Mass Spectra of Some Monocyclopentadienyl Derivatives of Titanium

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Fig. 1. Mass spectra

Figure 1: Fig. 1. Mass spectra

Abstract

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Mass Spectra of Some Monocyclopentadienyl Derivatives of Titanium

The assumption that, in certain cyclopentadienyl derivatives of titanium, there is to a considerable degree an ionic bond between titanium and the cyclopentadienyl ring, which we advanced earlier ([1]), was confirmed by an investigation of the IR ([2]) and NMR ([3]) spectra.

Fig. 1. Mass spectra of $C_5H_5TiCl_3$ *(I)*, $C_5H_5Ti(OC_2H_5)Cl_2$ *(II)*, $C_5H_5Ti(OC_2H_5)_2Cl$ *(III)*, $C_5H_5Ti(OC_2H_5)_3$ *(IV)*

The present work is devoted to the study of the mass spectra of compounds $C_5H_5Ti(OC_2H_5)_{3-n}Cl_n$, where $n = 0, 1, 2, 3$ (see Fig. 1).

For the spectra of all the monocyclopentadienyl derivatives of titanium studied by us, the following features are characteristic: the presence of a molecular ion; formation of the ions $(M - A)^+$ and $(M - 2A)^+$, where A = Cl or OC_2H_5; formation of the ion $C_5H_5^+$. In those cases where $n = 1$ and 2, the ion $(M-HCl)^+$ was recorded, and when $n = 0, 1, 2$, the ion $C_5H_5Ti^+ = O$.

The ratios $I_{M-C_5H_5}/I_M$ in the spectra of the titanium derivatives studied by us are given in Table 1. As can be seen, this ratio increases in the series: $C_5H_5TiCl_3$, $C_5H_5Ti(OC_2H_5)Cl_2$, $C_5H_5Ti(OC_2H_5)_2Cl$, $C_5H_5Ti(OC_2H_5)_3$. It was shown earlier ([4]) that in the mass spectra of cyclopentadienyl derivatives of various metals the ratio of the peaks $I_{M-C_5H_5}/I_M$ increases as the ionic character of the metal –cyclopentadienyl bond increases.

Table 1

No.	Substance	$I_{M-C_5H_5}/I_M$	$I_{M-C_5H_5}/I_{C5H_5}$
1	$C_5H_5TiCl_3$	0.00	0.00
2	$C_5H_5Ti(OC_2H_5)Cl_2$	0.00	0.00
3	$C_5H_5Ti(OC_2H_5)_2Cl$	0.81	0.35

No.	Substance	$I_{M-C_5H_5}/I_M$	$I_{M-C_5H_5}/I_{C5H_5}$
4	$C_5H_5Ti(OC_2H_5)_3$	2.75	0.96

The fragments $(M - C_5H_5)^+$ and $C_5H_5^+$ arise upon cleavage of the $Ti - C_5H_5$ bond in the molecular ion. It was to be expected that, in compounds with a more ionic character of the titanium–cyclopentadienyl bond, the probability of formation of the titanium-containing fragment $(M - C_5H_5)^+$ would increase. Indeed, the value of the ratio $I_{M-C_5H_5}/I_{C5H_5}$ increases in the same series (see Table 1).

Thus, from consideration of the mass spectra of $C_5H_5Ti(OC_2H_5)_{3-n}Cl_n$, where $n = 0, 1, 2, 3$, it may be concluded that the degree of ionicity of the $Ti - C_5H_5$ bond increases with decreasing n. The data obtained are in complete agreement with the chemical behavior, infrared spectra, and NMR spectra of the substances studied by us ([1–3]).

The mass spectra were recorded on an MX-1303 mass spectrometer, $U = 40$ V, $t = 175°$.

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Note: Figure translations are in progress. See original paper for figures.