## Supplemental material

## Biosensors

## Vibrational Spectra of Nucleotides in presence of the Au Cluster Enhancer in MD Simulation of a SERS Sensor

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Detailed tables of the calculated vibrational frequencies with high intensities for the DNA nucleobases and nucleotides, cytosine, thymine, adenine, and guanine, are collected in the present supporting information. The Green-Kubo method is used to obtain transient spectra in reaction coordinated in the molecular dynamics method.

The spectra of the bonds of atoms in the nucleotides reflect nucleobase structural differences. The spectra of all bonds have been calculated simultaneously at the same translocation through the graphene pore and arranged in the tables presented below. The highest amplitude frequencies of a particular bond are numbered in the sequence of decreasing intensities. They are collected into the spectral maps of molecular species and can be used as a fingerprint for the identification of nucleotides. The first four tables present frequencies for each bond between atoms that have numbers according to the Figs in the text of the paper. Tables 1-4 show results for four nucleobases in the nucleotides. The same frequencies that are present in spectra of many bonds belong to the cyclic ring modes of the particular nucleobase.

The remaining four tables, Tables 5-8, show calculations for the corresponding four nucleobases only, without the presence of the attached 2-deoxyribose.

All calculations of bond stretching in the adjacent tables were performed in the frequency region 100 - 2000 cm<sup>-1</sup>. The time step was 0.2 fs, calculations of spectra were done for 8192 time steps that correspond to approximately 16 ps duration, and to 40 cm<sup>-1</sup> resolution. All spectra of nucleotides or bases were obtained from the single MD run. The interaction interval with graphene during transient spectra sampling was sufficient to have intensities of vibrational modes amplified in calculations. The sampling time corresponds to several vibrational periods of bending and stretching modes that bring numerical errors in the computation of frequencies by FFT to a sufficient level.

Table 1 Frequencies of Cytosine nucleotide bonds, highest intensities. Frequencies are in cm<sup>-1</sup>.

	_	_	_	_	_	_	_	_	_	_	_	_	_	_	_	_	_	_	_								_		_							_	_	_	_
	第6ピーク	1638.9		1638.9		1638.9		1638.9		1638.9		1638.9		1638.9		1638.9		1638.9		1638.9		1638.9		1638.9		1638.9		1638.9		1638.9		1638.9		1638.9		1638.9		1638.9	
	第5ピーク	1270.2	1434.1	1270.2		1270.2	1434.1	1270.2	1434.1	1270.2	1434.1	1270.2	1434.1	1270.2	1434.1	1270.2	1434.1	1270.2	1434.1	1270.2	1434.1	1270.2	1434.1	1270.2	1434.1	1270.2	1434.1	1270.2	1434.1	1270.2	1434.1	1270.2	1434.1	1270.2	1434.1	1270.2	1434.1	1270.2	14341
	第4ピーク	1024.3	1188.2	1024.3		1024.3	1024.3	1024.3	1024.3	1024.3	1024.3	1024.3	1024.3	1024.3	1024.3	1024.3	1024.3	1024.3	1024.3	1024.3	1024.3	1024.3	1024.3	1024.3	1024.3	1024.3	1024.3	1024.3	1024.3	1024.3	1024.3	1024.3	1024.3	1024.3	1024.3	1024.3	1024.3	1024.3	1024.3
	第3ピーク	614.6	655.6	614.6	1434.1	614.6	655.6	614.6	655.6	614.6	655.6	614.6	655.6	614.6	655.6	614.6	655.6	614.6	655.6	614.6	655.6	614.6	655.6	614.6	655.6	614.6	655.6	614.6	655.6	614.6	655.6	614.6	655.6	614.6	655.6	614.6	655.6	614.6	655.6
cm – 1]	第2ピーク §	532.6	573.6	532.6	573.6	573.6	573.6	573.6	573.6	532.6	573.6	532.6	573.6	532.6	573.6	532.6	573.6	532.6	573.6	532.6	573.6	532.6	573.6	532.6	573.6	532.6	573.6	532.6	573.6	532.6	573.6	532.6	573.6	532.6	573.6	532.6	573.6	532.6	573.6
bend	育1ピーク 算	368.8	368.8	368.8	327.8	368.8	368.8	368.8	368.8	368.8	368.8	368.8	368.8	368.8	368.8	368.8	368.8	368.8	368.8	368.8	368.8	368.8	368.8	368.8	368.8	368.8	368.8	368.8	368.8	368.8	368.8	368.8	368.8	368.8	368.8	368.8	368.8	368.8	327.8
	ま準原子 う	C,1	N,6	C,1	N,7	C,2	C,3	C,2	N,5	C,2	N,6	C,3	C,2	C,3	C,4	C,4	C,3	C,4	N,7	N,5	C,2	N,6	C,1	N,6	C,2	N,7	0,1	N,7	C,4	H,8	N,5	6'H	N,5	H,10	C,3	Н,11	C,4	0,12	5
	子,番号	N.6		N.7		C,3		N,5		N,6		C,2		C,4		C,3		N,7		C,2		C,1		C,2		C,1		C,4		N,5		N,5		C,3		C,4		C,1	
	番号 対原																																			_	_	2	
_	原子. 3	C,1				C,2						C.3				C,4				N,5		N,6				N,7				H,8		6'H		H,10		H,1		0,1	
	6th peak			1720.9		1843.8										1843.8		1843.8								1843.8													17209
	5th peak	1638.9		1679.9		1720.9				1638.9	1720.9			1843.8		1720.9		1720.9							1720.9	1720.9								1843.8					1639.0
	4th peak	1393.1	1638.9	1557.0		1557.0				1393.1	1557.0	1761.8	1720.9	1720.9		1557.0		1557.0		1843.8		1720.9	1720.9	1761.8	1639.0	1639.0	1639.0		1720.9		1720.9		1720.9	1557.0	1720.9		1720.9	1720.9	13931
	3th peak	1270.2	1557.0	1270.2	1557.0	1393.1	1720.9	1393.1	1720.9	1270.2	1393.1	1557.0	1557.0	1557.0	1720.9	1393.1	1720.9	1270.2	1720.9	1557.0	1720.9	1639.0	1639.0	1557.0	1557.0	1557.0	1557.0		1557.0	1393.1	1557.0	1393.1	1557.0	1393.1	1557.0		1557.0	1639.0	1970.9
trech	2th peak	1188.2	1270.2	1188.2	1516.0	1147.2	1557.0	532.6	1557.0	1188.2	1270.2	1393.1	1393.1	1393.1	1557.0	1147.2	1557.0	1188.2	1557.0	1393.1	1557.0	1557.0	1557.0	1393.1	1270.2	1270.2	1270.2	1843.8	1270.2	532.6	1270.2	532.6	1270.2	1147.2	1270.2	1843.8	1270.2	1557.0	532.6
20	1th peak	532.6	532.6	573.6	1188.2	532.6	1188.2	450.7	1188.2	532.6	1188.2	532.6	1188.2	532.6	1188.2	532.6	1188.2	573.6	1188.2	532.6	1188.2	532.6	532.6	532.6	532.6	532.6	1188.2	1393.1	1188.2	450.7	1188.2	450.7	1188.2	532.6	1188.2	1393.1	1188.2	1270.2	450.7
	Ref atom	C.1	N,6	C,1	N,7	C,2	C,3	C,2	N,5	C,2	N,6	C,3	C,2	C.3	C,4	C,4	C,3	C,4	N,7	N,5	C,2	N,6	C,1	N,6	C,2	N,7	C,1	N,7	C,4	H,8	N,5	H,9	N,5	H,10	C,3	H,11	C,4	0,12	5
	Versus atom	N,6		N,7		C,3		N,5		N,6		C,2		C,4		C,3		N,7		C,2		C,1		C,2		C,1		C,4		N,5		N,5		C,3		C,4		C,1	
	atom & num	C,1				C,2						C,3				C,4				N,5		9'N				N.7				Н,8		6'H		H,10		Н,11		0,12	
	塩基名	CYT																																					

Column names for stretching (left columns) and bending (right columns) frequencies are in cm<sup>-1</sup> units and as follows:

Base, Atom & num., Bonding atom, Reference atom, 1st mode, 2nd mode, 3rd mode, 4th mode, 5th mode, 6th mode are shown in 2 sets of columns.

Table 2 Frequencies of Thymine nucleotide bonds, highest intensities. Frequencies are in cm<sup>-1</sup>.

