

A DFT Study of the *Cis*-dihydroxylation of Nitroaromatic Compounds Catalyzed by Nitrobenzene Dioxygenase

*Anna Pabis, Inacrist Geronimo, and Piotr Paneth**

Institute of Applied Radiation Chemistry, Lodz University of Technology, Zeromskiego 116, 90-924 Lodz, Poland

Supporting Information

Activation barriers for $\text{Fe}^{\text{III}}\text{-OOH}$ and $\text{HO-Fe}^{\text{V}}=\text{O}$ attacks on nitrobenzene and 2-nitrotoluene calculated using B3LYP and B3LYP-D functionals. Comparison between the Gibbs free activation energies and Gibbs free reaction energies for the O-O cleavage calculated for the stationary points optimized at B3LYP/LACVP* level with single-point corrections using B97D, B3LYP-D2 or B3LYP-D3, and the corresponding values calculated for the stationary points reoptimized using a given dispersion-corrected functional. Barriers for the Fe^{V} attacks on nitrobenzene ring calculated for the structures optimized using B97D functional. Activation energies for the formation of an epoxide intermediate for benzene and naphthalene; illustration of the transition state for the epoxide formation and the epoxide intermediate for benzene. Ketone intermediate formed from an epoxide intermediate and a preceding transition state for nitrobenzene. Stationary points along the O-C₂ pathway involving $\text{HO-Fe}^{\text{IV}}=\text{O}$ species.

Comparison between Mulliken and NBO spin densities calculated for selected species. XYZ coordinates of all stationary points.

Table S1. Gibbs free energies of activation (ΔG^\ddagger) for the initial attack of $\text{Fe}^{\text{III}}\text{-OOH}$ (concerted and non-concerted) or $\text{HO-Fe}^{\text{V}}=\text{O}$ species on nitrobenzene (NBZ) and 2-nitrotoluene (2-NT) ring calculated at B3LYP/LACV3P+*//B3LYP/LACVP* level of theory. In parenthesis barriers for the Fe^{V} attack calculated relative to Fe^{III} reactant complex are given.

		Fe^{III} non-concerted			Fe^{III} concerted			Fe^{V}		
		$\text{O}_1\text{-C}_2$ attack	O-C_1 attack	O-C_2 attack	$\text{O}_1\text{-C}_2$ attack	O-C_1 attack	O-C_2 attack	$\text{O}_1\text{-C}_2$ attack	O-C_1 attack	O-C_2 attack
NBZ	Model1	-	39.1	35.4	36.3	31.2	31.0	13.4 (29.7)	19.1 (34.3)	14.4 (30.7)
	Model2	-	40.7	35.5	-	33.6	-	9.5 (29.0)	15.3 (34.8)	12.6 (32.1)
	Model3	42.1	37.8	31.6	-	-	-	15.6 (34.7)	18.0 (37.1)	14.8 (33.9)
	Model4	40.8	39.2	30.3	-	-	-	15.6 (33.2)	18.3 (36.0)	14.4 (32.1)
2-NT	Model1	-	-	-	37.4	34.0	32.4	9.2	15.3	13.2
	Model2	-	-	-	-	-	-	7.5	-	-

Table S2. Gibbs free energies of activation (ΔG^\ddagger) for the initial attack of $\text{Fe}^{\text{III}}\text{-OOH}$ (concerted and non-concerted) or $\text{HO-Fe}^{\text{V}}=\text{O}$ species on nitrobenzene or 2-nitrotoluene (2-NT) ring calculated at B3LYP-D2/LACV3P+*//B3LYP/LACVP* level of theory. In parenthesis barriers for the Fe^{V} attack calculated relative to Fe^{III} reactant complex are given.

		Fe^{III} non-concerted			Fe^{III} concerted			Fe^{V}		
		$\text{O}_1\text{-C}_2$ attack	O-C_1 attack	O-C_2 attack	$\text{O}_1\text{-C}_2$ attack	O-C_1 attack	O-C_2 attack	$\text{O}_1\text{-C}_2$ attack	O-C_1 attack	O-C_2 attack
NBZ	Model1	-	37.9	34.8	35.7	24.9	27.3	7.7 (21.2)	13.0 (28.5)	9.2 (24.7)
	Model2	-	38.4	33.1	-	26.1	-	1.9 (21.0)	7.8 (27.0)	4.9 (24.0)

	Model3	35.7	33.6	24.3	-	-	-	7.4 (24.3)	9.1 (25.9)	5.3 (22.2)
	Model4	36.0	35.7	27.7	-	-	-	7.4 (22.1)	10.5 (25.2)	7.7 (22.4)
2-NT	Model1	-	-	-	-	-	-	1.1	15.8	13.9
	Model2	-	-	-	-	-	-	1.2	-	-

Table S3. Gibbs free energies of activation (ΔG^\ddagger) for the initial attack of $\text{Fe}^{\text{III}}\text{-OOH}$ (concerted and non-concerted) or $\text{HO-Fe}^{\text{V}}=\text{O}$ species on nitrobenzene or 2-nitrotoluene (2-NT) ring calculated at B3LYP-D3/LACV3P+*//B3LYP/LACVP* level of theory. In parenthesis barriers for the Fe^{V} attack calculated relative to Fe^{III} reactant complex are given.

		Fe^{III} non-concerted			Fe^{III} concerted			Fe^{V}		
		$\text{O}_1\text{-C}_2$ attack	O-C_1 attack	O-C_2 attack	$\text{O}_1\text{-C}_2$ attack	O-C_1 attack	O-C_2 attack	$\text{O}_1\text{-C}_2$ attack	O-C_1 attack	O-C_2 attack
NBZ	Model1	-	38.5	35.0	36.0	25.0	27.1	6.4 (23.4)	9.7 (26.8)	6.8 (23.9)
	Model2	-	38.4	33.1	-	25.7	-	0.2 (20.3)	5.1 (25.1)	3.4 (23.4)
	Model3	36.1	33.2	23.9	-	-	-	6.1 (23.5)	6.8 (24.2)	4.7 (22.1)
	Model4	35.6	34.7	26.7	-	-	-	4.7 (19.9)	6.2 (21.4)	5.8 (21.0)
2-NT	Model1	-	-	-	-	-	-	-0.5	8.1	6.2
	Model2	-	-	-	-	-	-	-0.3	-	-

Table S4. Comparison between the Gibbs free activation energies (ΔG^\ddagger) and Gibbs free reaction energies (ΔG_r) for the O-O cleavage leading from $\text{Fe}^{\text{III}}\text{-OOH}$ to $\text{HO-Fe}^{\text{V}}=\text{O}$ species calculated for the stationary points optimized at B3LYP/LACVP* level with single-point corrections using B97D, B3LYP-D2 or B3LYP-D3 functional with LACV3P+* basis set, and the corresponding values calculated for the stationary points reoptimized using a given dispersion-corrected functional. All values calculated for Model 1 with nitrobenzene, and in the absence of the substrate (Model 1').

	B97D				B3LYP-D2				B3LYP-D3			
	SP		OPT		SP		OPT		SP		OPT	
	ΔG^\ddagger	ΔG_r	ΔG^\ddagger	ΔG_r	ΔG^\ddagger	ΔG_r	ΔG^\ddagger	ΔG_r	ΔG^\ddagger	ΔG_r	ΔG^\ddagger	ΔG_r
Model 1'	16.4	7.4	18.9	5.9	26.7	17.8	26.5	16.5	28.1	19.0	28.0	17.9
Model 1	15.5	6.1	18.1	6.0	24.6	15.5	25.5	16.3	26.6	17.4	26.0	16.4

Table S5. Comparison between the Gibbs free energies of activation (ΔG^\ddagger) for the initial attack of HO-Fe^V=O species on nitrobenzene calculated for the stationary points optimized at B3LYP/LACVP* level with B97D/LACV3P+* single-point corrections, and the corresponding values calculated for the stationary points reoptimized at B97D/LACVP* level and corrected using LACV3P+* basis set. All values calculated for Model 1.

	ΔG^\ddagger [kcal/mol]		
	O ₁ -C ₂ attack	O-C ₁ attack	O-C ₂ attack
B97D/LACV3P+*/B3LYP/LACVP*	7.0	9.8	6.3
B97D/LACV3P+*/B97D/LACVP*	6.8	8.5	7.2

Table S6. Gas phase activation energies (ΔE^\ddagger) for the epoxide formation through the Fe^{III}-OOH attack on benzene and naphthalene, with concomitant O-O cleavage calculated for two models of the NBDO active site, relative to reactant complex. In parenthesis activation energies calculated relative to separate reactants are given. All barriers calculated at the B3LYP/LACV3P+*/B3LYP/LACVP level.

	ΔE^\ddagger [kcal/mol]	
	benzene	naphthalene
Model 1	22.2 (16.7)	20.1 (14.4)
Model 2	29.8 (12.3)	---

Table S7. Gibbs free energies of activation (ΔG^\ddagger) for the epoxide formation through the Fe^{III} -OOH attack on benzene and naphthalene, with concomitant O-O cleavage calculated for two models of the NBDO active site, relative to reactant complex. In parenthesis activation energies calculated relative to separate reactants are given. All values calculated at the B97D/LACV3P+*//B3LYP/LACVP* level in SMD continuum solvent model ($\epsilon=5.7$).

	ΔG^\ddagger [kcal/mol]	
	benzene	naphthalene
Model 1	16.0 (10.8)	13.5 (7.1)
Model 2	19.8 (8.2)	---

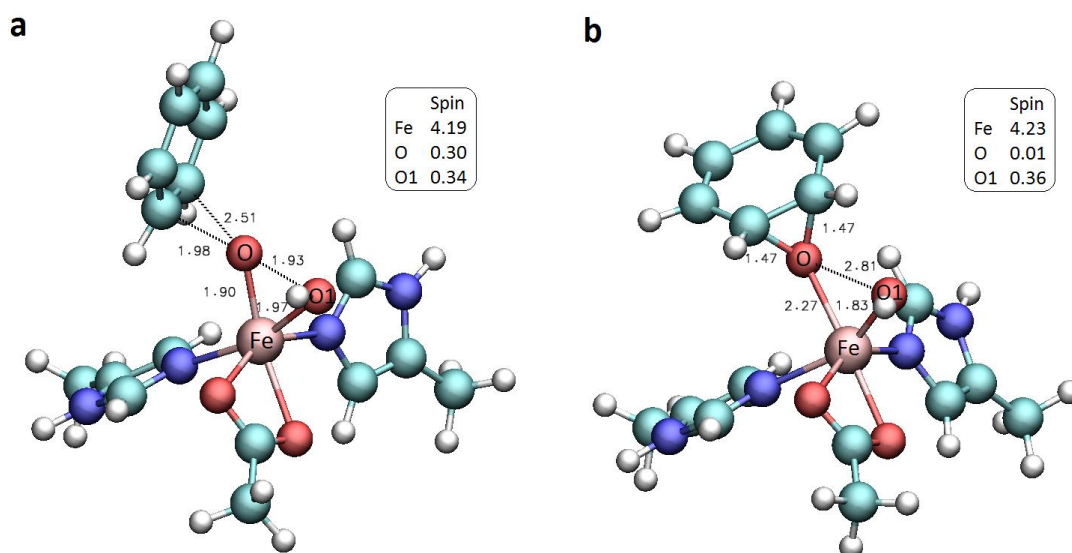


Figure S1. Optimized geometries, relevant Mulliken spin populations and bond lengths (\AA) of the transition state yielding the epoxide intermediate (**a**) and the epoxide intermediate (**b**) found for benzene in the smallest model of NBDO active site. Stationary points located at the B3LYP/LACV3P+*//B3LYP/LACVP* level in SMD continuum solvent model ($\epsilon=5.7$).

