptatriene (Figure 1) are not equivalent in the most stable conformation of the molecule<sup>12</sup> and can be attributed to the pseudo-axial and pseudo-equatorial C-H stretches. Although, the methylenic C-H progression was identified from the overtone spectrum only at the third and fourth overtones, it was possible to distinguish between these C-H oscillators. Overlap of the methylenic peaks with the broad and more intense olefinic absorptions made the interpretation of methylenic transitions complicated for low overtones. The observed absorptions of the methylenic progression were assigned to the pseudo-equatorial C-H oscillators with a mechanical frequency of  $3011 \pm 13 \text{ cm}^{-1}$  and an anharmonicity of  $-60.1 \pm 7.5 \text{ cm}^{-1}$  (Table 2). Low energy shoulders of  $\text{CH}_2$  pseudo-equatorial transitions were assigned to the pseudo-axial methylenic C-H stretch.

Olefinic C-H. Two progressions of the olefinic C-H stretches were identified. The progression of the most intense transition was assigned to the internal olefinic ( $\text{C-H}_{\text{in}}^{\text{O}}$ ) C-H oscillators of carbons 1, 2, 5, and 6 (Figure 1) and the high energy shoulder of these transitions was assigned to the terminal ( $\text{C-H}_{\text{ter}}^{\text{O}}$ ) C-H oscillators of carbons 3 and 4 (Figure 1) of the cycloheptatriene ring. For  $\text{C-H}_{\text{in}}^{\text{O}}$  the vibrational frequency and anharmonicity were  $3076 \pm 9$  and  $-59.3 \pm 2.2 \text{ cm}^{-1}$ , respectively.

Combination bands There are many other observed bands in the overtone spectrum of cycloheptatriene which must belong to different combinations of C-H stretch and other modes in the molecule. The most likely bands for these combinations involve the C-C stretches and C-H bends. Two peaks at  $7090 \text{ cm}^{-1}$  and  $12,520 \text{ cm}^{-1}$  are worth special

attention because these peaks fit a Birge-Sponer plot with the vibrational frequency of  $1486\text{ cm}^{-1}$  and an anharmonicity of  $-14\text{ cm}^{-1}$ . This progression, therefore, may belong to the fourth and eighth overtones of C-H bend.

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Table 1. Transition wavenumbers ( $\text{cm}^{-1}$ ) and assignments for cycloheptatriene.

Quantum number $\Delta v(\text{CH})$	Transition wavenumber	Intensity <sup>2</sup>	Assignment
2	5588	m	
	5640	h.en.sh.	
	5783	w	2v CH <sup>a</sup> <sub>eq</sub>
	5800	w	
	5867	l.en.sh.	
	5905	s	2v CH <sup>o</sup> <sub>in</sub>
	6029	w	2v CH <sup>o</sup> <sub>ter</sub>
	6820	w	
	6927	w	
	7090	w	
7227	w		
3	7948	vw	
	8102	w	
	8153	w	
	8227	w	
	8386	w	3v CH <sup>a</sup> <sub>eq</sub>
	8652	s	3v CH <sup>o</sup> <sub>in</sub>
4	11057	l.en.sh.	4v CH <sup>a</sup> <sub>ax</sub>
	11094	w	4v CH <sup>a</sup> <sub>eq</sub>
	11216	w	
	11313	l.en.sh.	
	11366	s	4v CH <sup>o</sup> <sub>in</sub>
	11437	h.en.sh.	4v CH <sup>o</sup> <sub>ter</sub>
5	12406	vw	
	12520	w	
	13080	m	
	13549	l.en.sh.	5v CH <sup>a</sup> <sub>ax</sub>
	13622	m	5v CH <sup>a</sup> <sub>eq</sub>
	13657	h.en.sh..	
	13864	l.en.sh.	
	13915	s	5v CH <sup>o</sup> <sub>in</sub>
	13981	h.en.sh.	5v CH <sup>o</sup> <sub>ter</sub>
6	16331	m	6v CH <sup>o</sup> <sub>in</sub>
	16375	h.en.sh.	6v CH <sup>o</sup> <sub>ter</sub>

1. Values are taken from reference 13.

2. vw-very weak, w-weak, m-medium, s-strong, l.en.sh.-low energy shoulder, h.en.sh.-high energy shoulder.

