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Molecular vibration of dopamine neurotransmitter: a relation between its normal modes

and harmonic notes

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ABSTRACT

Dopamine (3, 4-dihydroxyphenethylamine) is an important compound in the human brain for sending signals to other nerve cells. Dopamine plays major roles in controlling, motivation, arousal, reinforcement, and reward in the brain. Lactation, sexual gratification, and nausea are also results of dopamine pathways. In this study the normal modes analysis of dopamine has been exhibited for understanding their relation between those dopamine structure and harmonic notes. This work demonstrated details of the musical conversion of molecular vibrational based on normal modes analysis of dopamine. The normal modes can be mapped to a spectrum in the audible frequencies ranges, and it can also be mapped to musically useful parameters. **Keywords:** *dopamine; normal modes; harmonic notes.*

1. INTRODUCTION

In the past decades, several attempts have been done for converting the molecular specifics to acoustic and musical behavior. Axen and coworkers in 1996 used a pattern of acoustic conversion due to sonic phenomenon at time coordinates dependent on coordinates of cells [1]. Moreover, nucleic acids linkages of DNA have been converted into sonic musical notes via using a simple coding of DNA bases [2-5]. In another work, a method illustrated through acoustically converting mass-current oscillations based on the coherent quantum oscillations among the Helium atoms [6]. Based on converting of some molecular specifics such as frequency, amplitude and duration into sound dimensions the field of Sonification has been investigated by Albers 1994, Walker and Kramer 1996 [7, 8]. Although this method is applied for several other physical phenomena by Lunney and Foner, it has been reclaimed with analytical chemistry applications by Yeung and Frysinger in field of Sonification [9-12]. Electromagnetic ray's Sonification (such as infrared electromagnetic) is also a wonderful origin of musical acoustic which can be exhibited via spectral elements of light emitted [12, 13]. Based on base absorption band in DNA a vertical line corresponds to the central frequency of the band has been assigned, while the transposition of this frequency into the acoustic range produces a micro-tonality characteristic of the specific base. With this phenomenon a musical scales related to the DNA bases has been assigned and converted by Alexander, Lunney and Morrison [9-17]. Although the lines were subsequently depend to the notes of the chromatic scales, the data of an entire infrared spectrum being mapped into several octaves. In 1992, McMillan and coworkers [18] applied a neural network for the musical conversion of IR spectrum which the sound was applied for playing the acoustic foundation. In whether scientific and musical objectives necessitate different approaches to Sonification, or whether the same mapping can sometimes be useful for both. Non-scientist musicians may not understand that

molecules oscillate and play music under various conditions. In other words due to a very fast vibrate of the atoms in molecules that are orders of a large magnitude faster than acoustic vibrations cannot be possible to hear these frequencies physically. But, it is wondering how the vibrations would sound if mapped into the acoustic region. This perspective is become more amazing by the fact which each kind of molecules even each chemical reaction has a specific spectrum in a wide region. In any modeling of molecular properties towards musical Sonification any vibrations might be matched to the melodies, rhythms, pitch or duration of acoustic. This work demonstrated details of the musical conversion of molecular vibrational based on normal modes analysis. The normal modes can be mapped to a spectrum in the audible frequencies ranges, and it can also be mapped to musically useful parameters. In this study, a piece of music is considered to be a combination of elementary normal modes and depending on the time scale, the nature of the musical parameter, and the implementation, may be discrete or continuous including short or long durations. In the brain, dopamine (scheme 1) functions as an important neurotransmitter compounds released by nerve cells which are known as neurons for sending signals to adjacent nerve cells. Human brains have various pathways for distinct dopamine, for example one of which has a main role in the motivational components of reward-motivated behavior which increases the level of dopamine in the brain [19], and many addictive drugs increase dopamine release or block its reuptake into neurons following release. Other brain's dopamine pathway is consisting of motor control and for releasing of several hormones and this pathway of dopamine system is neuron- modulatory. Although dopamine is often known as the main chemical of pleasure, the current belief in pharmacologist is that dopamine confers motivational salience [20-23]. Dopamine signals the perceived motivational preferences such as musical notes of an outcome that in turn propels the organism's behavior toward that

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outcome [23]. Various diseases of the nervous are associated with invalidism of the dopamine system such as Parkinson's disease that is caused by a loss of dopamine-secreting neurons. There is strong witness that schizophrenia involves altered levels of dopamine activities, therefore dopamine as antipsychotic drug can be used for treating this kind disease.



Scheme 1. Dopamine optimized structure.