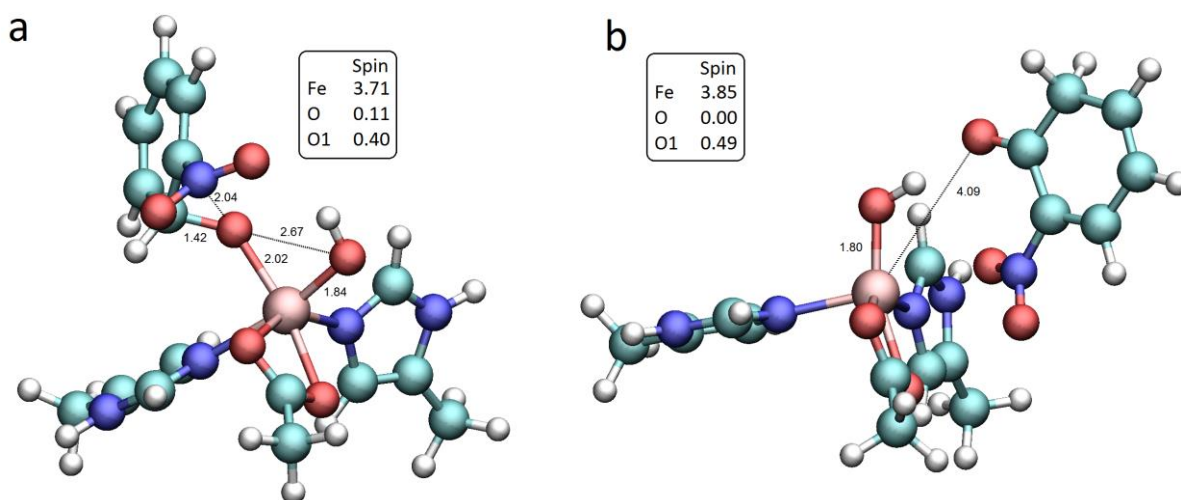


Figure S2. Optimized geometries, relevant spin populations (NBO) and bond lengths (\AA) of the transition state associated with the epoxide ring opening (**a**) and a ketone formed as a product of this reaction (**b**) found for nitrobenzene in the smallest model of NBDO active site. Stationary points located at the B97D/LACV3P+*//B3LYP/LACVP* level in SMD continuum solvent model ($\epsilon=5.7$).

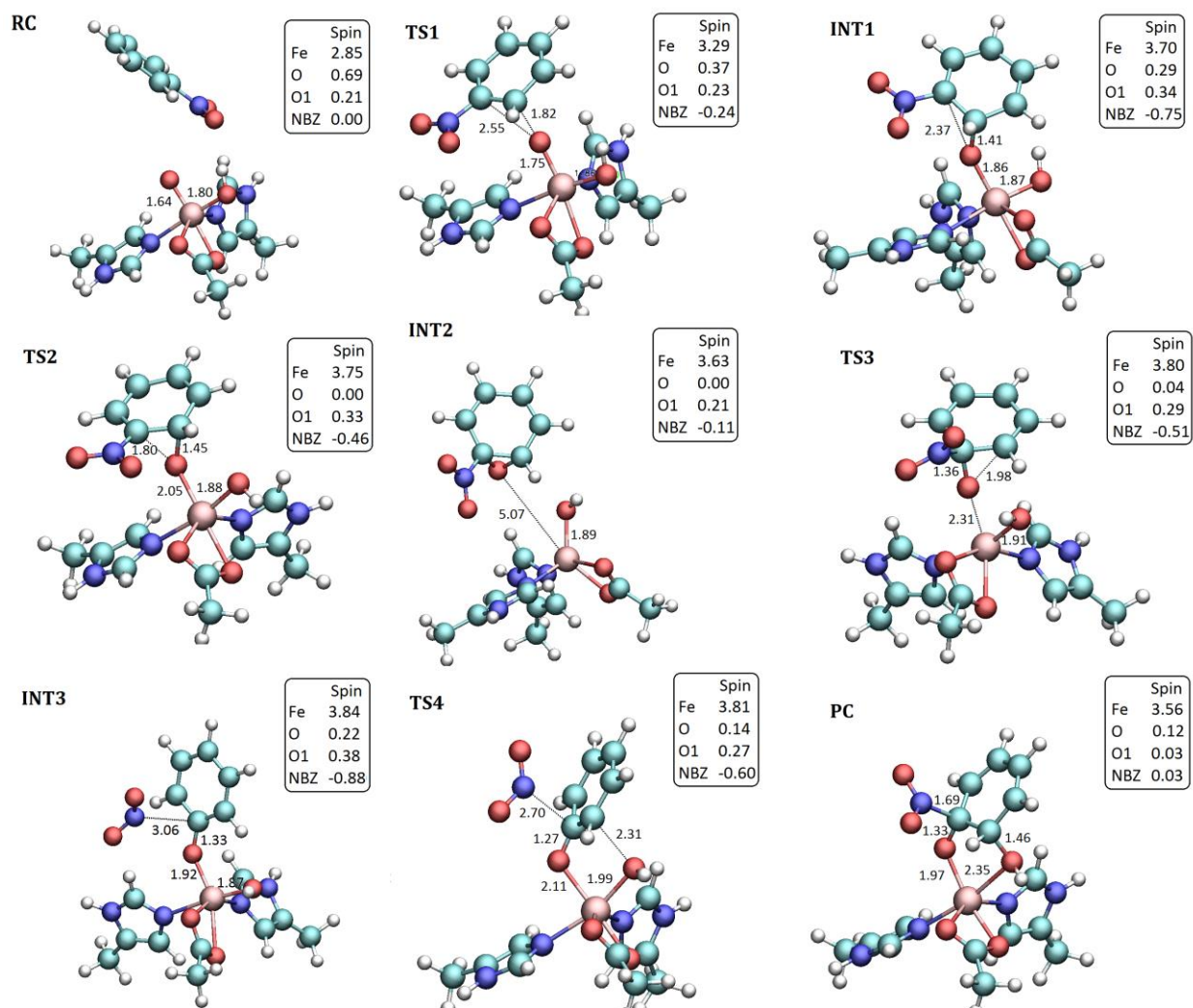


Figure S3. Optimized geometries of all stationary points along the O-C₂ pathway involving the HO-Fe^{IV}=O complex, calculated for Model 1. Key bond lengths and spin densities are given.

Table S8. Comparison of atomic spin densities calculated for the epoxide intermediates in Model 1 and 2 using Mulliken Population Analysis and Natural Bond Analysis. Reported densities are calculated at the B97D/LACV3P+* level for structures optimized using B3LYP/LACVP*.

	Model 1		Model 2	
	Mull.	NBO	Mull.	NBO
Fe	4.03	3.86	4.04	3.88
O	0.00	0.00	0.00	0.00
O1	0.42	0.45	0.42	0.45

Table S9. Comparison of atomic spin densities for the structures along the radical *cis*-dihydroxylation pathway of nitrobenzene calculated using Mulliken Population Analysis and Natural Bond Analysis. Reported densities are calculated at the B97D/LACV3P+* level for structures optimized using B3LYP/LACVP*.

Model 1											
	RC		TS1		INT		TS2		PC		
	Mull.	NBO	Mull.	NBO	Mull.	NBO	Mull.	NBO	Mull.	NBO	
Fe	3.16	2.89	3.15	2.89	3.07	2.87	3.50	3.14	4.17	3.85	
O	1.01	1.07	0.61	0.70	0.65	0.73	0.41	0.64	0.23	0.34	
O1	0.60	0.60	0.49	0.54	0.03	0.07	0.04	0.06	0.03	0.07	
NBZ	0.00	0.00	0.52	0.51	1.00	0.97	0.78	0.76	0.08	0.07	
Model 2											
	RC		TS1		INT		TS2		PC		
	Mull.	NBO	Mull.	NBO	Mull.	NBO	Mull.	NBO	Mull.	NBO	
Fe	3.18	2.90	3.09	2.85	3.06	2.88	3.45	3.14	4.19	3.85	
O	1.02	1.03	0.66	0.72	0.66	0.73	0.42	0.64	0.25	0.33	
O1	0.51	0.50	0.43	0.47	0.04	0.08	0.04	0.06	0.03	0.07	
NBZ	0.00	0.00	0.58	0.49	1.00	0.97	0.81	0.79	0.06	0.07	

XYZ coordinates of stationary points

Epoxide pathway

Nitrobenzene Model 1:

NBZ-FeIII-RC-modell:

C	-2.11593600	-1.23575200	4.33813500
N	-2.72207100	-0.89143800	3.13828200
H	-3.72178800	-0.86982300	2.96830000
C	-1.77557100	-0.60679000	2.22778100
H	-1.96974000	-0.31991000	1.20584100
N	-0.57140700	-0.74678200	2.77743900
C	-0.77161300	-1.14149800	4.09131400
H	0.05762100	-1.34014400	4.75275800
C	1.13853500	3.63359900	3.34462900
N	1.74139200	3.81972100	2.10778000
H	2.03664400	4.71093600	1.72322000
C	1.87220800	2.63720400	1.48748900
H	2.29130400	2.50140200	0.49918800
N	1.37625800	1.67285800	2.26547800
C	0.91683400	2.28549500	3.42488600
H	0.46016300	1.71910000	4.22207000
C	3.26632200	-1.52389200	2.50592600
O	2.19811400	-1.60504600	3.19536800
O	3.22644800	-0.78982700	1.45663700
C	3.07281100	-0.72547700	-2.88242100
C	3.05754500	-1.83697000	-3.72281200
C	2.04577200	-1.98289000	-4.67805700
C	1.04118400	-1.01729000	-4.79844400
C	1.03647200	0.09738000	-3.96254600
C	2.05704600	0.22417800	-3.01881600
N	2.05677900	1.38642200	-2.13060900
O	1.10484800	2.16447100	-2.17826800
O	3.02313400	1.53419200	-1.37165300
H	3.84874400	-0.58652400	-2.13942600
H	3.83801800	-2.58656300	-3.63420400
H	2.04251900	-2.85015600	-5.33187700
H	0.25951500	-1.13211200	-5.54293500
H	0.26609600	0.85529200	-4.03496300
O	0.60610600	-0.47254500	0.05211400
O	0.87012100	-1.89687100	0.10895200
H	1.72455600	-1.95537400	-0.36963000
H	5.33129400	-1.53776100	3.02707300
H	4.36837800	-2.83309700	3.80073300
H	4.80618600	-2.92431700	2.06815400

Fe	1.22225100	-0.32789000	1.82020500
C	4.51604600	-2.25594800	2.88653900
C	0.84391200	4.75725200	4.27997300
H	1.75756700	5.29218400	4.56565700
H	0.15876700	5.48419400	3.82705500
H	0.37719400	4.37156100	5.19002000
H	-3.55712900	-0.80413700	5.87492900
H	-3.50061200	-2.50493700	5.38378400
H	-2.20069900	-1.82804800	6.37944100
C	-2.88737300	-1.61223800	5.55664100

NBZ-FeIII-O-C1-concerted-TS1-model1:

