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ON THE STRUCTURE AND VIBRATIONAL SPECTRA OF CYCLOPENTADIENYLBERYLLIUM CHLORIDE

K.B. STAROWIEYSKI and J. LUSZTYK

Institute of Organic Chemistry and Technology, Warsaw Technical University (Politechnika), ul. Koszykowa 75, 00-662 Warszawa (Poland)

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Summary

The Raman spectra of solid and liquid C_5H_5BeCl and C_5D_5BeCl and also low temperature IR spectra of these compcunds have been measured. They indicate C_{5v} symmetry of the ring-metal moiety of the molecules. However, the data from mass spectra show an association of the compounds investigated, in the solid state.

The structure of cyclopentadienylberyllium chloride was investigated in the gas phase by electron diffraction [1]. It was found to be monomeric with C_{5v} symmetry of the molecule.

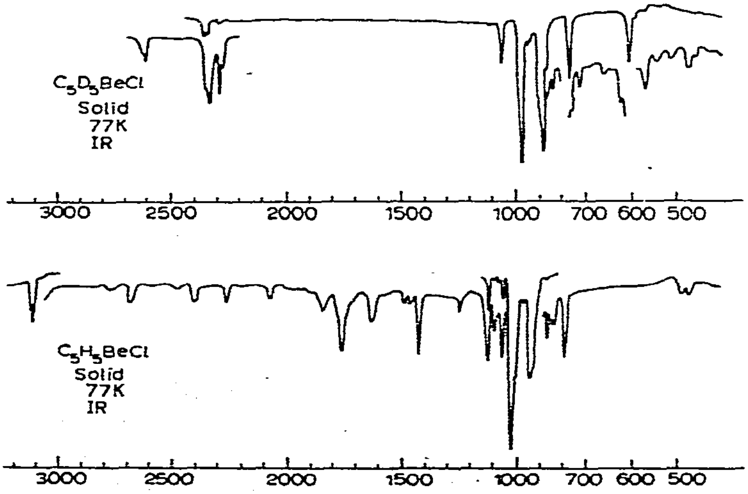

Fig. 1. Low temperature IR spectra of C_5D_5BeCl and C_5H_5BeCl.

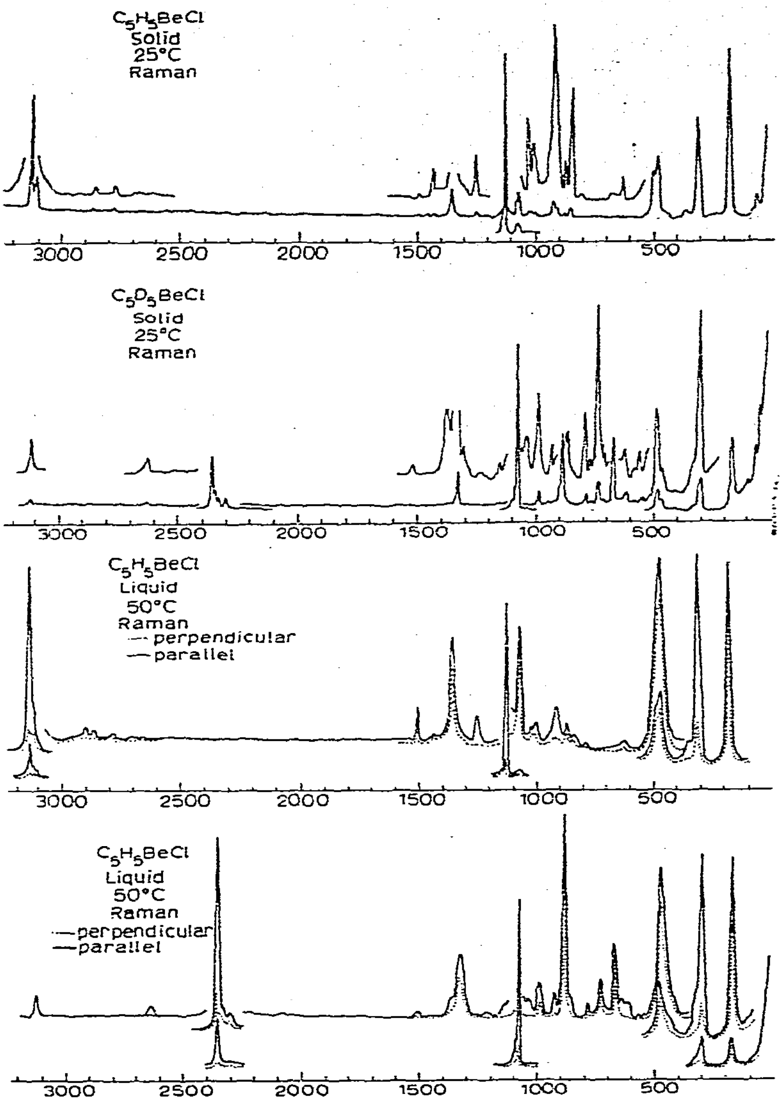

Fig. 2. Raman spectra of solid and liquid C_5H_5BeCl and C_5D_5BeCl.