1.1. Normal modes

In the classical movement of various vibrations, the normal modes are defined as a simple harmonic oscillator including; symmetric stretching, asymmetric stretching bending and improper, The total rules based on normal modes are suitable for musical Sonification of any vibrations which matched to the melodies, rhythms, pitch or duration of acoustic. The basic principles are abstracted as; (1) acts like a simple harmonic oscillator, (2) is a concerted motion of many atoms, (3) the center of mass doesn't move, (4) all atoms pass through their equilibrium positions at the same time and (5) Normal modes are independent without any interaction and are estimated using Newton's rule of motion. $\frac{d^2x}{dt^2} = -4\pi^2 \vartheta^2 X$ And m. $\frac{d^2 X}{dt^2} = -kX \rightarrow -4\pi^2 \vartheta^2 mX = -kX$ is the basis for the classical calculation of the normal modes of a molecule. Based on Wilson method [FG-\lambdaI]=0, F is a Matrix of force constants due to potential energies and G is a matrix involves masses and certain spatial relationships of the atoms due to kinetic energies. "I" is a unit matrix and λ is related to the frequency $\lambda = 4\pi^2 \vartheta^2 C^2$. As for instance for H₂O in C_{2v} character table the Γ_{3N} consists of E=9, $C_2=-1$, $\sigma_v(xz)=3$ and $\sigma_v(yz)=1$ which can be reduced to $\Gamma_{3N} = 3A_1 + A_2 + 3B_1 + 2B_2$ and $A_1 + A_2 + 2B_1 + 2B_2$ are belong to translation and rotation accounts, while 2A1+ B1 belongs to the vibrational modes. Displacements of the internal coordinates including O-H (Δd_1 and Δd_2) distances and HOH angle ($\Delta \theta$) are bases for the irreducible representation $(\Delta d_1, \Delta d_2) = A_1 + B_1$ and $\Delta \theta = A_1$. Applying projection operators to only one of the member of Δd_1 or Δd_2 yields: $\hat{p}^{A_1} \Delta d_1 = \{(1)\hat{E} + (1)\hat{C}_2 + (1)\hat{\sigma}_v(xz) + (1)\}$ $\hat{\sigma}_{\nu}(yz)$ $\Delta d_1 = \Delta d_1 + \Delta d_2$ and $\hat{p}^{B_1} \Delta d_1 = \Delta d_1 - \Delta d_2$. Consequently symmetry coordinates for vibrations are $A_1 = \{S_1 = \Delta \theta \text{ and } S_2 =$ $\frac{1}{\sqrt{2}}(\Delta d_1 + \Delta d_2)$ and $B_1 = \{S_3 = \frac{1}{\sqrt{2}}(\Delta d_1 - \Delta d_2)\}$ and $\frac{1}{\sqrt{2}}$ is the normalized factor to constitute an orthogonal set $(\Delta d_i \Delta d_j = \delta_{ij})$.

The potential energies can be written as $2V = \sum_{i,k} f_{ik} s_i s_k$ $(f_{ik} = force \ constants)$ (1), therefore for H₂O there are three internal coordinates and hence nine force constants including **Matrix**: $\Delta \mathbf{d_1} \quad \Delta \mathbf{d_2} \quad \Delta \boldsymbol{\theta}$

$$\Delta \mathbf{d_1} \quad f_d \qquad f_{dd} \quad f_{d\theta} \quad \text{where the force constants for (O-H)} \\ \Delta \mathbf{d_2} \quad f_{dd} \qquad f_d \quad f_{d\theta} \quad \text{where the force constants for (O-H)} \\ \Delta \boldsymbol{\theta} \quad f_{d\theta} \qquad f_{d\theta} \qquad f_{\theta} \quad f$$

stretching, (HOH)bending and interaction of one bond stretch to other bond stretch or angle bending are f_d , f_{θ} , f_{dd} and $f_{d\theta}$ respectively. Therefore the equation (1) can be written as: $2V = f_d(\Delta d_1)^2 + f_d(\Delta d_2)^2 + f_{\theta}(\Delta \theta)^2 + 2f_{dd}(\Delta d_1\Delta d_2) + 2f_{d\theta}(\Delta d_1\Delta \theta) + 2f_{d\theta}(\Delta d_2\Delta \theta) = \sum_{i,j} F_{ij} s_i s_j$

Here the F_{ij} are force constants described by symmetry coordinates of s_i and s_j which provides the easiest routs due to secular equations as 2v=s'fs or 2V=S'FS and it is also to find the relationship between internal coordinates and symmetry coordinates as: S=Us which U Matrix is defined as **UMatrix**: $\Delta d_1 \quad \Delta d_2 \quad \Delta \theta$

U' is the inverse matrix of U therefore $s=U^{-1}S=U'S$ and s' = (U'S)' = S'U and also it can be easily proved that UfU' = F and by transforming f matrix into F the F Matrix is :

