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## Non-planar distortion of terrylene molecules in a naphthalene crystal

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### Abstract

The ONIOM(B3LYP/6-31G(d,p):PM3) procedure was used for optimization of terrylene molecule embedded into a naphthalene crystal, which crystallographic lattice was described by the PM3 method. Experimentally observed appearance of the new (absent for isolated molecule) vibronic line in fluorescence excitation spectrum of terrylene in the crystal was attributed to lowering of the molecule symmetry from  $D_{2h}$  to  $C_i$ . Further refinement of the molecule coordinates was proposed in order to achieve the experimentally observed intensity distribution in the fluorescence excitation spectrum.

### 1. Introduction

The vibronic structure of fluorescence excitation spectrum of an organic molecule (as well as the vibrational structure of fluorescence spectrum) can serve as sensitive probe of interaction between the molecule and its local matrix environment. It is especially visible in case of highly symmetric molecules where limited number of  $a_g$  vibrations is allowed by the symmetry selection rules. Any lowering of the molecule symmetry, being the result of a site-specific molecule-matrix interaction, may activate appearance of additional vibronic lines.

In the present contribution we concentrate on terrylene (Tr), one of the most frequently used dye in single-molecule spectroscopic (SMS) studies at cryogenic temperatures. This molecule isolated in vacuum is planar ( $D_{2h}$  symmetry) and its lowest energy excited singlet  $S_1$  state is of the  $B_{1u}$  symmetry. The transition  $S_0 \rightarrow S_1$  is strongly allowed and polarized along the molecule long axis. In the low energy range, up to  $300 \text{ cm}^{-1}$  above the (0, 0) purely electronic origin, the fluorescence excitation spectrum of isolated Tr is composed of only one  $a_g$  transition, in which the constituting atoms oscillate along the long axis of the molecule. Such a spectrum, with single vibronic component separated from the (0, 0) origin by  $\sim 250 \text{ cm}^{-1}$ , was observed by us for single Tr molecules dispersed in *p*-terphenyl [1] and 2,3-

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