					strech									bena					
011         011 <th><b>東子</b>.</th> <th>番号 対原子.</th> <th>番号基</th> <th>连原子</th> <th>第1ピーク</th> <th>第2ピーク</th> <th>第3ピーク</th> <th>第4ピーク</th> <th>第5ピーク</th> <th>第6ピーク</th> <th>原子. 番号</th> <th>対原子,番号</th> <th>基準原子</th> <th>第1ピーク</th> <th>第2ピーク</th> <th>第3ピーク</th> <th>第4ピーク</th> <th>第5ピーク</th> <th>第6ピーク</th>	<b>東子</b> .	番号 対原子.	番号基	连原子	第1ピーク	第2ピーク	第3ピーク	第4ピーク	第5ピーク	第6ピーク	原子. 番号	対原子,番号	基準原子	第1ピーク	第2ピーク	第3ピーク	第4ピーク	第5ピーク	第6ピーク
	C.1	N,1	-	C,1	409.7	737.5	1024.3	1188.2	1270.2	1679.9	C,1	N,11	C,1	368.8	573.6	655.6	901.4	983.3	1147.2
				N,11	491.7	737.5	1270.2	1516.0	1638.9	1802.8			N,11	327.8	696.5	778.5	860.4		
C1         C1         C2         C1         C2         C1         C2         C1         C2         C1         C2         C1         C1 <thc1< th="">         C1         C1         C1<!--</td--><td></td><td>N,12</td><td>2</td><td>C,1</td><td>532.6</td><td>655.6</td><td>860.4</td><td>983.3</td><td>1270.2</td><td>1516.0</td><td></td><td>N,12</td><td>C,1</td><td>368.8</td><td>573.6</td><td>655.6</td><td>901.4</td><td>983.3</td><td>1147.2</td></thc1<>		N,12	2	C,1	532.6	655.6	860.4	983.3	1270.2	1516.0		N,12	C,1	368.8	573.6	655.6	901.4	983.3	1147.2
C2         C3         C3         C4         C3         C3 <thc3< th="">         C3         C3         C3<!--</td--><td></td><td></td><td></td><td>N,12</td><td>532.6</td><td>696.5</td><td>1270.2</td><td>1516.0</td><td>1720.9</td><td>1802.8</td><td></td><td></td><td>N,12</td><td>573.6</td><td>696.5</td><td>860.4</td><td>1024.3</td><td>1106.3</td><td></td></thc3<>				N,12	532.6	696.5	1270.2	1516.0	1720.9	1802.8			N,12	573.6	696.5	860.4	1024.3	1106.3	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C,2	C,3	~	C,2	696.5	1434.1	1516.0	1638.9	1761.8	1884.6	C,2	C,3	C,2	368.8	573.6	655.6	901.4	983.3	1147.2
$ \begin{array}{{ccccccccccccccccccccccccccccccccccc$				C,3	532.6	696.5	1270.2	1516.0	1720.9	1802.8			C,3	573.6	696.5	860.4	1024.3	1106.3	
		11,N	2	C,2	532.6	655.6	860.4	983.3	1270.2	1516.0		N,12	C,2	368.8	573.6	655.6	901.4	983.3	1147.2
C2         C2         TC2         C2         TC2         C2         TC2         C2         TC3         TC3 <thtc3< th=""> <thtc3< th=""> <thtc3< th=""></thtc3<></thtc3<></thtc3<>				N,12	532.6	696.5	1270.2	1516.0	1720.9	1802.8			N,12	573.6	696.5	860.4	1024.3	1106.3	
	C,3	C,2	~	C,3	573.6	860.4	1024.3	1434.1	1679.9	1761.8	C,3	C,2	C,3	368.8	573.6	655.6	901.4	983.3	1147.2
$ \begin{array}{{ccccccccccccccccccccccccccccccccccc$				C,2	532.6	696.5	1270.2	1516.0	1720.9	1802.8			C,2	573.6	696.5	860.4	1024.3	1106.3	
		C,4		C,3	737.5	860.4	1024.3	1434.1	1720.9			C,4	C,3	368.8	573.6	655.6	901.4	983.3	1147.2
C4         C3         C43         C43         C43         C43         C43         C43         C43         C44         C43         C44         C44 <thc44< th=""> <thc44< th=""> <thc44< th=""></thc44<></thc44<></thc44<>				C,4	532.6	696.5	1270.2	1516.0	1720.9	1802.8			C,4	573.6	696.5	860.4	1024.3	1106.3	
		C.5	5	C,3	696.5	819.5	1024.3	1147.2	1311.1	1516.0		C,5	C,3	368.8	573.6	655.6	901.4	983.3	1147.2
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$				C,5	532.6	696.5	1270.2	1516.0	1720.9	1802.8			C,5	573.6	696.5	860.4	1024.3	1106.3	
	C,4	C,3	~	C,4	696.5	1434.1	1516.0	1638.9	1761.8	1884.6	C,4	C,3	C,4	368.8	573.6	655.6	901.4	983.3	1147.2
				C,3	532.6	696.5	1270.2	1516.0	1720.9	1802.8			C,3	573.6	696.5	860.4	1024.3	1106.3	
C5         C3         C3         C3         C441         C441 <thc41< th=""> <thc41< th=""> <thc41< th=""></thc41<></thc41<></thc41<>		N,1	_	C,4	737.5	1270.2	1679.9					N,11	C,4	368.8	573.6	655.6	901.4	983.3	1147.2
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$				N,11	532.6	696.5	1270.2	1516.0	1720.9	1802.8			N,11	573.6	696.5	860.4	1024.3	1106.3	
	C,5	C.3	~	C,5	696.5	1434.1	1516.0	1638.9	1761.8	1884.6	C,5	C,3	C,5	368.8	573.6	655.6	901.4	983.3	1147.2
H6         M.12         H6         S226         6556         8004         9333         12703         15160         17203         15160         H6         M.12         H6         5326         6556         9014         9833           H7         C4         H3         7335         6965         17202         15160         17209         18028         H7         5736         6965         6004         10243         11003           H3         C5         H8         6655         8195         10243         11472         1141         1141         1141         9111         11003         9103         9014         9833           H9         C5         H3         6965         8195         10243         11472         13111         15160         H9         755         6965         8004         10243         11003           H10         C5         H3         6905         8195         10243         11003         11003         11003         11004         10243         11003         11003         11003         11003         11003         11003         11003         11003         11003         11003         11003         11003         110043         110043         11003	1			C.3	532.6	696.5	1270.2	1516.0	1720.9	1802.8			C.3	573.6	696.5	860.4	1024.3	1106.3	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	H,6	N,12	2	9'H	532.6	655.6	860.4	983.3	1270.9	1516.0	H,6	N,12	9'H	368.8	573.6	655.6	901.4	983.3	1147.2
H7         C4         H7         735         6664         17203         14341         17209         14341         17209         14341         17209         14341         17209         14341         17209         16013         508.8         573.6         6665.6         901.4         983.3           H8         C5         H8         665.5         819.5         1024.3         1147.2         1311.1         1516.0         H9         C5         H8         573.6         696.5         800.4         1024.3         1106.3           H0         C5         H3         696.5         819.5         1024.3         1147.2         1311.1         1516.0         H9         C5         F19         573.6         696.5         800.4         1024.3         1106.3           H10         C5         H10         696.5         819.5         1024.3         1106.3         100.4         983.3          H10         C5         H10         696.5         810.4         1024.3         1106.3           H11         C1         N11         C1         N11         C1         N11         265.6         901.4         983.3           C4         N11         C1         N11         C1				N,12	532.6	696.5	1270.2	1516.0	1720.9	1802.8			N,12	573.6	696.5	860.4	1024.3	1106.3	
H.8C.5H.8 $0.025$ $8195$ $10243$ $11472$ $1311.1$ $1516.0$ H.8C.5H.8 $363.8$ $573.6$ $696.5$ $901.4$ $983.3$ H.9C.5H.9 $595.5$ $696.5$ $8195$ $1024.3$ $1147.2$ $1311.1$ $1516.0$ H.9C.5 $696.5$ $696.5$ $690.4$ $1024.3$ $1106.3$ H.10C.5H.10G.5 $5120.6$ $6195.7$ $8195.7$ $1024.3$ $1147.2$ $1311.1$ $1516.0$ $H.9$ $C.5$ $C.5$ $573.6$ $696.5$ $800.4$ $1024.3$ $1106.3$ H.10C.5H.10G.5 $519.6$ $619.5$ $819.5$ $1024.3$ $1147.2$ $1311.1$ $1516.0$ $1720.9$ $1802.8$ $800.4$ $1024.3$ $1106.3$ N.11C.1N.11C.1N.11C.1N.11C.1N.11C.1N.11 $983.3$ $573.6$ $696.5$ $901.4$ $983.3$ N.12C.1N.11S60.4 $1516.0$ $1720.9$ $1802.8$ $N.11$ C.1N.11 $696.5$ $800.4$ $1024.3$ $1106.3$ N.12C.1N.11S60.4 $1516.0$ $1720.9$ $1802.8$ $N.11$ C.1 $N.11$ $C.1$ $N.11$ $S73.6$ $655.6$ $901.4$ $983.3$ N.12C.1N.12 $800.4$ $1516.0$ $1720.9$ $1802.8$ $N.12$ $C.1$ $N.11$ $S69.5$ $590.4$ $1024.3$ $1100.3$ N.12S61.6	Н.7	C.4	+	H.7	737.5	860.4 696.5	1024.3	1434.1 1516.0	1720.9	180.2 8	Н.7	C.4	H.7	368.8 573.6	573.6 696 5	655.6 860.4	901.4 1024.3	983.3 1106.3	1147.2
	H,8	C.5	15	6 H	696.5	819.5	1024.3	1147.2	1311.1	1516.0	H,8	C,5	H.8	368.8	573.6	655.6	901.4	983.3	1147.2
				C,5	532.6	696.5	1270.2	1516.0	1720.9	1802.8			C,5	573.6	696.5	860.4	1024.3	1106.3	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	Н,9	C,5	5	6'H	696.5	819.5	1024.3	1147.2	1311.1	1516.0	6'Н	C,5	6'H	368.8	573.6	655.6	901.4	983.3	1147.2
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$				C,5	532.6	696.5	1270.2	1516.0	1720.9	1802.8			C,5	573.6	696.5	860.4	1024.3	1106.3	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	Н,10	0 C,5	10	H,10	696.5	819.5	1024.3	1147.2	1311.1	1516.0	H,10	C,5	H,10	368.8	573.6	655.6	901.4	983.3	1147.2
N,I1         C,I         N,I1         860.4         1516.0         1720.9         1802.8         N,I1         C,I         N,I1         368.8         573.6         655.6         901.4         983.3           C,4         N,I1         860.4         1770.2         1516.0         1720.9         1802.8         1802.8         1802.8         1802.8         1736.5         606.5         860.4         1024.3         1106.3           C,4         N,11         860.4         1770.2         1516.0         1720.9         1802.8         73.6         655.6         901.4         983.3           N,12         C,1         N,12         6,1         1720.9         1802.8         N,12         C,1         73.6         655.6         901.4         983.3           N,12         C,1         N,12         573.6         696.5         800.4         1024.3         1106.3           C,2         N,12         573.6         696.5         1720.9         1802.8         N,12         C,1         573.6         696.5         800.4         1024.3         1106.3           C,2         N,12         573.6         696.5         800.4         1024.3         1106.3         800.4         1024.3         1106.3 <td></td> <td></td> <td></td> <td>C,5</td> <td>532.6</td> <td>696.5</td> <td>1270.2</td> <td>1516.0</td> <td>1720.9</td> <td>1802.8</td> <td></td> <td></td> <td>C,5</td> <td>573.6</td> <td>696.5</td> <td>860.4</td> <td>1024.3</td> <td>1106.3</td> <td></td>				C,5	532.6	696.5	1270.2	1516.0	1720.9	1802.8			C,5	573.6	696.5	860.4	1024.3	1106.3	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	N,1	1 C,1		N,11	860.4	1516.0	1720.9	1802.8			N,11	C,1	N,11	368.8	573.6	655.6	901.4	983.3	1147.2
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$				C,1	491.7	737.5	1270.2	1516.0	1638.9	1802.8			C,1	573.6	696.5	860.4	1024.3	1106.3	
N,12         C,4         491.7         737.5         1270.2         1516.0         1638.9         1802.8         N.12         C,4         573.6         666.5         860.4         1024.3         1106.3           N,12         C,1         N,12         532.6         696.5         1202.0         1720.9         1802.8         N,12         C,1         N,12         533.6         696.5         860.4         1024.3         1106.3           C,1         532.6         696.5         1270.2         1516.0         1720.9         1802.8         N,12         C,1         533.6         696.5         860.4         1024.3         1106.3           C,2         N,12         573.6         696.5         160.4         1224.2         1434.1         1679.9         1761.8         C,2         N,12         573.6         655.6         901.4         983.3           C,13         C,1         C,13         368.8         573.6         655.6         901.4         983.3           C,13         6,14         1229.2         1516.0         1720.9         1802.8         C,1         0,13         566.5         801.4         1024.3         1106.3           C,13         6,14         1229.2         1516.0 </td <td></td> <td>C,4</td> <td></td> <td>N,11</td> <td>860.4</td> <td>1516.0</td> <td>1720.9</td> <td>1802.8</td> <td></td> <td></td> <td></td> <td>C,4</td> <td>N,11</td> <td>368.8</td> <td>573.6</td> <td>655.6</td> <td>901.4</td> <td>983.3</td> <td>1147.2</td>		C,4		N,11	860.4	1516.0	1720.9	1802.8				C,4	N,11	368.8	573.6	655.6	901.4	983.3	1147.2
				C,4	491.7	737.5	1270.2	1516.0	1638.9	1802.8			C,4	573.6	696.5	860.4	1024.3	1106.3	
C,1         532.6         696.5         1270.2         1516.0         1720.9         1802.8         C,1         573.6         696.5         860.4         1024.3         1106.3           C,2         N,12         573.6         696.5         180.4         1024.3         1106.3         1106.3           O,13         C,2         N,12         573.6         696.5         860.4         1024.3         1106.3           0,13         C,1         0,13         G,1         1679.9         176.18         7.2         573.6         655.6         901.4         983.3           0,13         C,1         0,13         G,1         0,13         G,1         0,13         368.8         573.6         655.6         901.4         983.3           0,13         C,1         1229.2         1516.0         1720.9         1802.8         0,13         368.8         573.6         655.6         901.4         983.3           0,14         C,2         0,13         G,1         0,13         G,1         0,13         368.8         573.6         655.6         901.4         983.3           0,14         C,2         0,13         G,1         G,1         G,1         573.6         690.5	N.13	2 C,1		N,12	860.4	1516.0	1720.9	1802.8			N,12	C,1	N,12	368.8	573.6	655.6	901.4	983.3	1147.2
C.2         N.12         573.6         860.4         1024.3         1434.1         161.8         C.2         N.12         368.8         573.6         655.6         901.4         983.3           0,13         C.2         532.6         866.5         1720.2         1516.0         1720.9         1802.8         0.13         0.13         368.8         573.6         655.6         901.4         983.3           0,13         C,1         0,13         860.4         1229.2         1516.0         1720.9         1802.8         0.13         0,13         368.8         573.6         655.6         901.4         983.3           0,13         C,1         0,13         360.4         1229.2         1516.0         1720.9         1802.8         0,13         C,1         0,13         368.8         573.6         655.6         901.4         983.3           0,14         C,2         0,13         0,13         C,1         0,13         573.6         655.6         901.4         983.3           0,14         C,2         0,14         C,2         0,13         573.6         655.6         901.4         983.3           0,14         C,2         0,14         573.6         655.6         901.4 </td <td></td> <td></td> <td></td> <td>C.</td> <td>532.6</td> <td>696.5</td> <td>1270.2</td> <td>1516.0</td> <td>1720.9</td> <td>1802.8</td> <td></td> <td></td> <td>C,1</td> <td>573.6</td> <td>696.5</td> <td>860.4</td> <td>1024.3</td> <td>1106.3</td> <td></td>				C.	532.6	696.5	1270.2	1516.0	1720.9	1802.8			C,1	573.6	696.5	860.4	1024.3	1106.3	
C2         532.6         166.5         1720.2         1516.0         1720.9         1802.8         0.13         C.2         573.6         666.5         860.4         1024.3         1106.3           0,13         0,1         800.4         1229.2         1516.0         1720.9         1802.8         0.13         0,13         368.8         573.6         665.5         901.4         983.3           0,13         0,1         737.5         1516.0         1720.9         1802.8         0.14         033.3         669.5         860.4         1024.3         1106.3           0,14         573.6         656.4         1679.9         1802.8         0,14         C,1         573.6         655.6         901.4         983.3           0,14         C,2         0,14         573.6         655.6         901.4         983.3           0,14         C,2         0,14         C,1         0,13         368.8         573.6         655.6         901.4         983.3           0,14         C,2         0,14         C,2         0,14         C,2         573.6         655.6         901.4         983.3           0,14         73.7         163.9         1802.8         0,14         C,2 </td <td></td> <td>C,2</td> <td>0.</td> <td>N,12</td> <td>573.6</td> <td>860.4</td> <td>1024.3</td> <td>1434.1</td> <td>1679.9</td> <td>1761.8</td> <td></td> <td>C,2</td> <td>N,12</td> <td>368.8</td> <td>573.6</td> <td>655.6</td> <td>901.4</td> <td>983.3</td> <td>1147.2</td>		C,2	0.	N,12	573.6	860.4	1024.3	1434.1	1679.9	1761.8		C,2	N,12	368.8	573.6	655.6	901.4	983.3	1147.2
O.13         C.1         O.13         860.4         1229.2         1516.0         1720.9         1201.4         983.3           0.13         C.1         O.13         368.8         573.6         655.6         901.4         983.3           0.14         C.2         O.14         573.6         1516.0         1780.9         1802.8         0.14         265.5         901.4         983.3           0.14         C.2         O.14         368.8         573.6         655.6         901.4         983.3           0.2         491.7         737.5         1516.0         1632.8         1802.8         0.14         2.2         0.14         368.5         860.4         11024.3         1106.3				C,2	532.6	696.5	1270.2	1516.0	1720.9	1802.8			C,2	573.6	696.5	860.4	1024.3	1106.3	
C,1         491.7         737.5         1516.0         1638.9         1802.8         C,1         573.6         696.5         860.4         1024.3         1106.3           0,14         C,2         0,14         573.6         860.4         1679.9         1761.8         983.3           0,14         C,2         0,14         368.8         573.6         655.6         901.4         983.3           0,14         C,2         0,14         368.8         573.6         655.6         901.4         983.3           0,14         C,2         0,14         368.8         573.6         660.4         1024.3         1106.3	0,1	3 C,1	_	0,13	860.4	1229.2	1516.0	1720.9			0,13	C,1	0,13	368.8	573.6	655.6	901.4	983.3	1147.2
0,14         C,2         0,14         573.6         860.4         1679.9         1761.8         0.14         368.8         573.6         655.6         901.4         983.3           C,1         C,2         491.7         737.5         1516.0         1638.9         1802.8         1802.8         0.14         2,2         573.6         666.5         860.4         1024.3         1106.3				C,1	491.7	737.5	1516.0	1638.9	1802.8				C,1	573.6	696.5	860.4	1024.3	1106.3	
C2 491.7 737.5 1516.0 1638.9 1802.8 C2 573.6 696.5 860.4 1024.3 1106.3	0,1	4 C,2	01	0,14	573.6	860.4	1679.9	1761.8			0,14	C,2	0,14	368.8	573.6	655.6	901.4	983.3	1147.2
				C,2	491.7	737.5	1516.0	1638.9	1802.8				C,2	573.6	696.5	860.4	1024.3	1106.3	

