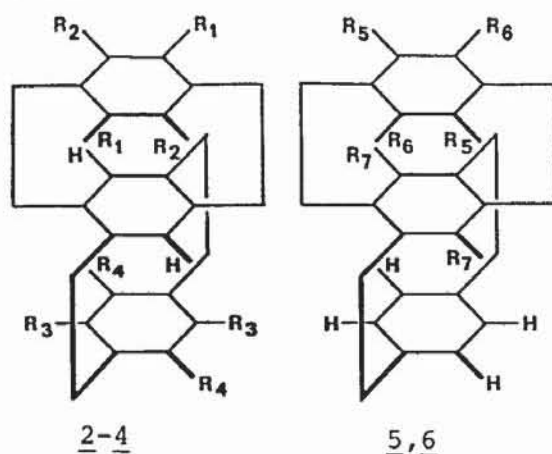


OPTICAL DETECTION OF MAGNETIC
RESONANCE (ODMR) OF TRIPLE-LAYERED PHANES

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The extension of [2.2]phanes into the z-direction (out of plane) by further subunits (triple-, quadruple-, etc. layered phanes) permits to study π -electron interactions through space in stack-like arrangements. The understanding of the π -electron interaction for instance in quasi one dimensional organic semiconductors or metals with alternating or segregated stacks is important, because it contains information about the energy and width of the substantial bands. The emission spectra and the zero field splitting parameters of the excited triplet state $|D|$ and $|E|$ (table 1) of some triple-layered cyclophanes (2-6, fig. 1) [1] with subunits of similar electron affinities were investigated at 1.3 K and compared with those of the monomer 1,4-dimethyl 2,5-dimethoxybenzene (1) and the pseudo-ortho (7) - and pseudo-geminal 4,7,12,15 tetramethoxy [2.2]paracyclophan (8) [2].

Fig. 1



- 2: $R_1=R_3=OCH_3$, $R_2=R_4=H$;
 3: $R_1=R_4=OCH_3$, $R_2=R_3=H$;
 4: $R_2=R_4=OCH_3$, $R_1=R_3=H$;
 5: $R_5=R_7=OCH_3$, $R_6=H$;
 6: $R_6=R_7=OCH_3$, $R_5=H$;

Table 1: Zero Field Splitting Parameters:

	$ D [cm^{-1}]$	$ E [cm^{-1}]$
<u>1</u>	0.1143	0.0351
<u>2</u>	0.0991	0.0218
<u>3</u>	0.0999	0.0256
<u>4</u>	0.1118	0.0286
<u>5</u>	0.0973	0.0301
<u>6</u>	0.1117	0.0289
<u>7</u>	0.0983	0.0281
<u>8</u>	0.0901	0.0226

The extension of the [2.2] phanes 7 and 8 in z-direction by another aromatic subunit leads to a further lowering of the first excited singlet- and triplet state due to the additional transannular interaction. This can be seen from the observed redshifts of the emission spectra. The dependence of the emission spectra of 2-6 on the relative orientations of the OCH_3 -groups is reduced with respect to 7 and 8. Although the D-parameters of 2-6 are reduced with respect to the monomer 1 the reduction is smaller than for the [2.2]-phanes 7 and 8 [2], while the dependence on the relative orientation of the OCH_3 -groups is comparable.

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