

Title: Synthesis and structural characterization of iron complexes with 2,2,2-tris(1-pyrazolyl)ethanol ligands: Application in the peroxidative oxidation of cyclohexane under mild conditions

Author(s): Silva, Telma F. S.¹; Guedes da Silva, M. Fátima^{1,2}; Mishra, Gopal S.^{1,3}; **Martins, Luísa M. D. R. S.**^{1,4}; Pombeiro, Armando J. L.¹

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Abstract: The reactions of FeCl₂ center dot 2H₂O and 2,2,2-tris(1-pyrazolyl) ethanol HOCH₂C(pz)(3) (1) (pz = pyrazolyl) afford [Fe{HOCH₂C(pz)(3)}₂][FeCl₄]Cl (2), [Fe{HOCH₂C(pz)(3)}₂](2)[Fe₂OCl₆](Cl)₂ center dot 4H₂O (3 center dot 4H₂O), [Fe{HOCH₂C(pz)(3)}₂] [FeCl{HOCH₂C(pz)(3)}(H₂O)(2)](2)(Cl)₄ (4) or [Fe{HOCH₂C(pz)(3)}₂]Cl-2 (5), depending on the experimental conditions. Compounds 1-5 were isolated as air-stable crystalline solids and fully characterized, including (1-4) by single-crystal X-ray diffraction analyses. The latter technique revealed strong intermolecular H-bonds involving the OH group of the scorpionate 2 and 3 giving rise to 1D chains which, in 3, are further expanded to a 2D network with intercalated infinite and almost plane chains of H-interacting water molecules. In 4, intermolecular pi center dot center dot center dot pi interactions involving the pyrazolyl rings are relevant. Complexes 2-5 display a high solubility in water (S-25 degrees C ca. 10-12 mg mL⁻¹), a favourable feature towards their application as catalysts (or catalyst precursors) for the peroxidative oxidation of cyclo-hexane to cyclohexanol and cyclohexanone, with aqueous H₂O₂/MeCN, at room temperature (TON values up to ca. 385). (C) 2011 Elsevier B. V. All rights reserved.

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Reprint Address: Pombeiro, AJL (reprint author), Univ Tecn Lisboa, Inst Super Tecn, Ctr Quim Estrut, Complexo 1, Av Rovisco Pais, P-1049001 Lisbon, Portugal.

Addresses:

1. Univ Tecn Lisboa, Inst Super Tecn, Ctr Quim Estrut, P-1049001 Lisbon, Portugal
2. Univ Lusofona Humanidades & Tecnol, ULHT Lisbon, P-1749024 Lisbon, Portugal
3. Univ Tras os Montes & Alto Douro UTAD, Ctr Quim, CQ VR, P-5001801 Vila Real, Portugal
4. ISEL, Area Dept Engn Quim, P-1959007 Lisbon, Portugal

E-mail Address: : pombeiro@ist.utl.pt

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