Table 2. Vibrational frequencies ( $w_e$ ) and unharmonicities ( $w_e x_e$ ) for cycloheptatriene.

Progression	$w_e$ , $\text{cm}^{-1}$	$w_e x_e$ , $\text{cm}^{-1}$	Fitting coeff.(R)
C-H <sup>a</sup> <sub>eq</sub>	3010±13	-60±8	0.982
C-H <sup>o</sup> <sub>in</sub>	3076±9	-59±2	0.997
C-H <sup>0</sup> <sub>ter</sub>	3137±10	-68±3	0.998

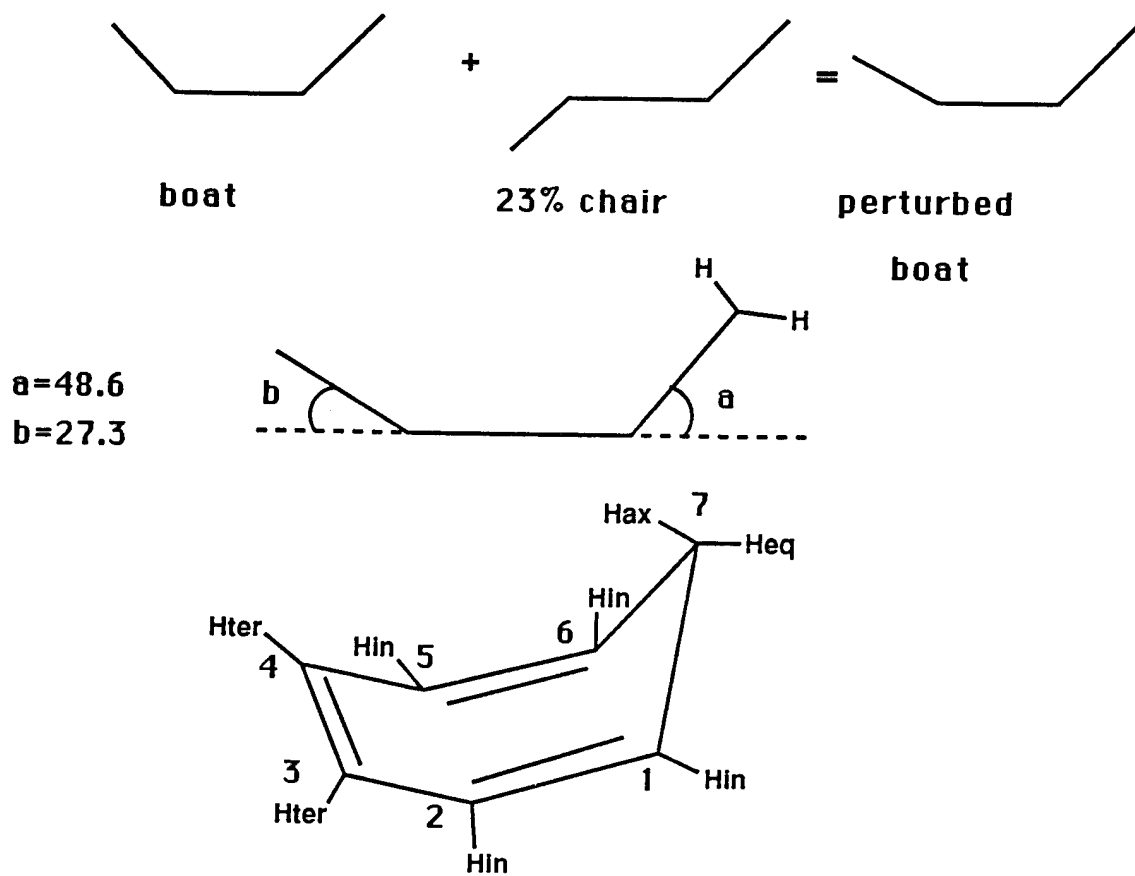


Figure 1. The most stable conformation of cycloheptatriene (Taken from ref. 12).

