Electronic Supplementary Information for

QM/MM calculations reveal a bridging hydroxo group in a vanadium nitrogenase crystal structure

Bardi Benediktsson, Albert Th. Thorhallsson and Ragnar Bjornsson

Main computational details

The computational model used was prepared analogously to our computational model of MoFe protein as previously described[1]. The crystal structure (PDB ID 6FEA) served as a starting structure and hydrogen positions were added via GROMACS[2]. Protonation states of titratable residues were determined via visual inspection (details in next section). A spherical QM/MM model centered on the carbide of FeVco present in chain D was used as a starting point and a 42 Å sphere cut out around it. Additionally, the whole chains of D, E and F were kept along with residues Ala12 to Arg19, Asn194 to Asp209 and Gly282 to Pro440 from chain B to keep structural integrity. 35 sodium ions were added to counter the total negative charge of the system of -35. In the QM/MM geometry optimizations the active region consisted of ~1000 atoms (approx. spherical region around the cofactor) and QM regions up to 106 atoms were used (details in SI). All QM/MM calculations were performed in Chemshell[3] using DL_POLY[4] as MM code with the CHARMM36 forcefield[5] and ORCA version 3.0.3[6] as QM code. The QM region contained the FeVco cofactor, singly protonated homocitrate (-3 charge) and the sidechains of residues Lys83D (+1 charge), Gln176D, His180D, Cys257D (-1 charge), Arg339D (+1 charge), Lys361D (+1 charge) and His423D as well. All QM/MM calculations used electrostatic embedding, and link atoms were used to terminate the QM/MM border together with the charge-shift procedure as implemented in Chemshell. The QM calculations used the TPSSh hybrid density functional,[7] ZORA scalar relativistic Hamiltonian,[8] the relativistically recontracted def2-TZVP basis set[9,10] on all metal, sulfur, carbide and XH atoms (def2-SVP on other atoms) and a D3 dispersion correction.[11] The RIJCOSX approximation[12] with a Coulomb auxiliary basis set by Weigend[13] was used. Analogous broken-symmetry solutions with M_s=3/2 as for FeMoco were found. The BS7-235 solution was used for all calculations, but alternative BS solutions were briefly explored and additional details can be found below.

---

[1] B. Benediktsson, R. Bjornsson, *Inorg. Chem.* **2017**, *56*, 13417-13429.

[2] a) B. Hess, C. Kutzner, D. van der Spoel, E. Lindahl, *J. Chem. Theory Comput.* **2008**, *4*, 435-47; b) S. Pronk, S. Páll, R. Schulz, P. Larsson, P. Bjelkmar, R. Apostolov, M. R. Shirts, J. C. Smith, P. M. Kasson, D. van der Spoel, B. Hess, E. Lindahl, *Bioinformatics* **2013**, *29*, 845-54; c) M. J. Abraham, T. Murtola, R. Schulz, S. Páll, J. C. Smith, B. Hess, E. Lindahl, *SoftwareX* **2015**, *1*, 19-25.

[3] a) P. Sherwood, A. H. de Vries, M. F. Guest, G. Schreckenbach, C. R. A. Catlow, S. A. French, A. A. Sokol, S. T. Bromley, W. Thiel, A. J. Turner, S. Billeter, F. Terstegen, S. Thiel, J. Kendrick, S. C. Rogers, J. Casci, M. Watson, F. King, E. Karlsen, M. Sjøvoll, A. Fahmi, A. Schäfer, C. Lennartz, *J. Mol. Struct.: THEOCHEM* **2003,** *632,* 1-28; b) S. Metz, J. Kästner, A. A. Sokol, T. W. Keal, P. Sherwood, *WIREs Comput. Mol. Sci.* **2014,** *4,* 101-110.

[4] W. Smith, T. Forester, *J. Mol. Graphics* **1996,** *14,* 136-141.

[5] R. B. Best, X. Zhu, J. Shim, P. E. Lopes, J. Mittal, M. Feig, A. D. Mackerell, *J. Chem. Theory Comput.* **2012**, *8,* 3257-3273.

[6] F. Neese, *WIREs Comput. Mol. Sci.* **2011**, *2,* 73-78

[7] a) J. Tao, J. Perdew, V. Staroverov, G. Scuseria, *Phys. Rev. Lett.* **2003**, *91,* 146401; b) V. N. Staroverov, G. E. Scuseria, J. Tao, J. P. Perdew, *J. Chem. Phys.* **2003**, *119,* 12129-12137.

[8] a) E. van Lenthe, E. J. Baerends, J. G. Snijders, *J. Chem. Phys.* **1993,** *99,* 4597-4610; b) C. van Wüllen, *J Chem Phys,* **1998**, *109,* 392.

[9] F. Weigend, R. Ahlrichs, *Phys. Chem. Chem. Phys.* **2005**, *7,* 3297-3305.

[10] D. A. Pantazis, X. Chen, C. R. Landis, F. Neese, *J. Chem. Theory Comput.* **2008**, *4,* 908-919.

[11] a) S. Grimme, J. Antony, S. Ehrlich, H. Krieg, *J. Chem. Phys.* **2010**, *132,* 154104; b) S. Grimme, S. Ehrlich, L. Goerigk, *J. Comput. Chem.* **2011**, *32,* 1456-1465.

[12] a) F. Neese, F. Wennmohs, A. Hansen, U. Becker, *Chem. Phys.* **2009**, *356,* 98-109; b) R. Izsák, F. Neese, *J. Chem. Phys.* **2011**, *135,* 144105.

[13] K. Eichkorn, F. Weigend, O. Treutler, R. Ahlrichs, *Theor. Chem. Acc.* **1997**, *97,* 119-124.

Amino acid protonation states and solvation

- No arginine or lysine were deprotonated and no glutamate was protonated. The following aspartates were protonated: Asp9A/D, Asp30C/F and Asp73C/F.

- For asparagine and glutamine, the amide functional group is flipped. As for histidine, the imidazole functional group is flipped. The following residues had their functional group flipped: His120A/D, His426A/D, 243B/E, Gln249A/D, Gln3C/F, Gln46C/F, Gln267B/E, Gln361B/E and Asn260B/E. As for histidine in the protein, the following were protonated on the epsilon nitrogen: His18A/D, His70A/D, His81A/D, His91A/D, His106A/D, His120A/D, His180A/D, His181A/D, His234A/D, His248A/D, His342A/D, His416A/D, His423A/D, His426A/D, His453A/D, His111C/F, His51E/B, His67E/B, His158E/B, His234E/B, His321E/B, His379E/B, His409E/B, His461E/B. The following histidine residues were protonated on the delta nitrogen: His364A/D, His448A/D, His5C/F, His110C/F, His80E/B, His177E/B, His334E/B, His386E/B. The only histidine found to be doubly protonated is His150E/B and no histidine is found to be deprotonated.

- As for the cysteine residues that are bound to the P-cluster, they were deprotonated and are as follows: Cys49A/D, Cys138A/D, Cys56E/B, Cys75A/D, Cys31B/E and Cys115B/E. The cysteine that is bound to FeVco is also deprotonated, Cys257A/D.

- After protonation and solvation, the system contained 7956 atoms and had 61- charge. The charge was neutralized with the addition of 61 Na^+ ions. The protonated system was then dissolved in approximately 5000 nm^3 cubic box with 151818 water molecules (TIP3P). Water molecules and hydrogen atoms were relaxed using the steepest descent algorithm whereas heavy atoms were constrained. The system was simulated for 2 ns in the canonical ensemble with a Berendsen thermostat with 4 chains. After 2 ns a 42 Å spherical cutout model centered on the carbide of FeVco in the DEF chains was extracted.

Hydrogen-bonding analysis

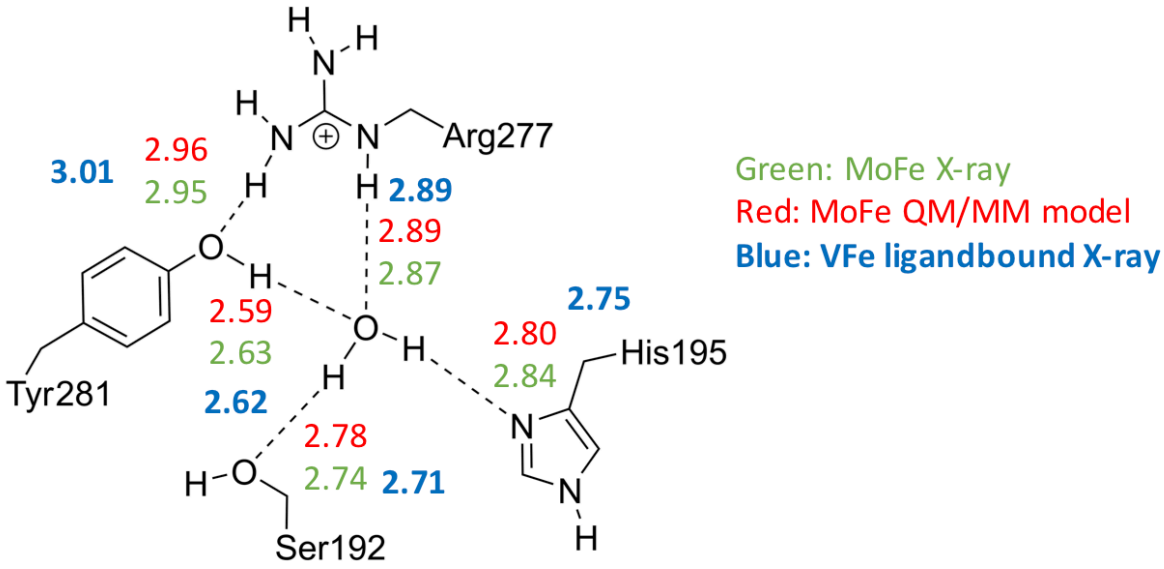

Figure S1. Comparison of hydrogen-bonded distances (Å) for residues His195, Ser192, Tyr281 and Arg277 and a crystallographic water molecule. The MoFe protein crystal structure (3U7Q) is compared to a QM/MM model of the same protein and to the analogous residues in the VFe ligandbound crystal structure

Metal-metal distance comparison between crystal structures

Table S1 demonstrates the reproducibility of metal-metal distances in various crystal structures of MoFe nitrogenase as well a comparison to calculated distances from the MoFe protein QM/MM model (from B. Benediktsson, R. Bjornsson, *Inorg. Chem.* **2017**, *56*, 13417-13429.)

Table S1. Difference in specific metal-metal distances (Å) between one of the cofactors of the 1.0 Å resolution 3U7Q MoFe structure and the cofactors from other MoFe crystal structures. A-D letters refer to different cofactors in each protein (1M1N has two proteins in the crystallographic cell and thus four cofactors).

