

Estimation of Vibrational Energy Levels of Diatomic Molecules (CN, CO and CS) Using Numerov Algorithm and Comparison with the Empirical Values

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Abstract: A general potential function which is suitable for all bound electronic states of all diatomic molecules has not been yet found, and in CN, CO and CS molecules as well. By comparisons with the experimental values, the potential function that more accurately describe the vibrations of these molecules is found. This work investigates the best-estimated vibrational energy levels of diatomic molecules observed in comets, which is in the best agreement with the empirical vibrational energies. Through this comparison, the best empirical potential function is offered which could be helpful in numerical and computer-based estimations. Empirical potential functions are listed and used to solve nuclear Schrodinger equation for some diatomic molecules namely CN, CO and CS, such as Morse, Rydberg, Lippincott, Frost-Musulin, Linnett, Poschl-Teller, Varshni and Hulbert-Hirschfelder are chosen to find the vibrational energy levels. Numerov algorithm has been employed for carrying out the calculations. The test is set, according to the ground state of the prementioned molecules. The ground state of CN is $X^2\tilde{\Lambda}^+$, and for CO and CS is $X^1\Sigma^+$. A detailed study of the performance of the empirical potential energy functions has been carried out by comparing them with the Rydberg-Klein-Rees potential energy curves for a ground electronic state of various diatomic molecules. Further, by employing the above potential energy functions, the Schrodinger nuclear equation has been solved for the vibrational energy levels, $G(v)$, and the vibrational wave functions, ψ_v . By comparisons with the experimental values, the potential function that more accurately describe the vibrations of CN, CO and CS molecules are found. Through the studies of this paper, which is mentioned as the estimation of the dissociation energies (D_e), the employed D_e for CN is 7.788 eV, and for CO and CS are 11.064 and 7.354 eV respectively; those are in good agreement with the literature values. Through Numerov-based estimations, it could be concluded that the five parameter Hulbert-Hirschfelder (H-H) empirical potential function is the best way to describe the vibrational energy levels of CN, CO and CS molecules.

Key words: comets, dissociation energy, diatomic molecules, vibrational energy levels, Numerov algorithm, empirical potential functions.

INTRODUCTION

Comets are of the most interesting objects in the sky, which is emphasized through fairy tales, which are quoted about the role of comets in our life, and our destiny. Spectacular display on the night sky that turned them into interesting objects, however comets are the most numerous objects in the solar system. We have heard about comets times and times but many issues regarding to them had yet to be set.

The ranges of comet nuclei are estimated from about 100 meters to more than 40 kilometers across. Some considerable components such as carbon monoxide, carbon monosulphide, cyanogen, carbon dioxide, methane and ammonia had been found in their frozen gases (Yeomans, D.K., 1991). Comets nuclei always have irregular shapes because their own gravity is not sufficient to give them a spherical shape.

Comets also contain methanol, hydrogen cyanide, formaldehyde, ethanol and ethane; as well as more complex molecules such as the amino acid glycine (Meech, M., 1997; NASA, 2006), which had been found in the comet dust recovered by NASA's Stardust mission.

It is too hard to detect cometary nuclei because in our solar system, those are among the least reflective objects. As well as in the outer solar system, because of their small size it is so difficult to detect from Earth.

The Hubble Space Telescope observations reported statistical detections of inactive comet nuclei, which are in the Kuiper belt (Cochran, A.L., 1995; Cochran, A.L., 1998). Not only there are many questions regarding to these observations (Brown, E. Michael, 1997; Jewitt, C. David, 1996), but also independent had not confirm them yet.

The comets that approach the inner solar system have different characteristics. The volatile materials within the comets start to vaporize and stream out of the nucleus and carrying dust away with them, as comets come closer to solar system.

The streams of dust and gas thus released form a huge, extremely tenuous atmosphere around the comet called the coma, and the force exerted on the coma by the Sun's radiation pressure and solar wind cause an enormous tail to form, which points away from the sun. Before the invention of the telescope, comets seemed to

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appear out of nowhere in the sky and gradually vanish out of sight. This circumstances made them so mysterious.

Isaac Newton explained that comets are compact and durable solid bodies moving in oblique orbits, and their tails look like a thin streams of vapor emitted by their heated by the sun. He described them as the origin of the life-supporting component of air.

Newton also described that the vapors given off by comets as replenish the planets' supplies of water, which was gradually being converted into soil. This changing is the result of the growth and decay of plants, and the sun's supply of fuel.

