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Single-crystal synchrotron X-ray diffraction study of new anthracene derivative compounds

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Anthracene derivative compounds have recently known an increasing scientific interest thanks to their unique physical properties (i.e., bright luminescence and large charge mobility)[1], making them ideal candidates for applications in new optoelectronic devices.

A structural study of new anthracene derivative compounds was carried out by single-crystal synchrotron X-ray diffraction to have insights on the structure-property relationships, characterize the crystal packing and the main aromatic interactions, and detect the presence of stacking arrangements (see, for example, Figure 1). Synchrotron data were collected at room temperature at the Swiss Light Source (SLS), Villigen, Switzerland, at the beamline X06DA-PXIII[2]. Structure solution was carried out by Direct Methods using SIR2019[3] and refined by SHELXL2014/7[4]. All non-hydrogen atoms were refined anisotropically; the carbon-bound H atoms were placed on geometrically calculated positions and refined using a riding-model approximation. The main crystallographic results are here presented.

References

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