Resolution:	1.00	1.16	1.16	1.16	1.16	1.43	2.00	2.00	2.00	1.08	1.08	QM/MM
Structure:	3U7Q B	1M1N A	1M1N B	1M1N C	1M1N D	4TKU A	4TKU B	4WNA A	4WNA B	4WES A	4WES B	
Fe1_Fe2	-0.01	0.00	0.01	-0.01	0.00	-0.01	0.00	-0.02	0.00	0.01	0.00	0.02
Fe1_Fe3	0.01	0.00	0.01	0.00	0.00	0.00	0.00	0.00	-0.04	0.00	-0.01	0.03
Fe1_Fe4	-0.01	0.00	0.00	-0.01	0.00	0.00	0.01	0.01	0.01	0.04	0.05	0.01
Mo_Fe6	0.01	0.00	0.00	0.01	0.00	0.02	0.01	0.03	0.01	-0.01	-0.01	0.03
Mo_Fe7	0.00	0.00	0.00	-0.01	-0.01	0.01	0.01	0.03	0.03	0.00	0.01	0.06
Mo_Fe5	0.00	0.00	0.00	0.01	0.00	0.01	0.00	0.01	0.01	0.03	0.03	0.02

Fe2-Fe3	0.00	0.00	0.01	0.00	0.01	0.01	0.01	0.01	0.02	0.00	0.00	0.02
Fe3-Fe4	0.00	0.00	0.00	0.00	-0.01	0.00	0.00	0.01	-0.02	-0.02	-0.02	0.03
Fe2-Fe4	0.00	0.00	0.01	0.00	0.00	0.02	0.02	0.03	0.02	0.00	0.00	0.03
Fe6-Fe7	0.00	0.00	0.01	0.02	0.01	0.01	0.00	-0.01	0.00	0.01	0.01	0.04
Fe5-Fe6	0.00	-0.01	0.00	0.02	0.00	0.00	-0.01	0.01	0.02	0.00	0.00	0.00
Fe5-Fe7	0.00	0.00	0.01	0.01	0.01	0.00	-0.01	0.02	0.02	0.00	0.00	0.01
Fe2-Fe6	0.00	0.00	0.00	0.00	0.00	0.00	-0.01	0.00	-0.01	0.00	0.00	-0.01
Fe3-Fe7	0.00	0.03	0.03	0.03	0.03	0.03	0.03	-0.01	-0.01	0.02	0.02	0.00
Fe4-Fe5	-0.01	-0.03	-0.04	-0.04	-0.03	-0.03	-0.03	-0.03	-0.05	0.00	0.00	-0.01

QM Cluster models

The QM cluster models did not include any protein environment apart from His180 and Gln176. The COSMO continuum solvation model with dielectric constant of 4 was used. Hydrogen capping atoms were used to saturate dangling bonds. Constraints on all CH3 groups in the model were used to keep residues in place.

ORCA input for all cluster models:

! TPSSH RIJCOSX D3BJ def2-TZVP def2-TZVP/J opt Grid5 FinalGrid6 tightscf cosmo slowconv

Table S2: Structural parameters of models, distances in Å and dihedrals in degrees.

Fe_2-Fe_3 lig.: **Fe_1-Fe_2 lig.:** **Redox state:**	NH CO_3^{2-} E0	NH NO_3^- E0	OH CO_3^{2-} E0	OH NO_3^- E0	*Crystal* *ABC, DEF*[a]
Q_{176}-X	2.90	2.75	3.20	2.89	2.51, 2.39
Q_{176}-H_{180}	3.93	3.91	2.84	2.82	2.85, 2.83
Q_{176}-HC	2.56	2.55	4.57	2.98	2.87, 2.91
Fe_2-X	1.95	1.88	1.98	1.95	2.01, 2.08
Fe_3-X	1.95	1.87	1.98	1.94	2.01, 2.05
Fe_2-Fe_3	2.43	2.43	2.69	2.51	2.64, 2.65
<Fe_2-Fe_3-Q_{176}-X.	-40.01	-37.77	-34.25	-29.70	4.30, 6.11
C-X	3.04	2.95	3.01	2.99	3.05, 3.15
V-Fe_2	2.68	2.66	2.76	2.65	2.71, 2.70
V-Fe_3	2.61	2.66	2.89	2.65	2.79, 2.78
V-Fe_4	2.70	2.69	2.82	2.65	2.77, 2.76
Fe_1-Fe_4	2.59	2.58	2.68	2.57	2.58, 2.59
Fe_1-Fe_2	2.57	2.55	2.70	2.55	2.64, 2.58
Fe_4-Fe_5	2.49	2.53	2.52	2.50	2.58, 2.64
Fe_4-Fe_6	2.63	2.59	2.70	2.59	2.79, 2.78
Fe_1-Fe_5	2.61	2.60	2.63	2.58	2.60, 2.60
Fe_1-Fe_6	2.60	2.63	2.74	2.64	2.69, 2.68
Fe_2-Fe_5	2.61	2.61	2.71	2.61	2.67, 2.67
Fe_2-Fe_6	2.61	2.58	2.68	2.63	2.59, 2.59
Fe_3-Fe_5	2.58	2.59	2.60	2.58	2.63, 2.64
Fe_3-Fe_6	2.60	2.60	2.69	2.58	2.64, 2.63
Fe_3-Fe_7	2.63	2.59	2.66	2.58	2.64, 2.65

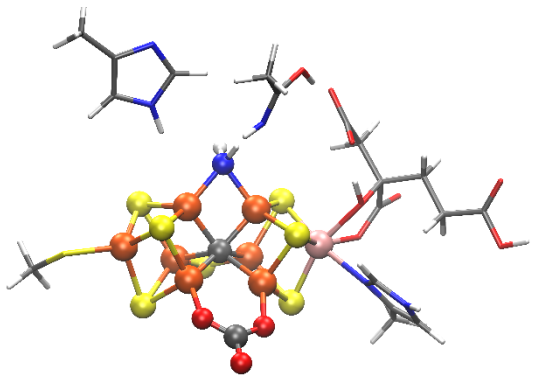

Figure S1: 83 atom cluster model with NH^{2-} and carbonate. NH group is protonated by amide group.

83
Fe7VC20N6H30S8O11

V	93.721179000	97.860666000	112.931460000
Fe	99.136203000	100.423885000	116.321876000
Fe	97.356170000	98.544548000	116.134683000
Fe	98.349972000	99.565821000	113.984819000
Fe	96.730764000	100.985404000	115.491676000
Fe	94.744634000	100.085160000	114.027134000
Fe	95.434867000	97.739567000	114.891737000
Fe	96.321338000	98.540925000	112.706364000
S	97.232364000	100.140303000	117.599488000
S	99.514073000	98.370502000	115.548548000
S	98.693754000	101.688634000	114.462440000
S	93.450983000	98.625334000	115.108461000
S	95.568767000	96.470437000	113.112788000
S	94.636645000	99.660223000	111.818435000
S	98.368263000	98.748056000	111.953420000
C	96.490497000	99.299992000	114.509923000
N	96.502459000	96.796713000	116.228295000
H	97.038998000	96.015615000	115.846442000
C	94.457706000	102.755666000	115.108843000
O	95.587987000	102.518172000	115.752073000
O	94.009969000	101.844027000	114.260799000
O	93.821551000	103.820853000	115.295273000
O	92.267984000	96.428649000	113.586558000
O	92.656577000	94.570004000	110.588973000
O	93.255082000	96.630561000	111.274512000
O	93.585136000	93.358612000	115.862871000
H	93.596102000	93.791842000	117.315377000
O	92.232721000	95.140604000	115.701605000
O	87.708810000	96.407047000	111.423195000
H	86.771850000	96.122463000	111.473394000
O	87.860895000	94.524189000	112.656158000
C	92.220219000	95.177478000	112.885695000
C	92.761413000	95.457993000	111.460916000
C	93.094609000	94.159467000	113.652699000
C	92.945879000	94.224904000	115.185787000
C	90.754980000	94.716071000	112.793277000
C	89.882689000	95.796208000	112.163682000
C	88.419983000	95.475478000	112.130885000
H	92.231934000	96.139029000	114.581562000
H	90.007017000	96.742285000	112.717081000
H	90.206249000	96.029711000	111.137159000
H	90.719337000	93.794486000	112.195760000
H	90.394931000	94.482319000	113.805780000
H	92.886515000	93.135484000	113.312008000
H	94.155339000	94.365450000	113.438674000
C	91.694000000	98.865997000	109.843002000
H	92.369191000	99.686823000	109.522905000
H	90.859001000	98.669998000	109.137001000
H	92.419998000	98.028000000	109.914001000
N	91.736407000	98.862551000	112.400876000
C	91.106168000	99.129631000	111.189321000
C	90.892779000	99.226896000	113.361380000
H	91.090381000	99.159663000	114.424852000
N	89.742703000	99.711931000	112.827448000
H	88.953717000	100.067522000	113.354388000

C	89.857070000	99.656370000	111.451409000
H	89.059240000	99.976470000	110.791532000
S	100.508600000	101.597461000	117.690051000
C	102.051003000	101.861000000	116.720001000
H	102.511194000	102.809634000	117.068832000
H	101.876999000	101.940002000	115.625999000
H	102.742996000	101.014999000	116.919998000
C	93.647003000	95.205002000	120.335999000
H	93.521004000	94.196357000	120.781934000
H	92.721001000	95.794998000	120.502998000
H	94.525002000	95.717003000	120.785004000
C	93.912891000	95.061214000	118.850493000
O	93.537780000	93.876779000	118.367496000
N	94.470007000	95.973521000	118.133204000
H	94.648580000	96.803285000	118.710673000
H	95.829680000	96.428332000	116.927100000
C	100.043999000	95.387001000	122.435997000
H	99.674004000	95.912003000	123.342003000
H	100.236514000	94.300820000	122.559484000
H	101.002998000	95.862999000	122.137001000
N	98.016079000	94.815160000	120.997387000
C	99.118470000	95.615847000	121.261067000
C	97.468562000	95.304671000	119.885364000
H	96.596246000	94.917616000	119.367003000
N	98.159464000	96.383595000	119.423135000
H	97.942791000	96.925018000	118.576787000
C	99.217089000	96.595213000	120.284222000
H	99.923712000	97.402612000	120.124319000

Constrained atoms
{ C 45 C }
{ C 46 C }
{ C 47 C }
{ C 48 C }
{ C 58 C }
{ C 59 C }
{ C 60 C }
{ C 61 C }
{ C 62 C }
{ C 63 C }
{ C 64 C }
{ C 65 C }
{ C 71 C }
{ C 72 C }
{ C 73 C }
{ C 74 C }

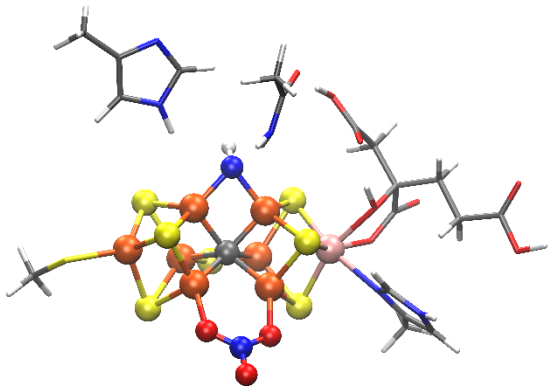

Figure S2: 83 atom cluster model with NH_2^- and nitrate.