C	-3.73081900	2.23058000	0.15109700
N	-2.69353800	3.12070800	-0.09182700
H	-2.77704900	4.13099200	-0.11034000
C	-1.56294700	2.43022400	-0.32295500
H	-0.60987200	2.87475900	-0.56252100
N	-1.80965700	1.12620600	-0.24022900
C	-3.15711400	0.99061300	0.05282600
H	-3.61768300	0.02027800	0.15561500
C	-0.34197200	-1.72582600	3.25813900
N	0.16455000	-2.81357100	2.56260900
H	0.47495600	-3.68557400	2.97728600
C	0.18357500	-2.53090700	1.24800000
H	0.54157000	-3.19694300	0.47925400
N	-0.28598400	-1.30235000	1.04360500
C	-0.61827200	-0.79366700	2.29217200
H	-1.03708300	0.19452800	2.40643500
C	-1.36261300	-2.41381800	-1.94141900
O	-2.16452900	-1.51343500	-1.54916400
O	-0.10826100	-2.23356600	-1.72759100
C	2.72156500	3.28449600	0.99591800
C	3.31260700	3.14735000	-0.27920300
C	3.40151600	1.90925500	-0.87316000
C	2.82370600	0.78109900	-0.21290800
H	2.67631300	4.26569500	1.45916200
H	3.71974800	4.01817100	-0.78258000
H	3.86828700	1.76869000	-1.84015900
O	1.16012700	0.67334400	-1.04688100
O	-0.08374200	0.52332700	-2.55456000
H	0.54217900	-0.02671800	-3.06395900
Fe	-0.46961400	-0.36433000	-0.84261100
C	-5.12953100	2.66656900	0.42898500
H	-5.18795500	3.29205000	1.32825800
H	-5.54337300	3.24371000	-0.40675900
H	-5.76565700	1.79102800	0.58339300
C	-0.49286900	-1.71345200	4.74210100

H	-1.16132500	-2.51223600	5.08545400
H	0.47236800	-1.84870000	5.24524700
H	-0.91357800	-0.75781800	5.06616300
C	-1.84000100	-3.65014300	-2.64359600
H	-1.46441900	-3.64757900	-3.67358500
H	-1.43415100	-4.53945400	-2.14982000
H	-2.93059500	-3.69340100	-2.65565000
C	2.22250600	2.17305700	1.67905300
H	1.79622700	2.28390200	2.67073500
C	2.31135000	0.90919600	1.10752500
H	1.98951100	0.02267400	1.63539900
N	3.27623100	-0.56586700	-0.66079800
O	3.75096600	-0.65490400	-1.78757300
O	3.14121500	-1.50090400	0.12475600

NBZ-FeIII-O-C1-concerted-INT1-modell (epoxide):

C	1.76942600	3.27993400	-1.66285400
N	0.40070400	3.06949900	-1.76893600
H	-0.22293100	3.55625900	-2.40381700
C	0.02424100	2.11433600	-0.90451400
H	-0.98141900	1.73414600	-0.80233700
N	1.09164000	1.68457800	-0.23002000
C	2.18258200	2.40802300	-0.69125800
H	3.17296700	2.24981500	-0.29275000
C	3.21623100	-2.62782800	-1.53548000
N	1.89983500	-3.04613600	-1.67921000
H	1.57725600	-3.76931500	-2.31337300
C	1.11356800	-2.34471700	-0.84901000
H	0.04174100	-2.45546400	-0.77777300
N	1.85728000	-1.47939300	-0.15859100
C	3.17010000	-1.65038700	-0.57714100
H	3.97527800	-1.06487900	-0.16029200
C	2.50248100	0.40290900	3.00392300
O	3.02587800	0.56775500	1.85950200
O	1.26493100	0.05116500	3.03699100
C	-6.01057000	0.12688800	0.96159500
C	-5.04675100	-0.74684100	1.60608100
C	-3.87430500	-1.08493000	1.02165400
C	-3.49571700	-0.40307000	-0.22179500
H	-6.96716000	0.27858600	1.45355300
H	-5.32328000	-1.20414100	2.55168100
H	-3.21507600	-1.84139900	1.42929200
O	-3.32260400	0.98055700	-0.23795900
O	-0.67824200	-0.35332800	1.03648400
H	-1.10403400	-0.35352700	1.91179900
Fe	1.10319400	0.03839400	0.98999200
C	2.50327500	4.26530200	-2.50880200
H	2.41287800	4.02243500	-3.57449700
H	2.12110500	5.28311500	-2.36469400

H	3.56495000	4.26094700	-2.24855900
C	4.33534400	-3.20005500	-2.33875100
H	4.45211200	-4.27532700	-2.15695900
H	4.16780700	-3.05772200	-3.41305600
H	5.27398600	-2.70692700	-2.07269500
C	3.25683200	0.59787600	4.28552200
H	2.74679900	1.35107500	4.89615600
H	3.25535000	-0.33986400	4.85240400
H	4.28404400	0.91026700	4.08997300
C	-5.79646500	0.64736100	-0.27074100
H	-6.58547100	1.15669800	-0.81585300
C	-4.49891500	0.48335300	-0.93198800
H	-4.42455900	0.59218200	-2.01108100
N	-2.50997600	-1.12867300	-1.09526200
O	-2.38743300	-2.33563100	-0.89773800
O	-1.92626600	-0.48967500	-1.96120700

NBZ-FeIII-O-C1-concerted-TS2-modell1:

C	-4.20925500	-0.61383900	-1.75507300
N	-3.46148300	-1.54135900	-2.46474600
H	-3.81094000	-2.12952000	-3.21252900
C	-2.20555200	-1.55941000	-1.97980200
H	-1.42882500	-2.22651500	-2.31718900
N	-2.08757000	-0.67788700	-0.99280300
C	-3.33051900	-0.08289200	-0.84521300
H	-3.51083600	0.66758000	-0.09044700
C	-0.55661300	3.68760700	0.54596400
N	-0.08116400	3.34174100	1.79858800
H	0.18484300	3.99211000	2.52923300
C	-0.03412900	1.99637400	1.89587400
H	0.31762400	1.46142100	2.76315200
N	-0.45808500	1.43765800	0.76847000
C	-0.78652100	2.48527300	-0.07951000
H	-1.17105100	2.30593300	-1.07289800
C	-0.87861600	-1.12472000	2.79131300
O	-1.81674100	-1.09391600	1.92987100
O	0.31210000	-0.89242700	2.40043600
C	3.16577400	1.24875000	-2.85664300
C	3.96805300	0.06463900	-2.85214700
C	3.98703400	-0.83293000	-1.78587800
C	3.23717700	-0.49912500	-0.67453200
H	3.19914200	1.89914900	-3.72404600
H	4.56823900	-0.16038600	-3.72962200
H	4.56327900	-1.74994600	-1.82607400
O	1.20644200	-0.30906300	-0.72627100
O	-0.10054100	-2.53264300	-0.03864100
H	0.84540400	-2.70509400	-0.18539700
Fe	-0.43085600	-0.76638900	0.36272900
C	-5.66215300	-0.39215800	-2.01488500

H	-5.84722300	-0.07728700	-3.04929600
H	-6.24230400	-1.30588000	-1.83611600
H	-6.04698400	0.38585800	-1.34997700
C	-0.71396700	5.10891900	0.11478600
H	-1.43167700	5.64477200	0.74806500
H	0.23846800	5.65121100	0.16155800
H	-1.07803500	5.15078700	-0.91554600
C	-1.18168600	-1.44534400	4.22808500
H	-2.08008600	-0.91132900	4.55202500
H	-1.38571600	-2.51961700	4.31606100
H	-0.33755700	-1.19379500	4.87400800
C	2.36354800	1.53262400	-1.79800700
H	1.73031600	2.41451300	-1.78951000
C	2.27598200	0.62240900	-0.60700100
H	2.28187000	1.18152200	0.33517700
N	3.30723000	-1.35835200	0.52017600
O	3.11892600	-2.56134400	0.36948100
O	3.58987200	-0.79048700	1.56720700

NBZ-FeIII-O-C1-concerted-INT2-model1 (ketone):

C	-2.24181900	-3.60892200	0.56521000
N	-1.81214200	-3.69331000	-0.75182500
H	-1.87962800	-4.51498100	-1.34203300
C	-1.28631800	-2.51128600	-1.12215600
H	-0.87543200	-2.29944600	-2.09693300
N	-1.35293200	-1.65347400	-0.10792200
C	-1.94187000	-2.32856100	0.94907600
H	-2.09879500	-1.84784300	1.90202200
C	-4.72499900	1.61020100	-0.97142200
N	-4.06798000	2.80412200	-0.71580500
H	-4.48617900	3.72714000	-0.75303800
C	-2.78326100	2.54695700	-0.40802200
H	-2.04689200	3.29559100	-0.16083400
N	-2.56805900	1.23608100	-0.44680600
C	-3.76945800	0.64296400	-0.79907900
H	-3.86731600	-0.42679200	-0.89976900
C	-0.22619300	1.46004100	2.01997400
O	-0.75300600	0.30757500	2.02048100
O	0.03490200	1.99682400	0.88163100
C	6.44882800	0.10241600	-1.12855800
C	6.33278900	0.09354000	0.21834300
C	5.03119700	0.06307700	0.82153800
C	3.87553700	0.02850300	0.09177500
H	7.42727300	0.10997200	-1.60159600
H	7.20290300	0.09660900	0.86561700
H	4.95500700	0.04939200	1.90467500
O	2.88260300	0.14853800	-2.09487200
O	0.06105100	0.42180300	-1.77097700
H	1.03124900	0.28664500	-1.84940700

Fe	-0.69889200	0.33984500	-0.13869400
C	-2.88031500	-4.74763800	1.28575800
H	-3.79483200	-5.08218100	0.78086100
H	-2.20552900	-5.60943700	1.35757600
H	-3.14621500	-4.44219100	2.30126300
C	-6.16708700	1.53778400	-1.34706400
H	-6.80873100	1.96908200	-0.56906200
H	-6.36666600	2.07804500	-2.28058300
H	-6.46192700	0.49472800	-1.49010200
C	0.04939100	2.20284100	3.29423100
H	0.25353500	1.50239600	4.10718700
H	0.88593300	2.89346700	3.16621900
H	-0.84039100	2.78798700	3.56066700
C	5.26090200	0.09859600	-2.02468000
H	5.31956100	-0.76313300	-2.70829800
C	3.87897800	0.08190900	-1.38219900
H	5.30070000	0.97137400	-2.69400300
N	2.62597100	-0.03915200	0.82658200
O	1.65625000	-0.56210300	0.25115900
O	2.58841700	0.39651400	1.97504400

Nitrobenzene Model 2:

NBZ-FeIII-RC-model2:

C	-2.12962700	-1.26313600	4.32162200
N	-2.73799400	-1.05846200	3.09057400
H	-3.73246200	-1.13470400	2.90612800
C	-1.80126300	-0.75898800	2.17516000
H	-1.99977400	-0.55994500	1.13368100
N	-0.60081800	-0.75564500	2.75175500
C	-0.79432600	-1.07308700	4.08744700
H	0.03314200	-1.14959600	4.77629800
C	1.29899000	3.54574000	3.54124000
N	2.55007900	3.44462900	2.94852500
H	3.26126200	4.16823400	2.94814200
C	2.67767000	2.23831500	2.37549400
H	3.55331400	1.89202000	1.84895500
N	1.55982200	1.53635900	2.56468600
C	0.69420000	2.34452800	3.28896400
H	-0.28718300	2.00661400	3.58296100
C	-0.36525000	5.89828200	-2.99099000
H	-1.19820500	5.64100600	-2.32224400
H	-0.40918500	5.17146100	-3.81323800
C	0.93942600	5.68123600	-2.22297400
O	1.72324700	6.59285100	-1.96460000
N	1.15563600	4.39773300	-1.81936500
H	2.04632400	4.17969400	-1.39155200
H	0.57990500	3.62234600	-2.13167000
C	3.25770300	-1.56287700	2.46492900