"From his huge vapouring train perhaps to shake Reviving moisture on the numerous orbs, Thro' which his long ellipsis winds; perhaps To lend new fuel to declining suns, To light up worlds, and feed th' ethereal fire." James Thomson, "The Seasons" (1730; 1748)

Comets deserve to be studied in scientific papers times and times because those reveal several useful information about the chemical history of solar system. Comets play a crucial role to answer a wide range of chemical physics questions in various important fields. The most important studies regarding comets reported in the cometary spectra rather than laboratory. Therefore comparative researches which bridging these two sides will afford a considerable achievements.

MATERIALS AND METHODS

Literature Review:

The role of diatomic molecules and their positive ions in astrophysical processes put them in the highest interest in recent years, which encourage both experimental and theoretical studies regarding to their chemical reactions.

Arpigny provided an Atlas of cometary spectra, which could be helpful for more detailed observations about diatomic molecules (Arpigny, C., 1994A; Arpigny, C., 1994B). Diatomic molecules such as CN (cyanogens), CO (Carbon monooxide) and CS (Carbon monosulphide) are of great interest in chem.-phys. In addition, other related disciplines.

Crovison and Encrenaz observed the most intense cometary band of the CN molecule. The CN molecule and radical has been studied in recent years, of its different various transitions. The most important achievements of that derived from 'C' stars, S-type and other important ones such as Se stars, Ba stars etc (Crovison, J. and T. Encrenaz, 2000). The cyanide radical - CN· has been identified in interstellar space (Pieniazek, A. Piotr, 2005).

In the comets spectra, CO is the most stable molecule and abundant one after H₂. Hyland observations about natural CO and its characteristics in the infrared spectra of cool stars are of most importance in literature review of CO (Hyland, A.R., 1974). CS is a common constituent in comets which deserve a scientific study. Astrophysical and chem.-phys. importance of CS molecules, besides its abundance, especially in several oxygen-rich stars is of the most important reasons which cause it has been chosen in this paper.

The potential energy curves display energy levels of diatomic molecules in a convenient way, through which those are known as the characteristics of molecular states. It may be expected that the kinetic mechanism, spectral phenomena through the role which played by them.

It should be noted that a general potential function, which is suitable for all bound electronic states of all diatomic molecules, has not been yet found.

Determination of reliable values of dissociation energies for the diatomic molecules is one of the interesting concerns of chemists as well as spectroscopists. The D₀ values are found to be 7.817, 10.95 and 7.27 eV for CN, CO and CS respectively. Here D₀=D_e-G(0). D_e is called the "equilibrium dissociation energy". It is an isotope independent property of the potential surface.

For many years, there has existed doubt about the values of the dissociation energies of CN, CO and CS.

Various investigators as shown in Table 1, 2 and 3 have reported the values of dissociation energies of CN, CO and CS obtained from different methods, through which the dissociation energies have been estimation to solve the Schrodinger nucleic equation.

To estimate vibrational energies, the molecular constants are needed, as well as dissociation energy. The molecular constants used in the present study are showed in table 4.

Research Question:

The paper is looking for the best-estimated vibrational energy levels of CN, CO and CS, which is in the best agreement with the empirical vibrational energies. The most well known empirical potential functions i.e. Morse, Varshni (VI), Rydberg, Frost-Musulin, Lippincott, Posch-Teller, Hulbert-Hirschfelder and Linnert are chosen for the test. The main question of the paper can be clarified as:

Which of empirical potential functions describe the vibrational energies of CN, CO and CS molecules in a better way?

Table 1: Values of dissociation energies of CN obtained from different methods.

Contributor	D ₀ (CN) (eV)	Explanations
Pauling, Linus and Sheehan, William F., Jr (1949)	6.28	1944
Gaydon (1968)	7.75 ± 0.2	1968
Grevesse and Sauval (1973)	7.5 to 8.4	1973
Ram <i>et al.</i> (1973)	7.90	1973
Rao <i>et al.</i> (1982)	8.05	1982
Snedden and Lambert (1982)	7.6	1982
Larsson <i>et al.</i> (1983)	7.4 to 7.7	At first step Larsson <i>et al.</i> (1983) get D ₀ (CN) = 7.00 eV and later it is corrected to 7.4 > D ₀ (CN) > 7.7 eV
Sinha and Tripathi (1986)	7.71 ± 0.06	Reanalysis of CN red system solar data, assumed f _{red 0-0} = 1.91 × 10 ⁻³ , 1986
Colket (1984)	7.92 ± 0.076	Shock tube study of CN violet absorption in C ₂ N ₂ -Ar mixtures, 1986
Lambert <i>et al.</i> (1986)	7.60	1986
Costes <i>et al.</i> (1990)	7.77 ± 0.05	Pulsed crossed supersonic molecular beam studies, 1990
Shavrina and Yakovina (1995)	7.85 to 7.90	1995
Reddy <i>et al.</i> (2003)	7.63 ± 0.18	2003

Table 2: Values of dissociation energies of CO obtained from different methods.