83
Fe7VC19N7H30S8O11

V	93.629555000	97.862345000	113.049074000
Fe	99.107423000	100.353127000	116.416215000
Fe	97.253953000	98.492131000	116.328295000
Fe	98.311737000	99.366716000	114.130400000
Fe	96.760500000	100.908419000	115.509669000
Fe	94.758870000	100.026795000	114.114879000
Fe	95.296996000	97.708664000	115.114942000
Fe	96.258128000	98.382890000	112.878553000
S	97.151000000	100.228668000	117.658914000

S	99.404861000	98.238754000	115.778695000
S	98.724529000	101.500329000	114.468252000
S	93.344185000	98.710497000	115.197403000
S	95.396013000	96.386499000	113.369967000
S	94.665489000	99.574293000	111.926218000
S	98.315495000	98.419246000	112.169185000
C	96.439791000	99.195006000	114.647137000
N	96.289808000	96.884151000	116.470129000
H	96.804714000	96.036014000	116.200064000
N	94.551022000	102.802438000	115.017920000
O	95.686103000	102.608185000	115.598659000
O	94.063224000	101.883345000	114.251727000
O	93.927226000	103.860117000	115.194202000
O	92.114260000	96.475909000	113.725708000
O	92.335095000	94.646157000	110.705278000
O	93.145191000	96.622358000	111.424187000
O	93.880786000	93.524915000	115.796179000
H	93.960276000	93.775744000	116.816770000
O	92.275527000	95.093385000	115.871638000
O	87.465607000	96.539180000	111.810492000
H	86.531577000	96.242977000	111.855358000
O	87.676879000	94.545622000	112.848320000
C	92.021879000	95.222025000	113.025414000
C	92.540280000	95.501871000	111.587607000
C	92.927980000	94.173840000	113.714470000
C	92.983709000	94.304590000	115.225687000
C	90.551795000	94.782785000	112.987993000
C	89.668524000	95.875334000	112.396159000
C	88.204874000	95.548938000	112.394686000
H	92.120337000	96.239765000	114.700314000
H	89.803688000	96.817957000	112.951063000
H	89.965633000	96.112698000	111.362174000
H	90.483016000	93.866152000	112.386269000
H	90.222833000	94.541657000	114.009923000
H	92.598830000	93.157190000	113.454887000
H	93.963968000	94.277984000	113.358488000
C	91.694000000	98.865997000	109.843002000
H	92.369191000	99.686822000	109.522905000
H	90.859001000	98.669998000	109.137001000
H	92.419998000	98.028000000	109.914001000
N	91.690389000	98.889018000	112.416502000
C	91.087608000	99.131294000	111.183488000
C	90.816327000	99.259098000	113.348904000
H	90.983772000	99.205946000	114.418245000
N	89.675888000	99.722086000	112.778639000
H	88.864232000	100.066443000	113.278278000
C	89.825615000	99.644979000	111.408162000
H	89.041814000	99.945873000	110.722977000
S	100.505495000	101.601807000	117.688470000
C	102.051003000	101.861000000	116.720001000
H	102.511194000	102.809634000	117.068832000
H	101.876999000	101.940002000	115.625999000
H	102.742996000	101.014999000	116.919998000
C	93.647003000	95.205002000	120.335999000
H	93.521004000	94.196357000	120.781934000
H	92.721001000	95.794998000	120.502998000
H	94.525002000	95.717003000	120.785004000
C	94.004477000	95.110743000	118.861460000
O	94.070561000	93.983036000	118.294755000
N	94.306654000	96.264506000	118.267485000
H	94.281507000	97.102300000	118.843591000
H	94.949651000	96.377700000	117.415717000
C	100.043999000	95.387001000	122.435997000
H	99.674004000	95.912003000	123.342003000
H	100.236514000	94.300820000	122.559484000
H	101.002998000	95.862999000	122.137001000
N	98.063545000	94.686611000	121.001617000
C	99.091025000	95.581263000	121.273960000
C	97.455799000	95.149700000	119.909928000
H	96.624069000	94.677902000	119.392963000
N	98.032648000	96.300563000	119.466580000
H	97.752368000	96.829921000	118.629385000
C	99.079746000	96.588870000	120.320555000
H	99.707668000	97.459784000	120.167699000

Constrained atoms
{ C 45 C }
{ C 46 C }
{ C 47 C }
{ C 48 C }

{ C 58 C }
{ C 59 C }
{ C 60 C }
{ C 61 C }
{ C 62 C }
{ C 63 C }
{ C 64 C }
{ C 65 C }
{ C 71 C }
{ C 72 C }
{ C 73 C }
{ C 74 C }

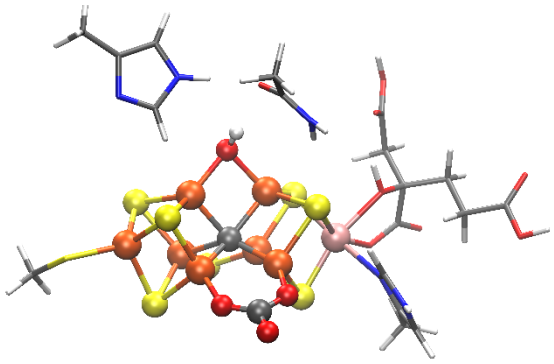

Figure S3: 83 atom cluster model with OH and carbonate.

83
Fe7VC20N5H30S8O12

V	93.728705219	97.245120836	112.574733631
Fe	99.154979439	100.229602512	116.397593835
Fe	97.558237432	98.009820429	116.182844394
Fe	98.356501340	99.216107954	114.016770967
Fe	96.605463005	100.453843763	115.589381226
Fe	94.591473792	99.262013877	114.249386176
Fe	95.649502484	96.840244884	114.695912077
Fe	96.415172770	98.095168003	112.643122855
S	97.271745206	99.664502824	117.690157431
S	99.804685658	98.222045952	115.555019088
S	98.436994712	101.416454994	114.532495162
S	93.463410408	97.320175260	114.949086124
S	95.769405788	95.877682492	112.626027426
S	94.623256047	99.274768461	111.929171282
S	98.456594991	98.563097088	111.913397619
C	96.496077627	98.710863605	114.577211599
O	96.782513316	96.187024264	116.184005040
H	96.249175122	95.844028363	116.917441514
C	93.949520736	101.721016946	115.576967189
O	95.241370373	101.780717192	115.828587935
O	93.501702979	100.679486225	114.902697175
O	93.177558970	102.613965431	115.958562192
O	92.501789722	95.455356429	112.765625130
O	92.632720285	94.990586093	109.273356155
O	93.456439824	96.513237118	110.695891642
O	93.719608488	91.412032049	112.965110209
H	93.686383492	91.030111130	113.860479147
O	92.956796886	93.178182199	114.114225950
O	87.718484943	95.792239896	111.288528245
H	86.819144178	95.422340893	111.311569867
O	88.187663099	93.608350613	111.504334856
C	92.430258260	94.579729742	111.625756482
C	92.860470333	95.420790776	110.408731373
C	93.451719337	93.441554168	111.767105668
C	93.327588098	92.693956958	113.057612075
C	91.000992363	94.062775554	111.476237997
C	90.006387082	95.211303087	111.384426450
C	88.579347578	94.752576679	111.399995423
H	92.686935291	94.907641936	113.558654838
H	90.147114703	95.910509308	112.213579770
H	90.162170035	95.796803647	110.473390645
H	90.952503033	93.446080715	110.577536490
H	90.755760921	93.429617157	112.333243251

H	93.386758028	92.764347951	110.916835897
H	94.456881794	93.890231163	111.782409625
C	91.694000006	98.865996899	109.843002088
H	92.369191014	99.686822041	109.522904958
H	90.859000993	98.669998025	109.137000968
H	92.419997986	98.028000031	109.914000993
N	91.745991831	98.366407606	112.325403304
C	91.198850522	99.053969155	111.239475924
C	91.078994798	98.768499299	113.395894792
H	91.284762061	98.465801581	114.407463565
N	90.130529355	99.663138349	113.060805994
H	89.535554578	100.151150080	113.710814481
C	90.191766399	99.858573966	111.698737419
H	89.532209694	100.540129591	111.189260453
S	100.502053231	101.587196947	117.672406677
C	102.051003048	101.860999932	116.720001068
H	102.511193989	102.809634021	117.068831980
H	101.876998997	101.940002021	115.625998965
H	102.742995971	101.014999027	116.919997990
C	93.647002842	95.205002075	120.335998882
H	93.521004050	94.196355952	120.781935053
H	92.721001050	95.794997977	120.502998008
H	94.525002049	95.717003001	120.785004047
C	93.979442130	95.135635158	118.852901844
O	95.072781890	94.701857363	118.455240231
N	93.055782596	95.596374523	117.996616232
H	92.231207249	96.065055763	118.335383669
H	93.298448581	95.746561643	117.019627089
C	100.043998986	95.387001027	122.435997005
H	99.674004001	95.912002994	123.342002994
H	100.236514009	94.300819985	122.559484000
H	101.002998004	95.862998998	122.137001000
N	98.801379991	96.869806908	120.856418931
C	99.028778165	95.604762154	121.359235887
C	97.825476112	96.736100259	119.976124701
H	97.412943403	97.530776339	119.370106621
N	97.408132364	95.449366996	119.889352420
H	96.635340589	95.100778478	119.316101899
C	98.168489476	94.711663847	120.769851186
H	98.027320766	93.650009603	120.891415281

Constrained atoms
{ C 45 C }
{ C 46 C }
{ C 47 C }
{ C 48 C }
{ C 58 C }
{ C 59 C }
{ C 60 C }
{ C 61 C }
{ C 62 C }
{ C 63 C }
{ C 64 C }
{ C 65 C }
{ C 71 C }
{ C 72 C }
{ C 73 C }
{ C 74 C }

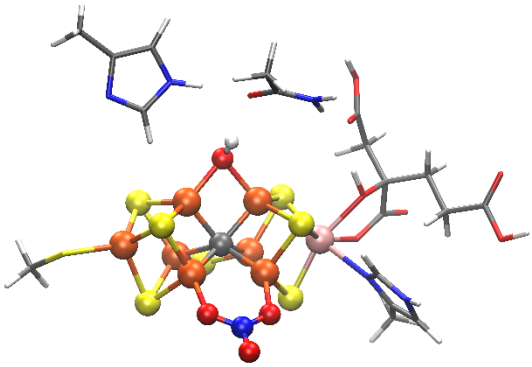

Figure S4: 83 atom cluster model with OH and nitrate

Fe7VC19N6H30S8O12

V	93.717566000	97.701914000	112.899207000
Fe	99.063541000	100.426751000	116.367000000
Fe	97.310622000	98.454819000	116.238868000
Fe	98.237994000	99.511538000	114.070560000
Fe	96.597164000	100.833896000	115.555401000
Fe	94.633783000	99.822034000	114.197457000
Fe	95.399249000	97.485638000	114.929892000
Fe	96.261109000	98.451156000	112.789371000
S	97.166320000	100.119570000	117.645586000
S	99.472119000	98.397088000	115.585797000
S	98.454043000	101.640466000	114.518497000
S	93.358498000	98.256494000	115.140516000
S	95.601222000	96.341851000	113.047298000
S	94.585009000	99.611272000	111.982310000
S	98.275143000	98.723533000	112.052249000
C	96.407751000	99.136101000	114.613181000
O	96.441605000	96.717964000	116.376149000
H	95.902905000	96.395697000	117.129632000
N	94.180535000	102.493049000	115.293037000
O	95.363989000	102.391768000	115.794614000
O	93.719119000	101.534732000	114.556215000
O	93.490550000	103.491920000	115.509375000
O	92.368305000	96.073438000	113.391296000
O	92.460795000	94.940757000	110.032796000
O	93.344590000	96.698819000	111.129366000
O	93.558269000	92.156476000	114.408285000
H	93.563367000	91.986658000	115.375690000
O	92.825357000	94.149568000	115.158416000
O	87.604994000	96.314354000	111.676240000
H	86.680637000	96.009775000	111.798467000
O	87.945952000	94.281984000	112.601593000
C	92.257281000	95.001404000	112.430345000
C	92.710814000	95.583217000	111.065447000
C	93.240464000	93.871070000	112.791597000
C	93.162563000	93.425382000	114.217818000
C	90.802916000	94.525813000	112.379148000
C	89.860603000	95.673307000	112.030196000
C	88.406355000	95.315462000	112.142973000
H	92.534368000	95.659438000	114.276777000
H	90.045131000	96.533211000	112.695101000
H	90.047611000	96.048788000	111.012690000
H	90.727004000	93.727495000	111.628481000
H	90.525186000	94.096105000	113.353674000
H	93.130544000	93.023931000	112.105117000
H	94.270938000	94.268603000	112.674216000
C	91.694000000	98.865997000	109.843002000
H	92.369191000	99.686822000	109.522905000
H	90.859001000	98.669998000	109.137001000
H	92.419998000	98.028000000	109.914001000
N	91.703856000	98.680932000	112.405014000
C	91.110646000	99.077743000	111.202968000
C	90.850058000	99.002168000	113.375757000
H	91.016524000	98.848493000	114.435088000
N	89.736540000	99.577351000	112.860859000
H	88.948087000	99.919450000	113.398509000
C	89.879907000	99.631862000	111.489664000
H	89.111733000	100.040644000	110.843922000
S	100.476764000	101.615768000	117.646559000
C	102.051003000	101.861000000	116.720001000
H	102.511194000	102.809634000	117.068832000
H	101.876999000	101.940002000	115.625999000
H	102.742996000	101.014999000	116.919998000
C	93.647003000	95.205002000	120.335999000
H	93.521003000	94.196356000	120.781935000
H	92.721001000	95.794998000	120.502998000
H	94.525002000	95.717003000	120.785004000
C	93.924644000	95.079206000	118.847580000
O	95.083603000	95.145546000	118.384357000
N	92.865582000	94.873352000	118.045966000
H	91.922885000	94.848167000	118.416657000
H	92.998098000	94.731360000	117.042244000
C	100.043999000	95.387001000	122.435997000
H	99.674004000	95.912003000	123.342003000
H	100.236514000	94.300820000	122.559484000
H	101.002998000	95.862999000	122.137001000
N	99.136816000	96.868239000	120.637819000
C	99.076034000	95.662878000	121.320952000
C	98.134598000	96.844487000	119.764650000
H	97.895438000	97.628998000	119.048234000

