

Table 1. B3LYP/LACVP:CHARMM calculated relative energies (Erel in kcal/mol), group spin densities (ρ), and charges (Q) for the spin states of compound 0 (A and B) and for the ferric-peroxo species (C and D).

Species		Fe	OO(H)	SH	Glu183	His105	Por
Erel							
A	ρ	0.9772	0.0998	-0.0143	0.0003	0.0000	-0.0630
Erel = 0.0	Q	0.5964	-0.3754	-0.6105	-0.0795	0.1152	-0.6462
B	ρ	3.3202	-0.4923	-0.0119	0.0005	0.0000	0.1835
Erel = 12.86	Q	0.7244	-0.2399	-0.6107	-0.0713	0.1176	-0.9201
C	ρ	3.7538	-0.939	0.0491	0.0054	0.0000	0.1307
Erel = 28.25	Q	0.7344	-0.1762	-0.7499	-0.0076	0.1512	-0.9519
D	ρ	0.1308	0.8931	-0.0001	-0.0014	-0.0001	-0.0223
Erel = 29.10	Q	0.5194	-0.1959	-0.7071	0.003	0.1513	-0.7707