The effect of Isotopic Substitution

When a particular atom in a molecule is replaced by its isotope — an element identical in every way except for its atomic mass — the resulting substance is identical chemically with the original. In particular there is no appreciable change in internuclear distance on isotopic substitution there is, however, a change in total mass and hence in the moment of inertia and B value for the molecule.

If $B = \frac{h}{8\pi^2 I c}$ $\quad B' = \frac{h}{8\pi^2 I' c}$

$$\frac{B}{B'} = \frac{h}{8\pi^2 I c} \times \frac{8\pi^2 I' c}{h} = \frac{I'}{I} = \frac{\mu'}{\mu}$$

For example

$^{12}C\,^{16}O \longrightarrow {}^{13}C\,^{16}O \longrightarrow$ mass increase

$\longrightarrow$ decrease in B value.

First Rotational absorption of $^{12}C^{16}O$ to be at 3.67337 cm^{-1} and $^{12}C^{16}$

3.84235 cm^{-1}

$^{13}C^{16}O$ 3.67337 cm^{-1}

The values of B determined from these figure

$$B = 1.92118\ cm^{-1}$$

$$B' = 1.83669\ cm^{-1}$$

$$\frac{B}{B'} = \frac{J'}{J} = \frac{\mu'}{\mu} = 1.046$$

where μ and the internuclear distance is considered unchanged by isotopic substitution. Taking the mass of oxygen to be 15.994 and that of carbon-12 to be 12.00, we have

$$\frac{\mu'}{\mu} = 1.046 = \frac{15.9994\, m'}{15.994 + m'} \times \frac{12 + 15.9994}{12 \times 15.9994}$$

from which m', the atomic weight of Carbon-13 is found to be 13.007.

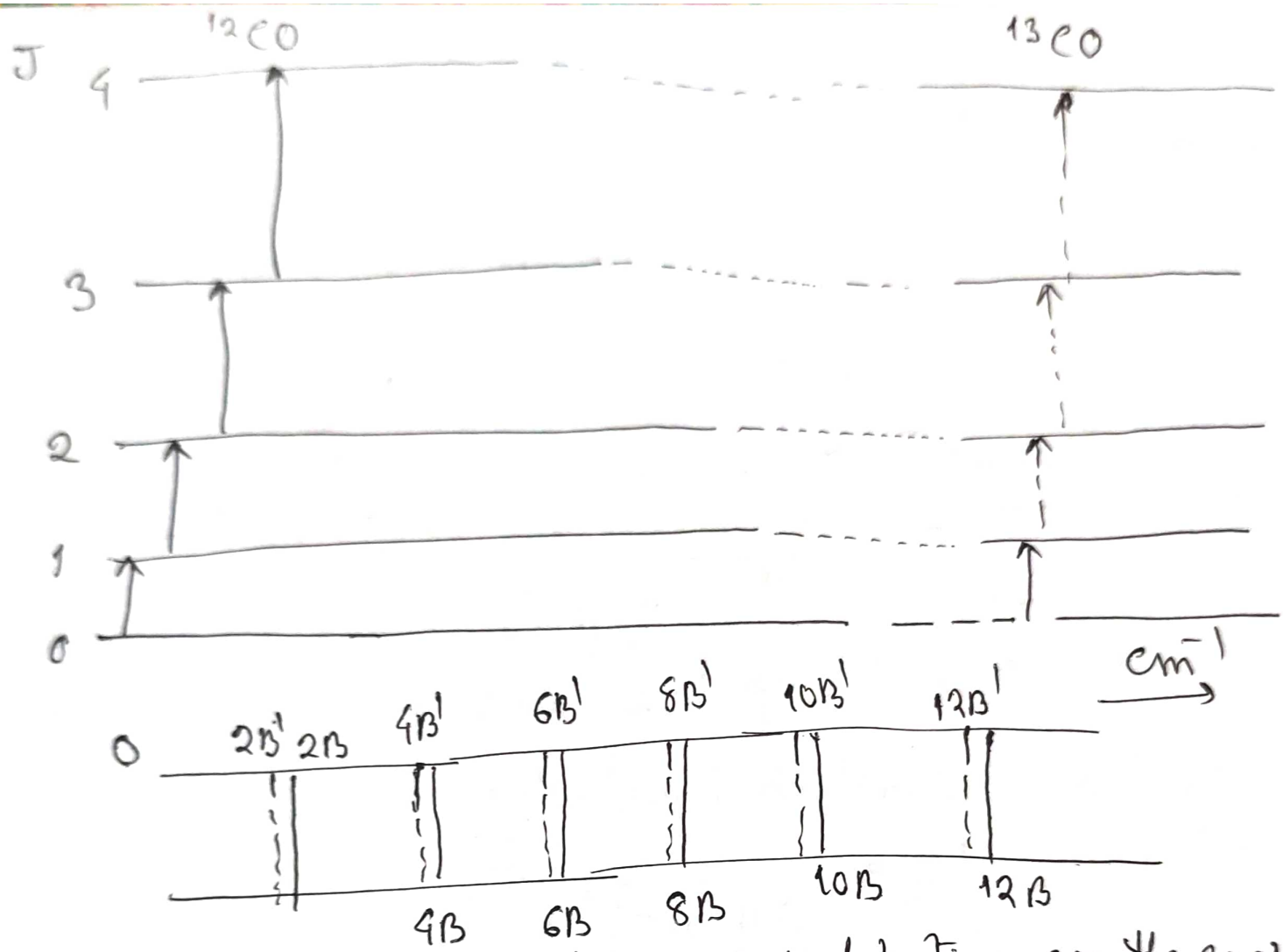

Fig The effect of isotopic substitution on the energy levels and rotational spectrum of a diatomic molecule such as carbon monoxide.