 $\begin{array}{ccc} f_{\theta} & \sqrt{2}f_{d\theta} & 0 \\ \sqrt{2}f_{d\theta} & f_d + f_{dd} & 0 \\ 0 & 0 & f_d - f_{dd} \end{array}$ The G Matrix can also be calculated

from UgU' = G

For finding a function of Eigen-vectors converting as a specific irreducible representation, the projection operator might be used in the related group theories and character tables. "F" is defined as an arbitrary function which can be expanded into various irreducible representations $F = \sum_{\alpha} \sum_{n} c_{\alpha}^{n} \xi_{\alpha}^{n}$ where α denotes the irreducible representation $\operatorname{and} c_{\alpha}^{n}$, ξ_{α}^{n} are the coefficients of the expansion and functions transforming according to the representation α , respectively. Therefore the projection operators " \hat{P} " presented as: $\hat{p}_{l(n)}^{\beta} = \frac{d_{\beta}}{g} \sum_{G} D_{l(n)}^{\beta} (G *)(G)$. In this equation d_{β} is degeneracy of irreducible representation of β and g is the symmetry order of group and G is the symmetrical operators operations for each l(n) element of $D(\beta)$ character table.

1.2. Projection Operators

From a given irreducible presentation, the functions can be produced along the irreducible presentation. In the orthonormal set L(i) of the functions including φ_1^i , φ_2^i , φ_3^i , ..., φ_L^i which is applied for forming the $i_{\rm th}$ irreducible representation of a group by order h, for the operators, \hat{R} , which defined as $\hat{R}\varphi_t^i = \sum_s \varphi_s^i \Gamma(R)_{st}^i$ (1), the multiply of this equation by $[\Gamma(R)_{s't'}^{i}]^*$ and a summation over the symmetrical function it can be written as $\sum_{R} [\Gamma(R)_{s't'}^{i}]^* \widehat{R} \varphi_t^{i}$ $= \sum_{R} \sum_{S} \Gamma \varphi_{S}^{i} \Gamma(R)_{st}^{i} \Gamma(R)_{s't'}^{i} = (2) \text{ Considering are functions}$ independent from R, the right side of the equation can be rewritten as: $\sum_{s} \varphi_{s}^{i} \sum_{R} [\Gamma(R)_{st}^{i} \Gamma(R)_{s't'}^{i}]^{*}$. So we have a series of L (i) terms with production of φ_s^i and coefficient of α . These coefficients are obey of orthogonally function: $\sum_{R} \left[\Gamma(\mathbf{R})_{st}^{i} \Gamma(\mathbf{R})_{s't'}^{i} \right] *= \left(\frac{h}{L_{i}L_{i}} \right)^{1/2} \delta_{ij} \delta_{ss'} \delta_{tt'} \quad (3) \text{ via using the}$ equation (3) the equation (2) will be simplified as follows: $\sum_{R} \left[\Gamma(R)_{s't'}^{i} \right] * \widehat{R} \varphi_{t}^{i} = \left(\frac{h}{L_{i}} \right) \varphi_{is'} \delta_{ij} \delta_{tt'} \quad (4) \text{ let us define the}$ projection operator as follows $\hat{P}_{s't'}^{j} = \frac{L_{j}}{h} \sum_{R} [\Gamma(R)_{st}^{i} \Gamma(R)_{s't'}^{i}] * \hat{R}$ (5) which yields $\hat{P}_{s't'}^{j} \varphi_{t}^{i} = \varphi_{is'} \delta_{ij} \delta_{tt'}$ (6). The application of the projection operator is projecting function φ_{t}^{i} from any function φ_{t}^{i} . In other words $\hat{P}_{t''t'}^{j} \varphi_{t}^{i} = \varphi_{t'} \delta_{ij} \delta_{tt'}$ (7). Through using projection operator linear combination of normal modes can be

2. MATERIALS AND METHODS

2.1. Wilson methods on dopamine.

In this work the Urey-Bradley force field has been applied and the calculation of normal mode frequencies have been done according to GF Wilson matrix. By this method F Matrix for dopamine has been calculated via UfU' = F transformation and G matrix or inverse kinetic energy matrix for dopamine has been estimated by the equation as follows: $G_{KL} = \sum_{i=1}^{66} B_{ki} B_{il} / m_i (k, l = 1, \dots, 3n - 1)$ 6) where m_i is the mass of the ith atom. The kinetic energy is given by: R'GR = 2T and R'FR = 2V which R' is transposing of *R*. The secular equation can be written as $[FG-\lambda I] = 0$ where the frequency $\lambda = 4\pi^2 \vartheta^2 C^2$ and the normal coordinate Q is related to the internal coordinate R with the equation R=LQ. And normal mode Q_k is described through the elements of the eigenvector L_k belonging to λ_k . The potential energy distribution helps for finding any coupling of normal modes which can be estimated with projection operator. Potential energy of Kth normal modes associating with ith internal coordinates can be written as: $PE_i^k =$ $\frac{L_{ik}^2 F_{ik}}{L_{ik}}$ Dopamine has 22 atoms or 3N-6=60 modes and the frequencies of these normal modes have been calculated with Wilson GF matrixes. Each assignment can be exhibited based on PED, line intensity and its group theory. Refined force constants and internal coordinate are listed in Table 1.