O	2.14521200	-1.78263500	3.04614500
O	3.25758800	-0.70584900	1.51124700
C	-3.31140000	0.24704900	-2.17133400
C	-4.07572900	-0.84156800	-2.58404200
C	-3.59716900	-1.69896900	-3.58052900
C	-2.35173300	-1.46945800	-4.17403700
C	-1.57554900	-0.38271500	-3.77748800
C	-2.07001900	0.45586600	-2.77680400
N	-1.26546900	1.59891200	-2.34911500
O	-0.21798500	1.83574600	-2.96412500
O	-1.66624000	2.28043400	-1.40513600
H	-3.66388000	0.92938800	-1.40752100
H	-5.04645700	-1.01754800	-2.13083300
H	-4.19796200	-2.54662500	-3.89694700
H	-1.98423600	-2.13594300	-4.94798600
H	-0.60987200	-0.18437600	-4.22554000
O	0.64602700	-0.32959200	0.04325400
O	0.89981800	-1.75781100	0.00836600
H	1.76859100	-1.79387200	-0.44643400
H	5.18024400	-1.52761900	3.36738000
H	4.30002500	-3.06540600	3.58578300
H	5.03902000	-2.64484200	2.00704100
Fe	1.20599400	-0.34766400	1.83333400
C	4.51604300	-2.25594700	2.88654000
C	0.84391200	4.75725100	4.27997400
H	1.50261100	4.97763500	5.12881500
H	0.82765200	5.64115600	3.63121800
H	-0.16686700	4.60038400	4.66532900
C	-0.52137000	7.32214800	-3.52064200
H	-3.61315100	-0.83263400	5.81809100
H	-3.43748300	-2.55353100	5.43773400
H	-2.19569400	-1.72769300	6.39521600
H	-0.49338200	8.05234800	-2.70563400
H	0.28321800	7.57653300	-4.21857700
H	-1.47625600	7.43164100	-4.04710400
C	-2.88737100	-1.61223800	5.55663900

NBZ-FeIII-O-C1-concerted-TS-model2:

C	-4.97999900	1.77479700	0.87001400
N	-4.12860700	2.70686200	0.29333500
H	-4.31226700	3.70133400	0.21909300
C	-3.03497900	2.07986600	-0.17296800
H	-2.21197000	2.55990600	-0.67789900
N	-3.12579400	0.77609800	0.07661700
C	-4.33607600	0.57402300	0.72158200
H	-4.66029200	-0.41165100	1.01842800
C	-0.20851500	-1.34607200	3.30695300
N	0.20274000	-2.46941500	2.60402300
H	0.75883900	-3.22928600	2.98097500

C	-0.25414600	-2.39913600	1.34140200
H	-0.07903200	-3.14269600	0.58030000
N	-0.95278300	-1.27836500	1.17514800
C	-0.93292600	-0.61709000	2.39780700
H	-1.44169700	0.32433000	2.53922400
C	5.99330100	0.70575800	0.35456100
H	5.12899400	0.60995400	1.02376600
H	5.63008500	1.23396300	-0.53918800
C	6.44425600	-0.68456100	-0.09601600
O	7.62518000	-0.97537900	-0.26840800
N	5.43732600	-1.58452000	-0.29276800
H	5.67215600	-2.46624500	-0.73166800
H	4.46016600	-1.31517200	-0.28761700
C	-2.65158600	-2.81741600	-1.51032900
O	-1.39443300	-2.55746800	-1.49679200
O	-3.43033100	-1.98489000	-0.94946000
C	-3.18353700	-4.02846200	-2.22994500
H	-3.37540500	-3.75176200	-3.27447900
H	-2.44970700	-4.83815100	-2.22026000
H	-4.12499100	-4.35772000	-1.78400100
C	0.14938200	-1.11024200	4.74025300
H	1.23634300	-1.06682700	4.87803400
H	-0.27616800	-0.16231900	5.07977700
H	-0.23725500	-1.90762900	5.38616600
C	-6.29001700	2.15287500	1.47455000
H	-6.95472900	2.61217500	0.73286500
H	-6.78845800	1.26414900	1.87046400
H	-6.16294800	2.86707500	2.29730100
C	7.11292300	1.50942400	1.01701300
H	6.76429800	2.51613200	1.27346000
H	7.45770000	1.02484800	1.93723400
H	7.97349200	1.60105400	0.34837000
Fe	-1.76699000	-0.63428400	-0.66553100
C	0.81106000	3.93223900	-0.34795700
C	1.20544300	3.54342600	-1.64748300
C	1.48465400	2.22497800	-1.92112000
C	1.29633500	1.24769500	-0.89175100
H	0.61364400	4.98034500	-0.14295100
H	1.31159200	4.29130900	-2.42650800
H	1.81141700	1.89790200	-2.90066100
O	-0.39389900	0.61523800	-1.29775400
O	-1.81767400	0.03297500	-2.51548900
H	-1.20488300	-0.50072900	-3.05738000
C	0.70234300	2.99360100	0.68190800
H	0.42670700	3.30785100	1.68330000
C	0.99211100	1.65710300	0.43750600
H	0.97391300	0.91946000	1.22794900
N	2.02840000	-0.03332200	-1.07267200
O	2.22997700	-0.42041700	-2.21526600
O	2.41281300	-0.61611000	-0.05332300

NBZ-FeIII-O-C1-concerted-INT1-model2 (epoxide):

C	2.87919500	-3.66730800	0.38759000
N	1.55929900	-3.38092100	0.07329500
H	0.78305100	-4.03071900	0.13702100
C	1.46561700	-2.10512000	-0.33811800
H	0.54002200	-1.62548300	-0.61728000
N	2.66875600	-1.53634200	-0.30944500
C	3.55772700	-2.50233600	0.13786000
H	4.61172600	-2.29196300	0.23607000
C	0.64544800	1.53083400	2.58878800
N	-0.03245800	2.17595200	1.56087600
H	-0.89127600	2.74530200	1.59880600
C	0.61873800	1.95176000	0.40781000
H	0.30316600	2.33804800	-0.54892400
N	1.68563100	1.18486700	0.62402300
C	1.71306100	0.92267800	1.98306200
H	2.48506300	0.31334300	2.43011300
C	-3.65627300	5.43291800	-0.22323700
H	-2.79362100	6.05834300	-0.48217300
H	-4.05661600	5.85614800	0.70703600
C	-3.08353900	4.06706700	0.15343300
O	-2.15884700	3.99153000	0.98011100
N	-3.62302700	2.98059900	-0.43286400
H	-3.29981300	2.04901800	-0.18923900
H	-4.38366700	3.05228000	-1.09362700
C	5.38844400	1.25539500	-0.72295800
O	4.39356300	2.00925200	-0.43104200
O	5.13165200	0.03566100	-0.98808500
C	6.77978900	1.80653600	-0.78661200
H	7.00980400	2.05102900	-1.83154900
H	6.86281600	2.71684900	-0.18932600
H	7.50134100	1.05748000	-0.45011600
C	0.23463000	1.53750500	4.02406300
H	-0.76482400	1.10671200	4.16119100
H	0.94424400	0.94799300	4.61050900
H	0.21410500	2.55462900	4.43372700
C	3.31236800	-5.00582500	0.88469300
H	3.10695900	-5.79274700	0.14873600
H	4.38750300	-4.99973600	1.08265400
H	2.79670400	-5.27490700	1.81437900
C	-4.71506300	5.50139300	-1.33295900
H	-5.01706700	6.54163100	-1.49273700
H	-4.32970700	5.11911400	-2.28561700
H	-5.61736500	4.93460400	-1.07340600
Fe	3.05457300	0.46616700	-0.75251400
C	-4.66326900	-4.70742400	-0.01595900
C	-4.74374200	-4.07433700	-1.31966600
C	-4.33338400	-2.80289500	-1.53246000

C	-3.61874000	-2.11681800	-0.44956000
H	-5.10313800	-5.69423400	0.09713300
H	-5.22902200	-4.61929700	-2.12403400
H	-4.51459900	-2.28058900	-2.46441200
O	-2.41232300	-2.62460800	0.03144800
O	2.34144800	0.80740000	-2.37864700
H	2.60524900	1.62720900	-2.83353400
C	-4.17441800	-4.05984000	1.06919700
H	-4.27720300	-4.47056000	2.06910900
C	-3.54731400	-2.74311900	0.92981500
H	-3.46594400	-2.08859700	1.79398300
N	-3.65098000	-0.61324100	-0.49451600
O	-4.56831100	-0.09767300	-1.12328500
O	-2.78130700	0.00043600	0.12232300

Separate reactants

NBZ:

C	-0.80365900	-0.98769400	-4.50633000
C	-0.80374200	-2.30492600	-4.96046900
C	0.23486000	-3.17132200	-4.60476300
C	1.28135500	-2.72436600	-3.79175500
C	1.29684400	-1.41022900	-3.32875400
C	0.25042200	-0.56294700	-3.69609300
N	0.25635500	0.82233800	-3.21106400
O	1.19216200	1.18158500	-2.49358900
O	-0.67528400	1.55744300	-3.54484000
H	-1.59666300	-0.29829000	-4.76821900
H	-1.61501900	-2.65409800	-5.59194800
H	0.22871300	-4.19713700	-4.96181600
H	2.08672900	-3.39861200	-3.51688700
H	2.09627500	-1.04218100	-2.69755000

Asn:

C	-1.81499100	-7.27773200	-1.71162500
H	-1.68398200	-8.31713400	-1.38527000
H	-2.18867700	-7.32682400	-2.74474700
C	-0.45600100	-6.58032500	-1.75758900
O	-0.30781700	-5.38859500	-1.49969200
N	0.58783200	-7.38380800	-2.11198400
H	1.48742500	-6.95787400	-2.29585800
H	0.44182200	-8.32989300	-2.43681900
C	-2.82454600	-6.54964400	-0.82630600
H	-2.93985400	-5.50941200	-1.14446200
H	-3.80371400	-7.03862100	-0.87758100
H	-2.50336400	-6.54327800	0.22145300

FeIII+ligands:

C	-3.25191100	-2.16702600	3.90329700
N	-3.91643000	-1.66920100	2.79058800
H	-4.92266500	-1.58447000	2.69424900
C	-3.01908100	-1.33182500	1.84999000
H	-3.26573500	-0.93071800	0.87907900
N	-1.78957100	-1.58301900	2.29729200
C	-1.92472800	-2.10638000	3.57425500
H	-1.06645700	-2.41005700	4.15375500
C	0.87967800	2.41542300	3.11601100
N	2.03594800	2.14163700	2.39816600
H	2.85236000	2.74168700	2.34473800
C	1.90894900	0.95803800	1.77930800
H	2.66251400	0.50138000	1.15683400
N	0.71470300	0.43574900	2.05963100
C	0.06543100	1.33822300	2.89136800
H	-0.92790600	1.14987700	3.26859700
C	1.82456500	-2.92911900	1.47171300
O	1.89036400	-1.95950800	0.63756700
O	0.76813800	-3.01331700	2.18042400
O	-0.73395100	-0.95762200	-0.44082400
O	-0.71236100	-2.38532300	-0.69412200
H	0.09916200	-2.47740400	-1.23784000
C	2.91940800	-3.94326900	1.58060300
H	2.80492700	-4.67070400	0.76671700
H	3.89595800	-3.46535700	1.46548600
H	2.86110100	-4.47404200	2.53300800
C	0.69649400	3.66069000	3.91437100
H	0.77135600	4.55458500	3.28365200
H	-0.28974200	3.65885900	4.38545000
H	1.45167000	3.74474700	4.70511300
C	-3.95660500	-2.63619800	5.12946700
H	-4.64561100	-3.45954200	4.90553000
H	-3.22801100	-2.99413200	5.86157800
H	-4.53870600	-1.83035000	5.59283700
Fe	-0.02324500	-1.30621600	1.26007500

