Ferrocenyl-substituted tris(pyrazolyl)borates – a new ligand type combining redox activity with resistance to hydrogen atom abstraction

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Supporting Information Available

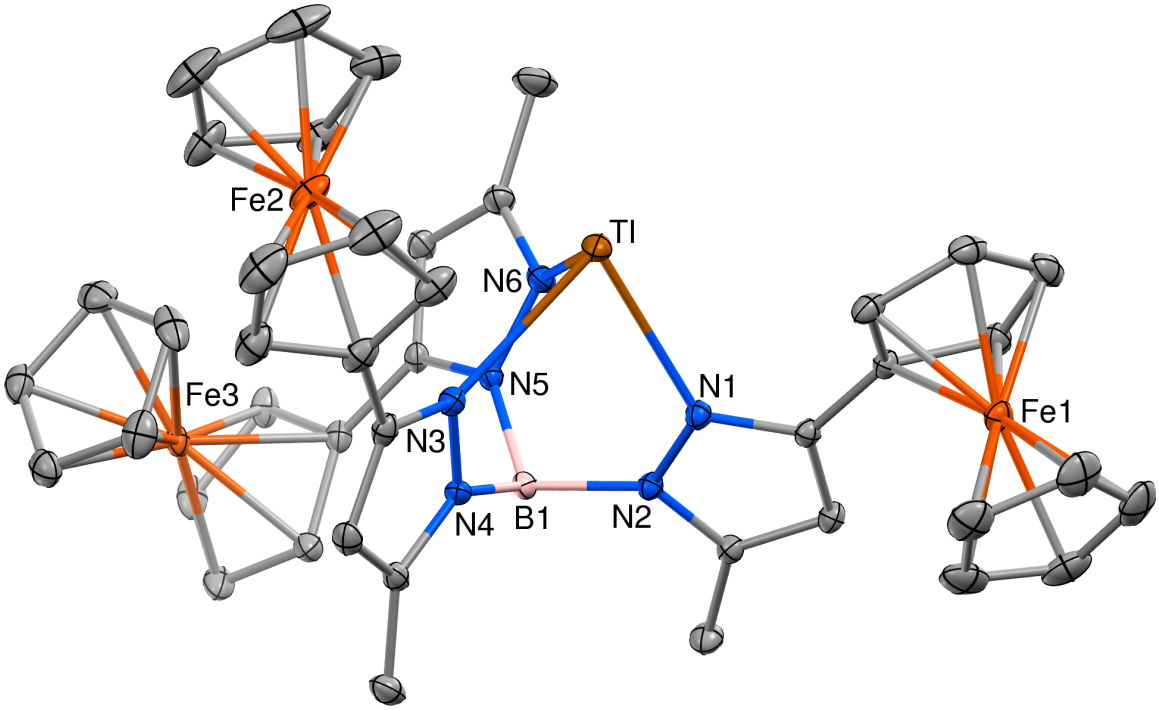

Figure 1S. The molecular structure of $Tp^{Fc,Me*}Tl$ (**2**) at the 30% probability level. Hydrogen atoms have been omitted for clarity. Selected interatomic distances and angles are listed in Table 2 of the manuscript and a comprehensive listing is available in the 'combined.cif' file submitted with this paper.