No	Internal	No	Internal	No	Internal	
	coordinate		coordinate		coordinate	
1	$\vartheta(\mathcal{C}_8\mathcal{O}_9)$	21	$\vartheta \left(O_9 H_{20} \right)$	41	$\vartheta[0.5(7+8)]$	
2	$\vartheta \overline{(C_6 O_7)}$	22	$\vartheta (O_7 H_{19})$	42	$\vartheta[0.5(12+13)]$	
3	$\vartheta(C_4C_5)$	23	$\emptyset(\overline{C_{10}C_{11}C_4})$	43	$\vartheta[0.5(12 - 13)]$	
4	$\vartheta(\mathcal{C}_5\mathcal{C}_6)$	24	$\phi(\overline{C_{11}C_4C_5})$	44	$\vartheta[0.5(21+22)]$	
5	$\vartheta(C_6\overline{C_8})$	25	$\phi(C_4C_5C_6)$	45	$\vartheta[0.5(21-22)]$	
6	$\vartheta (C_8 C_{10})$	26	$\phi(\overline{C_5C_6C_8})$	46	$\emptyset[0.5(23+24)]$	
7	$\vartheta(\mathcal{C}_{10}\mathcal{C}_{11})$	27	$\emptyset(C_6C_8C_{10})$	47	$\emptyset[0.5(24+25)]$	
8	$\vartheta(\mathcal{C}_{11}\mathcal{C}_4)$	28	$\phi(\overline{O_9C_8C_6})$	48	Ø[0.5(25 + 26)]	
9	$\vartheta(\mathcal{C}_4\mathcal{C}_3)$	29	$\phi(\overline{O_9C_8C_{10}})$	49	Ø[0.5(26 + 27)]	
10	$\vartheta(\mathcal{C}_3\overline{\mathcal{C}_2})$	30	$\phi(O_7C_6C_8)$	50	$\emptyset[0.5(28+29)]$	
11	$\vartheta(C_2N_1)$	31	$\phi(\overline{O_7C_6C_5})$	51	Ø[0.5(28 – 29)]	
12	$\vartheta(N_1H_{12})$	32	$\emptyset(\mathcal{C}_{11}\mathcal{C}_4\mathcal{C}_3)$	52	$\emptyset[0.5(30+31)]$	
13	$\vartheta (N_1 H_{13})$	33	$\emptyset(\overline{C_5C_4C_3})$	53	Ø[0.5(30 – 31)]	
14	$\vartheta(C_2H_{14})$	34	$\phi(C_4C_3C_2)$	54	$\emptyset[0.5(32+33)]$	
15	$\vartheta(C_2H_{15})$	35	$\phi(C_3C_2N_1)$	55	$\emptyset[0.5(33+34)]$	
16	$\vartheta(C_3H_{16})$	36	$\vartheta[0.5(1+2)]$	56	$\emptyset[0.5(34+35)]$	
17	$\vartheta(C_3H_{17})$	37	$\vartheta[0.5(2+3)]$	57	$\emptyset[0.5(14+15)]$	
18	$\vartheta(C_{11}H_{22})$	38	$\vartheta[0.5(3+4)]$	58	$\emptyset[0.5(14 - 15)]$	
19	$\vartheta(C_{10}H_{21})$	39	$\vartheta[0.5(5+6)]$	59	$\emptyset[0.5(16+17)]$	
20	$\vartheta(C_5H_{18})$	40	$\vartheta[0.5(6+7)]$	60	$\emptyset[0.5(16 - 17)]$	

Table 1. Internal coordinates of dopamine for 60 normal modes.