Contributor	D ₀ (CO) (eV)	Explanations
Faltings <i>et al.</i> (1938)	8.44 to 9.57	have studied the photodissociation of carbon monoxide, 1938
Hagstrum and Tate (1955)	9.61	1941
Gaydon and Penney [28]	11.11	1944
Pauling, Linus and Sheehan, William F., Jr. (1949)	9.77	1949
Schwarzschild <i>et al.</i> (1951)	9.5	1951
Kistiakowsky <i>et al.</i> (1952)	11.1	1952
Goldberg <i>et al.</i> (1953)	11.1	1953
Goldfinger (1955)	11.1	1955
Hagstun (1955)	11.1	1955
Cottrell (1958)	11.09	1958
Krupenie (1966)	11.108 to 11.074	1966
Gaydon (1968)	11.3	With usage Birge-Sponer extrapolation, 1968
Darwent (1970)	11.15	1970
Huber and Herzberg (1979)	11.092	1979
Herzberg (1989)	9.14	1989
Reddy <i>et al.</i> (2003)	10.95 ± 0.224	2003

Table 3: Values of dissociation energies of CS obtained from different methods.

Contributor	D ₀ (CS) (eV)	Explanations
Herzberg (1989)	7.8	1989
Lide (1993-1994)	7.39	1993
Jaschek and Jaschek (1995)	7.35	1995
Reddy <i>et al.</i> (2003)	7.27 ± 0.152	2003

Table 4: Molecular constants for different electronic states of CN, CO and CS (Reddy, R.R., 2003).

Molecule	μ	State	T _e (cm ⁻¹)	ω _e (cm ⁻¹)	ω _e x _e (cm ⁻¹)	B _e (cm ⁻¹)	α _e (cm ⁻¹)	r _e (Å°)	References
CN	6.4622	X ² Σ ⁺	0	2068.59	13.08	1.8997	0.01700	1.1718	Huber and Herzberg, 1979;
		A ² Π _i	9245.28	1812.56	12.60	1.7151	0.01708	1.2333	Sharp, 1984;
		B ² Σ ⁺	25752.0	2163.90	20.20	1.9730	0.02300	1.1500	Suchard et al., 1976.
CO	6.8562	X ¹ Σ ⁺	0	2169.82	13.29	1.9312	0.01751	1.1283	Huber and Herzberg, 1979;
		a ³ Π _r	48686.7	1743.41	14.36	1.6912	0.01904	1.2057	Eidelsberg et al., 1999;
		A ¹ Π	65075.7	1518.24	19.40	1.6115	0.02325	1.2358	Suchard et al., 1976.
		C ³ Π	93158.5	1804.72	11.70	1.9649	0.01811	1.1270	
CS	8.7252	X ¹ Σ ⁺	0	1285.08	6.46	0.8200	0.00592	1.5349	Huber and Herzberg, 1979;
		a ³ Π _r	2761.0	1135.10	7.73	0.7831	0.00720	1.5687	Suchard et al., 1976.

μ = Reduced mass.

T_e = Electronic energy above ground state (cm⁻¹).

ω_e = Vibrational spacing (cm⁻¹).

ω_ex_e = Anharmonic correction to vibrational spacing (cm⁻¹).

B_e = Rigid rotator rotational spacing (cm⁻¹).

α_e = Non rigid rotator correction to B_e (cm⁻¹).

r_e = Equilibrium inter nuclear distance (Å°).

Computer-based Numerical Techniques:

The development of modern computers has a lot to do with numerical methods. Before the advent of these modern computers, numerical methods often depended on hand interpolation in large printed tables, which was in need of long time and indefatigable efforts.

Since the mid 20th century, modern computers developed and undertook the required calculation functions instead. The interpolation algorithms and other necessities of solving differential equations are continued by the means of these modern machines.

The numerical analysis is based on techniques that are designed to give approximate but accurate solutions to hard problems. The goal of such techniques is to find the more accurate answer to the most complicated questions, i.e. the best-estimated vibrational energy levels of CN, CO and CS.

The numerical analysis techniques had previous records in numerical weather prediction, to solve ordinary differential equations, To run computer simulations e.g. car crashes simulations in order to test safety of the vehicles; all of these examples essentially consist of solving partial differential equations numerically.