Column names for stretching (left columns) and bending (right columns) frequencies are in cm<sup>-1</sup> units and as follows:

Base, Atom & num., Bonding atom, Reference atom, 1st mode, 2nd mode, 3rd mode, 4th mode, 5th mode, 6th mode are shown in 2 sets of columns.

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	ピーク	761.8	761.8	302.8	761.8	384.0 761 o	384.0	761.8	884.0 201 0	/01.8 884.0	761.8	384.0	761.8	384.0 761.8	384.0	761.8	384.0 761 8	884.0	761.8	384.0 761.0	84.0 884.0	761.8	384.0	761.8	584.U	384.0	761.8	584.U	384.0	761.8	384.0 761 e	384.0	761.8	384.0	/01.8 384.0	761.8	384.0	761.8 284.0	761.8	384.0	761.8
	第(	1.0		60	0	0.0	0	1	0.0	0.0	0	11	0.0	0.0	00	1.0	0.0	0	1	0.0	0.0	1.0	10	0.0	0.0	0	0.0	~ · ·	0	1.0	0.0	0.0	0	0.0	0.0	1.0	2 0 2	0.0	0	0.0	0.0
	5 第5ピ	1557	1884	1720	1557	1475	1475	1557	1475	1475	1557	1475	1557	14/5	1475	1557	1475	1475	1557	1475	1475	1557	1475	1557	14/5	1475	1557	1557	1475	1557	1475	1475	1557	1475	1475	1557	1475	1557	1557	1475	1557
	第4ピー/	1434.1	1679.9	1311.1	1434.1	901.4	901.4	1434.1	901.4	901.4	1434.1	901.4	1434.1	901.4 1434 1	901.4	1434.1	901.4 1434 1	901.4	1434.1	901.4	901.4	1434.4	901.4	1434.4	901.4	901.4	1434.4	14341	901.4	1434.1	901.4	901.4	1434.1	901.4	901.4	1434.1	901.4	1434.1	1434.1	901.4	1434.1
	き3ピーク	1311.1	1270.2	1065.3	1311.1	696.5	696.5	1311.1	696.5	696.5	1311.1	696.5	1311.1	696.5 1311 1	696.5	1311.1	696.5 1311 1	696.5	1311.1	696.5	696.5	1311.1	696.5	1311.1	0.060	696.5	1311.1 606 E	13111	696.5	1311.1	696.5	696.5	1311.1	696.5	696.5	1311.1	696.5	1311.1 Ror F	1311.1	696.5	1311.1
m – 1]	2ピーク §	188.2	514.6 188.2	983.3	188.2	514.6	100.Z 514.6	188.2	514.6	188.2 514.6	188.2	514.6	188.2	188 2	514.6	188.2	514.6 188 2	514.6	188.2	514.6	100.Z 514.6	188.2	514.6	188.2	100 0	514.6	188.2	188.0	514.6	188.2	514.6	514.6	188.2	514.6	188.2 514.6	188.2	514.6	188.2 *14 6	188.2	514.6	188.2
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q	「第己	1065	106	860	1065	491	491	1065	491	491	1065	491	1065	1065	491	1065	106	491	1065	491	491	1065	491	1065	1065	491	1065	1065	491	1065	1065	491	1065	491	491	1065	491	1065	1065	491	1065
	基準原子	C,1	C,2	N.11	C,	N,13	0.1 0.1	C,2	C,3	C,2 N,12	C,3	C,2	C,3	N,10	N.14	C,4	N,10	N.12	C,5	N,13	0.5 14	9'H	N,11	Н,7	z o	0.5 C.5	6'H	N 10	C.3	N,10	0,4 N 11		N,12	C,2	0,12 C.4	N,13	C,1	N,13	N,14	C,3	N,14
	対原子, 番号	C,2	N 11		N,13	ŗ	5	C,3		N,12	C,2		N,10	N 14		N,10	N 12	21,12	N,13	N 14	N, I 4	N,11		N,11	3 (	2	C,4	5	3	C,4	ŗ	5	C,2	. (	C,4	C,1		C,5	C,3		C,5
	原子, 番号	C,1				ç	2'0				C,3					C,4			C,5			Н,6		Н,7	0		6'H	N 10	2		N 11	,	N,12			N,13			N,14		
	第6ピーク		1843.8	1884.8		10420	1802.8		1802.8	1802.8		1802.8		1802.8 1802.8	1802.8		1802.8	1802.8		1802.8	1802.8		1802.8		1761 0	1802.8	1557.0	1802.8	1802.8	1557.0	1802.8	1884.8		1884.8	1884.8						
	第5ピーク	1802.8	1679.9	1720.9	1679.9	1670.0	1679.9		1679.9	1843.8	1802.8	1679.9	1638.9	16/9.9	1679.9	1638.9	1679.9 1843.8	1679.9	1679.9	1679.9	1679.9		1679.9	0 0 0 0	16200	1679.9	1311.1	8.8/01	1679.9	1311.1	1679.9	1720.9	1802.8	1720.9	1311.1	1802.8		1720.9			1720.9
	第4ピーク	1270.2	1516.0	1638.9	1188.2	1229.2	1434.1		1434.1	1638.9	1270.2	1434.1	1229.2	1434.1	1434.1	1229.2	1434.1 1638 g	1434.1	1188.2	1434.1	1434.1	1270.2	1434.1	1270.2	1434.1	1434.1	1147.2	1434.1	1434.1	1147.2	1434.1	1638.9	1270.2	1638.9	1638.9	1270.2	1229.2	1597.9	7.7.7	1229.2	1597.9
	第3ピーク	1106.3	1434.1 1106.3	1557.0	1065.3	901.4	1147.2	1638.9	1147.2	12/0.2	1106.3	1147.2	860.4	983.3	1147.2	860.4	1147.2	1147.2	1065.3	1147.2	903.3 1147.2	1106.3	1147.2	1106.3	1970.9	1147.2	983.3	1638 9	1147.2	983.3	1147.2	1557.0	1106.3	1557.0	983.3 1557.0	1106.3	901.4	1229.2	1638.9	901.4	1229.2
[cm – 1	第2ピーク	983.3	901.4 614.6	1147.2	901.4	614.6	901.4	1229.2	901.4	90.000	983.3	901.4	655.6	901.4 778.5	901.4	655.6	901.4 655.6	901.4	901.4	901.4	901.4	614.6	901.4	614.6	901.4	901.4	819.5	1020 2	901.4	819.5	901.4	1147.2	983.3	1147.2	6.919.5 1147.2	983.3	614.6	1065.3 614 6	1229.2	614.6	1065.3
strech	第1ピーク	532.6	614.6 368.8	532.6	368.8	532.6	614.6	1106.3	614.6	327.8 614.6	532.6	614.6	450.7	614.6 491.7	614.6	450.7	614.6 327.8	614.6	368.8	614.6	614.6	368.8	614.6	368.8	014.0	614.6	614.6	1106.3	614.6	614.6	614.6 522 6	532.6	532.6	532.6	014.0 532.6	532.6	532.6	860.4 530.6	1106.3	532.6	860.4
	基準原子	C,1	C'5	- 17 17	C.1	N,13	0.1 0.1	C,2	C'3	C,2	C,3	C,2	C,3	0,10 C.3	N.14	C,4	N,10	N.12	C,5	N,13	N.14	9'H	N,11	Н,7	z, s	C.5	6'H	N 10	C.3	N,10	C,4	- C	N,12	C,2	0,12 C.4	N,13	C,1	N,13	N,14	C,3	N,14
	対原子,番号	C,2	N 11		N,13	ċ	5	C,3		N,12	C,2		N,10	N 14		N,10	N 12	7	N,13		N, 14	N,11		11'N	u C	2	C,4	Ë	3	C,4	č	5	C,2		C.4	C,1		C,5	C.3		C,5
	原子.番号	C,1				ç	2'S				C,3					C,4			C,5			9'H		Н,7	0	2	6'H	N 10			11 N	Ż	N,12			N,13			N,14		
	塩基名	ADE																																							

Table 4 Frequencies of Guanine nucleotide bonds, highest intensities. Frequencies are in cm<sup>-1</sup>.