Nitrobenzene Model 1 GAS:

NBZ-FeIII-RC-model1-GAS:

C	-5.17690500	-1.63505100	-0.32375100
N	-4.70957500	-1.72212700	-1.64417200
H	-5.25319400	-2.03152200	-2.43618200
C	-3.40201800	-1.35380200	-1.68560000
H	-2.77546100	-1.34276100	-2.56081300
N	-3.00647500	-1.02638100	-0.44792900
C	-4.09701700	-1.20466700	0.40944100
H	-4.00303500	-1.04560100	1.46941000
C	-2.16396700	3.72966200	-0.05555500

N	-0.76167800	3.75016500	-0.06172800
H	-0.19107000	4.58200200	-0.08846300
C	-0.28904800	2.47546900	-0.03072800
H	0.74895400	2.18653600	-0.03212700
N	-1.32857000	1.63169900	-0.00618500
C	-2.49835600	2.39792400	-0.02335500
H	-3.47350700	1.94385500	-0.00657300
C	-0.25781100	-0.78236700	2.37630500
O	-1.45261900	-1.15473600	2.02274800
O	0.47033900	-0.22876400	1.44253700
C	7.40298800	-0.11433900	-0.07634300
C	6.78639500	-1.37270100	-0.13411200
C	5.40731100	-1.47071100	-0.31772800
C	4.66524000	-0.28814700	-0.43998400
H	8.47604100	-0.04631400	0.06510900
H	7.37906100	-2.27483000	-0.03799600
H	4.90889600	-2.42916800	-0.36862000
O	-0.38351600	-0.72949800	-1.73490600
O	0.06108000	-1.97628300	-0.97015900
H	1.05670600	-1.82030000	-0.88549300
Fe	-1.10528100	-0.41455100	0.03027100
C	-6.57606200	-1.96723700	0.06888500
H	-7.30657400	-1.32315100	-0.43562900
H	-6.82916500	-3.00833000	-0.16507600
H	-6.70256000	-1.83224300	1.14559000
C	-3.00274100	4.96198400	-0.07682800
H	-2.81578200	5.59833200	0.79656000
H	-2.82157600	5.56399600	-0.97543000
H	-4.06150700	4.69268100	-0.06790800
C	0.26390300	-1.00246500	3.75389600
H	0.69918000	-2.00783100	3.81897700
H	1.04408400	-0.27728700	3.99096700
H	-0.54849500	-0.94504300	4.48121300
C	6.64138000	1.05709900	-0.20234700
H	7.12301400	2.02698700	-0.15958300
C	5.26160500	0.97882200	-0.38591800
H	4.65287300	1.86682900	-0.48966300
N	3.22938900	-0.37397100	-0.63455800
O	2.71208800	-1.54076500	-0.69905500
O	2.55255500	0.68366700	-0.73878900

NBZ-FeIII-O-C1-concerted-TS-modell-GAS:

C	-3.66961500	2.36225100	0.29659900
N	-2.58788700	3.22885400	0.07778400
H	-2.63577800	4.23649900	0.10046100
C	-1.47709900	2.49859600	-0.21010400
H	-0.50831500	2.89688100	-0.45549800
N	-1.79322300	1.19870800	-0.17767400
C	-3.15361400	1.09918400	0.12974300

H	-3.65001100	0.14536700	0.16223300
C	-0.37943900	-1.87695700	3.17157500
N	0.23041000	-2.88633100	2.41367900
H	0.60379400	-3.74938700	2.78023900
C	0.25499400	-2.51934200	1.10560400
H	0.67865000	-3.09573100	0.30265400
N	-0.31036800	-1.31108900	0.97868800
C	-0.70947200	-0.90260900	2.25956000
H	-1.21311200	0.03408400	2.42095000
C	-1.53207100	-2.31313400	-2.01488300
O	-2.28911700	-1.37608600	-1.53359900
O	-0.24647800	-2.18693500	-1.79052200
C	3.09678200	3.24332600	0.86396100
C	3.64936200	2.95914500	-0.40866200
C	3.57334800	1.68501100	-0.93088300
C	2.86339000	0.67538800	-0.20366900
H	3.18574500	4.24487000	1.27133700
H	4.15837700	3.74000400	-0.96130500
H	4.00906700	1.42313500	-1.88619000
O	1.17614500	0.73111400	-0.95316200
O	-0.09030900	0.64315200	-2.49315100
H	0.58833600	0.26483700	-3.09377500
Fe	-0.53120900	-0.30218700	-0.83627000
C	-5.04385800	2.84092900	0.62274600
H	-5.06802800	3.41450300	1.55732600
H	-5.45239200	3.47653200	-0.17207300
H	-5.71665600	1.98818600	0.73964400
C	-0.57977600	-1.97149700	4.64750700
H	-1.21750400	-2.82187500	4.91728200
H	0.37087500	-2.08397300	5.18251700
H	-1.06446000	-1.06538100	5.01877100
C	-2.07563400	-3.44622700	-2.81584500
H	-2.07280100	-3.16969200	-3.87792800
H	-1.45070800	-4.33395500	-2.70026100
H	-3.10610800	-3.65902400	-2.52562900
C	2.47272000	2.24084500	1.61541500
H	2.08486900	2.46076900	2.60322700
C	2.38977200	0.94148400	1.11577700
H	1.97178900	0.13009400	1.69356100
N	3.14969000	-0.73694300	-0.57895500
O	3.55053800	-0.95493300	-1.74786800
O	2.95131100	-1.62764400	0.29382300

NBZ-FeIII-O-C1-concerted-INT1-model1-GAS (epoxide):

C	1.39077000	3.15755300	-1.93624700
N	0.01043200	2.94347700	-1.79689000
H	-0.70705200	3.38847200	-2.34932200
C	-0.21806300	2.04266600	-0.80875700
H	-1.18970400	1.67840000	-0.51418400

N	0.96396500	1.66118100	-0.29692300
C	1.97126800	2.35420000	-0.98445800
H	3.00961500	2.22333900	-0.73395500
C	3.03376900	-2.70239200	-1.57150700
N	1.71707000	-3.17966700	-1.48372300
H	1.34423200	-3.96379700	-1.99831700
C	1.01320000	-2.42382300	-0.60482200
H	-0.03057000	-2.56025000	-0.37240300
N	1.82117400	-1.46922900	-0.11545600
C	3.08368800	-1.63789600	-0.70344200
H	3.90706600	-0.99333500	-0.44914800
C	2.92407800	0.69087600	2.76572800
O	3.28711400	0.70018700	1.52326800
O	1.66433700	0.37732500	2.98681000
C	-6.05118100	0.16261300	0.88075900
C	-5.14745600	-0.65156100	1.67754800
C	-3.92570900	-1.02934000	1.22474900
C	-3.44005700	-0.46407100	-0.03432700
H	-7.04273000	0.35633300	1.27526300
H	-5.50536200	-1.02807000	2.62955700
H	-3.30397300	-1.74415100	1.74648000
O	-3.21490700	0.97229000	-0.14219500
O	-0.55533500	-0.32062300	1.34130300
H	-1.00032300	-0.31369200	2.20942000
Fe	1.18816700	0.11145900	1.00342400
C	1.96352300	4.07494400	-2.96597400
H	1.70808100	3.75177600	-3.98234800
H	1.60641600	5.10405800	-2.83984000
H	3.05306000	4.09224700	-2.88759400
C	4.05120800	-3.30901800	-2.48054500
H	4.23094200	-4.36478500	-2.24502100
H	3.74338000	-3.24592700	-3.53119800
H	5.00319000	-2.78231800	-2.38151600
C	3.83152600	1.00373200	3.90853800
H	3.42436400	1.84305600	4.48218600
H	3.87879600	0.14408600	4.58560200
H	4.83156900	1.24888900	3.55091500
C	-5.72633000	0.58093100	-0.37077100
H	-6.45782600	1.05576300	-1.01491500
C	-4.38546000	0.35445700	-0.90296900
H	-4.20860900	0.38121200	-1.97194700
N	-2.38666000	-1.25235800	-0.74762900
O	-2.21065200	-2.44272200	-0.37191600
O	-1.75573000	-0.70099300	-1.68394800

Nitrobenzene Model 2 GAS:

NBZ-FeIII-RC-model2-GAS:

C	5.08817600	-1.48820000	-1.87957400
---	------------	-------------	-------------

N	4.10511900	-1.30948900	-2.86410500
H	4.21618300	-1.52413100	-3.84392600
C	2.98773500	-0.78528300	-2.29750200
H	2.08267900	-0.52420800	-2.81764700
N	3.20344700	-0.62192700	-0.98510200
C	4.50804900	-1.04806500	-0.71285100
H	4.92204500	-0.98060900	0.27809500
C	0.25717300	-3.66678900	1.44343600
N	-0.88485700	-2.98322600	0.99280900
H	-1.85732700	-3.30962800	0.86116900
C	-0.54415300	-1.71870500	0.66872600
H	-1.23003300	-0.97191600	0.30605800
N	0.77730400	-1.53693500	0.88109100
C	1.28125000	-2.75055400	1.36788600
H	2.31929300	-2.87378200	1.62481800
C	-5.75738500	-3.36510500	-0.70244100
H	-6.10350300	-4.01240200	0.11414600
H	-5.35543000	-4.04503500	-1.46380900
C	-4.56596400	-2.58505200	-0.15509600
O	-3.53599600	-3.19748900	0.25915700
N	-4.65595000	-1.23958900	-0.12948100
H	-3.89720400	-0.66703300	0.22308400
H	-5.45972600	-0.74777600	-0.48556900
C	2.55264600	1.58631600	2.21070200
O	1.34241200	1.65434900	1.72238600
O	3.32294500	0.68582100	1.67014600
C	3.02827400	2.51053500	3.28073900
H	3.65662000	3.29102800	2.83382100
H	2.18418200	2.98003900	3.78672800
H	3.64696400	1.96717000	3.99952500
C	0.28166000	-5.09447800	1.89521700
H	-0.04607200	-5.77526300	1.10107800
H	1.29754800	-5.37407700	2.18369700
H	-0.37212900	-5.25562900	2.76008300
C	6.43641500	-2.05232200	-2.17924600
H	6.98076600	-1.44081000	-2.90881200
H	7.03696900	-2.08980000	-1.26741300
H	6.37176500	-3.07246800	-2.57658800
C	-6.93928100	-2.55673800	-1.27650300
H	-7.71023300	-3.24005800	-1.64455700
H	-7.40730300	-1.92126800	-0.51528600
H	-6.63107700	-1.92771200	-2.11998200
Fe	1.78377500	0.11434500	0.30192200
C	-0.92171800	5.48773100	-0.35408800
C	-0.44038900	4.43861500	0.44624300
C	-1.14865600	3.23686400	0.53608500
C	-2.33657700	3.11236800	-0.19505700
H	-0.36966900	6.41949100	-0.41314800
H	0.47090100	4.55785300	1.02169700
H	-0.78930400	2.42835100	1.15799800

