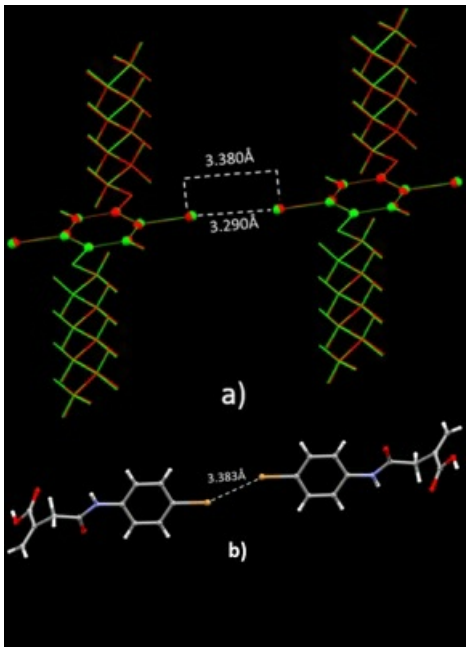
MS077.O04

Time-resolved study of molecular crystals, with anomalously short Br…Br contacts

Krishnayan Basuroy[1], Sounak Sarkar[2], Gage Bateman[1], Jason Benedict[1], Philip Coppens[1]
[1]*Chemistry Department, SUNY Buffalo, Buffalo, United States,* [2]*Solid State and Structure Chemistry Unit, Indian Institute of Science, Bangalore, India*
E-mail: kbasuroy@gmail.com

Purely organic luminescent molecules with long-lived excited states gained a certain amount of interest, due to their wide range of optoelectronic applications. The environment friendliness, non-toxicity and low cost also brought favourable attention over their inorganic counterparts. However, the benefit of using organic phosphorescent materials have been limited by their extreme sensitivity towards the surrounding environment (humidity and temperature) and fast non-radiative quenching. Nonetheless, a number of recent studies on purely organic phosphorescent molecules with unusually short Br...Br intermolecular contact distances have been reported.[1] We have also recently reported the excited state geometry of a Br containing purely organic phosphorescent molecule, studied by means of In-House Time Resolved X-Ray Diffraction.[2] The molecule shows strong luminescence only in solid state when excited at 355nm and does not show any emission in dilute dichloromethane solution. Shi et al. claims the presence of several deactivation processes (non-radiative decay, collisional quenching by oxygen and other impurities) caused this lack of luminescence in solution. We also observed an increment in the Br…Br intermolecular contact distance from 3.29Å (GS) to 3.38Å (ES), in crystals upon light induced excitation at 90K (Figure 1a). It seems that short Br…Br intermolecular interactions may have an important role in causing these molecules to be luminescent in solid state. Recently a series of molecules with short Br…Br intermolecular contacts have been reported (Figure 1b).[3] But most of these studies do not go beyond the crystal structure determination. We are synthesizing some and measuring their photo-physical properties. As the rapid improvement in the brightness of X-ray sources and the sensitivity of detectors, enables the use of laboratory equipment to explore short-lived excited state geometries in molecular crystals, the importance of this technique for the above mentioned class of purely organic luminophores cannot be ignored.

[1] Shi, H. F. et al. (2016). Cryst. Growth Des. 16, 808-813. [2] Basuroy, K. et al. (2017) Structural Dynamics (Manuscrit accepted). [3] Narayana, B. et al. (2014). Acta Cryst. E70, o779-o780.



Keywords: luminescence, time resolved crystallography, Br…Br intermolecular contact