and a summer	Income above	Out sham	Tels made	Onto another	John made	Ath and	Cals made	Rels name	han	and and the second	farmer at an	Duf sham	This make	Oak made	Take manula	Ath made	Esta man
unu.	Versus atom	Line atom	un pear	Vead un?	act peak	TOPO 1	Yead unc	otri peak	Date		versus arou	Line: atom	Veod UTI	vead un?	yead upp	ALL DOOM	and unc
_	c, c	5 0	368.8	450.7	1188.2	1302.1	1393.1	1638.9	<u>-</u> נ	5,5	5 0	245.8 163.9	0.32°C	696.5	1024.3	1302.1	038.9
	N,12	C,1	532.6	819.5	901.4	1557.0				N,12	C,1	245.8	532.6	1106.3	1188.2	1352.1	1638.9
		N,12	573.6	1188.2	1311.1	1393.1	1557.0	1638.9			N,12	286.8	368.8	573.6	655.6	1065.3	1188.2
2	N,11	C,2	450.7	614.6	1352.1				C,2	N,11	C,2	245.8	532.6	1106.3	1188.2	1352.1	1638.9
	N 10		0/3.0 E20.6	010 5	1.115	1393.1	0.7661			AL 10	Z, Z	280.8	308.8	0.5/0	0.00011	1 2 5 2 1	1 6 2 0 0
	N, 12	0,4 N 19	573.6	1188.2	301.4	1.2021	1557.0	1638 0		N,12	0,2 N 19	0.042	368.8	573.6	1 1 0 0. Z	1065.3	1188.2
	N 14	0.5	450.7	1024.3	1638.9			0.000		N 14	0.0	245.8	532.6	1106.3	1188.2	1352 1	1638.9
		N.14	573.6	1188.2	1311.1	1393.1	1557.0	1638.9			N.14	286.8	368.8	573.6	655.6	1065.3	1188.2
	C.1	C.3	450.7	1311.1	1557.0	1638.9	1802.8		C.3	C.1	C.3	245.8	532.6	1106.3	1188.2	1352.1	1638.9
		C,1	368.8	450.7	1188.2	1311.1	1393.1	1638.9			C,1	286.8	368.8	573.6	655.6	1065.3	1188.2
	C,4	C,3	532.6	1024.3	1393.1	1557.0	1638.9	1720.9		C,4	C'3	245.8	532.6	1106.3	1188.2	1352.1	1638.9
		C,4	368.8	450.7	1188.2	1311.1	1393.1	1638.9			C,4	286.8	368.8	573.6	655.6	1065.3	1188.2
	N,13	C,3	409.7	737.5	1188.2	1393.1	1720.9			N,13	C,3	245.8	532.6	1106.3	1188.2	1352.1	1638.9
		N,13	368.8	450.7	1188.2	1311.1	1393.1	1638.9			N,13	286.8	368.8	573.6	655.6	1065.3	1188.2
4	C,3	C,4	696.5	1024.3	1188.2	1352.1	1802.8		C,4	C,3	C,4	245.8	532.6	1106.3	1188.2	1352.1	1638.9
		C,3	368.8	450.7	1188.2	1311.1	1393.1	1638.9			C,3	286.8	368.8	573.6	655.6	1065.3	1188.2
	N,10	C,4	532.6	1188.2	1311.1	1557.0	1720.9			N,10	C,4	245.8	532.6	1106.3	1188.2	1352.1	1638.9
		N,10	368.8	450.7	1188.2	1311.1	1393.1	1638.9			N,10	286.8	368.8	573.6	655.6	1065.3	1188.2
	N,14	C,4	450.7	532.6	1024.3	1188.2	1638.9			N,14	C,4	245.8	532.6	1106.3	1188.2	1352.1	1638.9
		N,14	368.8	450.7	1188.2	1311.1	1393.1	1638.9			N,14	286.8	368.8	573.6	655.6	1065.3	1188.2
5	N,10	C,5	532.6	1188.2	1311.1	1557.0	1720.9		C,5	N,10	C,5	245.8	532.6	1106.3	1188.2	1352.1	1638.9
		N,10	368.8	450.7	1188.2	1311.1	1393.1	1638.9			N,10	286.8	368.8	573.6	655.6	1065.3	1188.2
	N,13	C,5	409.7	737.5	1188.2	1393.1	1720.9	0 0000		N,13	C,5	245.8	532.6	1106.3	1188.2	1352.1	1638.9
	110	N.13	300.0 E 20 6	400.1	010 5	1 100	1.093.1	1038.3	9	NI 10	N, IS	200.0	0.000	0/3.0	0.00011	10501	2.0011
•	N, IZ	0, L V	368.8	450.7	019.0	1311.1	1.2021	1638 0	o Ľ	N,12	0'H	240.0 286.8	368.8	573.6	655.6	1.302.1	1188.9
-	11N	H.7	450.7	614.6	860.4	942.3		6.000	H.7	N.11	H.7	245.8	532.6	1106.3	1188.2	1352.1	1638.9
		LI'N	368.8	450.7	1188.2	1311.1	1393.1	1638.9	1		N.11	286.8	368.8	573.6	655.6	1065.3	1188.2
	N,11	Н,8	450.7	614.6	860.4	942.3			Н.8	N.11	Н,8	245.8	532.6	1106.3	1188.2	1352.1	1638.9
		II,N	368.8	450.7	1188.2	1311.1	1393.1	1638.9			N,11	286.8	368.8	573.6	655.6	1065.3	1188.2
6	C,5	6'H	737.5	901.4	1270.2	1393.1	1720.9		6'H	C,5	6'H	245.8	532.6	1106.3	1188.2	1352.1	1638.9
		C,5	368.8	450.7	1188.2	1311.1	1393.1	1638.9			C,5	286.8	368.8	5/3.6	9.000	1065.3	1188.2
•	C,4	2'X	532.6 368.8	1024.3	1393.1	1.1121	1638.9	1/20.9	N,10	C,4	01'N	245.8	532.6 368.8	1106.3 573.6	1188.2 Refe	1352.1	1038.9
	C.5	10 10	737.5	9014	1270.2	1393.1	1720.9	0.000		C.5	10 10	245.8	532.6	1106.3	1188.2	1352.1	1638.9
	-	C.5	368.8	450.7	1188.2	1311.1	1393.1	1638.9			C.5	286.8	368.8	573.6	655.6	1065.3	1188.2
_	C,2	N,11	532.6	655.6	1557.0	1638.9	1720.9		N,11	C,2	N,11	245.8	532.6	1106.3	1188.2	1352.1	1638.9
		C,2	368.8	450.7	1188.2	1311.1	1393.1	1638.9			C,2	286.8	368.8	573.6	655.6	1065.3	1188.2
2	Ċ,1	N,12	450.7	737.5	1311.1	1638.9	1802.8		N,12	C,1	N,12	245.8	532.6	1106.3	1188.2	1352.1	1638.9
		C,1	573.6	1188.2	1311.1	1393.1	1557.0	1638.9			C,1	286.8	368.8	573.6	655.6	1065.3	1188.2
	C,2	N,12	532.6	696.5	1557.0	1638.9				C,2	N,12	245.8	532.6	1106.3	1188.2	1352.1	1638.9
-	ć	C'Z	3/3.0	1 1 8 8. Z	1.11.01	1393.1	0./001	038.9	N 12	ŝ	C,Z	200.0	308.8 E27.6	0.5/0	0.00011	1000.3	16200
2	r C	2.5	400./ 573.6	0.00011	0.4201	1 2 2 3 1	1567.0	16200	0'IN	5	2.5	0.042	0.200	673 A	1 1 0 0.Z	1065 2	11000
	5.5	5 N	0.0.0	1970.9	13931	17909	0./661	6.000		50	0 13 N 13	245.8	532 6	1106.3	1188.9	1359.1	1638.9
	2,2	2	573.6	1188.9	13111	13931	1557.0	1638.0		2	2 6	286.8	368.8	573 G	655.6	1065.3	1188.9
4	C.2	N.14	532.6	696.5	1557.0	1638.9	2.00	0.000	N.14	C.2	N.14	245.8	532.6	1106.3	1188.2	1352.1	1638.9
		C.2	573.6	1188.2	1311.1	1393.1	1557.0	1638.9			C.2	286.8	368.8	573.6	655.6	1065.3	1188.2
	C.4	N.14 0.14	532.6 573.6	1024.3	1393.1	1557.0	1638.9	1720.9		C.4	N.14 0.4	245.8 286.8	532.6 368.8	1106.3 573.6	1188.2 655.6	1352.1	1638.9
15	C,1	0,15	450.7	1311.1	1557.0	1638.9	1802.8		0,15	C,1	0,15	245.8	532.6	1106.3	1188.2	1352.1	1638.9
		5	409.7	1017	ALL R	13111	1879.0	10400			÷	0 000	0 000				

The numbering of the nucleotide atoms used in tables 1~4 and 5-8. Base atoms order is shown for each base, deoxyribose numbering is done consecutively after each base numbering as shown below for cytosine example.



deoxyribose numbering



## Comparison of calculated frequencies with experimentally measured IR spectra

(C. S. Peng, K. C. Jones, and A. Tokmakoff, "Anharmonic Vibrational Modes of Nucleic Acid Bases Revealed by 2D IR Spectroscopy," J. Am. Chem. Soc., 2011, **133**, 15650-15660)

 $\cdot$  CYT

CMP	C1	1651	9.2	1.0	1690	$\nu$ (C <sup>2</sup> =O), $\nu$ (N <sup>1</sup> =C <sup>6</sup> ), $\delta$ (C <sup>6</sup> -H)
	C2	1614	15	0.55	1624	$\nu$ (N <sup>3</sup> =C <sup>4</sup> -C <sup>5</sup> =C <sup>6</sup> ), $\nu$ (C <sup>2</sup> =O), $\delta$ (C <sup>5</sup> -H), $\delta$ (C <sup>6</sup> -H)
	C3	1583	17	0.21		
	C4	1524	6.1	0.57	1503	$\nu$ (C <sup>4</sup> -C <sup>5</sup> ), $\nu$ (N <sup>1</sup> -C <sup>6</sup> ), $\delta$ (C <sup>5</sup> -H), $\delta$ (C <sup>6</sup> -H), $\delta$ (N <sup>4</sup> D <sub>2</sub> )
	C5	1504	8.9	0.94	1483	$\nu (N^3 = C^4 - N^4), \nu (C^5 = C^6), \delta (C^5 - H), \delta (C^6 - H), \delta (N^4 D_2)$
		Calculated		E	xperimental	
	172	$21 cm^{-1} (C-C)$	; C-N)	16	$524 cm^{-1}$	$\rightarrow$ 93cm <sup>-1</sup> difference
	15	$57 cm^{-1} (C-N)$	1)	15	03 <i>cm</i> <sup>-1</sup>	$\rightarrow$ 54 <i>cm</i> <sup>-1</sup> difference
	• [	ГНҮ				
TMP	Т1	1690	11	0.74	1677	$\nu$ (C <sup>2</sup> =O), $\nu$ (C <sup>4</sup> =O), $\delta$ (N <sup>3</sup> -D)
	T2	1663	5.0	1.0	1657	$\nu$ (C <sup>4</sup> =O), $\nu$ (C <sup>5</sup> =C <sup>6</sup> ), $\delta$ (N <sup>3</sup> -D), $\delta$ (C <sup>5</sup> H <sub>3</sub> ), $\delta$ (C <sup>6</sup> -H)
	Т3	1629	10	0.94	1627	$\nu$ (C <sup>5</sup> =C <sup>6</sup> ), $\nu$ (C <sup>4</sup> =O), $\delta$ (C <sup>5</sup> H <sub>3</sub> ), $\delta$ (C <sup>6</sup> -H)
		Calculated		E	xperimental	
	172	$21 cm^{-1}(C-C)$	, N-C)	1	$657 cm^{-1}$	$64cm^{-1}$ difference
	17	$62 cm^{-1} (N-C)$	<u>()</u>	1	677cm <sup>-1</sup> —	$\rightarrow$ 85 <i>cm</i> <sup>-1</sup> difference
	• 1	ADE				
AMP	A1	1625	8.0	1.0	1588	$\nu$ (C <sup>4</sup> =C <sup>5</sup> , C <sup>5</sup> -C <sup>6</sup> out-of-phase), $\delta$ (C <sup>2</sup> -H), $\delta$ (N <sup>6</sup> D <sub>2</sub> ), Py
	A2	1578	9.8	0.41	1565	$\nu$ (C <sup>4</sup> =C <sup>5</sup> , C <sup>5</sup> -C <sup>6</sup> in-phase), $\nu$ (N <sup>1</sup> -C <sup>6</sup> ), $\nu$ (N <sup>3</sup> -C <sup>4</sup> ),
						$\nu$ (N <sup>7</sup> =C <sup>8</sup> ), $\delta$ (C <sup>8</sup> -H), Py + Im
		本 Calculate	d		Experimental	
	16	39 <i>cm</i> <sup>-1</sup> (C-C	; , C-N , N-C)		1588cm <sup>-1</sup>	$51cm^{-1}$ difference
	• (	GUA				
GMP	G1	1665	11	1.0	1692	$\nu$ (C <sup>6</sup> =O), $\delta$ (N <sup>1</sup> -D), Py
	G2	1579	4.0	0.63	1556	$\nu$ (C <sup>2</sup> =N <sup>3</sup> ), $\nu$ (C <sup>6</sup> =O), $\delta$ (N <sup>2</sup> -H), $\delta$ (N <sup>2</sup> D <sub>2</sub> ), Py
	G3	1565	7.8	0.62	1533	$\nu$ (C <sup>2</sup> =N <sup>3</sup> -C <sup>4</sup> =C <sup>5</sup> ), $\delta$ (C <sup>8</sup> -H), Py + Im
	G4	1539	18	0.29	1511	$\nu$ (C <sup>4</sup> =C <sup>5</sup> ), $\nu$ (N <sup>7</sup> =C <sup>8</sup> ), $\delta$ (C <sup>8</sup> -H), Py + Im
		Calculated		Ex	perimental	
	16	$39 cm^{-1} (C-N)$	I , N-C)		1692cm <sup>-1</sup>	$54cm^{-1}$ difference
	15	$57 cm^{-1}(C-C)$	, N-C)		$1556 cm^{-1}$	$1cm^{-1}$ difference