We also studied the vibrational spectra of C_5H_5BeCl and its derivative with a fully deuterated cyclopentadienyl ring (degree of deuteration 97%). Raman spectra of these compounds in the solid and liquid states, including polarization measurement and low temperature IR spectra, were carried out (Figs. 1 and 2).

Recently Coe et al. published a paper on the vibrational spectra of C_5H_5BeCl [2]. They measured the low temperature IR spectrum and the Raman spectra of the solid and melted compound and assigned the whole spectrum using a C_{5v} symmetry model for the molecule. Our spectra are in very good agreement with those reported in their work. We found three bands in the Raman spectra

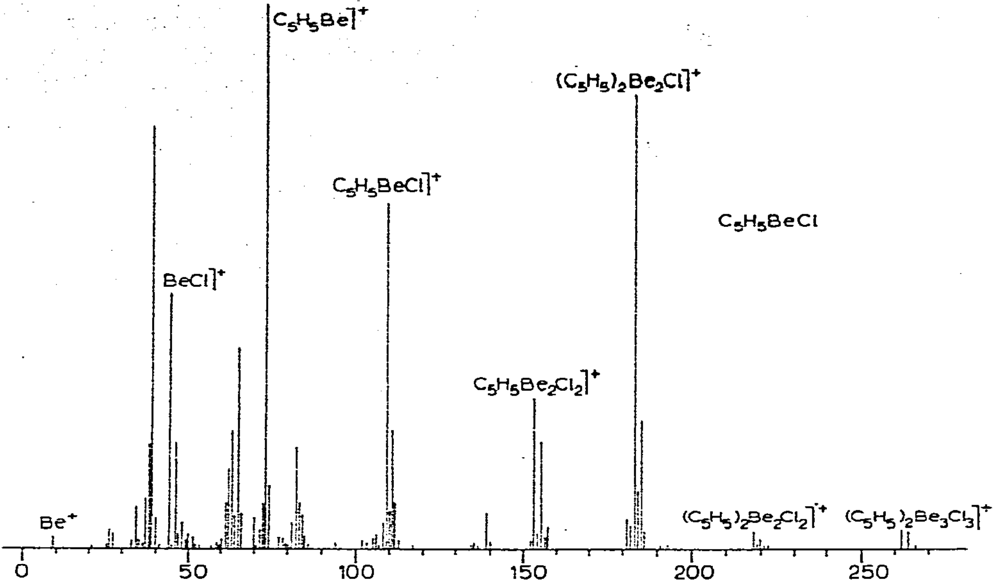

Fig. 3. Mass spectrum of C_5H_5BeCl. 75 eV, temp. of the sample 35° C.

and two in the IR spectrum in the region 3100 cm^{-1} corresponding to C—H stretching vibrations, a very strong Raman and a medium IR band at 1126 cm^{-1} corresponding to ring pulsation, and also bands at 479, 313 cm^{-1} corresponding respectively to ring tilt and ring-metal stretching vibrations. The assignment is confirmed by the relative positions of the bands in the spectra of C_5H_5BeCl and C_5D_5BeCl, the degree of depolarization, and the ratios of the intensities in the Raman and IR spectra. These bands indicate C_{5v} symmetry of ring-metal moiety. The region in which we expected bands corresponding to Be—Cl vibrations is still not solved and we cannot confirm the assignment made by Coe et al. [2].

In order to show whether the monomeric structure of the compound is retained in the solid phase, the mass spectrum of C_5H_5BeCl was measured and is shown in Fig. 3. The assignment was confirmed by the mass spectrum of C_5D_5-BeCl. The compounds were introduced directly into an ionisation chamber from the samples at 35° C. There are strong peaks in the spectrum indicating that the structure of cyclopentadienylberyllium chloride is not monomeric. The spectral evidence of deviation from a monomeric C_{5v} structure in the solid state and detailed discussion of the whole spectrum of C_5H_5BeCl will be the subject of our next paper.

Experimental

The cyclopentadienylberyllium chloride and its deuterated derivative were obtained by the equimolar reactions of $BeCl_2$ and sodium cyclopentadienide or deuterated sodium cyclopentadienide in diethyl ether. We used two methods to obtain deuterated sodium cyclopentadienide. One of these was the method proposed by Trifan and Nicholas [3]: by reduction of deuterated ferrocene. The other was direct synthesis from sodium and deuterated cyclopentadiene, the latter prepared by the method reported by Gallinella and Mirone [4]. The second method is more simple and gives a much better degree of deuteration than the first one.

Acknowledgements

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