Mean Amplitudes of Vibration in Certain Four-Atomic Molecules

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Mean amplitudes of vibration (u) for the interatomic distances in certain four-atomic molecules have been calculated from spectroscopic data (Table 1). When the instantaneous interatomic distance is denoted by R and R_e is the equilibrium distance, then u is defined by

$$u = [\overline{(R - R_e)^2}]^{\frac{1}{2}}$$

The average is taken over the molecules in the gaseous state by thermodynamic equilibrium at a given temperature T. The calculations are based on the assumption of small harmonic vibrations, the method being described by Morino *et al.*[1]

Informations concerning u-values from spectroscopic data are of great interest for electron diffraction investigations. As to studies of mean amplitudes both from electron diffraction data and spectroscopic calculations, references are made to Karle and Karle [2], Kimura *et al.*[3] and Bastiansen *et al.*[4-6]. Electron diffraction investigations of the molecules studied in this work would contribute appreciably to our knowledge of mean amplitudes and are under consideration.

Table 1. Calculated mean amplitudes of vibration (u).

Molecule	Interatomic distance	u (Å) $T = 0$	298°K
P_4	P—P	0.0478	0.0533
BF_3	B—F	0.0433	0.0437
	F—F	0.0408	0.0442
BCl_3	B—Cl	0.0485	0.0508
	Cl—Cl	0.0442	0.0569
BBr_3	B—Br	0.0494	0.0545
	Br—Br	0.0402	0.0585
PH_3	P—H	0.0862	0.0862
	H—H	0.1516	0.1521
AsH_3	As—H	0.0894	0.0894
	H—H	0.1586	0.1597
SbH_3	Sb—H	0.0944	0.0944
	H—H	0.1712	0.1736
PF_3	P—F	0.0410	0.0418
	F—F	0.0700	0.0788
PCl_3	P—Cl	0.0467	0.0526
	Cl—Cl	0.0770	0.1033
NF_3	N—F	0.0515	0.0535
	F—F	0.0751	0.0786
CH_2O	C—H	0.0801	0.0801
	C—O	0.0372	0.0372
	H—H	0.1170	0.1170
	O—H	0.0911	0.0912
CD_2O	C—D	0.0682	0.0682
	C—O	0.0365	0.0366
	D—D	0.0823	0.0824
	O—D	0.0727	0.0730
C_2H_2	C—C	0.0357	
	C—H	0.0743	
	C—C—H	0.0784	
	H—H	0.1049	
C_2D_2	C—C	0.0362	
	C—D	0.0637	
	C—C—D	0.0717	
	D—D	0.0951	
C_2HD	C—C	0.0358	
	C—H	0.0743	
	C—D	0.0634	
	C—C—H	0.0795	
	C—C—D	0.0687	
	H—D	0.0988	

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