						Re	action	Coordi	inate u	unit of [	cm – 1]							
strech	strech	strech	strech	strech										end				
atom & num Versus atom Ref atom 1th peak 2th peak 3th peak 4th p	m Versus atom Ref atom 1th peak 2th peak 3th peak 4th p	Ref atom 1th peak 2th peak 3th peak 4th p	1th peak 2th peak 3th peak 4th p	2th peak 3th peak 4th p	3th peak 4th p	4th p	eak	5th peak	6th peak	base	atom & num	<b>/ersus atom</b>	Ref atom	1th peak	2th peak	3th peak	4th peak	5th peak
C,1 N,6 C,1 532.6 942.4 1188.2 1516.0 N E 572.6 15570 1761.0	N,6 C,1 532.6 942.4 1188.2 1516.0 N.6 573.6 15570 1751.6	C,1 532.6 942.4 1188.2 1516.0 M.S. 573.6 15570 1761.0	532.6 942.4 1188.2 1516.0	942.4 1188.2 1516.0	1188.2 1516.0	1516.0	_			C,1	N,6	C,1	81.9 260 0	573.6 573.6	1638.9	1761.8	1 202 1	1667.0
N.7 C.1 573.6 942.4 1516.0	N.7 C.1 573.6 942.4 1516.0	C.1 573.6 942.4 1516.0	573.6 942.4 1516.0	942.4 1516.0	1516.0						N.7	0,1 0,1	81.9	573.6	303.3 1638.9	1761.8	1.050	0./001
N,7 614.6 983.3 1229.2 1557.0	N.7 614.6 983.3 1229.2 1557.0	N,7 614.6 983.3 1229.2 1557.0	614.6 983.3 1229.2 1557.0	983.3 1229.2 1557.0	1229.2 1557.0	1557.0		1638.9	1761.8			N,7	368.8	573.6	737.5	983.3	1557.0	
C,2 C,3 C,2 532.6 1106.3 1352.1 1516.0	C.3 C.2 532.6 1106.3 1352.1 1516.0	C.2 532.6 1106.3 1352.1 1516.0	532.6 1106.3 1352.1 1516.0	1106.3 1352.1 1516.0	1352.1 1516.0	1516.0	_	1761.8		C.2	C.3	C.2	81.9	573.6	1638.9	1761.8		
C,3 614.6 983.3 1229.2 1557.0	ME C,3 614.6 983.3 1229.2 1557.0	C,3 614.6 983.3 1229.2 1557.0	614.6 983.3 1229.2 1557.0	983.3 1229.2 1557.0	1229.2 1557.0	1557.0	_	1638.9	1761.8		1	0'3 0'3	368.8	573.6	737.5	983.3	1557.0	
N.3 C.2 332.0 342.4 1100.2 1332.1 N.5 614.6 983.3 1229.2 1557.0	N.3 V.2 332.0 342.4 1100.2 1332.1 N.5 614.6 983.3 1229.2 1557.0	N.5 614.6 983.3 1229.2 1557.0	614.6 983.3 1229.2 1557.0	983.3 1229.2 1557.0	1229.2 1557.0	1557.0		1638.9	1761.8		C'N	0'Z N.5	368.8	573.6	737.5	983.3	1557.0	
N,6 C,2 632.6 942.4 1188.2 1516.0	N,6 C,2 632.6 942.4 1188.2 1516.0	C,2 632.6 942.4 1188.2 1516.0	632.6 942.4 1188.2 1516.0	942.4 1188.2 1516.0	1188.2 1516.0	1516.0					N,6	C,2	81.9	573.6	1638.9	1761.8		
N.6 614.6 983.3 1229.2 1557.0	N.6 614.6 983.3 1229.2 1557.0	N.6 614.6 983.3 1229.2 1557.0	614.6 983.3 1229.2 1557.0	983.3 1229.2 1557.0	1229.2 1557.0	1557.0		1638.9	1761.8			N.6	368.8	573.6	737.5	983.3	1557.0	
C,3 C,3 C,3 1188.2 1393.1 1516.0 1720.9	C,2 C,3 1188.2 1393.1 1516.0 1720.9	C,3 1188.2 1393.1 1516.0 1720.9	1188.2 1393.1 1516.0 1720.9	1393.1 1516.0 1720.9	1516.0 1720.9	1720.9				C,3	C,2	C,3	81.9	573.6	1638.9	1761.8		
C.4 C.3 696.5 1106.3 1323.1 1516.0 C.4 C.3 696.5 1106.3 1393.1 1516.0	C.4 C.2 614.6 983.3 1229.2 1557.0 C.4 C.3 696.5 1106.3 1393.1 1516.0	C.2 614.6 983.3 1229.2 1557.0 C.3 696.5 1106.3 1393.1 1516.0	614.6 983.3 1229.2 1557.0 696.5 1106.3 1393.1 1516.0	983.3 1229.2 1516.0 1106.3 1393.1 1516.0	1229.2 1516.0 1393.1 1516.0	1516.0	-	1638.9	1 /61.8		C.4	C 23	308.8 81.9	5/3.6 573.6	737.5 1638.9	983.3 1761.8	0./ cc1	
C,4 614.6 983.3 1229.2 1557.0	C,4 614.6 983.3 1229.2 1557.0	C,4 614.6 983.3 1229.2 1557.0	614.6 983.3 1229.2 1557.0	983.3 1229.2 1557.0	1229.2 1557.0	1557.0	-	1638.9	1761.8			C,4	368.8	573.6	737.5	983.3	1557.0	
C,4 C,3 C,4 532.6 1106.3 1188.2 1352.1	C,3 C,4 532.6 1106.3 1188.2 1352.1	C.4 532.6 1106.3 1188.2 1352.1	532.6 1106.3 1188.2 1352.1	1106.3 1188.2 1352.1	1188.2 1352.1	1352.1		1516.0	1761.8	C.4	C.3	C,4	81.9	573.6	1638.9	1761.8		
C,3 614.6 983.3 1229.2 1557.0	C,3 614.6 983.3 1229.2 1557.0	C,3 614.6 983.3 1229.2 1557.0	614.6 983.3 1229.2 1557.0	983.3 1229.2 1557.0	1229.2 1557.0	1557.0	-	1638.9	1761.8			C,3	368.8	573.6	737.5	983.3	1557.0	
N,7 C,4 573.6 942.4 1516.0	N,7 C,4 573.6 942.4 1516.0	C,4 573.6 942.4 1516.0	573.6 942.4 1516.0	942.4 1516.0	1516.0 1000 0 1557 0	1667.0		1000	0 1221		N,7	C,4	81.9	573.6	1638.9	1761.8	102.0	
N.5 C.2 N.5 1188.2 1393.1 1516.0 1720.9	C.2 N.5 1188.2 1393.1 1516.0 1720.9	N.5 1188.2 1393.1 1516.0 1720.9	1188.2 1393.1 1516.0 1720.9	1393.1 1516.0 1720.9	1516.0 1720.9	1720.9		2.000	2.12.1	N.5	C.2	S'N	81.9	573.6	1638.9	1761.8	0.1001	
C,2 614.6 983.3 1229.2 1557.0	C,2 614.6 983.3 1229.2 1557.0	C,2 614.6 983.3 1229.2 1557.0	614.6 983.3 1229.2 1557.0	983.3 1229.2 1557.0	1229.2 1557.0	1557.0		1638.9	1761.8		ļ	C,2	368.8	573.6	737.5	983.3	1557.0	
N,6 C,1 N,6 532.6 1188.2 1516.0 1679.9	C,1 N,6 532.6 1188.2 1516.0 1679.9	N,6 532.6 1188.2 1516.0 1679.9	532.6 1188.2 1516.0 1679.9	1188.2 1516.0 1679.9	1516.0 1679.9	1679.9				N,6	C,1	N,6	81.9	573.6	1638.9	1761.8		
C,1 573.6 983.3 1229.2 1557.0	C,1 573.6 983.3 1229.2 1557.0	C,1 573.6 983.3 1229.2 1557.0	573.6 983.3 1229.2 1557.0	983.3 1229.2 1557.0	1229.2 1557.0	1557.0	_	1761.8				C,1	368.8	573.6	737.5	983.3	1557.0	
C,2 N,6 532.6 1188.2 1393.1 1516.0	C,2 N,6 532.6 1188.2 1393.1 1516.0	N,6 532.6 1188.2 1393.1 1516.0	532.6 1188.2 1393.1 1516.0	1188.2 1393.1 1516.0	1393.1 1516.0	1516.0		1720.9			C,2	9'N	81.9	573.6	1638.9	1761.8		
M7 C1 M7 525 1100 15100 15100 1510	C,2 573.6 983.3 1229.2 1557.0 C1 M7 529.6 11000 15160 15700	C,2 573.6 983.3 1229.2 1557.0 M7 529.6 1100.0 1516.0 1570.0	573.6 983.3 1229.2 1557.0	983.3 1229.2 1557.0	1229.2 1557.0	1557.0		1761.8		1 N	ć	C,2	368.8	573.6 573.6	737.5	983.3 1761 o	1557.0	
C1 614.6 983.3 1229.2 1557.0	C1 614.6 983.3 1229.2 1557.0	C.1 614.6 983.3 1229.2 1557.0	614.6 983.3 1229.2 1557.0	983.3 1229.2 1557.0	1229.2 1557.0	1557.0	_	1638.9	1761.8		ò	20	368.8	573.6	737.5	983.3	1557.0	
C,4 N,7 532.6 696.5 1393.1 1516.0	C,4 N,7 532.6 696.5 1393.1 1516.0	N,7 532.6 696.5 1393.1 1516.0	532.6 696.5 1393.1 1516.0	696.5 1393.1 1516.0	1393.1 1516.0	1516.0		1761.8			C,4	N,7	81.9	573.6	1638.9	1761.8		
C,4 614.6 983.3 1229.2 1557.0	C,4 614.6 983.3 1229.2 1557.0	C,4 614.6 983.3 1229.2 1557.0	614.6 983.3 1229.2 1557.0	983.3 1229.2 1557.0	1229.2 1557.0	1557.0		1638.9	1761.8			C,4	368.8	573.6	737.5	983.3	1557.0	
H,8 N,5 H,8 532.6 943.4 1188.2 1352.1	N,5 H,8 532.6 943.4 1188.2 1352.1	H,8 532.6 943.4 1188.2 1352.1	<b>532.6</b> 943.4 1188.2 1352.1	943.4 1188.2 1352.1	1188.2 1352.1	1352.1	-	1720.9	0 1011	Н,8	N,5	H,8	81.9	573.6	1638.9	1761.8		
H9 N5 H9 5326 9434 11882 13521	N.5 H.9 5326 943.4 1188.2 1352.1	H B 532 6 943 4 1188 2 1352 1	532 6 943 4 1188 2 1352 1	943.4 1188.2 1352.1	1188.2 1352.1	1352.1	_	1720.9	0.10/1	6 H	N.5	6 H	81.9	573.6	16.38.9	1761.8	0./001	
N.5 614.6 983.3 1229.2 1557.0	N.5 614.6 983.3 1229.2 1557.0	N.5 614.6 983.3 1229.2 1557.0	614.6 983.3 1229.2 1557.0	983.3 1229.2 1557.0	1229.2 1557.0	1557.0		1638.9	1761.8			N.5	368.8	573.6	737.5	983.3	1557.0	
H,10 C,3 H,10 532.6 901.4 1106.3 1352.1	C,3 H,10 532.6 901.4 1106.3 1352.1	H,10 532.6 901.4 1106.3 1352.1	532.6 901.4 1106.3 1352.1	901.4 1106.3 1352.1	1106.3 1352.1	1352.1		1516.0	1761.8	H,10	C,3	H,10	81.9	573.6	1638.9	1761.8		
C,3 614.6 983.3 1229.2 1557.0	C,3 614.6 983.3 1229.2 1557.0	C,3 614.6 983.3 1229.2 1557.0	614.6 983.3 1229.2 1557.0	983.3 1229.2 1557.0	1229.2 1557.0	1557.0	-	1638.9	1761.8			C,3	368.8	573.6	737.5	983.3	1557.0	
H,11 C,4 H,11 532.6 696.5 1393.1 1516.0	C,4 H,11 532.6 696.5 1393.1 1516.0	H,11 532.6 696.5 1393.1 1516.0	532.6 696.5 1393.1 1516.0	696.5 1393.1 1516.0	1393.1 1516.0	1516.0	_	1761.8		H,11	C,4	Н,11	81.9	573.6	1638.9	1761.8		
C,4 614.6 983.3 1229.2 1557.0	C,4 614.6 983.3 1229.2 1557.0	C,4 614.6 983.3 1229.2 1557.0	614.6 983.3 1229.2 1557.0	983.3 1229.2 1557.0	1229.2 1557.0	1557.0		1638.9	1761.8			C,4	368.8	573.6	737.5	983.3	1557.0	
0,12 C,1 0,12 532.6 1188.2 1516.0	C,1 0,12 532.6 1188.2 1516.0	0,12 532.6 1188.2 1516.0	532.6 1188.2 1516.0	1188.2 1516.0	1516.0					0,12	C,1	0,12	81.9	573.6	1638.9	1761.8		
C,1 81.9 573.6 1229.2 1638.9	C,1 81.9 573.6 1229.2 1638.9	C,1 81.9 573.6 1229.2 1638.9	81.9 573.6 1229.2 1638.9	573.6 1229.2 1638.9	1229.2 1638.9	1638.9		1761.8				C,1	368.8	573.6	737.5	983.3	1557.0	

Column names for stretching (left columns) and bending (right columns) frequencies are in cm<sup>-1</sup> units and as follows:

Base, Atom & num., Bonding atom, Reference atom, 1st mode, 2nd mode, 3rd mode, 4th mode, 5th mode, 6th mode are shown in 2 sets of columns.

