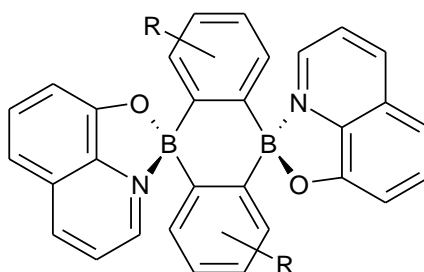




	<b>Experiment title:</b> High pressure crystallographic studies of new boroncontaining luminescent materials relevant for OLED applications	<b>Experiment number:</b> CH-4903
<b>Beamline:</b> ID15B	<b>Date of experiment:</b> from: 25/02/2017 to: 28/02/2017	<b>Date of report:</b> 31/03/2021
<b>Shifts:</b> 9	<b>Local contact(s):</b> Michael Hanfland	<i>Received at ESRF:</i>
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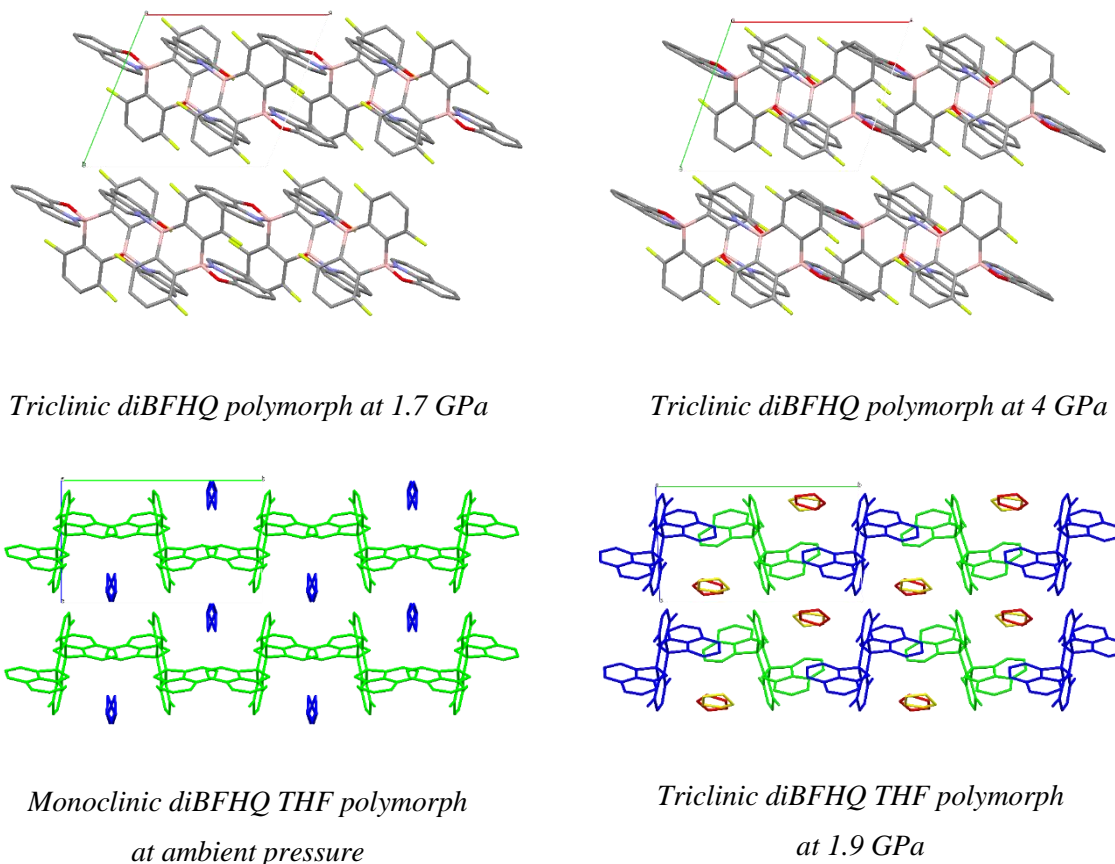
**Report:** Boron compounds were found to be more resistant to hydrolysis and more efficient emitters than their well-known and widely applied Al analogues.<sup>[1]</sup> Due to their high quantum yield values (up to about 60%) and potential applications in the construction of organic-light-emitting diodes (OLEDs) we have focused our attention on the synthesis and crystal structure of a family of bis-8-hydroxyquinoline DBA derivatives (dibenzosilaborins, dibenzoazaborins, dibenzophospha-borins and dibenzochalcogenaborins).

We have chosen three crystal systems for high pressure diffraction studies at ID15b High Pressure Beamline: parent DBA compound and the two polymorphic forms of its fluoro derivative (diBFHQ and tetrahydrofuran solvate, diBFHQ·THF).



**Figure 1.** General scheme of 5,10-bis(8-oxyquinolinato)-5,10-dihydroboranthrenes (R = various fluorine substituents).

High pressure single crystal diffraction experiments under hydrostatic and pseudo-hydrostatic conditions (using helium as the pressure transmitting medium) up to at least 18 GPa revealed series of pressure-induced phase transitions of diBFHQ and diBFHQ·THF crystals.



**Figure 2.** Molecular arrangement of diBFHQ and diBFHQ·THF at various pressure conditions.

Upon compression, diBFHQ undergoes at least to isostructural ( $P\bar{1}$  to  $P\bar{1}$ ) phase transitions, at 2 and 4 GPa respectively. Its tetrahydrofuran solvate forms monoclinic crystals at ambient pressure (space group  $P2_1/a$ ) and transforms to triclinic  $P\bar{1}$  polymorph at 1.9 GPa and at still elevated pressure again to monoclinic phase of  $P2_1$  space group.

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