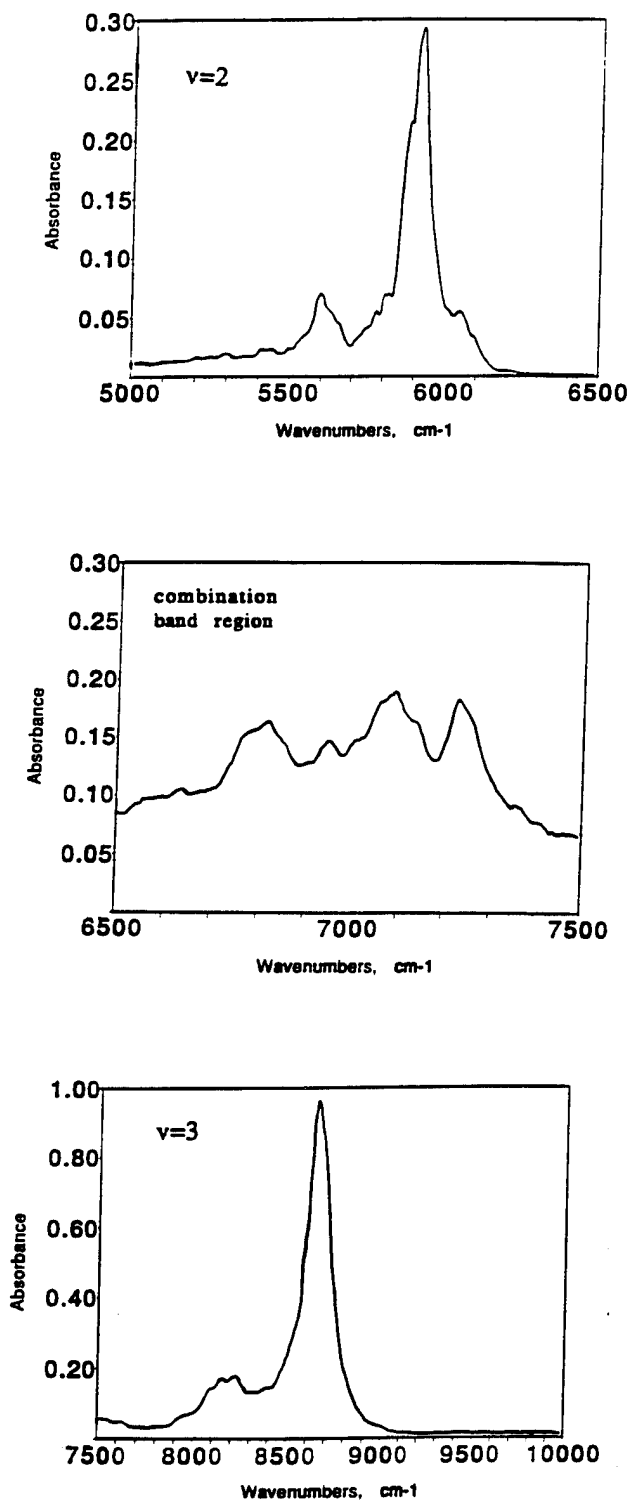


Figure 2. The first, second overtones and combinational band region of liquid cycloheptatriene.