Table 5. Frequencies of Cytosine base bonds, highest intensities. Frequencies are in cm<sup>-1</sup>.

1679.9         1761.8         N,12         N,12         N,12         0.65         942.4         11897.9         776.           1720.9         1843.7         C.2         C.3         368.8         942.4         1188.2         1761.           1720.9         1843.7         C.2         C.3         368.8         1393.1         1597.9         7761.           1720.9         1843.7         C.2         C.3         368.8         1393.1         1597.9         7761.           2827.1         2950.0         C.4         C.3         368.8         1393.1         1597.9         7761.           2827.1         2950.0         C.4         C.3         368.8         1393.1         1597.9         7761.           2827.1         2950.0         H43.7         C.4         C.3         368.8         1393.1         1597.9         7761.           1720.9         1843.7         C.4         C.3         368.8         1393.1         1597.9         7761.           1720.9         1843.7         C.4         C.3         368.8         1393.1         1597.9         7761.           1720.9         1843.7         C.4         C.4         C.3         368.8         192.4	Keactio           Strech           Versus atom         Ref atom         1th peak         2th peak         3th peak         4th peak           N.11         C,1         901.4         10065.3         1188.2         1352.1	Reaction           strech           Ref atom         1th peak         2th peak         3th peak         4th peak           C,1         901.4         1006.3         1188.2         1352.1	Reaction           strech           11h peak         2th peak         3th peak         4th peak           901.4         1065.3         1188.2         1352.1	Trech 2th peak 3th peak 4th pea 1065.3 1188.2 13521	Reaction           3th peak         4th peak           1188.2         1352.1	4th pea 1352.1		Coordir <sup>5th peak</sup>	nate u <sup>6th peak</sup>	nit of [ base C,1	cm – 1] atom & num N.11	ersus atom C,1	b Ref atom 368.8	end 1th peak 1393.1	2th peak 1597.9	3th peak 1761.8	4th peak 1884.7	5th peak
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		11,N	C, I, S	901.4 491.7	1065.3 1229.2	1188.2 1393.1	1352.1 1597.9	1679.9	1761.8	C,1	II.N SEM	C,1 N,11	368.8 327.8	1393.1 491.7	1597.9 778.5	1761.8 1065.3	1884.7	
C.3         C.2         Same         TSD         TSD <td></td> <td>N, IZ</td> <td>N,12</td> <td>1597.9</td> <td>942.4 1761.8</td> <td>1.265</td> <td>1434.1</td> <td>6.02/1</td> <td></td> <td></td> <td>N, I Z</td> <td>0,1 N,12</td> <td>368.8 368.8</td> <td>1393.1 942.4</td> <td>1188.2</td> <td>1311.1</td> <td>1884./</td> <td></td>		N, IZ	N,12	1597.9	942.4 1761.8	1.265	1434.1	6.02/1			N, I Z	0,1 N,12	368.8 368.8	1393.1 942.4	1188.2	1311.1	1884./	
	-	C,3	C.2 C.3	655.6 1597.9	1188.2 1761.8	1311.1	1475.0	1720.9	1843.7	C,2	C,3	C.2 C.3	368.8 368.8	1393.1 942.4	1597.9 1188.2	1761.8 1311.1	1884.7	
		N,12	C,2	737.5 1507 0	942.4 1761 8	1352.1	1434.1	1720.9			N,12	C,2	368.8 368.8	1393.1	1597.9	1761.8 1311 1	1884.7	
C4         C3         6656         10633         13521         11618         22771         25600         74.4         C3         3068         332.4         1182.2         1110           C5         5556         15973         17618         22771         25600         74.8         76.4         3088         92.4         1182.2         1111         14750         17209         184.7         C4         C3         3068         92.4         1182.2         1111         14750         17209         184.7         C4         C3         308.8         1397.3         1997.3         1761.           N11         C4         D31         1971.2         111.1         14750         17209         184.7         C5         C3         308.8         1397.3         1761.3           C1         D31         1971.2         1720.9         184.7         C5         C3         308.9         1781.1         1877.3         1761.3	-	C,2	C.3	409.7	655.6	1024.3	1188.2			C,3	C,2	C.3	368.8 368.8	1393.1	1597.9	1761.8	1884.7	
	_	C,4	C.S.	655.6 1507.0	1065.3	1352.1					C,4	2.00	368.8	342.4 1393.1 040.4	1597.9	1761.8	1884.7	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		C,5	0,3 C,4	450.7	1/01.0	1393.1	1761.8	2827.1	2950.0		CH3,5	0.4	368.8	342.4 1393.1	1597.9	1761.8	1884.7	
		C.3	C,5 C,4	1597.9 655.6	1761.8 1188.2	1311.1	1475.0	1720.9	1843.7	C.4	<b>C.</b> 3	C,5 C,4	368.8 368.8	942.4 1393.1	1188.2 1597.9	1311.1 1761.8	1884.7	
NII         C4         90.4         1063         1182         1321         1639         1720           C3         C5         6556         1188         1311         1475         17203         16837         15979         15973         15979         17618           C3         C5         6556         1188         13111         14750         17203         16847         C5         C3         15979         17618         13973         15979         17618         13973         15979         17618         13973         13979         17618         13973         13979         1761         13973         13973         1761         13973         13671         13973         13671         13973         13671         13973         1371         13973         1311         13572         1311         13572         1311         13631         13673         13631         13673         13671         13673         13671         13673         13617         13673         13617         13673         13617         13617         13617         13617         13617         13617         13617         13617         13617         13617         13617         13617         13617         13617         13617         1			C.3	1597.9	1761.8						)	C.3	368.8	942.4	1188.2	1311.1		
C.3         C.5         6556         1188.2         131.1         1475.0         1720.9         1843.7         C.5         C.3         369.3         1393.1         1597.9         1761.1           N112         H.6         N.12         H.6         N.12         H.6         N.12         H.6         139.3         1393.1         1597.9         1761.1           N.12         H.9         5556         1055.3         1352.1         143.41         170.0         147         C.4         H.7         6556         1065.3         1332.1         1397.1         1397.1         1397.1         1397.1         1397.1         1397.1         1397.1         1397.1         1397.1         1597.9         1761.           C.5         H.9         450.7         1065.3         1393.1         1761.8         2827.1         2950.0         H.9         C.5         H.1         2655.6         1397.9         1761.           C.5         H.90         450.7         1065.3         1393.1         1597.9         1761.         265         1393.1         1597.9         1761.         2765.7         259.9         333.1         1597.9         1761.         276.5         259.9         333.1         1597.9         1761. <t< td=""><td></td><td>N.11</td><td>C.4 N.11</td><td>901.4 1597.9</td><td>1065.3 1761.8</td><td>1188.2</td><td>1352.1</td><td>1638.9</td><td>1720.9</td><td></td><td>N,11</td><td>C.4 N.11</td><td>368.8 368.8</td><td>1393.1 942.4</td><td>1597.9 1188.2</td><td>1761.8 1311.1</td><td>1884.7</td><td></td></t<>		N.11	C.4 N.11	901.4 1597.9	1065.3 1761.8	1188.2	1352.1	1638.9	1720.9		N,11	C.4 N.11	368.8 368.8	1393.1 942.4	1597.9 1188.2	1761.8 1311.1	1884.7	
N12         H6         737.5         94.4         135.1         143.1         1720.9         H.6         N.12         H.6         368.8         139.1         1597.9         1761.           C.4         H7         556.1         1557.3         132.1         1434.1         1720.9         1761.           C.4         H3         557.9         1761.8         2827.1         2950.0         H.8         C.5         6.8         1333.1         1597.9         1761.           C.5         H.8         450.7         1065.3         1333.1         1761.8         2827.1         2950.0         H.8         C.5         6.88         1333.1         1597.9         1761.           C.5         1597.9         1761.8         2827.1         2950.0         H.9         C.5         6.88         1333.1         1597.9         1761.           C.5         1597.9         1761.8         2827.1         2950.0         H.10         C.5         568.8         392.4         1882.2         131.1           C.5         1597.9         1761.8         2827.1         2950.0         H.10         C.5         168.8         1761.8           C.5         1597.9         1761.8         2827.1 <td< td=""><td>_</td><td>C,3</td><td>C.5 C.3</td><td>655.6 1597.9</td><td>1188.2 1761.8</td><td>1311.1</td><td>1475.0</td><td>1720.9</td><td>1843.7</td><td>C,5</td><td>C,3</td><td>C.5 C.3</td><td>368.8 1597.9</td><td>1393.1 1761.8</td><td>1597.9</td><td>1761.8</td><td>1884.7</td><td></td></td<>	_	C,3	C.5 C.3	655.6 1597.9	1188.2 1761.8	1311.1	1475.0	1720.9	1843.7	C,5	C,3	C.5 C.3	368.8 1597.9	1393.1 1761.8	1597.9	1761.8	1884.7	
C.4         N12         1557.0         1761.8         1352.1         1188.2         1311.           C.5         H.8         450.7         1065.3         1352.1         2950.0         H.9         C.5         H.8         556.0         1065.3         1332.1         1597.9         1761.3           C.5         H.8         450.7         1065.3         1333.1         1761.8         2827.1         2950.0         H.9         C.5         H.8         360.8         1393.1         1597.9         1761.           C.5         H.9         450.7         1065.3         1393.1         1761.8         2827.1         2950.0         H.9         C.5         H.8         392.4         1188.2         1311.           C.5         H.10         450.7         1065.3         1393.1         1761.8         2827.1         2950.0         H.9         C.5         H.9         368.8         1393.1         1597.9         1761.           C.5         1597.9         1761.8         2827.1         2950.0         H.10         C.5         568.8         1393.1         1597.9         1761.           C.5         1597.9         1761.8         2827.1         2950.0         H.10         C.5         1391.9		N,12	H,6	737.5	942.4	1352.1	1434.1	1720.9		9'H	N,12	9'H	368.8	1393.1	1597.9	1761.8	1884.7	
