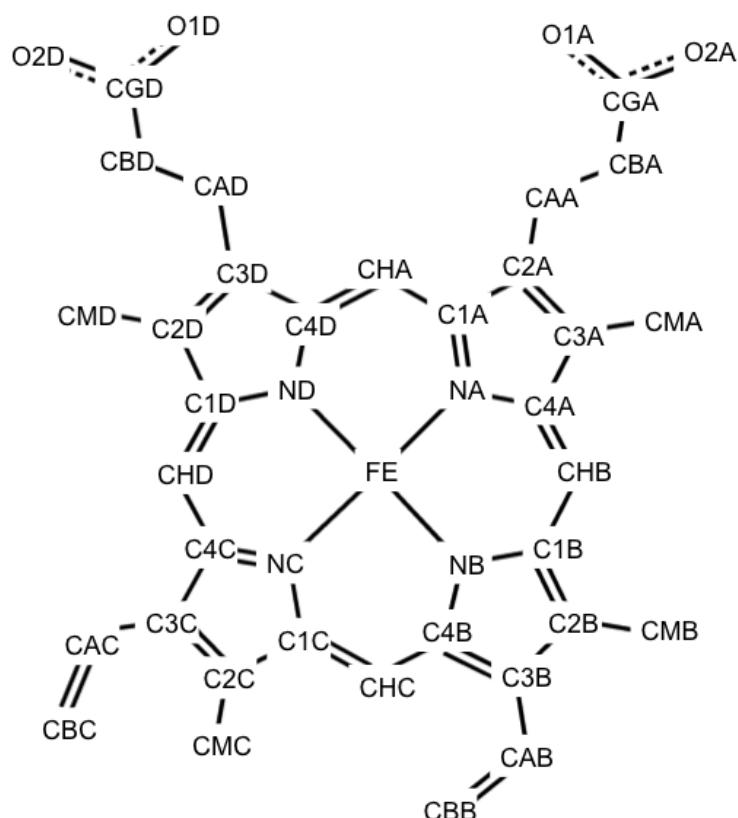


Supplementary information

Storage, transport, release: heme versatility in nitrite reductase electron transfer
studied by molecular dynamics simulations – heme charges

Anna Bauß and Thorsten Koslowski



Heme nonhydrogen atom identifiers

Hydrogen connectivities

HM81	CMA
HM82	CMA
HM82	CMA
HDM	CHB
HM11	CMB
HM12	CMB
HM13	CMB
HV2	CAB
HVC2	CBB
HVT2	CBB
HAM	CHC
HM31	CMC
HM32	CMC
HM33	CMC
HV4	CHC
HVC4	CBC
HVT4	CBC
HBM	CHD
HM51	CMD
HM52	CMD
HM53	CMD
HP61	CAD
HP62	CAD
HP63	CBD
HP64	CBD
HGM	CHA
HP71	CAA
HP72	CAA
HP73	CBA
HP74	CBA

Heme charges

atom ID	heme (Fe II)	heme (Fe III)
FE	0.2500	0.4473
NA	-0.1800	-0.2485
C1A	0.0300	0.0264
C2A	-0.0200	0.0205
CAA	-0.1600	-0.1761
HP71	0.1000	0.1000
HP72	0.1000	0.1000
CBA	-0.3000	-0.3094
HP73	0.1000	0.1000
HP74	0.1000	0.1000
CGA	0.3000	0.2925
O1A	-0.5000	-0.4814
O2A	-0.5000	-0.4773
C3A	0.0200	-0.0083
CMA	-0.2650	-0.2200
HM81	0.0750	0.0750
HM82	0.0750	0.0750
HM83	0.0750	0.0750
C4A	0.0200	0.0639
CHB	-0.1100	-0.0861
HDM	0.1500	0.1500
C1B	0.0300	0.0425
NB	-0.1800	-0.0453
C2B	0.0200	0.0098
CMB	-0.2650	-0.2136
HM11	0.0750	0.0750
HM12	0.0750	0.0750
HM13	0.0750	0.0750
C3B	-0.0500	0.0751
CAB	-0.1300	-0.1641
HV2	0.1500	0.1500
CBB	-0.3000	-0.2250
HVC2	0.1000	0.1000
HVT2	0.1000	0.1000
C4B	0.0200	-0.1197
CHC	-0.1100	0.0221
HAM	0.1500	0.1500
C1C	0.0300	-0.0383
NC	-0.1800	-0.1668
C2C	0.0200	0.0054
CMC	-0.2650	-0.2273
HM31	0.0750	0.0750
HM32	0.0750	0.0750
HM33	0.0750	0.0750
C3C	-0.0500	0.0243
CAC	-0.1200	-0.1512

HV4	0.1500	0.1500
CBC	-0.3000	-0.2199
HVC4	0.1000	0.1000
HVT4	0.1000	0.1000
C4C	0.0200	-0.0463
CHD	-0.1100	-0.0079
HBM	0.1500	0.1500
C1D	0.0300	-0.0815
ND	-0.1800	-0.0709
C2D	0.0200	0.1146
CMD	-0.2650	-0.2184
HM51	0.0750	0.0750
HM52	0.0750	0.0750
HM53	0.0750	0.0750
C3D	-0.0200	0.0882
C4D	0.0200	-0.0654
CHA	-0.1100	-0.0413
HGM	0.1500	0.1500
CAD	-0.1600	-0.1851
HP61	0.1000	0.1000
HP62	0.1000	0.1000
CBD	-0.3000	-0.2979
HP63	0.1000	0.1000
HP64	0.1000	0.1000
CGD	0.3000	0.3156
O1D	-0.5000	-0.4814
O2D	-0.5000	-0.4737