N	97.428982000	95.683006000	119.851330000
H	96.582443000	95.437676000	119.309690000
C	98.016158000	94.916091000	120.841256000
H	97.637372000	93.933844000	121.103605000

Constrained atoms
{ C 45 C }
{ C 46 C }
{ C 47 C }
{ C 48 C }
{ C 58 C }
{ C 59 C }
{ C 60 C }
{ C 61 C }
{ C 62 C }
{ C 63 C }
{ C 64 C }
{ C 65 C }
{ C 71 C }
{ C 72 C }
{ C 73 C }
{ C 74 C }

QM/MM model comparison of two broken symmetry solutions for NH containing model at E0 with carbonate

A smaller QM region of 80 atoms was used

Table S3: Structural parameters of BS models, distances in Å and dihedrals in degrees.

Fe_c-Fe_d lig.: **Fe_c-Fe_d lig** **Redox state** **BS state:**	NH carbonate E0 BS7-235	NH carbonate E0 BS10-135	*Crystal* *ABC, DEF*
Q_{1b}-X	2.96	2.98	2.51, 2.39
Q_{1b}-H_{188}	2.68	2.69	2.85, 2.83
Q_{1b}-HC	2.86	2.88	2.87, 2.91
Fe_c-X	1.80	1.82	2.01, 2.08
Fe_d-X	1.83	1.84	2.01, 2.05
Fe_c-Fe_d	2.50	2.42	2.64, 2.65
<Fe_c-Fe_d-Q_{1b}-X	5.44	6.70	4.30, 6.11
C-X	2.92	3.00	3.05, 3.15
V-Fe_3	2.74	2.72	2.71, 2.70
V-Fe_6	2.91	3.04	2.79, 2.78
V-Fe_7	2.74	2.67	2.77, 2.76
Fe_a-Fe_b	2.66	2.65	2.58, 2.59
Fe_a-Fe_3	2.73	2.70	2.64, 2.58
Fe_a-F_7	2.53	2.52	2.58, 2.64
Fe_b-Fe_3	2.73	2.77	2.79, 2.78
Fe_b-Fe_7	2.62	2.63	2.60, 2.60
Fe_c-Fe_2	2.66	2.63	2.69, 2.68
Fe_c-Fe_3	2.69	2.73	2.67, 2.67
Fe_c-Fe_6	2.59	2.70	2.59, 2.59
Fe_d-Fe_3	2.61	2.60	2.63, 2.64
Fe_d-Fe_6	2.64	2.75	2.64, 2.63
Fe_d-Fe_4	2.67	2.66	2.64, 2.65

BS7-235

23	93.174499965	97.704070652	113.162439658
26	98.974794637	100.486436412	116.206789879
26	96.986284624	98.738911534	116.470247090
26	98.063556240	99.070189015	114.113615634
26	96.639435844	101.039686965	115.224320114
26	94.363269997	99.948979591	114.182272061
26	94.941095295	97.698840862	115.470894116
26	95.906515878	97.945708580	113.142116922
16	97.057667080	100.797593855	117.469134082

16	99.156739682	98.298229637	115.998460939
16	98.667401043	101.324915453	114.051483758
16	92.833831799	98.585750081	115.313220384
16	94.770640945	96.055285342	113.899920529
16	94.441322863	99.206229871	112.010974707
16	97.966851781	97.747715197	112.322846515
6	96.115916695	99.207769218	114.714201781
7	95.955976132	97.343671578	116.953189615
1	96.059036995	96.401352218	117.322186048
6	94.275395468	102.704908166	115.089434968
8	95.562126239	102.628612605	115.212454921
8	93.618995784	101.718480994	114.523810165
8	93.653764288	103.726297927	115.492434415
8	91.640734707	96.295257295	113.552000250
8	92.228523345	94.709203216	110.428473817
8	93.064984652	96.510757124	111.446598125
8	90.279796576	92.903676817	114.732892443
8	91.371402525	94.728540417	115.460031993
8	87.534429709	95.237636155	110.704326598
8	87.023227617	96.886796356	112.127953071
6	91.462392425	95.207002293	112.636793970
6	92.317861225	95.483287915	111.408349219
6	91.961644494	93.918548052	113.335698658
6	91.155129215	93.795034176	114.626528452
6	89.983673531	95.078173254	112.242745351
6	89.338801423	96.377114292	111.764120906
6	87.851738953	96.165236097	111.495931006
1	91.687647495	95.835364171	114.471578895
1	89.471040051	97.158936022	112.513564179
1	89.811443517	96.715358504	110.836583156
1	89.897221347	94.319592195	111.459208698
1	89.438593905	94.695730366	113.111375126
1	91.831967181	93.066517433	112.666181218
1	93.024949778	94.048924760	113.574023371
6	91.583096250	98.650606748	109.923422791
1	90.828955359	98.382999117	109.175425535
1	92.192023010	97.775140817	110.155812910
7	91.418931821	98.862914792	112.447513561
6	90.909908004	99.101807191	111.181596929
6	90.522864368	99.330771193	113.304774506
1	90.644167461	99.332606694	114.379853836
7	89.459925354	99.858627893	112.659764724
1	88.600468130	100.138645366	113.143849677
6	89.683080746	99.719020352	111.309485450
1	88.969612501	100.030525970	110.563487516
6	102.001279181	101.898566237	116.784623097
1	101.818586452	102.057645865	115.719115437
1	102.673831706	101.045550648	116.906212321
16	100.386013329	101.633503775	117.621678265
6	100.090009610	95.418811806	122.380075946
1	99.823207492	95.947206776	123.303107789
1	100.996312836	95.885880145	121.975024873
7	98.049712105	96.625692369	121.723113230
6	98.908202855	95.582857284	121.478540777
6	97.084133755	96.517095774	120.826180508
1	96.257554131	97.207603230	120.697344409
7	97.290399912	95.466269823	119.998502500
1	96.585842716	95.143151296	119.302815451
6	98.454798414	94.854682716	120.393862636
1	98.871161905	94.003813386	119.874029832
6	93.469694430	93.710762701	120.628432211
1	94.318398396	93.127047020	120.268066439
1	92.558557315	93.237505190	120.247452250
6	93.600610972	95.142588737	120.088189599
1	92.669638352	95.695691736	120.183032161
1	94.386612087	95.708213960	120.599743821
6	94.049041367	95.052603475	118.641097861
8	95.248307164	94.844187356	118.375134369
7	93.123993297	95.143266203	117.684067172
1	92.122021056	95.234642296	117.866558780
1	93.392789625	95.040431149	116.711020633

BS10-135

23	93.186704311	97.679620964	113.120056130
26	98.958618634	100.497073828	116.265564883
26	96.990051672	98.763465271	116.444568646
26	98.023330203	99.138568849	114.090077619

26	96.601011519	101.141304473	115.117287393
26	94.285285703	99.909435660	114.230556327
26	94.981234288	97.739215092	115.575045794
26	95.844609206	97.952001559	113.221545299
16	97.071362672	100.866556546	117.379068258
16	99.066349413	98.242308289	115.923807546
16	98.634908414	101.400551595	114.085933372
16	92.815058440	98.518684404	115.321707490
16	94.721061374	96.092170704	114.024150519
16	94.431854495	99.236148698	112.060337833
16	97.872991665	97.800948658	112.295278367
6	96.130603131	99.235644861	114.717053098
7	96.011863821	97.352955826	117.050921508
1	96.139024114	96.378328407	117.315170303
6	94.204817318	102.718930327	115.123494590
8	95.489416290	102.684710470	115.243907546
8	93.583416289	101.691693484	114.590802534
8	93.554558565	103.731894073	115.500633841
8	91.634802466	96.298044375	113.505007799
8	92.261885789	94.685547575	110.403313784
8	93.122903759	96.474018086	111.425492051
8	90.288159459	92.916076854	114.719671820
8	91.379090462	94.747948859	115.431069919
8	87.530121583	95.230053055	110.697788371
8	87.030953725	96.879577996	112.126419011
6	91.473358538	95.201676057	112.599334374
6	92.350562490	95.461988739	111.380518364
6	91.970621755	93.919832943	113.314583677
6	91.162363905	93.807896411	114.606160862
6	89.997301525	95.064093050	112.196611653
6	89.342725026	96.367174843	111.742987222
6	87.853583299	96.157068355	111.488007943
1	91.682067340	95.852678458	114.431222653
1	89.480973701	97.137995741	112.502334989
1	89.804306512	96.720412029	110.815397672
1	89.918307147	94.319199838	111.399741356
1	89.454013808	94.660473424	113.057278147
1	91.843993448	93.060832166	112.653355393
1	93.032456417	94.051317561	113.558259186
6	91.588980247	98.637597505	109.923804822
1	90.839379470	98.367588554	109.172145735
1	92.199023476	97.763446976	110.158574372
7	91.418957165	98.836238287	112.443511533
6	90.910847087	99.086379408	111.180024198
6	90.523607883	99.295580986	113.305814837
1	90.644982970	99.281959106	114.380973372
7	89.462041480	99.831246728	112.664890539
1	88.603008636	100.109169353	113.151312865
6	89.685154379	99.704623004	111.312950440
1	88.971827600	100.023814445	110.569933505
6	102.088293001	101.864290588	116.798611219
1	101.915164843	102.011191035	115.730174474
1	102.775173757	101.025733613	116.936965277
16	100.472756766	101.556855670	117.606899020
6	100.089849030	95.419503886	122.382093830
1	99.826333755	95.947802654	123.306343554
1	100.995680958	95.885331460	121.974588383
7	98.058764001	96.639547696	121.713615429
6	98.905519321	95.582592406	121.483711939
6	97.084215808	96.519905631	120.827823852
1	96.270530345	97.221781489	120.683314947
7	97.272777113	95.450121873	120.022165278
1	96.572123525	95.126627653	119.324013702
6	98.436301405	94.837399223	120.418317284
1	98.843518830	93.975193124	119.910538950
6	93.469780152	93.706173830	120.633422943
1	94.318927760	93.122690106	120.273846495
1	92.558920693	93.231461845	120.253379560
6	93.600503055	95.136105525	120.089017815
1	92.671299727	95.692077868	120.184485887
1	94.389789021	95.701428083	120.596054776
6	94.045950619	95.035466052	118.641432652
8	95.239299479	94.801822637	118.376997780
7	93.119336790	95.144973009	117.685570603
1	92.117761627	95.227797043	117.872684879
1	93.381140530	95.028761840	116.712334627

