

1. Supplementary material

Table 1. Spin state and Stereochemical Relationships for (Porphinato)iron(III)complexes.

Coord. no.	Spin state	Axial ligand [†]	No. comp.	Fe-N _p [†]	Fe-Ct _N ^{††}
5	low	anionic	2 ^a	1.962,2.015	0.18,0.33
5	interm.	anionic	1 ^b	1.994	0.26
5	admix interm.	anionic	3 ^c	1.961-2.001	0.13-0.28
5	admix interm.	neutral	2 ^e	1.979,1.982	0.20,0.21
5	high	anionic	2 ^d	2.064,2.066	0.43,0.46
6	low	anionic	7 ^f	1.970-2.000	-0.03-0.04
		neutral	4 ⁱ	1.982-1.994	0-0.01
6	interm.	neutral	1 ^j	1.978	0
6	admix interm.	anionic	1 ^g	2.021	-0.01
6	admix interm.	neutral	1 ^k	2.006	0.01
6	high	anionic	1 ^h	2.048	0.18
6	high	neutral	3 ^l	2.041-2.045	0

^a Doppelt (1984); English *et al.* (1984). ^b Masuda *et al.* (1980). ^c Gupta, Lang, Lee *et al.* (1987); Shelly *et al.* (1985); Reed *et al.* (1979). ^d Tang *et al.* (1976); Zhang *et al.* (1994). ^e Cheng *et al.* (1994); Gupta, Lang, Reed *et al.* (1987); Scheidt *et al.* (1987). ^f Adams *et al.* (1979); Nasri *et al.* (1991, 1992); Quinn *et al.* (1983); Scheidt *et al.* (1980, 1983); Zhang *et al.* (1984). ^g Gimsmelseed *et al.* (1990). ^h Scheidt, Lee *et al.* (1982). ⁱ Collins *et al.* (1972); Mashiko *et al.* (1979, 1981); Scheidt, Geiger *et al.* (1982). ^j Masuda *et al.* (1982). ^k Scheidt *et al.* (1987). ^l Geiger *et al.* (1984); Mashiko *et al.* (1978); Scheidt *et al.* (1979).

[†] In the hexacoordination system anionic may involve one or two negatively charged ligands. [†] N_p is porphinato nitrogen atom. ^{††}Ct_N is centre of the best plane of the four N_ps.

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