O	0.60715900	0.77401400	-1.06016000
O	1.50951300	1.98508400	-1.21979300
H	0.92784000	2.70912200	-0.87627100
C	-2.11844800	5.34048800	-1.06908100
H	-2.49068000	6.15238800	-1.68277400
C	-2.83891500	4.14685600	-0.99310600
H	-3.76458800	4.00802000	-1.53591200
N	-3.07736000	1.86351300	-0.12700200
O	-2.57033900	0.88948900	0.52306700
O	-4.19330800	1.77996100	-0.71163700

NBZ-FeIII-O-C1-concerted-TS-model2-GAS:

C	-4.83479700	2.21614500	0.50530500
N	-3.91328300	3.00592100	-0.19955600
H	-4.04733500	3.97453900	-0.44804800
C	-2.83146600	2.25017800	-0.53006500
H	-1.98336000	2.58255100	-1.10263000
N	-3.00897500	1.00908400	-0.06225400
C	-4.25225000	0.97210100	0.57821800
H	-4.63757600	0.05976400	0.99835100
C	-0.28770900	-0.76682400	3.45013400
N	0.10394100	-1.99992700	2.90786100
H	0.65749000	-2.69780200	3.38179100
C	-0.36339200	-2.10471400	1.63523800
H	-0.19050300	-2.93128600	0.96879000
N	-1.04396300	-0.99422200	1.32495800
C	-1.00829300	-0.15750500	2.44960100
H	-1.50049600	0.79893600	2.45399800
C	6.88969900	0.03026000	-0.02120400
H	7.16647800	0.22846300	-1.06621800
H	7.49388200	-0.82372400	0.30800100
C	5.41028100	-0.33142400	-0.01333200
O	4.51080200	0.53669600	-0.16708800
N	5.11326500	-1.65130400	0.14820100
H	4.14550600	-1.94799200	0.12126800
H	5.83246000	-2.34981100	0.24443000
C	-2.81006100	-2.83733900	-1.11267300
O	-1.51324100	-2.62648700	-1.09982000
O	-3.54864500	-1.85605500	-0.70245700
C	-3.38615400	-4.11445500	-1.63632700
H	-3.50752400	-4.03153200	-2.72374000
H	-2.71234300	-4.95020400	-1.43717400
H	-4.36824700	-4.29721400	-1.19703000
C	0.08321000	-0.32333900	4.82888100
H	1.17064200	-0.26270300	4.95708500
H	-0.33123600	0.66808300	5.02672800
H	-0.30707100	-1.00364300	5.59524300
C	-6.14123900	2.74287300	1.00355100
H	-6.77072900	3.10797200	0.18321500

H	-6.69239300	1.94895400	1.51291400
H	-6.00624800	3.56523700	1.71655000
C	7.20296700	1.27160900	0.83122100
H	8.25009600	1.56549500	0.71118400
H	6.56621500	2.10653200	0.52529100
H	7.02307400	1.07813700	1.89460400
Fe	-1.76671700	-0.57253800	-0.59141000
C	1.76426800	3.41213100	-0.59461300
C	2.02608600	2.87732700	-1.87715500
C	2.00853200	1.51276200	-2.07574400
C	1.65033400	0.65793900	-0.98770300
H	1.80950900	4.48605000	-0.44613100
H	2.27281800	3.53990000	-2.69818700
H	2.23831600	1.06456100	-3.03272000
O	-0.21072900	0.41621600	-1.33379400
O	-1.77087300	-0.04704300	-2.48150100
H	-1.19686200	-0.53225400	-3.11281400
C	1.48858700	2.57293800	0.49150800
H	1.33219900	2.99206400	1.47851900
C	1.47470500	1.19163100	0.31850300
H	1.34316400	0.51307400	1.14701400
N	1.98996800	-0.77144400	-1.12280300
O	2.20052800	-1.22080900	-2.27366100
O	2.04443300	-1.47585200	-0.06899700

NBZ-FeIII-O-C1-concerted-INT1-model2-GAS (epoxide):

C	-2.71379000	3.49131300	0.16249300
N	-1.36093500	3.13966500	0.05574100
H	-0.55925100	3.74834600	0.14599800
C	-1.26243900	1.81659400	-0.22762900
H	-0.33119200	1.28854400	-0.32563600
N	-2.49215500	1.29253500	-0.31278000
C	-3.40639100	2.32481300	-0.07524200
H	-4.46638800	2.14116400	-0.09890400
C	-0.31185800	-1.45917000	2.59777700
N	0.33946000	-2.15921700	1.57526200
H	1.23945200	-2.65816600	1.58338800
C	-0.38069200	-2.04294700	0.43719900
H	-0.10461000	-2.47409200	-0.50803300
N	-1.47425700	-1.29653700	0.66872900
C	-1.44178100	-0.93274100	2.01702400
H	-2.21230200	-0.32773100	2.46331900
C	3.96944600	-5.30915300	-0.12305100
H	3.07310800	-5.93418800	-0.21646500
H	4.40234900	-5.56615200	0.85309100
C	3.46762800	-3.87437500	0.00070100
O	2.56004700	-3.59527900	0.83449700
N	4.02542900	-2.92748000	-0.79093600
H	3.72951500	-1.96052700	-0.72190200

H	4.75106700	-3.15290400	-1.45240400
C	-5.16803200	-1.60224600	-0.52192100
O	-4.13950000	-2.38980600	-0.45769600
O	-4.89684400	-0.32669900	-0.66971400
C	-6.56519900	-2.11112100	-0.46221500
H	-7.17982700	-1.45952000	0.16459800
H	-6.99991300	-2.10036000	-1.46940800
H	-6.58167500	-3.13292300	-0.08226500
C	0.18331100	-1.34010300	4.00066400
H	-0.50647400	-0.72874100	4.58763000
H	0.26164000	-2.31846100	4.48937900
H	1.17372900	-0.87115200	4.04514300
C	-3.17074100	4.87347900	0.49566600
H	-2.83079000	5.60649500	-0.24596200
H	-4.26248600	4.90985300	0.51863300
H	-2.80673600	5.19676700	1.47857200
C	4.96885800	-5.63683100	-1.24779400
H	5.21404200	-6.70262000	-1.22549300
H	4.55366000	-5.41819000	-2.23871900
H	5.91183800	-5.08826300	-1.13239700
Fe	-2.82211000	-0.71281900	-0.74172900
C	4.22412300	4.91855300	-0.02716300
C	4.28801900	4.22761400	-1.30503300
C	3.73277300	3.00430700	-1.49345600
C	2.90302000	2.44248800	-0.42653200
H	4.76531400	5.85314900	0.07250700
H	4.86821300	4.67980900	-2.10168700
H	3.88696300	2.42711400	-2.39566400
O	1.66975700	3.11732600	-0.03546200
O	-2.03159600	-1.05581500	-2.31342900
H	-2.20832800	-1.34793400	-3.22229100
C	3.61021100	4.37306900	1.05628900
H	3.70014200	4.81908500	2.04036700
C	2.85389100	3.13072500	0.93145800
H	2.63919800	2.53003400	1.80787600
N	2.76152500	0.94784500	-0.42263400
O	3.68112500	0.29485500	-0.98708600
O	1.77938500	0.43436600	0.16921600

Separate reactants GAS

NBZ-gas:

C	0.43101400	-1.22380200	0.00000100
C	1.82734800	-1.21575200	0.00000200
C	2.52495000	0.00000000	0.00000000
C	1.82734800	1.21575200	-0.00000100
C	0.43101400	1.22380200	-0.00000200
C	-0.24357700	0.00000000	0.00000000
N	-1.71008100	0.00000000	-0.00000100

O	-2.30585600	1.11552400	0.00000400
O	-2.30585600	-1.11552400	-0.00000300
H	-0.13595500	-2.14523800	0.00000200
H	2.36885600	-2.15515300	0.00000300
H	3.60989100	0.00000000	0.00000100
H	2.36885600	2.15515300	-0.00000300
H	-0.13595500	2.14523800	-0.00000300

Asn-GAS:

C	0.69291600	-0.72436500	0.21426700
H	0.59863000	-1.64963200	-0.37013400
H	0.74215700	-1.02928300	1.27055700
C	-0.56200300	0.12696000	0.04225100
O	-0.54199900	1.37505600	0.07699700
N	-1.73046700	-0.57130500	-0.12486500
H	-2.59359200	-0.05539800	-0.20607200
H	-1.75884300	-1.57671300	-0.17310100
C	1.96905000	0.03412200	-0.16770900
H	2.01568500	0.98513600	0.36925400
H	2.85902600	-0.55621300	0.07389300
H	1.98642300	0.26049100	-1.23917000

FeIII+ligands-GAS:

C	-3.32676100	-1.45326300	-0.69608500
N	-3.39348000	-1.51663500	0.70444900
H	-4.13231200	-1.95649800	1.23349100
C	-2.32713900	-0.86735800	1.23824000
H	-2.13345200	-0.73465800	2.28876000
N	-1.56698100	-0.39217800	0.23983400
C	-2.18194400	-0.74409300	-0.96652300
H	-1.77727400	-0.43438800	-1.91399700
C	2.77304400	-2.47137600	-0.16491200
N	3.61858200	-1.35250000	-0.19435300
H	4.62005700	-1.38215200	-0.32011500
C	2.88565900	-0.22287400	-0.02404700
H	3.26977000	0.78278400	-0.00619100
N	1.59458500	-0.56242900	0.11561600
C	1.51399200	-1.95792500	0.02994400
H	0.57541600	-2.47683000	0.11008300
C	0.56714000	2.67380100	-1.10709900
O	1.33219700	2.41230600	-0.07412900
O	-0.44162200	1.86923300	-1.26896100
O	-0.04878300	0.99209900	2.37331000
O	-0.94807800	2.17770200	2.04337700
H	-0.42863900	2.93667100	2.40257800
C	0.81023400	3.83424800	-2.00417300
H	0.26922600	4.70801000	-1.61834400
H	1.87245800	4.08333300	-2.03380400

H	0.43413200	3.62534800	-3.00735300
C	3.26062700	-3.87192600	-0.32534500
H	3.97330400	-4.14673300	0.46127000
H	2.42103500	-4.56839900	-0.26847600
H	3.75291300	-4.02324400	-1.29332100
C	-4.34911500	-2.06432800	-1.59144200
H	-5.34568500	-1.63994000	-1.42059400
H	-4.08754600	-1.87957200	-2.63582800
H	-4.41845100	-3.14997900	-1.45265200
Fe	0.09469200	0.78008800	0.48059800

Benzene Model 1

BNZ-FeIII-RC-modell:

