Circular Dichroism of (+)-3-Methylcyclopentanone†

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Summary The circular dichroism of (+)-3-methylcyclopentanone is reported down to 165 nm, using a newly developed instrument capable of resolution of 0·8 nm and sensitivity of 1 part in 10^4.

THE circular dichroism of (+)-3-methyl-cyclopentanone in the gas phase has previously been reported[1] down to about 166 nm. We describe here the c.d. of the same compound obtained in our laboratory, using a McPherson vacuum spectrometer, a modified Hinteregger hydrogen source, a magnesium fluoride Rochon prism as polarizer, and a stress-plate modulator[2] of fused quartz (1/8 in. thickness) as 1/4-wave retardation element.

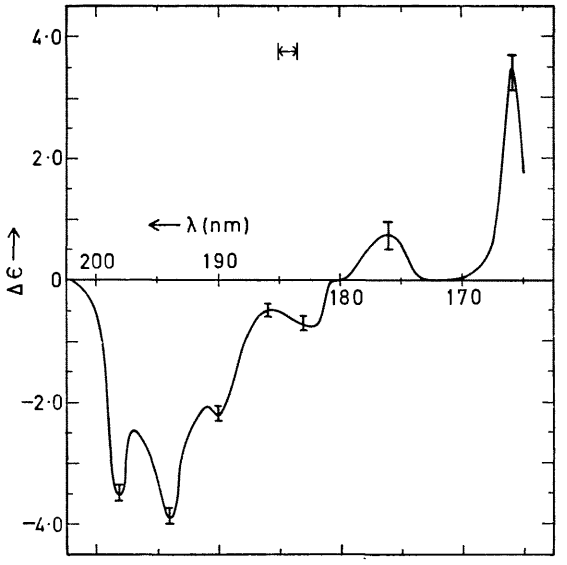

FIGURE 1. *Circular dichroism of* (+)-3-*methyl-cyclopentanone in the gas phase. Spectral slit width* 1·6 *nm. Vertical bars indicate noise level.*

The c.d. spectrum consists of four distinct spectral regions (Figure 1):

(a) An intense negative system between 200—186 nm containing two intense and one weaker vibronic bands with a spacing of about 1150 cm^{-1}.

(b) A weak single band has been observed at 185—182 nm which is also negative in sign.

(c) A weak positive system is found at 178—174 nm. In this region the ratio $\Delta\epsilon/\epsilon = 10^{-4}$ and therefore the error in this measurement is relatively large.

(d) A relatively narrow peak has been observed at 166 nm.

Figure 2 presents a higher resolution run for the region 200—180 nm. The vibronic bands of the first intense

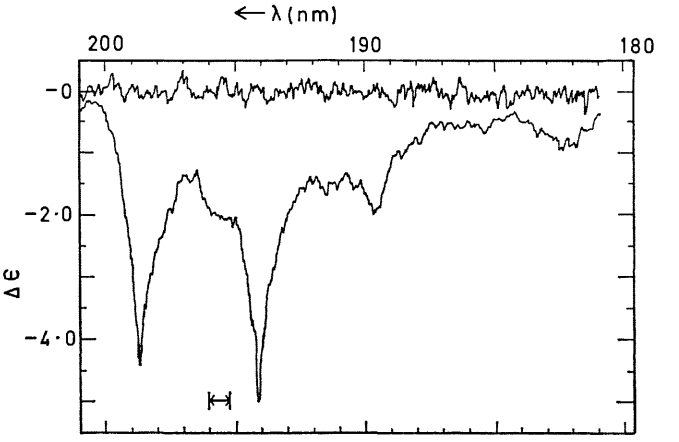

FIGURE 2. *Circular dichroism of* (+)-3-*methyl-cyclopentanone in the gas phrase. Spectral slit width* 0·8 nm. *The base line is also given.*

system are narrower than they appear in Figure 1, indicating that they were not resolved at the lower resolution. Correspondingly, the peaks are also higher. In Figure 3 we present the absorption coefficient curve.

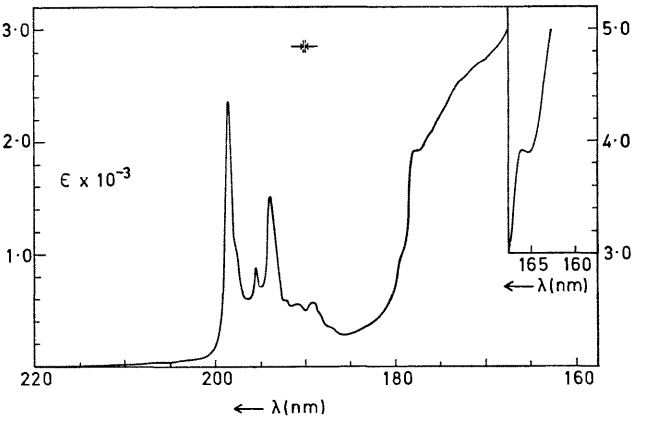

FIGURE 3. *Absorption coefficient of* (+)-3-*methyl-cyclopentanone in the gas phase. Spectral slit width* 0·16 *nm.*

The present instrument is capable of higher resolution than the one used previously[1] as is indicated by the width of the vibronic bands in the first intense system, by the high degree of resolution of the vibronic bands, and by the observation of a third weak band of the vibronic progression. Also a shoulder is clearly resolved at 196 nm.

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This shoulder corresponds to a resolved absorption peak. Further fine structure is probably to be found in the region 190—192 nm. We also find that there is disagreement between the present results and those in ref. 1 in the region 185—170 nm. We find two distinct systems, both weak and of opposite sign. Our results confirm the peak reported by the previous authors, which we find to be located at 166 nm. However, our record is considerably sharper. The $\Delta\epsilon$ values are in reasonably good agreement.

We have also investigated the c.d. of *trans*-cyclo-octene to 165 nm.[3]

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[2] J. C. Kemp, *J. Opt. Soc. Amer.*, 1969, **59**, 950.
[3] O. Schnepp, E. F. Pearson and E. Sharman, *J. Chem. Phys.*, submitted for publication.