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Spin-resolved electron density on a tri-radical borazine

The first experimental electron density study of a borazine core was conducted by Guzman et al.[1]. This study allowed for the analysis of charge delocalization (Figure 1.b) in the core of an unsubstituted borazine and confirmed the very low aromaticity of this core compared to a benzene ring.\\\\
Recently, the D. Luneau team focused on the magneto-structural properties of radicals based on a borazine core by performing substitutions on the boron atoms, thereby enabling the study of the influence of these substituents on the borazine core [2]. This work led to the synthesis of new compounds, including a tri-phenyl borazine (B, B', B"-trimethyl-N, N', N"-triphenylborazine) and an open-shell (nitroxide radical) borazine (Figure 1a). In collaboration with our team, a charge density study was conducted on the tri-phenyl borazine using the Hansen and Coppens multipolar model [3]. From a magnetic perspective, spin density maps derived through maximum entropy methods based on polarized neutron diffraction data (ILL Grenoble) collected on a borazine with nitroxide radical groups provided key insights. On the one hand, no intramolecular couplings were observed (no spin density on the borazine core), but inter-molecular ferromagnetic couplings between nitroxide radicals located on parallel layers were identified (Figure 1.c).\\\\
To further analyze these couplings, we are currently refining the experimental electron density, which will serve as a starting point for joint refinement using polarized neutron and high-resolution X-ray diffraction data with the spin split model [4]. This study will allow us to map the spin-resolved electron density of the tri-radical borazine and perform charge integration using Bader's theory, thus leading to a more precise analysis of the influence of nitroxide radicals on the borazine core and its crystalline magnetic behavior.

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