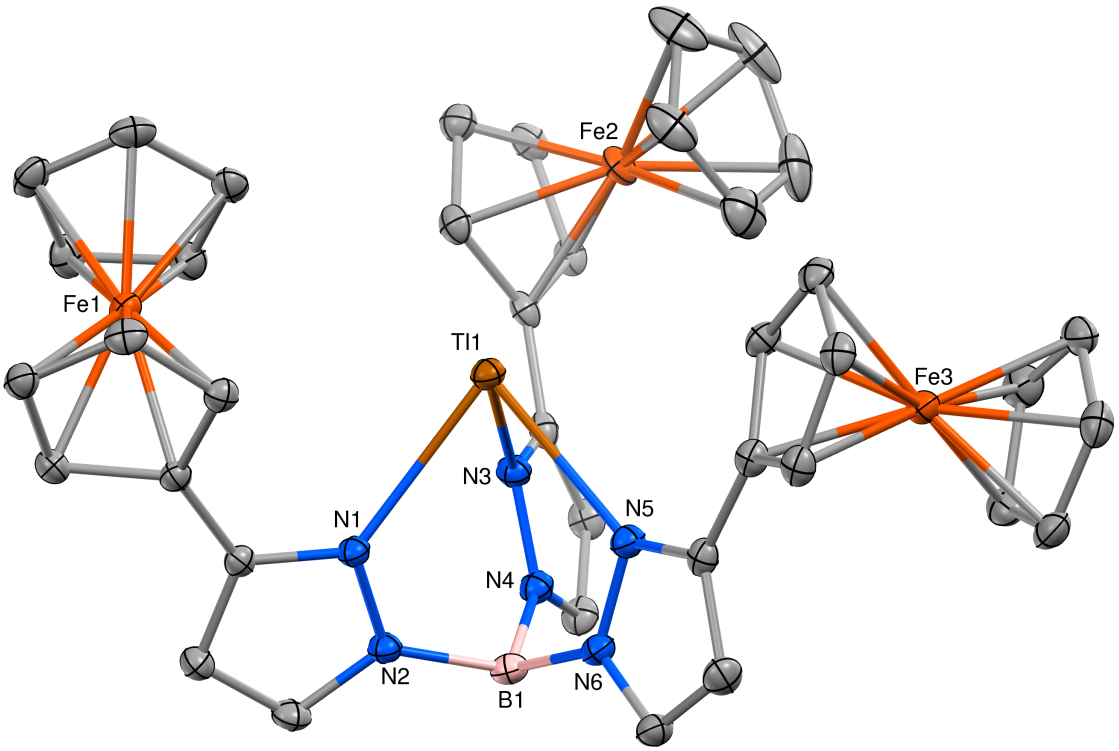

Figure 2S. The molecular structure of $Tp^{Fc}Tl$ (**6**) at the 30% probability level. Hydrogen atoms have been omitted for clarity. Selected interatomic distances and angles are listed in Table 2 of the manuscript and a comprehensive listing is available in the 'combined.cif' file submitted with this paper.

X-ray structural analysis for $Bp^{Fc,CF3}Tl$: A data crystal was selected and mounted on plastic mesh using viscous oil flash-cooled to the data collection temperature. Data were collected on a Bruker-AXS APEX CCD diffractometer with graphite-monochromated Mo-Kα radiation (λ=0.71073 Å). Unit cell parameters were obtained from 60 data frames, 0.3° ω, from three different sections of the Ewald sphere. The systematic absences in the data and the unit cell parameters were consistent to *C*2/*c* and *Cc*. The centrosymmetric space group option yielded chemically reasonable and computationally stable results of refinement. The data were treated with SADABS absorption corrections based on redundant multiscan data. The structure was solved using direct methods and refined with full-matrix, least-squares procedures on F^2. One molecule of cocrystallized solvent chloroform was located in the asymmetric unit. All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were treated as idealized contributions. Atomic scattering factors are contained in the SHELXL-97 (SHELXTL 6.12) program library (Sheldrick, G.M. 2008. Acta Cryst. A64, 112-122). Structural information has been deposited with the Cambridge Structural Crystallographic Centre under depositary number CCDC 1011377.

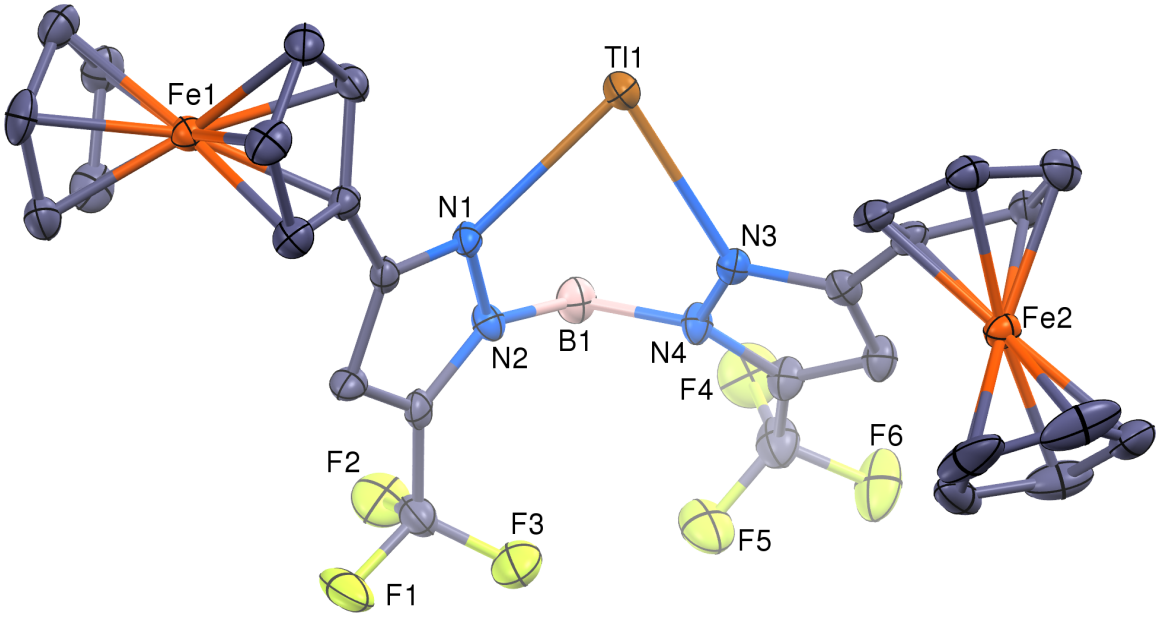

Figure 3S. The molecular structure of $Bp^{Fc,CF3}Tl$ at the 30% probability level. Hydrogen atoms have been omitted for clarity. Selected interatomic distances: Tl1-N1, 2.578(5); Tl1-N3, 2.593(5) Å; and angles: N1-Tl1-N3, 76.54(15)°. Crystallograpic detail and a comprehensive listing of metric parameters is available in the file 'Bp(Fc,CF3)Tl.cif' submitted with this manuscript.