C.5         H.8         450.7         1065.3         133.1         1761.8         282.7.1         2950.0         H.8         568.8         1333.1         1597.9         1761.3           C.5         C.5         1957.9         1761.8         282.7.1         2950.0         H.9         568.8         1393.1         1597.9         1761.           C.5         1950.7         1065.3         1393.1         1761.8         2827.1         2950.0         H.9         568         1393.1         1597.9         1761.           C.5         1957.9         1761.8         2827.1         2950.0         H.9         568         1393.1         1597.9         1761.           C.5         1597.9         1761.8         2827.1         2950.0         H.10         C.5         H.9         368.8         1393.1         1597.9         1761.           C.5         1597.9         1761.8         2827.1         2950.0         H.10         C.5         1761.8         1761.8           C.5         1741         1882         1333.1         1597.9         1761.8         231.1         1761.8         1761.8           C.4         0.11         100.3         1332.1         1587.9         1761.8 <t< td=""><td></td><td>C.4</td><td>N,12 H,7 C,4</td><td>1597.9 655.6 1597.9</td><td>1761.8 1065.3 1761.8</td><td>1352.1</td><td></td><td></td><td></td><td>Н.7</td><td>C,4</td><td>N.12 H.7 C.4</td><td>368.8 655.6 368.8</td><td>942.4 1065.3 942.4</td><td>1188.2 1352.1 1188.2</td><td>1311.1 1311.1</td><td></td><td></td></t<>		C.4	N,12 H,7 C,4	1597.9 655.6 1597.9	1761.8 1065.3 1761.8	1352.1				Н.7	C,4	N.12 H.7 C.4	368.8 655.6 368.8	942.4 1065.3 942.4	1188.2 1352.1 1188.2	1311.1 1311.1		
C.5         H.9         450.7         1065.3         1393.1         1761.8         2827.1         2950.0         H.9         C.5         H.9         368.8         1393.1         1597.9         1761.8           C.5         1597.9         1761.8         2827.1         2950.0         H.10         C.5         1597.9         1761.8         1393.1         1597.9         1761.8           C.5         1597.9         1761.8         2827.1         2950.0         H.10         C.5         1597.9         1761.8           C.1         1053         1761.8         2827.1         2950.0         H.10         C.5         167.9         1761.           C.1         N11         491.7         1229.2         1393.1         1597.9         1761.8         267.1         268.8         333.1         1597.9         1761.           C.4         N.11         409.7         655.6         1024.3         1188.2         1761.8         764         1188.2         1761.8           C.1         491.7         12292         1393.1         1597.9         1761.8         764         1188.2         1761.9           C.1         1106.3         1555.6         17209.0         2130.6         1761.8 <t< td=""><td>_</td><td>C.5</td><td>H.8 C.5</td><td>450.7 1597.9</td><td>1065.3 1761.8</td><td>1393.1</td><td>1761.8</td><td>2827.1</td><td>2950.0</td><td>Н.8</td><td>C.5</td><td>H.8 C.5</td><td>368.8 368.8</td><td>1393.1 942.4</td><td>1597.9 1188.2</td><td>1761.8 1311.1</td><td>1884.7</td><td></td></t<>	_	C.5	H.8 C.5	450.7 1597.9	1065.3 1761.8	1393.1	1761.8	2827.1	2950.0	Н.8	C.5	H.8 C.5	368.8 368.8	1393.1 942.4	1597.9 1188.2	1761.8 1311.1	1884.7	
C.5         H,10         450.7         1065.3         1393.1         1761.8         2827.1         2950.0         H,10         56.8         1393.1         1597.9         1761.           C.1         1166.3         1352.1         1516.0         1720.0         1701.0         56.8         1393.1         1597.9         1761.           C.1         N.11         1106.3         1352.1         1516.0         1720.0         2130.1         1597.9         1761.           C.4         N.11         409.7         655.6         1024.3         1188.2         1761.8         7.1         368.8         333.1         1597.9         1761.           C.4         N,11         409.7         655.6         1024.3         1188.2         1761.8         7.1         368.8         333.1         1597.9         1761.           C.1         N,12         106.3         1555.6         1024.3         1188.2         7.4         1188.2         1331.1         1597.9         1761.           C.1         N,12         106.3         1555.6         1024.3         1188.2         1331.1         1597.9         1761.           C.1         N,12         106.3         1556.6         1074.3         1188.2		C.5	H.9 C.5	450.7 1597.9	1065.3 1761.8	1393.1	1761.8	2827.1	2950.0	6'H	C.5	H.9 C.5	368.8 1597.9	1393.1 1761.8	1597.9	1761.8	1884.7	
C.1       N.11       1106.3       1352.1       1516.0       17209.0       2130.6       N.11       C.1       N.11       368.8       1393.1       1597.9       1761.         C.4       N.11       1106.3       1352.1       1516.0       17209.0       2130.6       1761.8       1311       1597.9       1761.3       368.8       1393.1       1597.9       1761.3         C.4       N.11       655.6       1024.3       1597.9       1761.8       C.1       368.8       1393.1       1597.9       1761.3         C.1       N.12       1106.3       1352.1       1516.0       17209.0       2130.6       1761.8       C.1       368.8       1393.1       1597.9       1761.3         C.1       N.12       I.1       C.1       N.12       C.1       N.12       S.1       1679.9       1761.3         C.1       N.12       I.1       S.2       1361.6       17209.0       2130.6       1761.8       1761.3       1782.3       1761.3       1761.3       1761.3       1761.3       1761.3       1761.3       1761.3       1761.3       1761.3       1761.3       1761.3       1761.3       1761.3       1761.3       1761.3       1761.3       1761.3       1761.3 <td></td> <td>C,5</td> <td>H,10 C,5</td> <td>450.7 1597.9</td> <td>1065.3 1761.8</td> <td>1393.1</td> <td>1761.8</td> <td>2827.1</td> <td>2950.0</td> <td>H,10</td> <td>C,5</td> <td>H,10 C,5</td> <td><mark>368.8</mark> 368.8</td> <td>1393.1 942.4</td> <td>1597.9 1188.2</td> <td>1761.8 1311.1</td> <td>1884.7</td> <td></td>		C,5	H,10 C,5	450.7 1597.9	1065.3 1761.8	1393.1	1761.8	2827.1	2950.0	H,10	C,5	H,10 C,5	<mark>368.8</mark> 368.8	1393.1 942.4	1597.9 1188.2	1761.8 1311.1	1884.7	
C,1         491.7         1229.2         1333.1         1597.9         1679.8         1761.8         C,1         368.8         942.4         1188.2         1311.           C,4         N,11         490.7         655.6         1024.3         1188.2         1597.9         1761.8         C,4         N,11         368.8         942.4         1188.2         1331.1         1597.9         1761.           C,1         N,12         190.7         655.6         1024.3         1188.2         1331.1         1597.9         1761.           C,1         N,12         190.3         155.0         1750.0         2130.6         N,12         C,4         N,11         368.8         942.4         1188.2         1761.           C,1         N,12         409.7         655.6         1024.3         1188.2         1761.		C,1	11,N	1106.3	1352.1	1516.0	17209.0	2130.6		N,11	C,1	N,11	368.8	1393.1	1597.9	1761.8	1884.7	
C,4         491.7         1229.2         1393.1         1597.9         1679.9         1761.8         54.4         1188.2         1311.1           C,1         N,12         1106.3         1352.1         1516.0         17209.0         2130.6         1761.8         1697.9         1761.8         1761.2         1697.9         1761.2         1761.2         1597.9         1761.2         1597.9         1761.2 <t< td=""><td></td><td>C.4</td><td>L'O'N</td><td>491.7 409.7</td><td>1229.2 655.6</td><td>1393.1 1024.3</td><td>1597.9 1188.2</td><td>1679.9</td><td>1761.8</td><td></td><td>C.4</td><td>L'O</td><td>368.8 368.8</td><td>942.4 1393.1</td><td>1188.2 1597.9</td><td>1311.1 1761.8</td><td>1884.7</td><td></td></t<>		C.4	L'O'N	491.7 409.7	1229.2 655.6	1393.1 1024.3	1597.9 1188.2	1679.9	1761.8		C.4	L'O	368.8 368.8	942.4 1393.1	1188.2 1597.9	1311.1 1761.8	1884.7	
C,1         N,12         1160.3         1557.1         1516.0         17209.0         2130.6         N,12         C,1         N,12         368.8         1333.1         1597.9         1761.           C,1         1597.9         1761.8         2130.6         1720.9         2130.6         1761.1         201.1         201.2         368.8         1333.1         1597.9         1761.1           C,2         N,12         409.7         655.6         1024.3         1188.2         2         1311.2         368.8         1393.1         1597.9         1761.1           C,1         0,13         1106.3         1720.9         1781.8         1188.2         1761.1         2         2         1371.1         1597.9         1761.1         1761.1         1597.9         1761.1         1761.1         1761.2         368.8         1393.1         1597.9         1761.1         1761.1         1761.2         1761.1         1761.2         1761.1         1761.1         1761.2         1761.1         1761.2         1761.1         1761.1         1761.1         1761.1         1761.1         1761.1         1761.1         1761.1         1761.1         1761.1         1761.1         1761.1         1761.1         1761.1         1761.1 <t< td=""><td></td><td></td><td>C,4</td><td>491.7</td><td>1229.2</td><td>1393.1</td><td>1597.9</td><td>1679.9</td><td>1761.8</td><td></td><td>ł</td><td>C,4</td><td>368.8</td><td>942.4</td><td>1188.2</td><td>1311.1</td><td></td><td></td></t<>			C,4	491.7	1229.2	1393.1	1597.9	1679.9	1761.8		ł	C,4	368.8	942.4	1188.2	1311.1		
C.2         N.12         409.7         655.6         1024.3         1188.2         7101           C.1         O.13         1106.3         1761.8         0.13         0.13         0.68.8         1393.1         1597.9         1761.4           C.1         O.13         1106.3         1720.9         1761.8         0.13         0.13         0.68.8         1393.1         1597.9         1761.4           C.1         O.13         1106.3         1720.9         1761.8         0.13         0.13         368.8         1393.1         1597.9         1761.4           C.1         O.13         1106.3         1720.9         1761.8         0.13         0.13         368.8         1393.1         1597.9         1761.7           C.1         O.13         368.8         107.4         1188.2         1761.7         0.14         1761.7		C,1	N,12	1106.3	1352.1 1761 8	1516.0	17209.0	2130.6		N,12	C,1	N,12	368.8 368.8	1393.1	1597.9 1188.2	1761.8	1884.7	
C.2         1597.9         1761.8         542.4         1188.2         1311.           C,1         O,13         1106.3         1720.9         1761.8         0,13         0,13         368.8         1393.1         1597.9         1761.           C,1         491.7         1516.0         1761.8         356.8         365.8         1393.1         1597.9         1761.           C         1         491.7         1516.0         1761.8         356.1         1786.2         1311.	_	C,2	N,12	409.7	655.6	1024.3	1188.2				C,2	N,12	368.8	1393.1	1597.9	1761.8	1884.7	
C,1 O,13 1106.3 1720.9 159.9 1761.8 0,13 C,1 O,13 368.8 1393.1 1597.9 1761. C,1 491.7 1516.0 1679.9 1761.8 1557 1775.0 1, C,1 368.8 942.4 1188.2 1311. C,1 400.7 1555.6 100.4 1761.9 1757 1775.0 1, C,1 366.8 1942.4 1188.2 1311.			C,2	1597.9	1761.8							C.2	368.8	942.4	1188.2	1311.1		
		Ċ,1	0,13	1106.3	1516.0	1670 0	1761 8			0,13	C,1	0,13	368.8 368.8	1393.1	1597.9	1761.8	1884.7	
0,14 403.7 0,14 403.7 033.0 1024.3 1100.2 1332.1 1413.0 0,14 0,14 0,14 000.0 1330.0 1330.1 1337.3 1101.		C,2	0,14	409.7	655.6	1024.3	1188.2	1352.1	1475.0	0,14	C,2	0,14	368.8	1393.1	1597.9	1761.8	1884.7	

