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Resolving the challenging magnetic and electronic structure of thiophene-based heterophenoquinones

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Close-shell ground-state of thiophene-based heterophenoquinones can mysteriously exhibit biradicaloid character. The electronic structure of some examples of these types of molecules have been studied by a combination of Electron Paramagnetic Resonance (EPR), Nuclear Magnetic Resonance (NMR), Raman, Infrared (IR) and synchrotron single crystal X-ray diffraction measurements. This combined approach resolved and provided a detailed picture of the electronic structure of the molecules. Indeed these molecules exhibit response to magnetic fields typical of paramagnets, and may represent a good choice when stable molecules with paramagnetic characters are required.