Numerov Algorithm:

Vibrational energies of diatomic molecules could be inferred through Schrodinger nuclear equation. In order to solve this equation, there are some choices such as Numerov (Blatt, J.M., 1967), Cooley Numerov (Cooley, J.W., 1961), Renormalized Numerov (Johnson, B.R., 1977), Discrete Variable Representation (DVR) (Light, J.C., T. Carrington, 2003) and Finit-element methods. Numerov Algorithm has been employed in this paper.

Numerov's method is a numerical method to solve ordinary differential equations of second order in which the first-order term does not appear. It is a fourth-order linear multistep method. The method is implicit, but can be made explicit if the differential equation is linear.

Boris Vasil'evich Numerov developed Numerov's method. The Numerov method can be used to solve differential equations of the form

$$\left(\frac{d^2}{dx^2} + f(x) \right) y(x) = 0$$

The function $y(x)$ is sampled in the interval $[a..b]$ at equidistant positions x_n . The one-dimensional and time-independent Schrodinger Equation is of this kind:

$$\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2} [V(x) - E] \psi$$

Here $V(x)$ is the potential energy function, m is the reduced mass of the problem, and \hbar is Planck's constant divided by 2π .

Starting from function values at two consecutive samples x_{n-1} and x_n the remaining function values can be calculated as

$$\psi_{n+1} \approx \frac{2\psi_n - \psi_{n-1} + \frac{5}{6}G_n \psi_n s^2 + \frac{1}{12}G_{n-1} \psi_{n-1} s^2}{1 - \frac{1}{12}G_{n+1} s^2}$$

Where

$$\psi'' = \frac{2m}{\hbar^2} [V(x) - E] \psi$$

$$\psi'' = G \psi \quad \Rightarrow \quad G = \frac{m}{\hbar^2} [2V(x) - 2E]$$

$\psi_n = \psi(x_n)$ and $G_n = G(x_n)$ are the function values at the positions x_n and $s = x_n - x_{n-1}$ is the distance between two consecutive samples.

This paper is based on solving Schrodinger nuclear equation with Numerov's method through Excel codes.

Case Studies:

The Numerov algorithm is employed to solve nuclear Schrodinger equation for diatomic molecules (CN, CO, CS) with several empirical potential functions as: Frost- Musulin, Hulbutr- Hirschfelder, Linnet, Lippincott, Morse, Poschl-Teller, Rydberg, and Varshni (VI) to obtain the vibrational energy levels of these molecules. It results in calculated vibrational energies, which the first-eight lower levels are presented here.

Table 5: Energy values using empirical potentials for the ground electronic state of CN molecule (cm^{-1}).

Standard Deviation (s)	E ₇	E ₆	E ₅	E ₄	E ₃	E ₂	E ₁	E ₀	Vibrational Levels (v)	Energy
0	14778.2	12892.9	10981.3	9043.6	7079.7	5089.7	3073.4	1031	Empirical energies (cm^{-1})	
112.10040	14556.45	12726.29	10862.07	8963.79	7031.44	5065.03	3064.57	1030.04	Morse	Calculated energies using empirical potential functions
62.97060	14652.63	12799.47	10915.09	8999.63	7053.26	5076.11	3068.34	1030.09	Varshni (VI)	
74.57319	14630.00	12782.15	10902.48	8991.10	7048.10	5073.56	3067.59	1030.27	Rydberg	
109.82215	14561.06	12729.65	10864.41	8965.32	7032.37	5065.54	3064.80	1030.15	Frost-Musulin	
19.22311	14740.13	12864.87	10961.41	9029.95	7070.69	5083.82	3069.54	1028.02	Lippincott	
112.07150	14556.49	12726.33	10862.11	8963.83	7031.48	5065.07	3064.61	1030.08	Poschl-Teller	
11.16355	14753.45	12876.83	10971.69	9038.39	7077.31	5088.81	3073.26	1031.02	Hulbert-Hirschfelder	
54.03461	14671.78	12812.48	10923.49	9004.74	7056.18	5077.72	3069.29	1030.82	Linnet	

Table 6: Energy values using empirical potentials for the ground electronic state of CO molecule (cm^{-1}).