QM-region coordinates of QM/MM models featured in the manuscript

NH at E_o with carbonate

23	93.218135909	97.738015849	113.167508348
26	99.009050264	100.355277868	116.352015979
26	96.986794386	98.604373090	116.573109052
26	98.064060123	99.020701349	114.239003974
26	96.661040971	100.971012253	115.459381884
26	94.412775384	99.956122399	114.210162705
26	94.892142367	97.694955900	115.512288901
26	95.913537198	97.978027237	113.219906938
16	97.144742432	100.577969898	117.699593780
16	99.160840053	98.161688432	116.078974130
16	98.644077627	101.250026130	114.234890532
16	92.823253661	98.638384628	115.298853995
16	94.783209620	96.073166499	113.914611178
16	94.509658234	99.243336013	112.022894019
16	97.965117135	97.723986487	112.412797873
6	96.110864459	99.180296317	114.828793784
7	95.877358254	97.232430346	116.976106789
1	96.016457344	96.267017909	117.260251982
6	94.329152836	102.697361917	115.144378179
8	95.610876678	102.590898904	115.315763937
8	93.671365475	101.727545169	114.559628091
8	93.716842480	103.734936117	115.522162752
8	91.653051427	96.337469768	113.544007436
8	92.307878347	94.689302271	110.464236041
8	93.106961041	96.522335345	111.457573197
8	90.276716028	92.936621975	114.745779213
8	91.331783985	94.786023102	115.467468620
8	87.539227622	95.249997380	110.704856070
8	87.043585408	96.880178514	112.154967578
6	91.486524439	95.237220384	112.643137367
6	92.368219228	95.491305232	111.427166793
6	91.969796226	93.954460420	113.365273938
6	91.142107696	93.839469614	114.642237073
6	90.010021273	95.102297084	112.234427365
6	89.357274124	96.393260138	111.741669972
6	87.866377057	96.172208895	111.499381660
1	91.678858674	95.894755951	114.465687174
1	89.497035984	97.185979828	112.478507152
1	89.817808179	96.716736291	110.802545519
1	89.932071915	94.334432472	111.458871296
1	89.459227691	94.726437559	113.103165058
1	91.849134063	93.095697677	112.702461114
1	93.029761260	94.085662373	113.618290899
6	91.693395449	98.644439260	109.896714366
1	90.950241154	98.320469069	109.159182463
1	92.358518550	97.815814267	110.142674705
7	91.478109039	98.887660971	112.415997104
6	90.985111248	99.092866952	111.139047153
6	90.569734404	99.370661584	113.252119310
1	90.674086004	99.394907861	114.328168981
7	89.512060741	99.877355955	112.581515220
1	88.646252995	100.156517938	113.052767951
6	89.751681031	99.705371036	111.236965605
1	89.044487691	99.997307504	110.475929258
6	102.066920597	101.779085103	116.880400928
1	101.876896919	101.870307278	115.809252036
1	102.765444091	100.954156125	117.047621627
16	100.464727458	101.485593044	117.731344255
6	99.991381799	95.472058171	122.428813360
1	99.674567073	95.943225181	123.367157302
1	100.904188025	95.983169045	122.096595225
7	98.134439038	96.839200683	121.505518061
6	98.873257103	95.674250375	121.448062429
6	97.236212566	96.746508068	120.533440518
1	96.491005739	97.488551002	120.267286295
7	97.363557489	95.585137681	119.852091133
1	96.649713525	95.230723494	119.183388030
6	98.403466532	94.888343835	120.414289099
1	98.749870957	93.943968055	120.021764059
6	93.481358929	93.705728066	120.642244957
1	94.323818108	93.117821865	120.275006030
1	92.564586000	93.238505869	120.267108692
6	93.619165437	95.135213619	120.098038112
1	92.693441257	95.698322783	120.196276659
1	94.417685179	95.698074672	120.595091410

6	94.058808059	95.018773507	118.650488480
8	95.247848514	94.758720275	118.388424250
7	93.130754345	95.132351405	117.698158450
1	92.136642486	95.252906709	117.891320051
1	93.390996570	95.038886451	116.721668102
6	89.592788658	98.405877032	117.085597113
1	89.528815326	99.301894284	116.464097749
1	90.365253541	98.552543086	117.835788234
7	90.044133326	97.272533498	116.234128706
1	90.965764115	97.504113641	115.804792513
1	90.161835126	96.387925228	116.787354458
1	89.350578807	97.097494962	115.480162349
6	95.926496811	93.350740062	111.462582901
1	94.915186105	93.289416926	111.873686891
1	96.578630027	92.664160246	112.006719959
7	96.441337524	94.728046961	111.689621900
1	96.030092882	95.158819001	112.564146119
1	97.481984171	94.763912585	111.795618198
1	96.165661780	95.405808551	110.947802914
6	95.147142269	103.518827259	112.015002572
1	94.242516030	103.133729807	112.500630379
1	94.903171553	103.818074140	110.992286320
7	96.184777666	102.489950424	111.991934429
1	96.762554692	102.373388775	112.825482529
6	96.367761813	101.601069672	111.019365788
7	95.528358772	101.584213429	109.967716733
1	94.582998134	101.943269329	110.099467163
1	95.589107942	100.827736671	109.287462662
7	97.451726600	100.808830145	111.044613918
1	98.021329641	100.831843184	111.892616946
1	97.390763250	99.878112805	110.646907703

NH at E_0 with nitrate

23	93.225083941	97.723768678	113.122248154
26	99.015305558	100.366701457	116.378132344
26	97.065943527	98.578122851	116.738756997
26	98.000560531	99.028827925	114.329519310
26	96.621506114	100.922561565	115.517822890
26	94.354759052	99.904558269	114.252360755
26	94.930017801	97.737034650	115.641417537
26	95.866439936	98.006880900	113.311396804
16	97.151565535	100.590530961	117.747471886
16	99.183737328	98.155905535	116.110840466
16	98.580239596	101.235998770	114.263726432
16	92.834483964	98.588636504	115.330232618
16	94.734219612	96.147798909	114.042650120
16	94.502309164	99.275761034	112.088937563
16	97.917327335	97.736765513	112.547111637
6	96.068170645	99.155304018	114.869719095
7	95.904266818	97.210379926	117.024493017
1	95.887473195	96.250422340	117.372298858
7	94.336869570	102.684961662	115.237683360
8	95.563738977	102.539025867	115.516784170
8	93.674505366	101.743545167	114.616231724
8	93.719646049	103.740938152	115.571402504
8	91.666765337	96.350486552	113.494782454
8	92.390266884	94.685092403	110.442878804
8	93.185854633	96.509323897	111.451485634
8	90.342201618	92.985538904	114.779116099
8	91.408939935	94.851459405	115.447474959
8	87.526308056	95.267805285	110.723161571
8	87.074203311	96.891115773	112.191499709
6	91.521304387	95.235098042	112.604737226
6	92.428107864	95.480800433	111.404003819
6	92.014135166	93.970190210	113.354007502
6	91.201682712	93.882354570	114.643206533
6	90.048908010	95.075232006	112.182315604
6	89.375408809	96.375764645	111.742636388
6	87.877505491	96.175970476	111.522774259
1	91.700951420	95.913748680	114.428701450
1	89.528480047	97.143877093	112.502086919
1	89.812917675	96.729742323	110.803299665
1	89.993651943	94.329700370	111.381537368
1	89.506157587	94.656302612	113.037082900
1	91.887672148	93.092956299	112.719963334
1	93.075112873	94.101036679	113.598968539
6	91.609786690	98.632482531	109.925501317
1	90.864249483	98.350962761	109.173917074
1	92.224610780	97.764092752	110.167430117

7	91.449357302	98.869049475	112.444173568
6	90.932173125	99.093793144	111.178149147
6	90.545799441	99.322498399	113.303631674
1	90.648440478	99.305873911	114.379707829
7	89.476864242	99.835337511	112.658245138
1	88.612978720	100.103217690	113.144751613
6	89.698757201	99.696848180	111.307939958
1	88.982556748	100.003111579	110.562233024
6	102.035111564	101.808360554	116.877117289
1	101.848356243	101.906226478	115.806557734
1	102.722841497	100.975112052	117.043915270
16	100.429222297	101.527071015	117.729136251
6	99.993081153	95.466967610	122.413265620
1	99.677499583	95.945352969	123.347984031
1	100.904654706	95.975360002	122.074735507
7	98.112964430	96.809771479	121.498640963
6	98.870582794	95.657299272	121.435095168
6	97.201006178	96.698862107	120.544203091
1	96.431775047	97.423580796	120.299524041
7	97.339236801	95.537946206	119.860667371
1	96.623499622	95.179286343	119.201764490
6	98.400875307	94.861352782	120.409220208
1	98.759134126	93.922148228	120.016120574
6	93.464931437	93.690780244	120.671603407
1	94.293575237	93.092455733	120.291294794
1	92.536658542	93.244043969	120.300421485
6	93.619237597	95.130309687	120.159309203
1	92.714529223	95.714969320	120.314158814
1	94.455879681	95.656730715	120.631442707
6	93.982685311	95.037700495	118.694919488
8	95.167977619	94.836423852	118.364202227
7	92.996012872	95.115578078	117.798077556
1	92.012074504	95.154466229	118.060987696
1	93.176607426	94.974308358	116.809059473
6	89.582258343	98.291521547	117.169024435
1	89.570389866	99.188226699	116.545025930
1	90.343156460	98.399580078	117.937106044
7	89.989119546	97.136148579	116.323321327
1	90.918586864	97.308457769	115.902519182
1	90.053885649	96.239429954	116.867855013
1	89.295789743	97.002586372	115.558644997
6	95.858691354	93.484340275	111.423781923
1	94.836718353	93.440863854	111.806970651
1	96.490522523	92.806805795	112.002142883
7	96.386738987	94.867098392	111.631921056
1	96.011543659	95.293791783	112.510607004
1	97.428812453	94.876124742	111.734209040
1	96.118142486	95.539316004	110.880863140
6	95.214615245	103.468509486	112.041316229
1	94.300038611	103.069492947	112.497069643
1	94.981219001	103.796982091	111.026273178
7	96.253306860	102.441182116	111.992043003
1	96.883919954	102.342193146	112.789723405
6	96.413781632	101.549839275	111.014198153
7	95.553358737	101.519527514	109.979636400
1	94.609611411	101.886964980	110.115490675
1	95.601208939	100.733438334	109.334997088
7	97.494516989	100.756529624	111.020630116
1	98.081179241	100.761897482	111.855576792
1	97.447889822	99.851387966	110.569883266

NH at E_{ox} with carbonate

23	93.291982660	97.709231386	113.198649949
26	99.038467882	100.389522065	116.363276688
26	97.010903119	98.640838635	116.750790284
26	98.148683741	99.104819779	114.221259397
26	96.679816689	100.966069302	115.469943182
26	94.459043658	99.902742641	114.267308909
26	95.082019105	97.610098813	115.513276020
26	96.040962101	98.025416144	113.242631148
16	97.179100682	100.619318287	117.717966852
16	99.167834014	98.193517545	116.058168182
16	98.648755016	101.285306180	114.257542419
16	92.988885060	98.514663703	115.313773341
16	94.899662824	96.108362758	113.828160203
16	94.551071238	99.243008175	112.100085788
16	98.064525431	97.838823826	112.450376283
6	96.237305982	99.136471390	114.878707873
7	95.956992576	97.236230511	117.060619834