C	-1.81952800	0.27016500	1.88121700
N	-2.31087100	0.36772400	0.58648000
H	-3.26380300	0.61676500	0.33084500
C	-1.33332800	0.06556300	-0.28238600
H	-1.44923600	0.04863700	-1.35491500
N	-0.21613200	-0.22480200	0.38403600
C	-0.51043300	-0.10256100	1.73387900
H	0.22999800	-0.30284500	2.49285400
C	3.23423900	3.13725600	-0.13983000
N	4.27199400	2.40409800	-0.69824600
H	5.18227100	2.77466800	-0.94998700
C	3.89063800	1.12602300	-0.84156100
H	4.51146900	0.33653200	-1.23470100
N	2.63965700	0.98455800	-0.40248300
C	2.22136400	2.23325700	0.03550500
H	1.23683000	2.38999600	0.44828100
C	3.17494700	-2.23027300	0.78199600
O	2.07423700	-1.84116500	1.29897200
O	3.40456100	-1.88960100	-0.42894700
C	-6.09397900	-0.44651500	0.53504400
C	-5.74244100	-1.21847600	-0.57635200
C	-5.25212600	-0.60116900	-1.73113700
C	-5.11336500	0.79012900	-1.77558300
H	-6.48184300	-0.92669600	1.42963500
H	-5.85358900	-2.29903900	-0.54389000
H	-4.98508900	-1.20170400	-2.59678100
O	1.04299300	-1.25056800	-2.16568400
O	0.79422900	-2.58438700	-1.65155700
H	1.59148700	-3.06742900	-1.95820900
Fe	1.59302800	-0.78266000	-0.43432600
C	-2.65156900	0.52706400	3.09089800
H	-3.04900500	1.54916700	3.09867100
H	-3.50326500	-0.16143000	3.14407600
H	-2.04833500	0.39011100	3.99212200
C	3.34186800	4.59328600	0.15586300

H	4.16085400	4.80118500	0.85480100
H	3.52544400	5.17511300	-0.75544600
H	2.41255800	4.95182200	0.60605800
C	4.13770000	-3.06927000	1.55986000
H	3.82874100	-4.11982500	1.48497700
H	5.14821800	-2.97614100	1.15624900
H	4.11779300	-2.78937700	2.61624200
C	-5.95501100	0.94507400	0.49282800
H	-6.23640800	1.54640600	1.35349200
C	-5.46378000	1.56392300	-0.66296000
H	-5.36486000	2.64578600	-0.70008900
H	-4.74081500	1.27132800	-2.67627000

BNZ-FeIII-O-C1-concerted-TS-model1:

C	-2.93496600	2.78542500	0.76336500
N	-1.72013500	3.45640500	0.75764500
H	-1.58380500	4.42821800	1.01282200
C	-0.75420400	2.61912700	0.33789500
H	0.28380700	2.88796300	0.21959100
N	-1.27853300	1.42615700	0.07329200
C	-2.63645100	1.51964000	0.33261600
H	-3.29806200	0.68229500	0.17354000
C	-0.42461600	-2.32031500	2.83947100
N	-0.21853700	-3.33267700	1.91614500
H	-0.15106200	-4.32133500	2.13164800
C	-0.13061900	-2.79758300	0.68388900
H	0.02279900	-3.36151100	-0.22256700
N	-0.26661800	-1.47580100	0.75345400
C	-0.45165600	-1.17004100	2.09382800
H	-0.60337000	-0.15530400	2.42804600
C	-1.59769100	-1.70481400	-2.34947800
O	-2.19721900	-0.76577600	-1.74697300
O	-0.32964600	-1.82418300	-2.17441300
C	4.67782200	1.92194800	0.20450400
C	4.87368200	0.94797900	-0.79461500
C	4.04600200	-0.15667200	-0.84876700
C	2.96945300	-0.28936900	0.07513100
H	5.33473700	2.78670600	0.24203100
H	5.68040700	1.06611400	-1.51169300
H	4.18637300	-0.91902800	-1.60922300
O	1.50751400	0.48969900	-1.01593600
O	0.27619800	1.03316700	-2.40001200
H	0.73187200	0.48977000	-3.07015600
Fe	-0.28274200	-0.14066400	-0.91416400
C	-4.21877600	3.43465000	1.15629100
H	-4.18354700	3.81236800	2.18552000
H	-4.45768100	4.27939800	0.49861800
H	-5.03583400	2.71137000	1.08857700

C	-0.57465700	-2.57498800	4.30126100
H	-1.43589100	-3.22115800	4.51062800
H	0.31508600	-3.06226800	4.71839600
H	-0.72388800	-1.63066700	4.83142700
C	-2.32401800	-2.65981100	-3.25165900
H	-1.92651700	-2.57109700	-4.26929200
H	-2.14682500	-3.68941300	-2.92174100
H	-3.39534400	-2.45109500	-3.25859400
C	3.66082300	1.78471200	1.15412000
H	3.53591100	2.53459700	1.92956500
C	2.82338700	0.67456900	1.10867900
H	2.04175400	0.53930300	1.84941500
H	2.47127700	-1.24656300	0.16746500

BNZ-FeIII-O-C1-concerted-INT-model1 (epoxide):

C	-1.87739000	3.34465200	1.18061200
N	-0.53350500	3.59120600	0.94512600
H	-0.02924100	4.42513500	1.22470500
C	0.00107400	2.54646100	0.28801800
H	1.03717000	2.47716800	-0.00219200
N	-0.93121500	1.62017100	0.08044200
C	-2.10694600	2.11024300	0.62905700
H	-3.02364300	1.54336500	0.58269400
C	0.52730200	-1.92815900	2.85277500
N	0.11771700	-3.06559400	2.17478200
H	0.12228800	-4.00812600	2.54809300
C	-0.29661300	-2.71934800	0.94060400
H	-0.67546900	-3.41055100	0.20522300
N	-0.18030600	-1.40573000	0.77464600
C	0.33571600	-0.90587800	1.96091300
H	0.53239500	0.14586000	2.09485300
C	-2.70867600	-1.68279400	-1.34220800
O	-2.78140400	-0.53444700	-0.78574000
O	-1.55966300	-2.11530200	-1.67840300
C	4.49654800	0.13769600	-0.01435900
C	4.33755300	1.41696000	-0.68739500
C	3.39300600	1.60643900	-1.63879000
C	2.39026900	0.56453600	-1.90437300
H	5.33522900	0.01904500	0.66632300
H	5.06656600	2.19624500	-0.48206200
H	3.37788300	2.50271800	-2.25223100
O	1.53645500	0.20110600	-0.76227000
O	-0.49694300	0.22546500	-2.69873100
H	-0.86599600	-0.42944900	-3.31588800
Fe	-0.69105200	-0.22254600	-0.93516300
C	-2.75528500	4.31166100	1.90377700
H	-2.38155700	4.51455800	2.91475300
H	-2.82052000	5.26956500	1.37331500
H	-3.76603800	3.90450300	1.99137600

C	1.04613200	-1.95285700	4.25140600
H	0.29903100	-2.34546800	4.95208100
H	1.94392400	-2.57711600	4.33820000
H	1.30698300	-0.93930900	4.56762200
C	-3.95188300	-2.49021400	-1.59576000
H	-4.61302900	-1.93486800	-2.27062800
H	-3.70500200	-3.45712100	-2.03797900
H	-4.49355200	-2.63690600	-0.65492500
C	3.70820700	-0.92193500	-0.30919000
H	3.92510300	-1.91468700	0.07393900
C	2.55542000	-0.75613600	-1.20629500
H	2.11763800	-1.64305300	-1.65670700
H	1.81421000	0.60177700	-2.82289000

Benzene Model2

BNZ-FeIII-RC-model2:

C	3.65148900	-3.23171200	-1.86810000
N	2.77085700	-2.73274000	-2.81717200
H	2.71486100	-3.03349100	-3.78410800
C	2.01823500	-1.76776900	-2.26108500
H	1.25842300	-1.20420400	-2.77983000
N	2.36418400	-1.61109500	-0.98581000
C	3.38117600	-2.51697900	-0.73086700
H	3.85257900	-2.57869500	0.23795400
C	-1.62745700	-3.09131900	1.40157600
N	-2.33718000	-2.02272400	0.87444500
H	-3.34923800	-1.92995700	0.72607100
C	-1.47557300	-1.05467200	0.53029300
H	-1.77211100	-0.11407600	0.09283100
N	-0.22729500	-1.43347700	0.80484700
C	-0.31219100	-2.70573400	1.34942700
H	0.56604200	-3.25202500	1.66111200
C	-6.13012200	0.76283900	-0.98792300
H	-5.57948900	0.69415500	-1.93469300
H	-5.62538200	1.54559000	-0.40868600
C	-5.85412800	-0.54281300	-0.24999300
O	-4.68746600	-0.86841600	0.01449600
N	-6.90879400	-1.31144600	0.08858000
H	-6.75173400	-2.18265000	0.57973900
H	-7.86245600	-1.04982100	-0.11772200
C	2.75858900	0.60642000	2.23407800
O	1.50037000	0.81698200	2.08486500
O	3.33528900	-0.10839500	1.35708900
C	3.51119900	1.21032500	3.38103700
H	3.73051400	2.25961800	3.14608600
H	2.90145400	1.19240800	4.28862500
H	4.45414900	0.68428500	3.54327300
C	-2.27093100	-4.34787600	1.88707600

H	-2.83536900	-4.84446100	1.08843100
H	-1.50679800	-5.04265600	2.24582200
H	-2.96556500	-4.15064200	2.71257700
C	-7.58832300	1.15107700	-1.24927600
H	-7.62870600	2.10787700	-1.78011500
H	-8.10262900	0.41017600	-1.87288500
H	-8.15154000	1.26960400	-0.31606900
Fe	1.44785200	-0.30306400	0.34245000
C	0.54086200	5.53364000	-1.57185400
C	1.80467400	5.51751100	-0.97481800
C	2.00213900	4.82654100	0.22449000
C	0.93267800	4.14885800	0.82660300
H	0.38831200	6.07176300	-2.50367500
H	2.63345100	6.04306700	-1.44132300
H	2.98300700	4.81870000	0.69276300
O	0.57596700	0.80700700	-0.91067400
O	1.78685300	1.60010000	-0.89681700
H	1.50354300	2.40135000	-0.39431000
C	-0.52710300	4.85824100	-0.97376200
H	-1.50864700	4.87224800	-1.43986800
C	-0.33255700	4.16445300	0.22384700
H	-1.16147400	3.64101700	0.69265300
H	1.08077400	3.61390500	1.76100300
C	4.63259000	-4.31488000	-2.16330700
H	4.13086300	-5.24018100	-2.47183200
H	5.32093800	-4.02580700	-2.96679000
H	5.22608400	-4.53219500	-1.27129700

BNZ-FeIII-O-C1-concerted-TS-model2:

C	-4.30530900	-2.74380400	-1.40615400
N	-3.07160900	-3.36376100	-1.54390100
H	-2.90388500	-4.24130700	-2.02291500
C	-2.13378100	-2.62503900	-0.92167900
H	-1.08940700	-2.88679700	-0.85377900
N	-2.69585600	-1.54641500	-0.38656700
C	-4.04761300	-1.61178700	-0.67937900
H	-4.73629800	-0.85286300	-0.34100600
C	-2.73894300	2.82748900	-2.05224600
N	-2.58237000	3.58017100	-0.89868000
H	-2.69914600	4.58510600	-0.82957200
C	-2.26044300	2.76424800	0.12254900
H	-2.08521800	3.08724100	1.13665600
N	-2.19648100	1.50707600	-0.30537700
C	-2.49446600	1.53676300	-1.66024500
H	-2.51790500	0.63527300	-2.25343000
C	8.37545000	0.45439800	-0.72645200
H	9.12240200	0.05961800	-1.42750200
H	8.87080100	1.27722900	-0.19222500
C	8.04708100	-0.63064500	0.29774100

