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Technical Report No. 5

**Octahedral Metallomesogens:  
Liquid Crystallinity in Low Aspect Ratio Materials**

by

**Hanxing Zheng and Timothy M. Swager**

*J. Am. Chem. Soc.* in press

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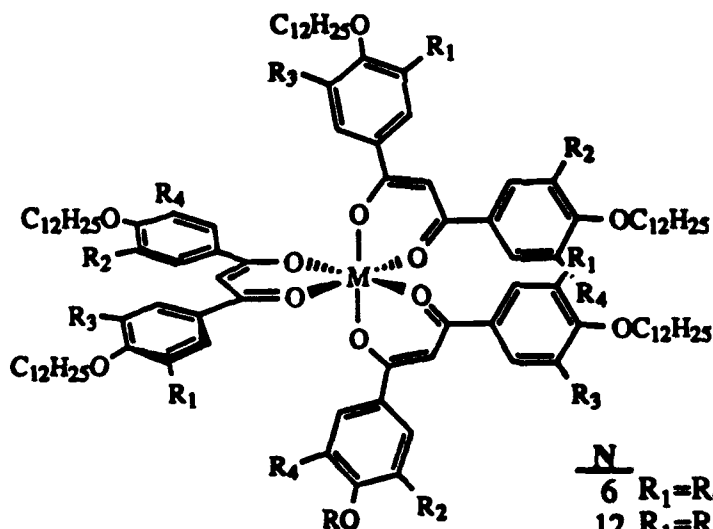
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# Octahedral Metallomesogens: Liquid Crystallinity in Low Aspect Ratio Materials

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## Abstract:

A new class of metallomesogens with octahedral structures 1, 2, and 3 are described. The observation of liquid crystallinity in these materials was unexpected as a result of their low aspect ratios. To better understand these materials, the dependence of the mesomorphism upon the number of sidechains (N) and metal center was investigated. Complexes of 1 (N=6) appear to exhibit a highly ordered smectic phase. However, all of the complexes investigated with N=12, 15, and 18 display columnar mesomorphism. Columnar phases with hexagonal and rectangular symmetry were observed which display optical textures similar to known discotic phases. In addition it was found that the conformational preferences of the alkoxyphenyl groups attached to the 1,3-diketone ligands are coupled to the stability of different phases. Although these phases show textural and structural similarities with known discotic columnar phases, they are not miscible with discotic compounds having similar lattice parameters and regions of mesomorphism. It is proposed that the octahedral complexes exhibit clefts necessary to accommodate sidechains which can not be directed outside the columns core. As a result of the differences from regular discotics, these new columnar phases have been labeled as octahedral hexagonal  $O_h$  and octahedral rectangular  $O_r$ .



1 M=Fe, 2 M=Mn, 3 M=Cr

| N  |                                       |
|----|---------------------------------------|
| 6  | $R_1=R_2=R_3=R_4=H$                   |
| 12 | $R_1=R_2=OC_{12}H_{25}$ , $R_3=R_4=H$ |
| 15 | $R_1=R_2=R_3=OC_{12}H_2$ , $R_4=H$    |
| 18 | $R_1=R_2=R_3=R_4=OC_{12}H_2$          |