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THE USE OF POLYMETHINE DYES (PMD) AS THE SENSOR HARMFUL GASES

On the one hand, PMD have good stability, thanks to the rigid structure of the polymethine chain, on the other - are known facts of their fading. Research PMD sensitivity to the presence of harmful gases, in particular ammonia, devoted to this work.

One of the easiest types of the trimethine cyanine dye with substituents: $R_1 = H$ and $R_2 = OCF_3$, $OCCl_3$, $COOH$, NO_2 was used as the model object for research. To find the optimal structure of the PMD complex with ammonia molecule, we set two positions. The first position is associated with the NH group, near to the R_2 substituent, and the second one – with the *NH* group, near to the R_1.

The hazardous gas sensor can detect the change in optical density of the layer or the light intensity, transmitted through the sensor layer.

The ammonia molecule interacts with PMD not only due to the hydrogen bond between the *H* atom and *N* of ammonia molecule, but due to one between the ammonia *H* and *O* atom of R_2-substituent, that distinguishes the results found for the $OCCl_3$ and NO_2 from the other PMD (Tab.1). $OCCl_3$ and NO_2 substituents show the spectrum shift and more sensitivity to the presence of ammonia PMD.

Table 1

The spectral position of the long-wavelength absorption band of PMD complex with ammonia molecule.

PMD molecule		λ_1 ($\Delta\lambda$), first position of NH_3	λ_2 ($\Delta\lambda$), second position of NH_3	The oscillator strength in the second case
($R_1 = H$)	PMD - I OCF_3	472.54 (+0.02)	466.44 (-6.08)	0.959
	PMD -II $OCCl_3$	460.07 (-4.09)	455.47 (-8.69)	0.992
	PMD -III $COOH$	470.65 (-0.38)	465.76 (-5.27)	0.983
	PMD -IV NO_2	468.15 (+3.35)	455.34 (-9.46)	1.020
($R_1 = O$)	PMD - V OCF_3	535.40 (+0.22)	530.61 (-4.57)	0.800
	PMD -VI $OCCl_3$	529.00 (+0.76)	523.70 (-4.54)	0.864
	PMD-VII $COOH$	535.10 (-0.26)	529.58 (-5.78)	0.838
	PMD -VIII NO_2	536.43 (+0.20)	531.42 (-4.81)	0.882