

This article was downloaded by:

On: 30 January 2011

Access details: *Access Details: Free Access*

Publisher *Taylor & Francis*

Informa Ltd Registered in England and Wales Registered Number: 1072954 Registered office: Mortimer House, 37-41 Mortimer Street, London W1T 3JH, UK



Spectroscopy Letters

Publication details, including instructions for authors and subscription information:

<http://www.informaworld.com/smpp/title~content=t713597299>

A New Relation Free From Electronegativity For Vibrational Constant Of Diatomic Molecules

S. S. L. Surana^a; P. C. Mehta^{ab}

^a Department of Physics, University of Jodhpur, Jodhpur, India ^b Instrument Research and Development, DehraDun, India

To cite this Article Surana, S. S. L. and Mehta, P. C.(1974) 'A New Relation Free From Electronegativity For Vibrational Constant Of Diatomic Molecules', *Spectroscopy Letters*, 7: 4, 189 — 192

To link to this Article: DOI: 10.1080/00387017408067235

URL: <http://dx.doi.org/10.1080/00387017408067235>

PLEASE SCROLL DOWN FOR ARTICLE

Full terms and conditions of use: <http://www.informaworld.com/terms-and-conditions-of-access.pdf>

This article may be used for research, teaching and private study purposes. Any substantial or systematic reproduction, re-distribution, re-selling, loan or sub-licensing, systematic supply or distribution in any form to anyone is expressly forbidden.

The publisher does not give any warranty express or implied or make any representation that the contents will be complete or accurate or up to date. The accuracy of any instructions, formulae and drug doses should be independently verified with primary sources. The publisher shall not be liable for any loss, actions, claims, proceedings, demand or costs or damages whatsoever or howsoever caused arising directly or indirectly in connection with or arising out of the use of this material.

A NEW RELATION FREE FROM ELECTRONEGATIVITY FOR
VIBRATIONAL CONSTANT OF DIATOMIC MOLECULES

S.S.L.SURANA and P.C.MEHTA*

Department of Physics, University of Jodhpur, Jodhpur, India.

Most of the previous relations¹⁻³ for the calculation of vibrational constant of diatomic molecules are electronegativity dependent. Electronegativity (χ) is a complex quantity containing an atomic term depending on the charge and hybridization of the atom, and a molecular term depending on the length and the nature of the bonds in the molecule and as such it is not as precise as the bond length r_e or the reduced mass μ of the molecule. Thus the formule dependent on the electronegativity are expected to yield divergent results. Though there is a relation given by Varshni and Guggenheimer⁴ which is free from electronegativity but the drawback is that it depends on too many quantities and also contains two empirical constants. Therefore it was thought to propose a new relation free from electronegativity, containing a single constant A , depending only on r_e and μ .

* Present address: Instrument Research and Development
Establishment, Dehra Dun, India.

The proposed relation is

$$\omega_e = \frac{A}{\sqrt{\mu} r_e^3} \quad \dots(1)$$

whereas the previous relation of Varshni and Guggenheimer⁴ is

$$\omega_e = a(Z_1 Z_2)^{\frac{1}{2}} \mu^{-\frac{1}{2}} r_e^{-b} \quad \dots(2)$$

and that of Tandon et al³ and Hussain's² are

$$\log \omega_e = m \log X / \mu^2 + c \quad \dots(3)$$

and

$$\omega_e = \frac{q X}{\mu^p} \quad \dots(4)$$

respectively. a , b , m , c , q , and p are empirical constants to be determined by the experimental observations.

As a test case of the proposed relation, computations have been carried out in the case of twenty diatomic halides of atoms of IIIb group. The results have been compared with those derived from eqns. (3) and (4). The results have been collected in Table 1.

For the calculation of the constant A , the ω_e values of GaF, InF, and TlBr were not considered to make a fair comparison with earlier reported values^{2,3}. The present formula yields ω_e values for these molecules to be 635.4, 545.0, and 192.4 cm^{-1} respectively, which are quite agreeable to the experimentally reported values 623.2, 534.7, and 192.1 cm^{-1} respectively. However, Tandon et al³ and Hussain² predicted ω_e values for these molecules to be 644.5, 561.3, and 182.7 cm^{-1} ; and 695.4, 598.9, and 165.9 cm^{-1} respectively, which are much divergent from the experimental values. ω_e

TABLE 1*

Molecule	$r_e (\text{\AA})$	$\mu (\text{a.m.u.})$	$\omega_e (\text{cm}^{-1})$			
			Observed	Calculated		
				ZH	TMP	P
BF	1.262	6.9724	1400.6	1696.0	1696.0	1442.0
BCl	1.716	8.3758	839.1	723.6	839.9	829.6
BBr	1.880	9.6644	684.3	684.3	684.3	673.3
BI	2.110	9.9610	-	352.9	504.3	557.8
AlF	1.654	11.1520	801.9	728.3	814.0	820.6
AlCl	2.130	15.2350	481.3	368.4	453.3	480.6
AlBr	2.295	20.1129	378.0	328.9	378.7	374.0
AlI	2.530	22.2578	316.1	215.5	288.4	307.1
GaF	1.775	14.9102	623.2	695.4	644.5	635.4
GaCl	2.202	23.2069	365.0	365.0	365.0	368.6
GaBr	2.352	37.2320	263.0	271.4	265.7	263.4
GaI	2.575	44.6820	216.4	216.4	216.4	210.3
InF	1.985	16.3020	534.7	598.9	561.9	545.0
InCl	2.401	26.8179	317.4	317.4	325.7	319.5
InBr	2.543	47.4920	221.0	221.1	221.0	220.3
InI	2.754	60.3200	177.1	189.2	180.9	173.4
TlF	2.123	17.3880	477.3	475.0	472.4	480.9
TlCl	2.485	29.8690	287.5	252.8	287.4	289.9
TlBr	2.618	57.9790	192.1	165.9	182.7	192.4
TlI	2.814	78.3120	150.0	150.1	150.0	148.6
Average error				11.8%	5.1%	1.6%

* Data have been taken from Ref. 4.

for BI is also predicted to be 557.8 cm^{-1} , yet to be experimentally determined.

The proposed relation though depends on only two measurable quantities, yields better results (average error 1.6%) as compared to the earlier X independent relation⁴ (average error 5%) and X dependent relation³ (average error 5.1%).

ACKNOWLEDGEMENT

Authors are thankful to Dr. S.P.Tandon for his critical comments on the manuscript prior to its publication. Dr. M.P.Bhuttra is also thanked for helpful discussions. Authors wish to thank CSIR, India for providing financial assistance

REFERENCES

1. Z.Herzberg, 'Molecular Spectra and Molecular Structure. I. Spectra of Diatomic Molecules', D-Van Nostrand Co. Inc., New York, 1950.
2. Z.Hussain, Can. J. Phys., 44, 917 (1966).
3. S.P.Tandon, M.P:Bhuttra and P.C.Mehta, Spectrosc. Letts., 2, 213 (1969).
4. K.S.Krasnov, V.S.Timoshinin, T.G.Danilova and S.V.Khandozhko, 'Handbook of Molecular Constants of Inorganic Compounds', Israel Program for Scientific Translations, Jerusalem, 1970, p.12.

Received March 19, 1974

Accepted April 1, 1974