UREY-BRADLEY FORCE FIELD: BORINE CARBONYL AND BORINE CARBONYL-d_3

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Abstract

A normal co-ordinate treatment has been carried out to calculate the force constants of BH_3CO and BD_3CO molecules, on the basis of a Urey-Bradley potential force field.

Introduction

A symmetric C_{3v} structure for the BH_3CO molecule has been established by the electron diffraction work of Bauer[1] and by the micro wave experiments of Gordy *et al.*[2] The molecule has $4a_1 + 4e$ vibrations. BH_3CO and BD_3CO have been subjected to normal co-ordinate analysis by Bethke and Wilson,[3] Taylor,[4] Sundaram and Cleveland.[5] Here an attempt has been made to calculate the Urey-Bradley force constants.

Symmetry Co-ordinates, F and G Matrices

Symmetry co-ordinates used in this investigation are the same as those given by Bethke and Wilson,[3] except for S_4 which has been taken from Sundaram and Cleveland.[5] The Urey-Bradley potential function in the general form was taken and after the elimination of the q co-ordinates, the elements of the potential energy matrices are obtained in the usual way. The elements of the kinetic energy matrices are derived by the method of Wilson.

Results

The F and G matrix elements derived are used for the evaluation of force constants of the molecule. The molecular parameters and observed frequencies used in the calculation are the same as those given by Bethke and Wilson.[3] The values of the force constants obtained here together with the stretching and bending force constants as reported by Sundaram and Cleveland[5] are given in Table I, where K_D, K_R and K_r are the C–O, B–C and B–H stretching H_a, H_β and $H\phi$ are the H–B–H, H–B–C and B–C–O bending F_a, F_β and F_{OH} are the H–H, C–H and O–H repulsion constants respectively.

TABLE I

Force constants (10^5 dynes/cm.) of BH_3CO and BD_3CO

Force constant	K_D	K_R	K_r	H_α	H_β	H_ϕ	F_α	F_β	$F_{\alpha\alpha}$
Present values ..	17·5429	1·782	2·7508	0·2919[5]	0·1534	0·1722	−0·0211	0·3227	0·0411
Sundaram and Cleveland[5]	18·0450	2·7283	3·20589	0·29194	0·32335	0·40598	..	..	..

The observed and calculated frequencies of BH_3CO and BD_3CO are given in Table II.

TABLE II

Observed and calculated frequencies of BH_3CO and BD_3CO ($cm.^{-1}$)

Molecule		a_1				e			
BH_3CO ..	Observed	2380	2169	1073	692	2434	1101	816	317
	Calculated	2382	2167	1073	692	2447	1114	823	311
BD_3CO ..	Observed	1679	2169	862	625	1837	801	709	266
	Calculated	1679	2170	862	625	1844	798	709	266

From Table II it can be seen that the calculated frequencies are in good agreement with those observed.

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