S-H bond cleavage in molecules of biological interest with CpFe(dppe)I

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The reaction of CpFe(dppe)I (Cp, cyclopentadienyl; dppe, Ph2P(CH2)2PPh2) with biologically active RSH molecules (L-cysteine hydrochloride, dithiothereitol and 2-mercaptoethanol) in the presence of NH4PF6 and in methanol as solvent afforded the new iron(III) thiolate complexes [CpFe(dppe)SR]PF6. The blue-black paramagnetic complexes were characterized by elemental analysis and IR, EPR and UV-visible spectroscopy. The selective S-H bond cleavage in the thiols suggests a possible utilization of the organometallic iron(II) complexes as inhibitors in some cysteine proteases. The spectroscopic properties of the new complexes have been compared with those of other Fe-S models as well as with Fe-S proteins. Copyright (C) 2000 John Wiley and Sons, Ltd.