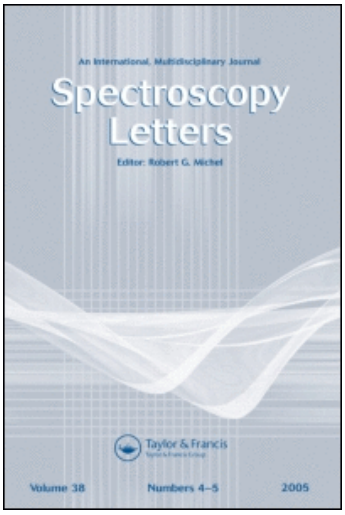

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Mean Amplitudes Of Vibration For Aluminum And Ferric Chloride Dimers

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MEAN AMPLITUDES OF VIBRATION FOR ALUMINUM AND FERRIC CHLORIDE DIMERS

Keywords: Mean amplitude, Al_2Cl_6, Fe_2Cl_6

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ABSTRACT

Mean amplitudes of vibration were calculated from spectroscopic data for all the types of interatomic distances in Al_2Cl_6 and Fe_2Cl_6.

INTRODUCTION

In a previous paper[1] normal coordinate analyses were reported for Al_2Cl_6 and Fe_2Cl_6. The purpose of the present work is to calculate mean amplitudes of vibration[2] for the molecules. These quantities are of great value in connection with electron diffraction studies. Modern gas electron diffraction investigations have actually been performed for these molecules, viz. Al_2Cl_6 [3] and Fe_2Cl_6,[4] among others of the bridged M_2X_6 metal-halogen type: Al_2Br_6,[3] Ga_2Cl_6 [5] and Ga_2Br_6.[5]

COMPUTATIONS

The structural parameters and force fields adopted in this work are reported elsewhere.[1] The computations of mean amplitudes were performed by standard methods[2] using an

ALGOL program series designed for the UNIVAC-1108 computer at the Computing Centre of The University of Trondheim.

The results of the calculations for Al_2Cl_6 and Fe_2Cl_6 at absolute zero and room temperature are collected in Table 1. The nine types of interatomic distances are identified in accord with previous reports.[6,7]

DISCUSSION AND CONCLUSION

The applied force fields[1] were reported to be uncertain for some reasons. Nevertheless we believe that they give mean amplitudes of significant value in electron diffraction studies. The obtained results (Table 1) all seem to have reasonable orders of magnitude.

Generalized mean-square amplitudes of vibration[2] have been reported previously for Al_2Cl_6.[8] The mean amplitudes of vibration which we have deduced from these data are rather different from our results (Table 1). The previous data, how-

TABLE 1

Mean Amplitudes of Vibration (Å units)

Distance	Al_2Cl_6		Fe_2Cl_6	
	0 K	298 K	0 K	298 K
M-X_t	0.047	0.054	0.043	0.049
M-X_b	0.051	0.060	0.050	0.063
M···X	0.070	0.117	0.085	0.235
M-M	0.058	0.074	0.055	0.089
X_b···X_b	0.055	0.071	0.063	0.091
X_b···X_t	0.069	0.112	0.082	0.170
com(X···X)	0.064	0.097	0.070	0.124
cis(X···X)	0.094	0.203	0.144	0.527
trans(X···X)	0.072	0.122	0.088	0.202

ever, were obtained from a force field[9] based on an old vibrational assignment, which presumably was improved in our previous work.[1]

Mean amplitudes of vibration for Fe_2Cl_6 from spectroscopic data are given here (Table 1) for the first time.

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