1	95.407474079	96.573945327	117.640521179
6	94.379962309	102.653603436	115.186559896
8	95.662841127	102.572815078	115.382499195
8	93.758320278	101.637927801	114.615646586
8	93.737620633	103.670666488	115.515183271
8	91.760320769	96.379907865	113.604900546
8	92.423359855	94.701470016	110.553083084
8	93.147671657	96.578678550	111.504996801
8	90.420841415	92.998388047	114.941365194
8	91.392778747	94.940353695	115.553775359
8	87.577929416	95.284458239	110.762345251
8	87.074134545	96.905828618	112.209190482
6	91.563860859	95.260580167	112.722395845
6	92.436905087	95.506464916	111.498590131
6	92.049629258	94.004714087	113.487851228
6	91.228652879	93.924552260	114.774822629
6	90.079539732	95.109806733	112.320519495
6	89.395423958	96.397084844	111.856708062
6	87.901179485	96.186476007	111.576951764
1	91.747321629	95.953981932	114.553909637
1	89.506994620	97.171828070	112.618379835
1	89.858669893	96.754213595	110.930653997
1	90.019609191	94.348066546	111.533999818
1	89.541830077	94.705270386	113.184375863
1	91.923615146	93.118213801	112.866367764
1	93.110502844	94.126865804	113.737289544
6	91.604635392	98.648948946	109.972195909
1	90.829797237	98.392942893	109.241810137
1	92.210512589	97.764636451	110.170700726
7	91.529007205	98.881524488	112.511059972
6	90.975423850	99.098485557	111.254301097
6	90.642705039	99.335773595	113.393992347
1	90.761613313	99.314166214	114.467954330
7	89.558396535	99.838161033	112.772759643
1	88.699065745	100.116794320	113.273313349
6	89.744505393	99.697073279	111.419111735
1	89.000264979	99.989906169	110.694387220
6	102.037110557	101.816929103	116.876664967
1	101.867038601	101.917597608	115.804400054
1	102.712244750	100.977028962	117.056445594
16	100.418225477	101.547627118	117.704770736
6	99.974990518	95.458707389	122.389845048
1	99.565349231	95.911860104	123.298331294
1	100.903641901	95.989495001	122.145299893
7	98.102009826	96.744530189	121.379596264
6	98.968038568	95.670036921	121.294011072
6	97.397439830	96.748563265	120.261813353
1	96.619630884	97.451873291	119.986434732
7	97.769131875	95.722178087	119.453697602
1	97.374156758	95.533272650	118.538421629
6	98.773068998	95.024329292	120.088506145
1	99.252726466	94.167343039	119.640091434
6	93.474617826	93.812918522	120.672585007
1	94.286860751	93.245548101	120.214531036
1	92.533589118	93.388141040	120.306520922
6	93.593076380	95.293431741	120.269745867
1	92.882777380	95.916696738	120.818940581
1	94.604107218	95.680274484	120.434172053
6	93.302717826	95.368871012	118.783331345
8	94.215308998	95.387493779	117.943692700
7	92.004052643	95.322418884	118.449554094
1	91.303340942	95.317693535	119.208491591
1	91.748835898	95.103847983	117.486142781
6	89.443597535	97.970527125	117.253066238
1	89.724143658	98.798897243	116.599998965
1	90.170426504	97.855450130	118.055873858
7	89.441567106	96.702038041	116.464337482
1	90.346019603	96.379839977	116.085804502
1	89.135270525	95.907321599	117.083616849
1	88.755569787	96.771180760	115.682730001
6	95.980450305	93.420639692	111.327647436
1	94.972789559	93.397140515	111.749207487
1	96.625950060	92.745632844	111.892951187
7	96.529308229	94.802688144	111.491060657
1	96.163121040	95.234095601	112.365260677
1	97.571883213	94.804282674	111.593680664
1	96.239511004	95.470135302	110.743813820
6	95.137533387	103.488577998	112.036561819
1	94.262315099	103.081004556	112.554216755
1	94.839830433	103.799824726	111.033978993

7	96.194511837	102.478249255	111.941948258
1	96.881909208	102.441919918	112.690498473
6	96.368091942	101.625235517	110.933526350
7	95.471019291	101.563153317	109.936963382
1	94.536443450	101.957209211	110.071310689
1	95.521088282	100.795265260	109.271644434
7	97.477983317	100.877660872	110.885306515
1	98.127650748	100.879337290	111.665494433
1	97.559479270	100.105221999	110.240999985

NH at E_{ox} with nitrate

23	93.194525631	97.739448264	113.243544079
26	99.025122511	100.326103968	116.289762363
26	96.951127898	98.628566036	116.673529309
26	98.119494298	99.008200594	114.168442411
26	96.728855162	100.920529258	115.323160590
26	94.541102796	99.942191508	114.200553065
26	94.894148779	97.736663830	115.568195972
26	95.978575491	98.045147374	113.089624348
16	97.125494396	100.668060037	117.563976403
16	99.093382747	98.112453454	116.062771407
16	98.681880393	101.173062800	114.162429495
16	92.937757050	98.790299629	115.338782391
16	94.911168727	96.186262631	113.938338565
16	94.474963234	99.298986153	112.066383511
16	98.017639977	97.830064846	112.364712145
6	96.223030217	99.073154474	114.775047385
7	95.803306003	97.332886171	117.058817515
1	95.425114340	96.557485727	117.638422175
7	94.378401865	102.711022039	115.179680694
8	95.618273798	102.629080305	115.381162643
8	93.740333126	101.766072982	114.615661056
8	93.763147642	103.721292672	115.534928679
8	91.807957914	96.405385993	113.703737711
8	92.270631091	94.806769243	110.561631057
8	93.117738145	96.616246567	111.549748049
8	90.752461031	92.809839133	114.999185674
8	91.590325691	94.803975846	115.608752147
8	87.579176536	95.292709304	110.810729432
8	87.053801195	96.918496415	112.245091666
6	91.555281035	95.342114647	112.806582463
6	92.354625638	95.580420540	111.528695687
6	92.117923236	94.032008425	113.434668452
6	91.425390352	93.788733145	114.749939103
6	90.053576211	95.165934005	112.489284182
6	89.376869458	96.417810372	111.927788885
6	87.889892474	96.197985472	111.623504669
1	91.906434888	95.579915014	115.020473798
1	89.472232510	97.238841397	112.640502740
1	89.863726975	96.713635943	110.991788669
1	89.949221060	94.341932101	111.772477660
1	89.546998804	94.853459784	113.412931033
1	91.982038374	93.186045203	112.761601559
1	93.189691919	94.175135464	113.625525816
6	91.559204652	98.698819211	109.979682829
1	90.791499254	98.439940901	109.243178081
1	92.167475384	97.816567218	110.183509390
7	91.443557731	98.909278107	112.524767860
6	90.915513209	99.140405949	111.258685327
6	90.532648479	99.344776199	113.392030338
1	90.622661922	99.302836107	114.467725567
7	89.458994039	99.853559188	112.754806263
1	88.593808196	100.139344660	113.238730509
6	89.677341250	99.730101683	111.404548634
1	88.952451574	100.031247944	110.664761667
6	102.022800135	101.809317248	116.861201804
1	101.905875160	101.894866429	115.781120996
1	102.679974508	100.963998734	117.076663055
16	100.362888523	101.558681577	117.617953326
6	99.936560708	95.458570914	122.360585703
1	99.601202263	95.942160975	123.284556750
1	100.843243265	95.978242332	122.027547498
7	98.026891834	96.752855263	121.425803472
6	98.827224753	95.627282421	121.355912583
6	97.146715138	96.652137787	120.446991379
1	96.354822556	97.356804607	120.217306558
7	97.344425349	95.513957729	119.729817547
1	96.728730191	95.183565200	118.990889442
6	98.416703872	94.851552457	120.290103092

1	98.816110098	93.938739165	119.878938513
6	93.499525968	93.804140506	120.743633379
1	94.323372414	93.255344728	120.283619565
1	92.564992819	93.392871947	120.347829264
6	93.623097864	95.303059156	120.412548782
1	92.865123084	95.898210544	120.927153852
1	94.612830880	95.698518611	120.659069444
6	93.444610465	95.398464423	118.922321672
8	94.423625106	95.336729155	118.153392843
7	92.172546362	95.441527305	118.504501068
1	91.429099095	95.434772901	119.222321011
1	91.950748346	95.185683890	117.545195942
6	89.442693433	98.072250919	117.181650151
1	89.557549788	98.963438762	116.561498207
1	90.240942692	98.013537891	117.919919889
7	89.542198378	96.861707861	116.304490143
1	90.417434216	96.803522515	115.775830985
1	89.440065486	95.986558530	116.880657447
1	88.762924182	96.882617383	115.608967548
6	95.949322262	93.355423740	111.371987321
1	94.935349125	93.321109396	111.776805245
1	96.589195834	92.670613851	111.931338826
7	96.494305847	94.735950506	111.573232021
1	96.156391503	95.136475301	112.468353344
1	97.540673119	94.738531643	111.645359433
1	96.187649773	95.425768986	110.850909771
6	95.200102616	103.514952165	111.987316312
1	94.336663691	103.073724064	112.497789262
1	94.866503674	103.865729503	111.009692954
7	96.267110841	102.521993988	111.823125503
1	97.083955529	102.604739335	112.418396920
6	96.378321248	101.682544282	110.784477616
7	95.415942494	101.618330678	109.860042895
1	94.506690573	102.058830095	110.022498029
1	95.398734433	100.827201904	109.216500141
7	97.471731592	100.920051728	110.663611765
1	98.216636584	100.957824530	111.348812285
1	97.655943569	100.406455580	109.813102857

OH at E_0 with carbonate

23	93.198069064	97.751371841	113.196312853
26	99.013365479	100.348755659	116.422787843
26	96.980680199	98.607490669	116.700018322
26	98.017910699	99.015400970	114.375816018
26	96.622686549	100.959505822	115.537589197
26	94.385295728	99.960572031	114.309840254
26	94.791507233	97.654900984	115.511388981
26	95.895565805	98.022700086	113.288577493
16	97.147095595	100.572629335	117.769829583
16	99.146599229	98.143880593	116.162215360
16	98.597571853	101.216119971	114.314118310
16	92.778392228	98.619045109	115.333303312
16	94.799532725	96.086668340	113.886424676
16	94.489882534	99.295356750	112.119928276
16	97.964766298	97.777718133	112.556064021
6	96.080800972	99.146059922	114.942214742
8	95.764639283	97.210789628	117.083459643
1	95.633825359	96.323416865	117.492411121
6	94.314371870	102.691345415	115.198932555
8	95.594864709	102.568916165	115.392012155
8	93.656909512	101.716632884	114.616679001
8	93.709325559	103.733244047	115.549506563
8	91.678065625	96.336202673	113.592182317
8	92.307970728	94.740202750	110.481820696
8	93.094798763	96.569684347	111.489275820
8	90.394997018	92.940707025	114.821901763
8	91.485566011	94.783375203	115.519923486
8	87.543963055	95.271744993	110.757349672
8	87.040267156	96.904130542	112.198747355
6	91.504898372	95.243562337	112.677588282
6	92.365325408	95.524612353	111.452556907
6	92.023700409	93.962909097	113.378567473
6	91.253032972	93.838929471	114.690007546
6	90.024056314	95.097984948	112.288778000
6	89.355424437	96.394667618	111.833645153
6	87.866379779	96.184968460	111.561391694
1	91.758948619	95.876148711	114.508540366
1	89.478254990	97.167459418	112.594844301
1	89.820960641	96.751635123	110.908830386

