Determination of Force Constants of Octahedral XY_6 Molecules by the GF Matrix Method

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The force constants of the internal coordinates of octahedral XY_6 molecules and complex ions were calculated by using the GF matrix method. The matrix solutions were found by means of a computer program using the Newton-Raphson method. From the calculations it has been observed that the bond stretch force constants of octahedral XF_6 molecules and XY_6 complex ions having the same centre X atom decrease with the increasing molar mass of the centre X atom for the former and the ligand Y atom for the latter, respectively. This was attributed to the slowing down of the molecule with increasing molar mass of the molecule as the whole. In addition we have concluded that the difference of squares of the vibration frequencies ν_1 and ν_2 of octahedral XY_6 complex ions decreases with the increasing mass of the Y atom since the interaction force constant of these ions decreases with the increasing mass.

Key words: GF Matrix Method; Force Constants; XY_6 Molecules; XY_6 Ions.