2.2. Description of method.

Some of the types of wave function and frequencies as normal modes are listed in table 2 and Fig.1, which can be investigated for any waveforms based on inverse Fourier transforms of vibrational spectra. This spectrum of dopamine is easily transposed down into the audible frequencies area, and its inverse Fourier transform can be taken for yielding a time -domain wave form. A transposition calculated. This linear combination consists of normal mode combinations which matched with melodies, rhythms, pitch or duration of acoustic.

of about 60 notes in around 8 octaves (Table 3 &4) from normal modes yields the spectrum down to the musically useful ranges. (The frequency ratios corresponding to these octaves are approximately 3×10^{10}) (Speed of light cm/second). This procedure converts a vibrational perspective into the acoustic standpoint, or substitution of vibrational into the acoustic region. The spectrum can be converted such a molecular sound via computer software. In another methodology based on inverse Fourier transform of the molecular vibrational, the data of the spectrum will be converted to standard sound frequencies or acoustic notes. It is notable, the resulting wave shape might be present any time-varying musical data. The transposition frequencies for dropping the molecular vibrational waves into the lower-frequencies spectrum yield musical note forms that are important for controlling rhythm and also pitch or timbre. Based on our previous theoretical work and basic of molecular simulation, this work we has been simulated for any further resulting and discussing [24-54].

 Table 2. Number of normal modes (No.), Degeneracy (D), Frequency (F) and Intensity (I) of 60 normal modes, Hyper-Chem calculating.

No	Ď	F	Ι	No	D	F	Ι
1	1	20.29	0.077	31	1	608.83	2.025
2	1	32.6	0.185	32	1	643.42	1.931
3	1	47.00	3.263	33	1	662.91	0.882
4	1	57.5	0.638	34	1	685.57	2.476
5	1	70.21	4.531	35	1	713.27	0.200
6	1	89.65	8.005	36	1	734.43	3.927
7	1	129.0	0.201	37	1	759.14	1.184
8	1	149.3	2.963	38	1	816.47	0.330
9	1	160.5	0.528	39	1	827.27	3.450
10	1	188.7	0.206	40	1	933.12	3.075
11	1	213.7	0.612	41	1	1073.0	2.876
12	1	230.5	0.396	42	1	1131.9	0.737
13	1	270.4	0.139	43	1	11.923	2.205
14	1	277.8	1.454	44	1	1226.4	1.373
15	1	286.3	0.253	45	1	1256.8	0.741
16	2	320.3	0.810	46	1	1309.6	2.077
17	2	321.6	1.975	47	1	1319.5	2.177
18	1	352.2	0.370	48	1	1327.1	1.043
19	1	367.4	0.131	49	1	1362.4	10.37
20	1	376.0	0.081	50	1	1373.3	5.423
21	1	386.1	0.073	51	1	1419.8	6.311
22	1	398.2	0.491	52	1	1429.7	10.10
23	1	442.9	0.336	53	1	1492.3	2.901
24	2	454.3	1.360	54	1	1550.4	15.55
25	2	454.9	1.536	55	1	1573.5	32.60
26	1	465.3	2.724	56	1	1648.5	0.064
27	1	498.5	0.070	57	1	1698.6	13.05
28	1	518.5	1.827	58	1	1756.6	127.7
29	1	547.1	2.460	59	1	1790.2	15.62
30	1	575.9	1.448	60	1	1794.2	17.79

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Figure 1. The normal modes analysis of dopamine.

Table 3. Harmonic frequencies (**F**, cm⁻¹), Red Mass (**R**), force constant (**K**, m Dyne/A) and IR intensities (**I**, KM Mole⁻¹), for Dopamine with B3LYP/6-31g* method.