1	89.948019540	94.348522348	111.494581957
1	89.490518777	94.693871719	113.155039341
1	91.879417465	93.103575387	112.722472599
1	93.092394250	94.092953571	113.588748651
6	91.587630424	98.653338500	109.948854465
1	90.834682809	98.386572944	109.199879498
1	92.195616744	97.777841025	110.178418961
7	91.431530595	98.895017633	112.475217453
6	90.916455648	99.110551994	111.205532780
6	90.528198282	99.367225185	113.327128553
1	90.633827419	99.378066932	114.402592475
7	89.461190759	99.873467146	112.674424402
1	88.601988302	100.166737077	113.155207880
6	89.684851856	99.718929295	111.326879193
1	88.970099376	100.017380904	110.576746756
6	102.040084243	101.799189738	116.888398291
1	101.848879637	101.895362671	115.818624127
1	102.728625489	100.966871807	117.055198958
16	100.438818296	101.516339102	117.746331015
6	99.994460519	95.463319804	122.405696922
1	99.680879996	95.945289499	123.338981577
1	100.906540591	95.968389129	122.063963976
7	98.102231079	96.798981686	121.514069470
6	98.870988112	95.655420593	121.429469798
6	97.194345307	96.701214922	120.556255992
1	96.418466805	97.423744915	120.328107642
7	97.345599809	95.555188749	119.848991876
1	96.645076476	95.220102413	119.171811940
6	98.413157709	94.875937359	120.385516733
1	98.780584607	93.948605632	119.973175597
6	93.470768890	93.727281598	120.689842858
1	94.291915599	93.131918908	120.288302462
1	92.536158347	93.305534880	120.306003811
6	93.636354953	95.186449136	120.240059052
1	92.755575957	95.781618372	120.477470334
1	94.514218106	95.667708640	120.682929955
6	93.896834273	95.161999167	118.755597576
8	95.074384750	95.058466702	118.336371418
7	92.842208804	95.187780751	117.944678638
1	91.892414679	95.204154743	118.309870577
1	92.910948039	95.035121196	116.939114436
6	89.489435435	98.236438162	117.126778189
1	89.467681367	99.133095639	116.503618668
1	90.295785973	98.319436536	117.851763167
7	89.795246374	97.062712437	116.256375960
1	90.692703584	97.189737403	115.767781526
1	89.861121099	96.172942177	116.811870367
1	89.040938743	96.951953843	115.546514635
6	95.896971006	93.506270397	111.354935797
1	94.876541357	93.482012829	111.745472274
1	96.524481987	92.834640421	111.944899099
7	96.433634540	94.887156239	111.531036998
1	96.050254657	95.323085258	112.407430974
1	97.474045601	94.897287532	111.638270602
1	96.149096625	95.551157892	110.779737413
6	95.155823990	103.482781114	112.047297653
1	94.255919266	103.088204819	112.533334640
1	94.904661899	103.782733392	111.027852715
7	96.201782382	102.460554349	112.009947152
1	96.804859042	102.368131310	112.826313613
6	96.387554897	101.569610988	111.038911623
7	95.547526004	101.528384939	109.988302763
1	94.601435699	101.898332481	110.100501532
1	95.612280147	100.742011608	109.346648754
7	97.475133309	100.783657402	111.064175823
1	98.047231142	100.790602783	111.907980347
1	97.440398051	99.876394905	110.616588030

OH at E_0 with nitrate

23	93.256035088	97.740031501	113.199611285
26	99.025526019	100.338751076	116.436769819
26	97.001474130	98.574488751	116.773564569
26	98.109925390	98.943431018	114.399205345
26	96.690235445	100.851018748	115.503577784
26	94.540637873	99.859301177	114.303783118
26	94.891381555	97.531837743	115.553002000
26	95.990272049	97.955529106	113.278978958
16	97.120438121	100.599661871	117.747165681
16	99.188932367	98.144260989	116.231539848

16	98.627961126	101.165188498	114.302380916
16	92.925950775	98.634968523	115.352722163
16	94.862317519	96.058621240	113.854934318
16	94.598078423	99.270588748	112.129283750
16	98.060794952	97.724255243	112.590605393
6	96.186828950	99.039055111	114.958498555
8	95.948893680	97.054989206	117.106865744
1	95.327681451	96.477674837	117.652787054
7	94.369773169	102.666781050	115.200032332
8	95.606304855	102.585326311	115.412226855
8	93.732432158	101.713878385	114.651018734
8	93.757462815	103.694039622	115.531012800
8	91.707847884	96.395210386	113.600384723
8	92.396847250	94.694313408	110.563284420
8	93.126324336	96.570060304	111.518346576
8	90.388826834	93.012874579	114.951914820
8	91.369098975	94.945639287	115.580944578
8	87.566723099	95.271135253	110.747160627
8	87.053653420	96.907224965	112.173718035
6	91.533257224	95.263834945	112.729574555
6	92.415246719	95.504771876	111.507747987
6	92.023565906	94.018540447	113.507814266
6	91.202205484	93.937835950	114.792701931
6	90.054728902	95.104136704	112.315603051
6	89.376947636	96.391184695	111.840685608
6	87.886084710	96.181470892	111.553670970
1	91.726497635	95.987858577	114.541825827
1	89.487736898	97.169779464	112.598333271
1	89.847893247	96.742290163	110.916111492
1	90.002639051	94.340503738	111.530720832
1	89.509159356	94.703408536	113.176548711
1	91.906067844	93.127440419	112.890857421
1	93.082808659	94.153999153	113.757829930
6	91.614584152	98.651481611	109.968325322
1	90.854031801	98.390470090	109.224741108
1	92.214749718	97.768284100	110.190269373
7	91.496141522	98.897831433	112.497005203
6	90.959893206	99.110496541	111.234174135
6	90.590837652	99.338597027	113.365143516
1	90.690729211	99.301586110	114.440783723
7	89.509570774	99.834810446	112.728820167
1	88.645515568	100.109842909	113.216298055
6	89.720116807	99.697828569	111.377167377
1	88.986190933	99.984597667	110.640183742
6	102.019057334	101.820599936	116.888417521
1	101.838157597	101.918579309	115.817463686
1	102.696865819	100.981340650	117.061198326
16	100.408432912	101.551825914	117.736237501
6	99.980179361	95.454331481	122.383874851
1	99.563529872	95.908314253	123.288625018
1	100.910855789	95.984728291	122.145796277
7	98.106226487	96.729788001	121.360840335
6	98.983713872	95.664343195	121.278225957
6	97.422661808	96.739979592	120.230400003
1	96.643082296	97.439305260	119.950931648
7	97.816603657	95.725270627	119.417668493
1	97.452012411	95.552813427	118.486353846
6	98.815391159	95.029953850	120.062654146
1	99.307838265	94.180276670	119.614375216
6	93.472453341	93.812274795	120.656351672
1	94.282322084	93.238144370	120.202545106
1	92.530918120	93.384571052	120.296040326
6	93.592471158	95.289350314	120.238655425
1	92.892294735	95.917693050	120.795742216
1	94.606037355	95.675342584	120.387957467
6	93.270579894	95.377545328	118.758836550
8	94.161079061	95.506453805	117.895054175
7	91.984283569	95.224771214	118.439332272
1	91.287660456	95.208138480	119.201408648
1	91.720038990	95.062409536	117.464126889
6	89.446485770	98.017494082	117.216066222
1	89.796160804	98.825236314	116.570598722
1	90.133272708	97.881069812	118.050514017
7	89.430080214	96.741656160	116.439746335
1	90.333252829	96.398726216	116.072035833
1	89.104924650	95.960034743	117.065914247
1	88.752239278	96.810556325	115.650526341
6	95.951318418	93.405377748	111.346254826
1	94.939567650	93.378976907	111.757939391
1	96.592351679	92.728478579	111.914481323

7	96.497279206	94.785267298	111.521280422
1	96.131101789	95.213820177	112.401195951
1	97.539902632	94.786699403	111.616866152
1	96.205972869	95.456872578	110.779046279
6	95.250720781	103.480984241	112.004108706
1	94.342211865	103.073224586	112.464725162
1	94.996031468	103.814253761	110.996157917
7	96.296337700	102.460172464	111.935618295
1	96.993146098	102.426957318	112.675968291
6	96.444479357	101.567413529	110.951714458
7	95.555595467	101.517605246	109.947942721
1	94.628947305	101.930175358	110.073968966
1	95.578475221	100.725435868	109.308775119
7	97.527841086	100.782266483	110.939196190
1	98.131753736	100.747172736	111.756941311
1	97.557211038	99.962980968	110.349375986

OH at E_{ox} with carbonate

23	93.268950423	97.767535534	113.223704631
26	99.028068173	100.322844070	116.419525458
26	96.979643262	98.564407088	116.818500233
26	98.109052713	99.002019908	114.295252471
26	96.645079988	100.894246048	115.504760691
26	94.476859816	99.902921675	114.430454136
26	94.869809438	97.519105639	115.640321544
26	95.982408992	98.076571647	113.206914222
16	97.149235756	100.548223068	117.743874839
16	99.121526841	98.102552299	116.155003351
16	98.617388935	101.164368512	114.312200897
16	92.914323576	98.543833091	115.387701403
16	94.927316614	96.146207952	113.869803912
16	94.517522056	99.392878528	112.219983636
16	98.006635853	97.875404406	112.463354748
6	96.193865715	98.974025064	114.980509487
8	95.864782185	97.137061342	117.225578208
1	95.189471410	96.501626685	117.742963186
6	94.370993420	102.619294456	115.241359817
8	95.663889478	102.492520698	115.400937848
8	93.705378125	101.601514540	114.730305735
8	93.781683143	103.663454414	115.550992467
8	91.748798399	96.416497402	113.622627182
8	92.462046673	94.742027425	110.585503913
8	93.165850994	96.612470750	111.568434506
8	90.441257309	93.039034891	114.988491734
8	91.411183138	94.988963352	115.588410425
8	87.589979735	95.278020055	110.755960944
8	87.077418733	96.902954446	112.196417061
6	91.564077967	95.289655828	112.745475226
6	92.452279198	95.539022352	111.534592149
6	92.056486879	94.042270815	113.520290689
6	91.241012816	93.964192827	114.811427835
6	90.084697294	95.127190083	112.333860576
6	89.400832258	96.405529840	111.845081861
6	87.906009260	96.185196477	111.565555535
1	91.735516975	95.996927697	114.573709373
1	89.506684493	97.192230246	112.595158949
1	89.866505490	96.746534108	110.913906194
1	90.032668594	94.352885812	111.558981486
1	89.542147249	94.734680562	113.200712137
1	91.933511613	93.150102357	112.906419576
1	93.117946561	94.166219189	113.766826052
6	91.616015841	98.663386669	109.980629569
1	90.843706655	98.411665990	109.246340939
1	92.213092281	97.773787221	110.181278911
7	91.519830991	98.901990797	112.524270342
6	90.981221815	99.117666804	111.258519698
6	90.616874478	99.352746430	113.394406420
1	90.711336113	99.329758869	114.470113515
7	89.541129675	99.851483969	112.758120680
1	88.675258257	100.130132548	113.249208952
6	89.746170758	99.711320538	111.407993953
1	89.011614050	100.000714040	110.672027030
6	101.991718916	101.819176161	116.868861415
1	101.813992016	101.930034764	115.799518873
1	102.663513565	100.975565731	117.040471795
16	100.377580066	101.535375591	117.704907529
6	99.981005425	95.456348278	122.390916296
1	99.573455152	95.913742235	123.297770390
1	100.908118794	95.985482988	122.139103074

