

Supplementary Materials: Catalytic Performance of Fe(II)-scorpionate Complexes towards Cyclohexane Oxidation in Organic, IonicLiquid and/or Supercritical CO₂ Media: A Comparative Study

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Table S1 – Selected data^a for the cyclohexane oxidation using FeCl₂·2H₂O as catalyst.

Entry	Medium	Yield (%) ^b			Total TON ^c	Total TOF ^d (h ⁻¹)	Selectivity towards cyclohexanone ^e (%)
		Cyclohexanol	Cyclohexanone	Total			
1	CH ₃ CN	1.3	2	3.3	16.5	3	61
2	[bmim][PF ₆]	1.1	2.5	3.6	18	3	69
3	[bmim][FAP]	0.4	2	2.4	12	2	83
4	scCO ₂	2.5	1.7	4.2	21	4	40
5	scCO ₂ -[bmim][PF ₆]	1.9	3.2	5.1	25.5	4	63
6	scCO ₂ -[bmim][FAP]	1.7	2.6	4.3	21.5	4	60

^a Reaction conditions, unless stated otherwise: liquid solvent (3.0 mL), CyH (5.0 mmol), TBHP (10.0 mmol), FeCl₂·2H₂O (10.0 μmol, 0.2 mol% vs. CyH), 70 °C, 6 h and *p*(CO₂)=90 bar. ^b Based on GC analysis, after treatment with PPh₃; total yields in moles of cyclohexanol + cyclohexanone per 100 moles of cyclohexane. ^c Total turnover number (moles of cyclohexanol+cyclohexanone per mol of catalyst). ^d TOF (h⁻¹) = TON/time (h). ^e Moles of cyclohexanone per 100 moles of cyclohexanol+cyclohexanone.