Standard Deviation (s)	E ₇	E ₆	E ₅	E ₄	E ₃	E ₂	E ₁	E ₀	Vibrational Levels (v)	Energy
0	15525.9	13542.2	11531.9	9495	7431.5	5341.5	3224.8	1081.6	Empirical energies (cm^{-1})	
2.93710	15531.72	13546.56	11535.01	9497.09	7432.79	5342.11	3225.05	1081.61	Morse	Calculated energies using empirical potential functions
48.99460	15622.26	13615.12	11584.45	9530.36	7452.93	5352.26	3228.45	1081.58	Varshni (VI)	
32.57519	15589.97	13590.65	11566.81	9518.52	7445.82	5348.76	3227.41	1081.79	Rydberg	
2.67571	15520.80	13538.18	11528.91	9492.95	7430.28	5340.86	3224.68	1081.69	Frost-Musulin	
71.42706	15667.41	13648.64	11607.99	9545.55	7461.44	5355.76	3228.61	1080.08	Lippincott	
2.98708	15531.78	13546.62	11535.08	9497.16	7432.86	5342.18	3225.12	1081.68	Poschl-Teller	
1.24357	15528.50	13543.99	11533.09	9495.77	7432.00	5341.77	3225.04	1081.78	Hulbert-Hirschfelder	
5.21835	15536.80	13549.81	11536.97	9498.20	7433.41	5342.50	3225.38	1081.96	Linnet	

Table 7: Energy values using empirical potentials for the ground electronic state of CS molecule (cm^{-1}).

Standard Deviation (s)	E ₇	E ₆	E ₅	E ₄	E ₃	E ₂	E ₁	E ₀	Vibrational Levels (v)	Energy
0	9274.7	8080.1	6872.5	5652	4418.6	3172.3	1913.1	640.9	Empirical energies (cm^{-1})	
14.86764	9245.29	8057.97	6856.69	5641.45	4412.23	3169.05	1911.91	640.79	Morse	Calculated energies using empirical potential functions
6.63902	9287.58	8089.98	6879.76	5656.96	4421.63	3173.80	1913.51	640.81	Varshni (VI)	
0.92117	9276.33	8081.45	6873.61	5652.83	4419.15	3172.58	1913.16	640.89	Rydberg	
14.68616	9245.68	8058.23	6856.86	5641.55	4412.30	3169.10	1911.95	640.84	Frost-Musulin	
23.64940	9321.63	8115.37	6897.70	5668.67	4428.33	3176.73	1913.93	639.97	Lippincott	
14.85333	9245.31	8057.99	6856.71	5641.47	4412.25	3169.07	1911.93	640.81	Poschl-Teller	
0.84322	9272.81	8078.87	6871.82	5651.70	4418.52	3172.34	1913.16	641.01	Hulbert-Hirschfelder	
4.20919	9283.16	8086.28	6876.88	5654.92	4420.38	3173.25	1913.49	641.09	Linnet	

Results and Discussions:

The vibrational energy levels are calculated by varying the potential functions. Standard deviations (s) is determined between the calculated E_v and the experimental $G(v)$ values. The most useful empirical potentials are the ones those Standard deviations are minimum.

An accurate estimation of the dissociation energy (D_0) requires an empirical potential function, which gives the best reproduction of the experimental energy values.

Table 5 demonstrates calculated vibrational energies of the CN molecule as well as empirical potentials. Table 5 also indicates that the empirical potential functions of Hulbert-Hirschfelder, Lippincott and Linnet, are

in the best order to describe the molecular vibrations of CN, because those Standard deviations (s) 11.16355, 19.22311 and 54.03461 respectively.

Table 6 shows that the empirical potential functions of Hulbert-Hirschfelder, Frost-Musulin and Morse respectively are in the best agreement with the empirical vibrational energies of CO. In the case of CO, s of Hulbert-Hirschfelder is 1.24357 Frost-Musulin is 2.67571, and Morse is 2.93710.

In the case of CS molecule (table 7), the estimations show that the empirical potential functions of Hulbert-Hirschfelder (s:0.84322), Rydberg (s: 0.92117), and Linnet (s: 4.20919) are respectively in the best agreement with the empirical vibrational energies of CS.

Through Numerov -based estimations, it could be concluded that empirical potential function of Hulbert-Hirschfelder is the best way to describe the vibrational energies of CN, CO and CS molecules (Table 8).

Table 8: Final Scores of various empirical potential functions.

Empirical Potentials	CN	CO	CS	Final Score
Morse	8	3	7	7
Varshni (VI)	4	7	4	5
Rydberg	5	6	2	3
Frost-Musulin	6	2	5	3
Lippincott	2	8	8	7
Poschl-Teller	7	4	6	6
Hulbert-Hirschfelder	1	1	1	1
Linnet	3	5	3	2

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