7	98.089042770	96.709083982	121.361374026
6	98.971599970	95.647205901	121.296029170
6	97.374269643	96.673731899	120.252784908
1	96.575630489	97.353731290	119.978845000
7	97.757097967	95.631405471	119.465193851
1	97.359346324	95.393734367	118.564631342
6	98.778715728	94.968581100	120.109425986
1	99.270844190	94.108922934	119.680968053
6	93.457672470	93.844370520	120.632736479
1	94.261327753	93.263504013	120.175354300
1	92.510984086	93.423231368	120.279259984
6	93.586451434	95.325586174	120.219353419
1	92.898064756	95.954221426	120.791294552
1	94.603840855	95.702623799	120.362114397
6	93.234379937	95.439969555	118.752074125
8	94.104969726	95.637501364	117.859331167
7	91.963673475	95.241243177	118.437700758
1	91.270338826	95.194989935	119.206061968
1	91.693516625	95.102410031	117.458464522
6	89.408190494	97.995939044	117.248781652
1	89.738141976	98.809043118	116.599663216
1	90.104041433	97.860239494	118.075891884
7	89.378835570	96.721818204	116.468107280
1	90.274958106	96.377849283	116.087499767
1	89.056157636	95.938014698	117.093747599
1	88.692141115	96.799110782	115.685543690
6	95.987438825	93.362322100	111.336857846
1	94.976588862	93.338869246	111.750075628
1	96.627330924	92.676896175	111.895402406
7	96.545347293	94.740266932	111.523009887
1	96.215433257	95.143287920	112.418119950
1	97.591306427	94.736105260	111.594070672
1	96.237213240	95.433185290	110.803822979
6	95.169108776	103.436532477	112.038573902
1	94.334355237	102.978295774	112.579510559
1	94.810245064	103.776374355	111.066272911
7	96.257340749	102.468348611	111.848543058
1	97.016373991	102.484350952	112.520327027
6	96.403986391	101.656028139	110.800769565
7	95.462848109	101.590809583	109.853869986
1	94.540888482	102.010334446	110.005403075
1	95.491767392	100.834289871	109.174128409
7	97.510797728	100.901888234	110.686388720
1	98.276227964	101.012137451	111.339331604
1	97.737568049	100.463085099	109.804079081

OH at E_{ox} with nitrate

23	93.105335192	97.677995762	113.234399107
26	98.996887195	100.382438561	116.415314302
26	96.964808320	98.600336133	116.809575880
26	98.160756366	99.060194850	114.259767418
26	96.668788034	100.863191481	115.433379949
26	94.488774070	99.814659707	114.300877501
26	94.933612526	97.527329940	115.541346755
26	96.047436276	97.982900751	113.264877996
16	97.080138445	100.627285526	117.689969277
16	99.115483732	98.168710528	116.162994756
16	98.627791197	101.233598526	114.312373596
16	92.939561435	98.576094921	115.392295169
16	94.908957531	96.106882019	113.790913714
16	94.511366718	99.193659527	112.154656557
16	98.054874307	97.839358191	112.491369857
6	96.221835247	99.027555239	114.936832590
8	95.902504285	97.114625686	117.136235922
1	95.236042845	96.513858597	117.671311964
7	94.361497672	102.635835438	115.212589207
8	95.602620696	102.575678336	115.413869058
8	93.734569212	101.652048723	114.688957147
8	93.738147461	103.648467782	115.520650281
8	91.844862753	96.371372696	113.630469707
8	92.342648870	94.743334917	110.527434138
8	93.082343939	96.610400602	111.500893625
8	90.723382807	92.784610575	114.968228738
8	91.537722829	94.771051710	115.607751705
8	87.587858989	95.301458157	110.805776275
8	87.078842319	96.922781927	112.253237148
6	91.566403719	95.287627832	112.749029127
6	92.375970635	95.533019066	111.478105338
6	92.109754051	94.000466798	113.419865631

6	91.391187082	93.760801178	114.723972046
6	90.060322894	95.148131728	112.449859591
6	89.397739927	96.415168848	111.906753470
6	87.902697877	96.203165038	111.618438353
1	91.954138041	95.518705590	115.103650817
1	89.505487463	97.228680038	112.627670203
1	89.876699203	96.710529852	110.966629954
1	89.937058401	94.329705795	111.729280394
1	89.556957829	94.837433378	113.375765404
1	91.980620513	93.147312988	112.754653993
1	93.180726664	94.132106137	113.622846395
6	91.557060687	98.698368615	109.983625521
1	90.779511356	98.472281243	109.247193627
1	92.139845939	97.796183256	110.168475110
7	91.472540160	98.921238689	112.535994076
6	90.930631818	99.141214820	111.269353027
6	90.570407973	99.367925191	113.414864843
1	90.669600147	99.329866113	114.490096658
7	89.493944396	99.864643878	112.782242475
1	88.626201557	100.146749561	113.272548741
6	89.696844775	99.733041208	111.430370010
1	88.963275043	100.030595077	110.696979484
6	101.947883887	101.861497342	116.851596897
1	101.747358580	101.996301931	115.789217560
1	102.614850151	101.009530603	116.998127659
16	100.345305031	101.571308013	117.704158796
6	99.982692891	95.454127826	122.388506754
1	99.565279293	95.910163483	123.291311308
1	100.910149931	95.985806251	122.144115622
7	98.092088093	96.688083467	121.325771653
6	98.984903352	95.633791541	121.281989862
6	97.388855109	96.632753563	120.211032509
1	96.583345396	97.299660933	119.925338090
7	97.789356143	95.584436061	119.438977485
1	97.403135277	95.325171132	118.539674958
6	98.810327473	94.939733240	120.101678024
1	99.314735183	94.078975557	119.690423318
6	93.476764035	93.851338399	120.643748293
1	94.272393449	93.258840239	120.187624879
1	92.524411863	93.447592155	120.285940346
6	93.634653177	95.334419414	120.239932146
1	92.960897417	95.971378384	120.821736295
1	94.660124372	95.690084878	120.376721355
6	93.264000748	95.461522738	118.780242277
8	94.104930657	95.646570305	117.861868511
7	91.975719831	95.286215962	118.508563860
1	91.299187344	95.246765447	119.297618758
1	91.677516333	95.086602823	117.558884891
6	89.398187628	98.049247773	117.263841758
1	89.639098695	98.907849088	116.634455095
1	90.135480355	97.927050691	118.055611375
7	89.426878993	96.810496113	116.422363121
1	90.321528224	96.638442208	115.961341765
1	89.210566587	95.967278650	117.019049064
1	88.691047317	96.874347996	115.681769931
6	96.028979263	93.340762325	111.305299326
1	95.024334585	93.326486824	111.734165295
1	96.672379260	92.653824416	111.857445544
7	96.596939478	94.717323028	111.474096480
1	96.271681928	95.131662304	112.363146414
1	97.643370314	94.705316332	111.543989176
1	96.286281472	95.403405268	110.750278796
6	95.231748044	103.477459742	111.990802861
1	94.390532909	103.002241345	112.508179172
1	94.871312673	103.837581951	111.026005181
7	96.327600594	102.519885735	111.794406543
1	97.171199041	102.664160304	112.336533732
6	96.428765204	101.670631588	110.762445744
7	95.428416399	101.546765383	109.890968585
1	94.531971738	102.021030850	110.029946080
1	95.420859725	100.768816937	109.231871444
7	97.539236078	100.929777953	110.610702670
1	98.330175872	101.062379177	111.228979746
1	97.752813108	100.525949122	109.706561445

QM-region coordinates of QM/MM doubly protonated homocitrate model at E0 with NH and carbonate ligand

23	93.276939440	97.775007899	113.087076481
26	99.045682907	100.520431772	116.136639241
26	97.059762112	98.806934326	116.632857219
26	98.074690062	99.135769839	114.050591878
26	96.660645871	101.066491250	115.202965931
26	94.391278374	99.959983834	114.205927844
26	95.035424889	97.753392963	115.596853166
26	95.901303243	98.039186878	113.233600746
16	97.155230814	100.892361330	117.432761279
16	99.152475823	98.307596003	115.918336520
16	98.639356566	101.320938188	114.004485903
16	92.913960655	98.570257032	115.302374363
16	94.817826330	96.159994206	113.950824436
16	94.527903069	99.312583171	112.035221747
16	97.911139557	97.806427477	112.337704079
6	96.189159630	99.209214465	114.778772859
7	95.985963683	97.458515756	117.125406819
1	95.957990877	96.529397882	117.547838759
6	94.348910498	102.728402334	115.099731511
8	95.641711281	102.679945975	115.202894680
8	93.712446634	101.708108507	114.560928501
8	93.704340961	103.727887241	115.489338719
8	91.724204836	96.356035322	113.555175706
8	92.360132722	94.661186450	110.507738292
8	93.141238983	96.528149702	111.448147665
8	90.705310703	92.676379381	114.787040233
8	91.360681567	94.677910490	115.569249903
8	87.577369347	95.279879451	110.611102220
8	87.032532587	96.969999534	112.092675478
6	91.585882037	95.209318488	112.703988139
6	92.426751415	95.475599013	111.450817705
6	92.169323854	93.974845454	113.435716201
6	91.398716874	93.808135524	114.712800691
6	90.104885167	94.996512968	112.361333466
6	89.381300718	96.266906293	111.923566663
6	87.890344175	96.048555321	111.815732284
1	91.800287070	96.036258464	114.481000511
1	89.559056267	97.050868390	112.664139095
1	89.784259773	96.629761464	110.964473302
1	90.037522933	94.227619795	111.582895856
1	89.584644213	94.601597075	113.245164185
1	92.101196523	93.100638440	112.785280743
1	93.220722114	94.181165771	113.683788375
6	91.542883164	98.626337116	109.929700412
1	90.779783920	98.370768893	109.188032206
1	92.157057742	97.748352209	110.133507695
7	91.473801854	98.897346349	112.455584539
6	90.897483058	99.067803200	111.204280185
6	90.608732748	99.394435740	113.333781661
1	90.780330951	99.462546169	114.399164761
7	89.506735395	99.865777508	112.714903396
1	88.657992177	100.162884200	113.218447556
6	89.666422539	99.665725350	111.365417964
1	88.914897408	99.939336959	110.642677632
6	102.057945171	101.815205260	116.830197340
1	101.915021609	101.922973005	115.754958541
1	102.734935624	100.978544638	117.019025387
16	100.420942585	101.526890068	117.612077123
6	100.113718524	95.399533080	122.352381467
1	99.840098844	95.942990747	123.263962721
1	101.024225904	95.854205713	121.945132343
7	98.040837392	96.546702283	121.688010602
6	98.939882691	95.538908649	121.438634815
6	97.083949661	96.410311063	120.791881587
1	96.235554663	97.073717869	120.670870927
7	97.332450541	95.375403632	119.954101135
1	96.653612085	95.059261923	119.249488524
6	98.520332792	94.803668488	120.346010577
1	98.967652423	93.969187386	119.826233664
6	93.462499534	93.743491960	120.675751101
1	94.293431527	93.153615902	120.284482274
1	92.533809231	93.317303948	120.282240028
6	93.627483480	95.204098865	120.228308104
1	92.735414287	95.793007802	120.433726118
1	94.479986696	95.690331195	120.710992804

6	93.961074081	95.195534483	118.756818367
8	95.126684434	95.009988453	118.369785414
7	92.949769735	95.336896355	117.886889121
1	91.978277243	95.396303391	118.178322575
1	93.141434759	95.261632917	116.896008553
6	89.511081552	98.594532986	117.087617840
1	89.469816473	99.487367060	116.461790022
1	90.274010083	98.722163959	117.849460435
7	89.945970222	97.439929228	116.247190199
1	90.892147737	97.623510868	115.855937498
1	89.980784186	96.562283383	116.821054246
1	89.267047982	97.306994264	115.469058308
6	95.932403754	93.491454135	111.377197964
1	94.918564646	93.458613904	111.783424998
1	96.571755915	92.813585215	111.946825134
7	96.468030600	94.873163964	111.562931209
1	96.090643109	95.307941530	112.437451100
1	97.510374884	94.878169176	111.669943075
1	96.193330911	95.538843186	110.808300071
6	95.126508108	103.538765186	111.961514394
1	94.274089203	103.119635938	112.507641980
1	94.790548073	103.840011828	110.968406854
7	96.188815072	102.540649731	111.832956383
1	96.895745133	102.502328947	112.564064478
6	96.316778077	101.663549375	110.839572994
7	95.390270617	101.601823613	109.867954379
1	94.456727777	101.980197098	110.047625939
1	95.403693814	100.804015723	109.234721483
7	97.416034826	100.901113862	110.766808682
1	98.072910016	100.897790320	111.542789296
1	97.430603664	100.077829775	110.182976071
1	87.223401116	95.950728994	109.999227441
1	90.118929587	92.634749879	115.572915808