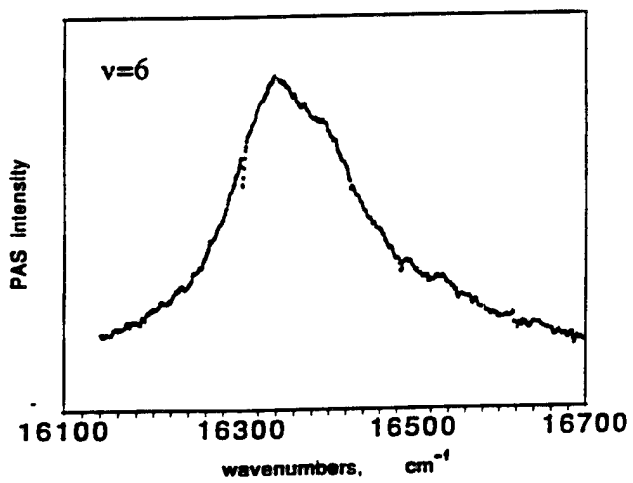
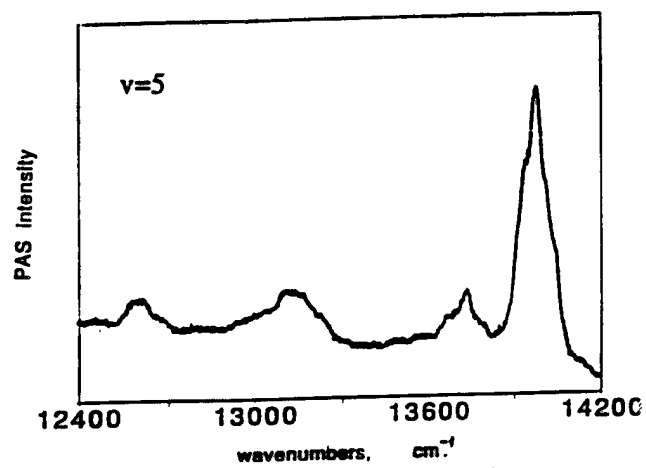
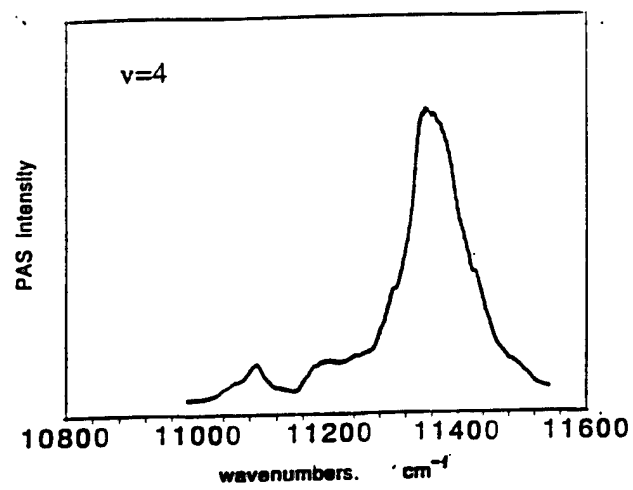


Figure 3. The third, fourth and fifth and overtones of gaseous cycloheptatriene.

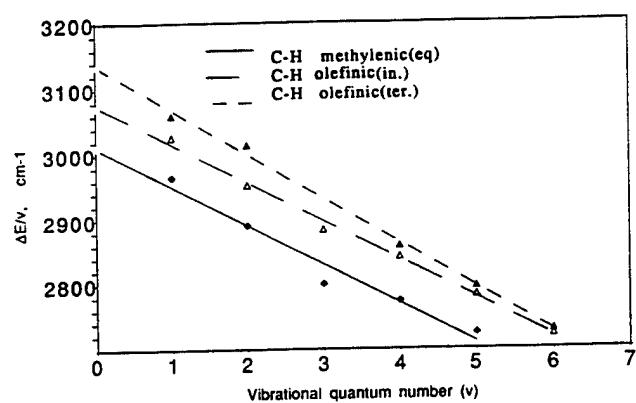


Figure 4. The Birge-Sponer plot for cycloheptatriene.

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