EFFECT OF TEMPERATURE AS WELL AS MOLECULAR AND CRYSTAL STRUCTURE ON PHOSPHORESCENCE SPECTRA OF BROMO-SUBSTITUTED BENZOPHENONE ISOMERS

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Using the single-crystal x-ray diffraction technique, we have established the room-temperature structure of ortho-bromobenzophenone (2-bromobenzophenone, OBBP) to be monoclinic with space group P21/a (Z=4). The molecular packing in the crystal under study is compared to that in the crystal of para-bromobenzophenone (4-bromobenzophenone, PBBP) with the same space group [a]. We carried out a comparative study of phosphorescence spectra of liquid solutions and crystals of mono-bromo-substituted benzophenone isomers over a wide temperature range. It has been found that phosphorescence spectra of PBBP solutions and crystals are close to those of molecules and crystals of unsubstituted benzophenone, which is an ideal testing field for studying the photophysical and photochemical properties of flexible molecules, as well as to those of symmetric di-halogeno-substituted benzophenones[b]. The peculiarities of the phosphorescence spectra of OBBP both in solutions and in the solid are discussed versus the specific features of molecular geometry (transformation of the excited triplet state from $n\pi*$ to $\pi\pi*$) and molecular packing in the crystal (triplet eximer emission).

[a] S. Ebbinghaus, D. Abeln, M. Epple, Z. Kristallogr. 212, 339 (1997).
[b] S. Dym, R. M. Hochstrasser, J. Chem. Phys. 52, 2458 (1969).