No	F	R	K	I	No	F	R	K	I
1	32.6	2.8	0.02	3.7	31	1166.0	1.3	1.0	3.03
2	79.8	4.96	0.02	0.98	32	1178.3	1.5	1.2	11.5
3	93.4	2.26	0.01	5.4	33	1194.3	1.4	1.2	88.2
4	181.3	4.34	0.08	24.9	34	1228.2	1.4	1.3	40.9
5	204.7	1.15	0.03	133.	35	1272.4	1.4	1.4	8.97
6	253.5	1.32	0.05	47.9	36	1303.7	1.9	1.9	37.2
7	264.2	3.22	0.13	2.48	37	1325.6	2.7	2.8	131.
8	297.2	3.34	0.17	2.81	38	1335.8	1.4	1.4	35.0
9	314.1	4.04	0.23	4.09	39	1366.9	1.4	1.6	9.39
10	331.2	3.38	0.21	19.0	40	1369.8	1.5	1.6	141.
11	389.7	5.46	0.48	3.05	41	1406.4	3.2	3.7	22.9
12	432.7	1.19	0.13	70.2	42	1437.7	1.4	1.7	18.8
13	460.1	2.67	0.33	5.86	43	1516.9	2.8	3.8	4.84
14	471.3	3.88	0.50	2.75	44	1520.	1.0	1.5	1.40
15	555.7	4.77	0.86	27.4	45	1545.9	1.0	1.5	3.42
16	594.7	5.30	1.10	2.06	46	1566.5	3.3	4.7	153.
17	638.4	4.75	1.14	5.82	47	1661.7	6.4	10.	42.9
18	702.9	5.14	1.49	0.31	48	1681.4	6.2	10.	3.28
19	764.7	4.04	1.39	12.8	49	1695.5	1.0	1.8	24.9
20	792.7	1.63	0.60	8.50	50	2960.1	1.0	5.5	70.9
21	803.9	1.46	0.55	23.2	51	3030.9	1.0	5.8	29.7
22	806.5	2.26	0.86	19.3	52	3070.6	1.0	6.0	28.9
23	881.6	1.39	0.63	13.7	53	3096.3	1.0	6.2	30.0
24	885.2	1.29	0.59	139.	54	3166.4	1.0	6.4	19.8
25	905.6	1.30	0.62	1.27	55	3194.2	1.0	6.6	16.9
26	963.7	2.60	1.42	10.2	56	3198.0	1.0	6.5	3.3
27	985.1	2.59	1.48	7.63	57	3456.6	1.0	7.4	3.5
28	1061.	2.19	1.45	39.5	58	3541.9	1.0	8.0	1.0
29	1099.	2.13	1.51	5.19	59	3717.4	1.0	8.7	82.0
30	1137.	1.92	1.46	93.5	60	3773.6	1.0	8.9	62.0

3. RESULTS

In this study, the possibility controlling of physical properties such as density of states versus normal mode energies (Fig.2) allows the construction of more molecular wave forms, with different time-domain shapes but with the same timbres based on the inverse Fourier transform of a vibrational spectrum. According to the normal modes principles, each mode form is static for a stable and homogeneous musical samples (Tables 4 and 5). Therefore, it is possible to acoustically convert each normal modes of frequency to the relative intensity mapped acoustic notes. A molecular vibrational spectrum is independent of

