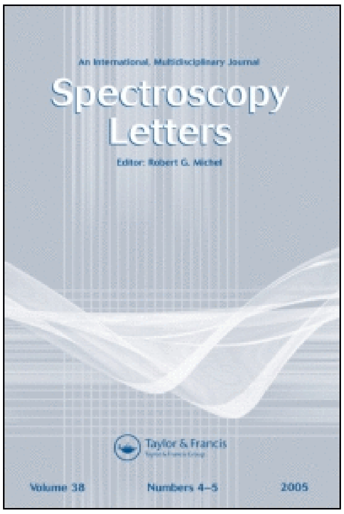

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A New Relation Free From Electronegativity For Vibrational Constant Of Diatomic Molecules

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

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Most of the previous relations[1-3] for the calculation of vibrational constant of diatomic molecules are electronegativity dependent. Electronegativity (X) 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 Guggenheimer[4] 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.

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The proposed relation is

$$\omega_e = \frac{A}{\sqrt{\mu\, r_e^3}} \qquad ...(1)$$

whereas the previous relation of Varshni and Guggenheimer[4] is

$$\omega_e = a(Z_1Z_2)^{\frac{1}{2}} \mu^{-\frac{1}{2}} r_e^{-b} \qquad ...(2)$$

and that of Tandon et al[3] and Hussain's[2] are

$$\log \omega_e = m \log X/\mu^2 + C \qquad ...(3)$$

and

$$\omega_e = \frac{q\,X}{\mu^p} \qquad ...(4)$$

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 al[3] and Hussain[2] 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(A°)	μ(a.m.u.)	ω_e (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 relation[4] (average error 5%) and X dependent relation[3] (average error 5.1%).

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