Table 6. Frequencies of Thymine base bonds, highest intensities. Frequencies are in  $\rm cm^{-1}$ .

Column names for stretching (left columns) and bending (right columns) frequencies are in cm<sup>-1</sup> units and as follows:

Base, Atom & num., Bonding atom, Reference atom, 1st mode, 2nd mode, 3rd mode, 4th mode, 5th mode, 6th mode are shown in 2 sets of columns.

		5th peak			1 7 0 0	8.0211												8°/801	1507 0	8.1801	1507 0	2.122	1597.9																						1 5 0 7 0	8.1801		
		4th peak	1720.9		1/20.9	0.7661	1393.1	1720.9	1393.1	1720.9	1393.1	1720.9	1393.1	1720.9	1393.1	1720.9	1393.1	1434.1	1.050.1	12021	1434.1	1393.1	1434.1	1393.1	1720.9	1393.1	1720.9	1393.1	1720.9	1790 0	1393.1	1720.9	1393.1	1720.9	1393.1	1393.1	1720.9	1393.1	1720.9	1393.1	1393.1	1720.9	1393.1	1720.9	1393.1	13031	1720.9	1393.1
		3th peak	1597.9	1270.2	9.7861	15070	819.5	1597.9	819.5	1597.9	819.5	1597.9	819.5	1597.9	819.5	1597.9	6.918	0105	019.0	810 5	1147.9	819.5	1147.2	819.5	1597.9	819.5	1597.9	819.5	1597.9	15070	819.5	1597.9	819.5	1597.9	819.0	819.5	1597.9	819.5	1597.9	819.5	819.5	1597.9	819.5	1597.9	819.5	8105	1597.9	819.5
		2th peak	1147.2	819.5	114/.2	903.3 1117 9	655.6	1147.2	655.6	1147.2	655.6	1147.2	655.6	1147.2	655.6	1147.2	0.000	819.5	0.000	655 6	8105	655.6	819.5	655.6	1147.2	655.6	1147.2	655.6	1147.2	0.000	655.6	1147.2	655.6	1147.2	0.000	655.6	1147.2	655.6	1147.2	655.6	655.6	1147.2	655.6	1147.2	655.6	655.6	1147.2	655.6
	end	1th peak	819.5	573.6	819.5	0.000	573.6	819.5	573.6	819.5	573.6	819.5	573.6	819.5	573.6	819.5	0/3.0	0.000.0	013.0	673 B	655.6	573.6	655.6	573.6	819.5	573.6	819.5	573.6	819.5	0/3.0 810.5	573.6	819.5	573.6	819.5	0/3.0 010 E	573.6	819.5	573.6	819.5	5/3.6	573.6	819.5	573.6	819.5	573.6	673.6	819.5	573.6
	ق	Ref atom	491.7	327.8	491./	7 1 0	327.8	491.7	327.8	491.7	327.8	491.7	327.8	491.7	327.8	491.7	321.8	81.9	010	8 L 0 L 0	810	327.8	81.9	327.8	491.7	327.8	491.7	327.8	491.7	0.125 A017	327.8	491.7	327.8	491.7	321.8	327.8	491.7	327.8	491.7	327.8	327.8	491.7	327.8	491.7	327.8	2.07 g	491.7	327.8
		rsus atom F	C,1	C,2	C.1	2	N.13	C.2	C,1	C.2	C,3	C,2	N,12	C,3	C,2	C,3	N,10	C.3	† •	N 10	1	N.12	C.5	N,13	C,5	N.14	9'H	N,11	H.7	, a	2 2	6, H	C,4	N,10	5°.0	0.4	N,11	C,1	N,12	C,2 M 13	0.4	N.13	C,1	N,13	C.5	* °	N.14	C,5
Ŧ		& num Vei	C,2		=	1 3	2	C.1		C.3		1,12		C,2		1,10		,14			1.0	-	1.13		1,14		E,		<u> </u>	2	2	C,4	_	C3		t	C,1		C,2		r.	C,1		C,5		¢.	C.5	
of [cm		atom				2						2				2			-		~	-	2		2		~						_															
unit o		base	C,1					C.2						C,3						* 5			C.5				9'H		Н,7	п	-	6' Н		N,10			11,N		N,12			N.13				2		
inate		6th peak			1/20.9		1557.0		1884.8						1884.8		1884.8	1004 0	0.4.0	1884 8		1884 8		1884.8	1557.0	1884.8	1720.9	1884.8	1720.9	1790.0	1884.8	1679.9	1884.8		1670.0	1884.8		1884.8		1834.8	1884.8		1557.0	1720.9	1557.0	1557 0	1720.9	1557.0
Coord		5th peak	2171.7	1884.8	1393.1	1 2 0 2 1	1434.1		1597.9		1597.9	1393.1	1597.9	2171.7	1597.9	1597.9	6.1861	0.7031	1231.3	15070	13031	1597.9	1393.1	1597.9	1270.2	1597.9	1393.1	1597.9	1393.1	15070	1597.9	1393.1	1597.9		6./801	1597.9	1884.8	1557.0	1884.8	1557.0	1557.0		1434.1	1597.9	1434.1	14341	1597.9	1434.1
action		4th peak	1884.8	1597.9	819.5	0.7661	819.5		1393.1		1393.1	1270.2	1393.1	1884.8	1393.1	1311.1	1393.1	114/.2	10201	1 2 0 2 1	1.970.9	1393.1	1147.2	1393.1	1147.2	1393.1	819.5	1393.1	819.5	1 2 0 2 1	1393.1	1106.3	1393.1		1106.0	1393.1	1557.0	1393.1	1557.0	1393.1	1393.1		819.5	1393.1	819.5	8105	1393.1	819.5
Re		3th peak	1557.0	1393.1	0.0001	002.2	655.6	1557.0	1147.2	1557.0	1147.2	1147.2	1147.2	1557.0	1147.2	1147.2	114/.2	819.5	2.1411	1147 9	2.1711	1147.9	983.3	1147.2	819.5	1147.2	6.5.5.6	1147.2	655.6	7785	1147.2	819.5	1147.2	1557.0	010 5	1147.2	1393.1	655.6	1393.1	655.6 010.5	655.6	1557.0	655.6	819.5	655.6 1 E E 7 A	655.6	819.5	655.6
	rech	2th peak	1106.3	655.6	532.6 e e e e	01050	368.8	1393.1	655.6	1393.1	655.6	778.5	655.6	1106.3	655.6	819.5	0.000	614.0 665.6	01010	8 5 5 8	778.5	655.6	819.5	655.6	614.6	655.6	532.6	655.6	532.6	0.000 614 6	655.6	614.6	655.6	1393.1	0.000	655.6	614.6	491.7	614.6	491.7 614.6	491.7	1393.1	368.8	614.6	368.8	368.8	614.6	368.8
	st	1th peak	532.6	532.6	321.8	431.1 535 8	81.9	532.6	532.6	532.6	532.6	327.8	532.6	532.6	532.6	532.6	0.32.0	491./	0.700	0.700 529.6	327.8	532.6	532.6	532.6	491.7	532.6	327.8	532.6	327.8	7 104	532.6	327.8	532.6	532.6	0.32.0	532.6	532.6	327.8	532.6	327.8	327.8	532.6	81.9	491.7	81.9	81 0	491.7	81.9
		Ref atom	C,1	C,2	C.1	2	N.13	C.2	C,1	C.2	C,3	C,2	N,12	C,3	C,2	C,3	N,10	C'3		M 10	0.4	N.12	C.5	N.13	C,5	N.14	9'H	11'N	H.1	Z A	9 0	6, H	C.4	N,10	5 °	0.4	N,11	C,1	N,12	C,2	0.4	N.13	C,1	N,13	C.5	* °	N.14	C.5
		Versus atom F	C,2		I.	N 13	2	C.1		C.3		N,12		C,2		N,10	:	N.14	M 10	2	N 12	41.1	N.13		N.14		N,11	:	11.N	5	2	C.4		C 3		t. D	C,1		C,2	č	r. D	C.1		C,5	ç	°. 5	C.5	
		atom & num 1	C.1					C.2						C.3						†.			C.5				9°H		Н.7	a I	2	6'H		N.10			N.11		N,12			N.13				†  2		
		base	ADE																																													

Table 7. Frequencies of Adenine base bonds, highest intensities. Frequencies are in cm<sup>-1</sup> .

		5th peak																																												
		4th peak																																												
		3th peak	1679.9	1229.2	1679.9	1270.2	10/9.9	1679.9	1270.2	1679.9	1270.2	1679.9	1270.2	1679.9	2.0121	8.8/01 1970.9	1670.0	1270.2	1679.9	1270.2	1679.9	1270.2	16/9.9	12/0.2	1270.2	1679.9	1270.2	1679.9	1679.9	1270.2	1679.9	1679.9	1270.2	1679.9	1270.2	1270.2	1679.9	1270.2	01010	1679.9	1270.2	1679.9	12/0.2	1270.2	1270.2	1679.9 1270.2
		2th peak	1557.0	737.5	1557.0	860.4	0./661	1557 0	860.4	1557.0	860.4	1557.0	860.4	1557.0	800.4	0./ C C I	1557 0	860.4	1557.0	860.4	1557.0	860.4	0./661	860.4	860.4	1557.0	860.4	1557.0	1557.0	860.4	1557.0 860.4	1557.0	860.4	1557.0	860.4	860.4	1557.0	860.4	0./001	1557.0	860.4	1557.0	860.4 1557.0	860.4 1557.0	860.4	1557.0 860.4
	end	1th peak	614.6	614.6	614.6	737.5	014.0 727 5	614.6	737.5	614.6	737.5	614.6	737.5	614.6	0.151	0   4.0 727 5	614 G	737.5	614.6	737.5	614.6	737.5	614.6	131.5 614.6	737.5	614.6	737.5	614.6 797 E	614.6	737.5	614.6 737 5	614.6	737.5	614.6	737.5 614 6	737.5	614.6	737.5	014.0 727.5	614.6	737.5	614.6	614.6	737.5 614.6	737.5	614.6 737.5
	-	Ref atom	368.8	327.8	368.8	614.6	308.8	368.8	614.6	368.8	614.6	368.8	614.6	368.8	0.4.0	308.8 614.6	2,62,0	614.6	368.8	614.6	368.8	614.6	368.8	262.8	614.6	368.8	614.6	368.8	368.8	614.6	368.8 614.6	368.8	614.6	368.8	614.6 368.8	614.6	368.8	614.6	308.8	368.8	614.6	368.8	614.6 368.8	614.6 368.8	614.6	368.8 614.6
		ersus atom	C,1	C,3	C,1	N,12	G,2 M 11		N.12	C.2	N.14	C, 3	C,1	C'3	4 0 0	C,3 N 13	2.0	t 0	C.4	N,10	C,4	N,14	C.5	N,10	N.13	9'H	N,12	Н.7	8 H	N,11	6 H O	N.10	C,4	N,10	C.5	C.2	N,12	0'1	N,12	N,13	C,3	N,13	0.5 N,14	C.2 N.14	C.4	0,15 C,1
m – 1]		atom & num /	C,3		N,12		11.N	N 12		N.14		C,1		C ,4		N,13	6.0	2	N.10		N.14		01,N	N 12		N.12		N,11	N.11		C.5	C.4		C.5	6 0	4	C.1	0	C,2	C.3		C.5	C,2	C.4		C,1
<u>nit of [c</u>		base	C,1				C,2					C ,3						r.					¢,5			9'H		Н,7	H.8		6' H	N.10			N 11		N,12			N.13			N,14			0,15
nate ur		6th peak	2048.6	1638.9		1557.0	1557 0	0.1001	1557.0	2253.5	1557.0	1802.8	1557.0		0.1001	1557 0	0.100	1557.0		1557.0		1557.0		0./661	1557.0		1557.0	1667.0	0.100	1557.0	1557.0	0.100	1557.0		1557.0	1557.0		1557.0	1557 0	0.100	1557.0		0./661	1557.0	1557.0	
Coordir		5th peak	1352.1	1557.0		1352.1	1959 1	1.2001	1352.1	1638.9	1352.1	1638.9	1352.1	2253.5	1.302.1	13591	1188.9	1352.1		1352.1		1352.1		1352.1	1352.1		1352.1	1311.1	1311.1	1352.1	1679.9	2253.5	1352.1	1679.9	1352.1	1352.1	1802.8	1352.1	1 / 61.8	1352.1	1352.1	1679.9	1352.1	1352.1	1352.1	1638.9
iction (		4th peak	1188.2	1352.1		1229.2	1311.1	7.8221	1229.2	1188.2	1229.2	1516.0	1188.2	1638.9	2.8811	1188.2	1106.1	1188.2		1188.2		1188.2		1188.2	1188.2		1188.2	860.4	860.4	1188.2	1557.0	1638.9	1188.2	1557.0	1188.2	1188.2	1638.9	1229.2	0./001	1188.2	1229.2	1557.0	1557.0	1229.2	1229.2	1516.0
Rea		3th peak	1106.3	1188.2	983.3	778.5	860.4 770 F	983.3	778.5	983.3	778.5	1352.1	860.4	1557.0	800.4	860.4	1.000	860.4	1229.2	860.4	983.3	860.4	1229.2	860.4	860.4	983.3	860.4	778.5	778.5	860.4	1229.2 860 4	1557.0	860.4	1229.2	860.4	860.4	1516.0	778.5	779.5	1106.3	778.5	1229.2	1/18.5	778.5	778.5	1352.1
	crech	2th peak	860.4	860.4	860.4	614.6	5/3.0 614.6	860.4	614.6	860.4	614.6	901.4	778.5	860.4	0.811	8 1 9 . 0 7 7 8 5	572.6	778.5	860.4	778.5	860.4	778.5	860.4	1/8.5 810 5	778.5	860.4	778.5	573.6 770 c	573.6	778.5	860.4 778 5	860.4	778.5	860.4	178.5	778.5	1352.1	614.6	614.6	860.4	614.6	860.4	614.6 1188.2	614.6 860.4	614.6	737.5 614.6
	S.	1th peak	737.5	614.6	532.6	81.9	450./	532.6	81.9	573.6	81.9	614.6	614.6	737.5	0.4.0	614.6	0.710	614.6	737.5	614.6	573.6	614.6	131.5	614.6 7275	614.6	532.6	614.6	450.7	450.7	614.6	737.5 614.6	737.5	614.6	737.5	614.6 522.6	614.6	614.6	81.9	0.32.0	737.5	81.9	737.5	81.9 532.6	81.9 737.5	81.9	614.6 368.8
		Ref atom	C,1	C.3	C,1	N,12	G,2	C 0	N.12	C.2	N.14	C.3	c.1	0'3	+ c	C.3	2.0		C.4	N,10	C,4	N,14	C.5	N,10	N.13	9'H	N,12	1.H	8 H	11,N	6'H	N.10	C ,4	N,10	0'2 N 11	0.2	N,12	C.1	N,12	N,13	C.3	N,13	0.5 N,14	C.2 N.14	C.4	0,15 C,1
		Versus atom	C,3		N,12		LI.N	N 12	4	N.14		C,1		C ,4		N, I &		2, 2	N.10		N,14	:	N,10	N 12		N.12		N,11	N.11		C,5	C.4		C,5	° 0	4	C,1		C,2	C ,3		C,5	C,2	0.4		C,1
		atom & num	C,1				C,2					C,3						t,					c,5			9'H		Н,7	H.8		6' H	N.10			N 11		N,12			N.13			N,14			0,15
		base	GUA																																											

Table 8. Frequencies of Guanine base bonds, highest intensities. Frequencies are in cm<sup>-1</sup> .

				stretch	[cm <sup>-1</sup> ]								st	retch [cm <sup>-1</sup>	ני			
base	atom	Versus	Ref.	1 <sup>st</sup>	2 <sup>nd</sup>	3 <sup>rd</sup>	4 <sup>th</sup>	5 <sup>th</sup>	6 <sup>th</sup>	atom	Versus	Ref.	1 <sup>st</sup>	2 <sup>nd</sup>	3 <sup>rd</sup>	4 <sup>th</sup>	5 <sup>th</sup>	6 <sup>th</sup>
	&	atom	atom	peak	peak	peak	peak	peak	peak	&	atom	atom	peak	peak	peak	peak	peak	peak
	num									num								

bend atom & num Versus atori Ref atom 11th peak 2th peak 3th peak 4th peak 5th peak

strech atom & num Versus atom | Ref atom | 1th peak | 2th peak | 3th peak | 5th peak | 6th peak