Table 4.	Frequencies	for equal-te	empered sca	ale $A_4 = 440 H$	ΗZ.
Note	F (HZ)	λ(cm)	Note	F (HZ)	λ(cm)
C ₀	16.35	2109.89	$F_{4}^{\#}/G_{4}^{b}$	369.99	93.24
$C_{0}^{\#}/D_{0}^{b}$	17.32	1991.47	G_4	392.00	88.01
0	18.35	1879.69	$G_{4}^{\#}/A_{4}^{b}$	415.30	83.07
$D_{0}^{\#}/E_{0}^{b}$	19.45	1774.20	A_4	440.00	78.41
E	20.60	1674.62	$A_{4}^{\#}/B_{4}^{b}$	466.16	74.01
F ₀	21.83	1580.63	B_4	493.88	69.85
F [#] 0/G ^b 0	23.12	1491.91	C ₅	523.25	65.93
G	24.50	1408.18	$C^{\#}_{5}/D^{b}_{5}$	554.37	62.23
G [#] 0/A ^b 0	25.96	1329.14	D ₅	587.33	58.74
A	27.50	1254.55	D [#] 5/E ^b 5	622.25	55.44
$\mathbf{A}^{\#}_{0}/\mathbf{B}^{\mathbf{b}}_{0}$	29.14	1184.13	E ₅	659.25	52.33
Bo	30.87	1117.67	F ₅	698.46	49.39
$\frac{-3}{C_1}$	32.70	1054.94	$F^{\#}_{5}/G^{b}_{5}$	739.99	46.62
$\frac{\mathbf{C}_{1}^{\#}}{\mathbf{C}_{1}^{\#}}$	34.65	995.73	G	783.99	44.01
$\frac{\mathbf{D}_{1}}{\mathbf{D}_{1}}$	36.71	939.85	$G^{\#}_{5}/A^{b}_{5}$	830.61	41.54
$\frac{D^{\dagger}}{D^{\sharp}}$	38.89	887.10	A	880.00	39.20
E.	41.20	837.31	$A^{\#}_{\epsilon}/B^{b}_{\epsilon}$	932 33	37.00
<u> </u>	43.65	790.31	B _e	987.77	34.93
$\frac{F_{1}}{F_{1}^{\#}/G_{1}^{b}}$	46.25	745.96	C ₆	1046.50	32.97
<u>G</u>	49.00	704.09	$C^{\#}_{\epsilon}/D^{b}_{\epsilon}$	1108.73	31.12
$\frac{G_1}{G_1^{\#}/A^b}$	51.91	664 57	D.	1174.66	29.37
<u>A</u> ,	55.00	627.27	$D_{b}^{\#}/E_{c}^{b}$	1244 51	27.72
$A^{\#}_{1}/B^{b}_{1}$	58.27	592.07	E _c	1318 51	26.17
B.	61 74	558.84	E ₆ F₄	1396.91	24.70
$\frac{\mathbf{L}_1}{\mathbf{C}_2}$	65.41	527.47	$F^{\#}_{\epsilon}/G^{b}_{\epsilon}$	1479.98	23.31
$\frac{C_2}{C^{\#}_2/D^b_2}$	69.30	497.87	G ₆	1567.98	22.00
$\frac{0}{D_2}$	73.42	469.92	$G^{\#}_{6}/A^{b}_{6}$	1661.22	20.77
$\frac{\mathbf{D}_2}{\mathbf{D}_2^{\#} \mathbf{P}_2}$	77.78	443.55	A ₆	1760.00	19.60
<u>E₂</u>	82.41	418.65	$A^{\#}_{6}/B^{b}_{6}$	1864.66	18.50
<u> </u>	87.31	395.16	B _€	1975.53	17.46
$\frac{-2}{F^{\#}}$, G^{b} ,	92.50	372.98	C7	2093.00	16.48
$\frac{1}{G_2}$	98.00	352.04	$C^{\#}_{7}/D^{b}_{7}$	2217.46	15.56
$\frac{G_2}{G_2^{\#}/A_2^{b}}$	103.83	332.29	D_7	2349.32	14.69
<u>A</u> 2	110.00	313.64	$D^{\#}_{7}/E^{b}_{7}$	2489.02	13.86
$A^{\#}_{2}/B^{b}_{2}$	116.54	296.03	E ₇	2637.02	13.08
B ₂	123.47	279.42	F ₇	2793.83	12.35
$\frac{-2}{C_3}$	130.81	263.74	F [#] 7/G ^b 7	2959.96	11.66
C [#] ₃ /D ^b ₃	138.59	248.93	G ₇	3135.96	11.00
D ₃	146.83	234.96	$G^{\#}_{7}/A^{b}_{7}$	3322.44	10.38
D [#] ₃ /E ^b ₃	155.56	221.77	A ₇	3520.00	9.80
E ₃	164.81	209.33	$A^{\#}_{7}/B^{b}_{7}$	3729.31	9.25
<u> </u>	174.61	197.58	B ₇	3951.07	8.73
$\frac{1}{F_{3}^{\#}/G_{3}^{b}}$	185.00	186.49	C ₈	4186.01	8.24
Ga	196.00	176.02	C [#] ₈ /D ^b ₈	4434.92	7.78
G [#] 3/A ^b 3	207.65	166.14	D ₈	4698.63	7.34
<u>A</u> ₁	220.00	156.82	$D^{\#}_{\circ}/E^{b}_{\circ}$	4978.03	6.93
A [#] 3/B ^b 3	233.08	148.02	E ₈	5274.04	6.54
<u> </u>	246.94	139.71	F ₈	5587.65	6.17
<u> </u>	261.63	131.87	F [#] ₈ /G ^b ₈	5919.91	5.83
$\frac{C^{\#}}{C^{\#}}$	277.18	124.47	G ₈	6271.93	5.50
$\overline{\mathbf{D}}_4$	293.66	117.48	$G^{\#}_{8}/A^{b}_{8}$	6644.88	5.19
$\overline{\mathbf{D}^{\#}_{4}/\mathbf{E}^{b}_{4}}$	311.13	110.89	A ₈	7040.00	4.90
<u> </u>	329.63	104.66	A [#] ₈ /B ^b ₂	7458.62	4.63
 F_4	349.23	98.79	B ₈	7902.13	4.37

the other physical properties, so it can be separately described versus time and any other conversions of the musical notes spectrum. As a simplified item of that mechanism, it is also feasible for limiting such conversions to the musical's peaks. Such conversions produce a series of simplified normal modes forms. Consequently, each of those normal modes forms can be based either directly on the extracted peaks, or else on their inverse Fourier transforms. If the normal modes of dopamine describe acoustic or molecular sounds, this method is helpful to listen of the specific frequency proportion of the vibrational spectral peaks.

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As an instance, each sound of the group corresponds and assigned to a separate key of a musical instrument's keyboard. In other words for the simple item of a series of sinusoidal components, each sound can be considered one note of a normal modes. Once a conversion is produced, the individual acoustic note of the family might be considered as independent notes, which can be composed in any further sequence for producing the large varieties of musical combinations.

Table 5 shows the series notes based on normal modes technique. The dopamine spectrum has been applied for generating group notes of molecular sounds which are played using sine oscillators. Furthermore the rhythms are derived from these sequences and the pitches are played repetitively at a rate symmetrical to the corresponding normal modes frequency. Although the normal modes described in this paper were constructed using theoretical data, other wave based on experimental vibrational ranges could also be used.



