

**1,1'-Diethyl-2,2',3,3',4,4',5,5'-octamethylferrocenium Tetracyanoethylenide,
[Fe(C₅EtMe₄)₂]⁺[TCNE]⁻, a Charge-Transfer Salt Magnetic Solid with a Novel Structural
Motif**

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Abstract

1,1'-Diethyl-2,2',3,3',4,4',5,5'-octamethylferrocene has been utilized as a one-electron donor in the synthesis of a tetracyanoethylene charge-transfer salt, [Fe(C₅EtMe₄)₂]⁺[TCNE]⁻. Structural characterization shows that it adopts an arrangement of anions and cations completely different from the usual π stacking seen in analogous decamethylferrocenium compounds. The TCNE radical sits along side of the ferrocene, nearly perpendicular to the planes of the C₅ rings. It crystallizes in the triclinic space group *P*-1 with unit cell dimensions *a* = 10.4024(9) Å, *b* = 10.7491(9) Å, *c* = 12.9992(11) Å and α = 75.656(2)°, β = 77.715(2)° and γ = 67.9460(10)° and *Z* = 2. The nearly square geometry of the TCNE anion creates disorder over two orientations. [Fe(C₅EtMe₄)₂]⁺[TCNE]⁻ is a simple paramagnet exhibiting neither long range magnetic order nor slow paramagnetic relaxation to the lowest measured temperatures (*ca.* 1.8 K) as determined by both ac and dc magnetic susceptibility and Mössbauer spectroscopy (*ca.* 1.3 K).

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