Figure 2. Density of states versus 40 normal modes energies.

4. CONCLUSIONS

The present method explained a sonification ways for normal mode analysis. In other words by this invistegation, the sonification which is application of a non-speech audio to convey information or perceptualize data has been used for normal modes of dopamine. Auditory perception has advantages in temporal, spatial, amplitude, and frequency resolution that open possibilities as an alternative or complement to visualization techniques[55-57].

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Table. 5. Harmonic frequencies (**F**, cm⁻¹), IR intensities (**I**, KM Mole⁻¹), and Acoustic frequencies (**A**, HZ) for Dopamine with B3LYP/6-31g*

	method.						
F	Ι	pitch	Α	F	Ι	pitch	Α
32.6	3.7	C ₁	32.70	1166.0	3.03	D ₆	1174.6
79.8	0.98	D ₂	73.42	1178.3	11.5	D ₆	1174.6
93.4	5.4	$F_{2}^{\#}/G_{2}^{b}$	92.50	1194.3	88.2	D ₆	1174.6
181.3	24.9	$F_{3}^{\#}/G_{3}^{b}$	185.0	1228.2	40.9	$D_{6}^{\#}/E_{6}^{b}$	1244.5
204.7	133.	$G_{3}^{\#}/A_{3}^{b}$	207.6	1272.4	8.97	$D_{6}^{\#}/E_{6}^{b}$	1244.5
253.5	47.9	B ₃	246.9	1303.7	37.2	E ₆	1318.5
264.2	2.48	C_4	261.6	1325.6	131.	E ₆	1318.5
297.2	2.81	D_4	293.6	1335.8	35.0	E ₆	1318.5
314.1	4.09	$D_{4}^{\#}/E_{4}^{b}$	311.1	1366.9	9.39	F ₆	1396.9
331.2	19.0	E_4	329.6	1369.8	141.	F ₆	1396.9
389.7	3.05	G ₄	392.0	1406.4	22.9	F ₆	1396.9
432.7	70.2	A_4	440.0	1437.7	18.8	$F_{6}^{\#}/G_{6}^{b}$	1479.9
460.1	5.86	$A^{\#}_{4}/B^{b}_{4}$	466.1	1516.9	4.84	G ₆	1567.9
471.3	2.75	B_4	493.8	1520.	1.40	G ₆	1567.9
555.7	27.4	$C_{5}^{\#}/D_{5}^{b}$	554.3	1545.9	3.42	G ₆	1567.9
594.7	2.06	D ₅	587.3	1566.5	153.	G ₆	1567.9
638.4	5.82	$D_{5}^{\#}/E_{5}^{b}$	622.2	1661.7	42.9	$G_{6}^{\#}/A_{6}^{b}$	1661.2
702.9	0.31	F ₅	698.4	1681.4	3.28	$G_{6}^{\#}/A_{6}^{b}$	1661.2
764.7	12.8	$F_{5}^{\#}/G_{5}^{b}$	739.9	1695.5	24.9	$G_{6}^{\#}/A_{6}^{b}$	1661.2
792.7	8.50	G ₅	783.9	2960.1	70.9	F [#] 7/G ^b 7	2959.9
803.9	23.2	$G_{5}^{\#}/A_{5}^{b}$	830.6	3030.9	29.7	F [#] 7/G ^b 7	2959.9
806.5	19.3	$G_{5}^{\#}/A_{5}^{b}$	830.6	3070.6	28.9	G ₇	3135.9
881.6	13.7	A ₅	880.0	3096.3	30.0	G ₇	3135.9
885.2	139.	A ₅	880.0	3166.4	19.8	G ₇	3135.9
905.6	1.27	$A_{5}^{\#}/B_{5}^{b}$	932.3	3194.2	16.9	G ₇	3135.9
963.7	10.2	$A_{5}^{\#}/B_{5}^{b}$	932.3	3198.0	3.3	G ₇	3135.9
985.1	7.63	B ₅	987.7	3456.6	3.5	A ₇	3520.0
1061.	39.5	C ₆	1046.	3541.9	1.0	A ₇	3520.0
1099.	5.19	C ₆	1046.	3717.4	82.0	$A^{\#}_{7}/B^{b}_{7}$	3729.3
1137.	93.5	D_6	1174.	3773.6	62.0	$A^{\#}_{7}/B^{b}_{7}$	3729.3

It can be applied with the following goals: 1. Audio character of a molecular substance, after adopting an efficacious musical coding which is identical for all those analyzing of the same category. For controlling audio real-time of the evolution the chemical sample's properties might be applied for time or analysis zone.

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