O	6.89792400	-0.93612100	0.61811500
N	9.13060500	-1.24800900	0.83978500
H	8.99355500	-1.91748000	1.58627500
H	10.07466400	-0.94790600	0.63830600
C	-2.94009400	0.65071900	2.91615900
O	-1.76483100	1.05674700	2.58920500
O	-3.51744600	-0.18252600	2.15711800
C	-3.57812100	1.13543100	4.18524200
H	-4.65581200	0.95931100	4.17023500
H	-3.14456200	0.58464800	5.02952500
H	-3.36666700	2.19736600	4.33997400
C	-3.09730800	3.42505700	-3.37126900
H	-2.34297700	4.14935100	-3.70215000
H	-3.16743700	2.63988200	-4.12878100
H	-4.06200700	3.94500000	-3.32979100
C	-5.56529100	-3.30007200	-1.97590100
H	-5.78070500	-4.29936500	-1.57866500
H	-6.40635900	-2.64848900	-1.72428700
H	-5.51358900	-3.38093200	-3.06879900
Fe	-1.73514800	-0.19251900	0.90163300
C	3.71761600	-0.19464200	-0.06462800
C	3.11617200	0.90281700	0.56919400
C	1.83680800	1.29565300	0.20440100
C	1.11616700	0.55877400	-0.77468900
H	4.72799200	-0.48892600	0.21103000
H	3.65808600	1.44627600	1.33762900
H	1.36384900	2.14903500	0.68067200
O	0.09963300	-0.53060700	0.56482300
O	-0.78254600	-1.63276900	1.86531200
H	-0.25602400	-1.24268200	2.58788000
C	3.03776700	-0.90168200	-1.07299200
H	3.52472500	-1.73933700	-1.56365100
C	1.76005100	-0.51966100	-1.44254400
H	1.22671100	-1.05045500	-2.22594600
H	0.21914700	0.98612600	-1.20718700
C	7.15172000	0.97219200	-1.47801700
H	7.44720300	1.74994100	-2.19114400
H	6.65886500	0.16980100	-2.03694200
H	6.41717400	1.40236400	-0.79081000

BNZ-FeIII-O-C1-concerted-INT-model2 (epoxide):

C	-4.43215500	2.06137800	1.10454300
N	-3.46453000	2.94508900	0.65088400
H	-3.48592400	3.95181400	0.76863100
C	-2.49010100	2.25723500	0.03040000
H	-1.60851500	2.70402700	-0.39991800
N	-2.77007400	0.95678300	0.05571400
C	-3.98224000	0.82451400	0.71752500
H	-4.44240000	-0.14170700	0.85624700

C	0.36216700	-1.38592900	2.89351800
N	0.44572600	-2.61933400	2.26503100
H	0.89967100	-3.44355900	2.64247600
C	-0.16471100	-2.55010100	1.06667700
H	-0.24229500	-3.36808700	0.36839800
N	-0.65024500	-1.32748500	0.87538300
C	-0.32752700	-0.59601400	2.01064700
H	-0.60241100	0.44181100	2.11159800
C	5.98958000	0.52769500	-0.73119300
H	5.35926700	1.34139100	-0.35723600
H	5.76050900	0.44073400	-1.80248100
C	5.46177600	-0.74605800	-0.07363500
O	4.25479600	-0.91656700	0.12045300
N	6.37773100	-1.68582700	0.27043900
H	6.05306300	-2.56491900	0.65234500
H	7.36308900	-1.58885600	0.07294700
C	-2.74821400	-2.76201600	-1.43178200
O	-1.49258100	-2.64523600	-1.61547700
O	-3.36260300	-1.80095800	-0.85785600
C	-3.49653700	-3.96963200	-1.93710300
H	-3.90250800	-3.73496300	-2.92917300
H	-2.82669400	-4.82740200	-2.02999000
H	-4.33473200	-4.20725100	-1.27686100
C	0.95783000	-1.11347600	4.23738900
H	2.04159000	-1.28210400	4.23567300
H	0.77591100	-0.07320400	4.52018700
H	0.52062900	-1.75771700	5.01002700
C	-5.64321300	2.52165500	1.84689300
H	-6.25980500	3.19048600	1.23395500
H	-6.25701100	1.66267300	2.13092700
H	-5.37096500	3.06222400	2.76158300
C	7.47165800	0.86732300	-0.54050600
H	7.69277500	1.84000800	-0.99314600
H	7.74049100	0.92550100	0.52052800
H	8.13070400	0.13436500	-1.02208300
Fe	-1.62136100	-0.56802600	-0.86517400
C	2.14693700	2.98438200	0.33563500
C	1.47882800	3.66904500	-0.75993100
C	0.93565400	2.98859100	-1.79717500
C	0.86477100	1.51954400	-1.76225100
H	2.64797000	3.59036500	1.08617800
H	1.51302900	4.75535800	-0.78082200
H	0.58065400	3.49988400	-2.68753400
O	0.10444100	0.94498200	-0.65199600
O	-1.55505300	-0.08257600	-2.62643100
H	-1.48980000	-0.83452200	-3.23965700
C	2.26153800	1.63572800	0.36534700
H	2.90233700	1.12664400	1.07653500
C	1.56313900	0.81089300	-0.63266000
H	1.90142900	-0.21076000	-0.77235100

H	0.67798900	0.98614500	-2.68815700
---	------------	------------	-------------

Separate reactants

BNZ:

C	1.21702300	0.68782000	-0.00004100
C	0.01280300	1.39788600	0.00001700
C	-1.20419500	0.70999300	-0.00001400
C	-1.21704100	-0.68782500	-0.00002600
C	-0.01278800	-1.39786300	0.00004400
C	1.20419000	-0.71000200	-0.00001200
H	2.14057500	-1.26222200	0.00008100
H	2.16355000	1.22244100	-0.00008500
H	0.02290000	2.48498700	0.00007700
H	-2.14055400	1.26220800	0.00006800
H	-2.16354700	-1.22251300	-0.00002100
H	-0.02287700	-2.48494900	0.00006800

Asn:

C	-1.81499100	-7.27773200	-1.71162500
H	-1.68398200	-8.31713400	-1.38527000
H	-2.18867700	-7.32682400	-2.74474700
C	-0.45600100	-6.58032500	-1.75758900
O	-0.30781700	-5.38859500	-1.49969200
N	0.58783200	-7.38380800	-2.11198400
H	1.48742500	-6.95787400	-2.29585800
H	0.44182200	-8.32989300	-2.43681900
C	-2.82454600	-6.54964400	-0.82630600
H	-2.93985400	-5.50941200	-1.14446200
H	-3.80371400	-7.03862100	-0.87758100
H	-2.50336400	-6.54327800	0.22145300

FeIII+ligands:

C	-3.25191100	-2.16702600	3.90329700
N	-3.91643000	-1.66920100	2.79058800
H	-4.92266500	-1.58447000	2.69424900
C	-3.01908100	-1.33182500	1.84999000
H	-3.26573500	-0.93071800	0.87907900
N	-1.78957100	-1.58301900	2.29729200
C	-1.92472800	-2.10638000	3.57425500
H	-1.06645700	-2.41005700	4.15375500
C	0.87967800	2.41542300	3.11601100
N	2.03594800	2.14163700	2.39816600
H	2.85236000	2.74168700	2.34473800
C	1.90894900	0.95803800	1.77930800
H	2.66251400	0.50138000	1.15683400
N	0.71470300	0.43574900	2.05963100

C	0.06543100	1.33822300	2.89136800
H	-0.92790600	1.14987700	3.26859700
C	1.82456500	-2.92911900	1.47171300
O	1.89036400	-1.95950800	0.63756700
O	0.76813800	-3.01331700	2.18042400
O	-0.73395100	-0.95762200	-0.44082400
O	-0.71236100	-2.38532300	-0.69412200
H	0.09916200	-2.47740400	-1.23784000
C	2.91940800	-3.94326900	1.58060300
H	2.80492700	-4.67070400	0.76671700
H	3.89595800	-3.46535700	1.46548600
H	2.86110100	-4.47404200	2.53300800
C	0.69649400	3.66069000	3.91437100
H	0.77135600	4.55458500	3.28365200
H	-0.28974200	3.65885900	4.38545000
H	1.45167000	3.74474700	4.70511300
C	-3.95660500	-2.63619800	5.12946700
H	-4.64561100	-3.45954200	4.90553000
H	-3.22801100	-2.99413200	5.86157800
H	-4.53870600	-1.83035000	5.59283700
Fe	-0.02324500	-1.30621600	1.26007500

Benzene Modell GAS

BNZ-FeIII-RC-modell-GAS:

C	-1.78200400	0.51513200	2.01543400
N	-2.35146100	0.53503400	0.73483100
H	-3.31897500	0.75900600	0.51949000
C	-1.42124600	0.16577200	-0.17655100
H	-1.59130700	0.06541600	-1.23386300
N	-0.26293000	-0.08566500	0.45865100
C	-0.47901800	0.12244800	1.82571800
H	0.29557400	-0.06040100	2.54969500
C	3.38040000	3.00080100	-0.26061900
N	4.37818500	2.15356600	-0.76351100
H	5.31677800	2.43716600	-1.00438600
C	3.88869400	0.89267000	-0.87745600
H	4.43662800	0.03192700	-1.22028700
N	2.60996900	0.88719800	-0.47072100
C	2.28302100	2.19325800	-0.08766200
H	1.30597800	2.44597800	0.28422600
C	3.00687800	-2.32263300	0.82040000
O	1.93731300	-1.82536100	1.37027100
O	3.19820100	-2.00224700	-0.43432400
C	-5.88008800	-0.10485200	0.56949800
C	-5.51217100	-1.17312000	-0.26004000
C	-4.95760200	-0.92208400	-1.52253800
C	-4.76924700	0.39779100	-1.95748800
H	-6.32974000	-0.29955000	1.53799400

H	-5.66795900	-2.19472100	0.07026600
H	-4.68684300	-1.75001000	-2.16959400
O	0.72318400	-1.13389600	-2.15467300
O	0.38556700	-2.50108900	-1.56652400
H	0.97646000	-3.10052300	-2.08303200
Fe	1.43614100	-0.78928200	-0.41363300
C	-2.53902500	0.86374300	3.25074100
H	-2.87957500	1.90621800	3.24090200
H	-3.42189600	0.22619400	3.37643700
H	-1.90404200	0.72910700	4.12944300
C	3.59640700	4.45151000	0.00200700
H	4.38732700	4.61736200	0.74321000
H	3.87142300	4.99480000	-0.90990600
H	2.67994600	4.90163000	0.39038100
C	3.93417900	-3.21408900	1.56528100
H	3.54827600	-4.24130800	1.54036700
H	4.92456700	-3.21106500	1.10780500
H	3.99205900	-2.91100900	2.61303200
C	-5.69148300	1.21768500	0.13681100
H	-6.00224900	2.04533000	0.76696200
C	-5.13569200	1.46890900	-1.12834000
H	-5.01208800	2.49061800	-1.47340600
H	-4.36248200	0.59131100	-2.94519000

BNZ-FeIII-O-C1-concerted-TS-model1-GAS:

C	-2.48173100	3.09326100	0.91629000
N	-1.19866300	3.62404200	0.71397800
H	-0.93252000	4.58334200	0.87824500
C	-0.38229000	2.65303600	0.22260800
H	0.64769900	2.78065900	-0.06171500
N	-1.08058300	1.51716200	0.10841500
C	-2.38776300	1.77756000	0.53029900
H	-3.15142900	1.02157800	0.48040500
C	-0.50039800	-2.33830700	2.81739400
N	-0.35401900	-3.35621500	1.86732500
H	-0.32425100	-4.34444900	2.07041900
C	-0.27533000	-2.80603400	0.62389200
H	-0.18228200	-3.35047200	-0.29998700
N	-0.36005200	-1.47345300	0.72770900
C	-0.50021200	-1.17192700	2.08782500
H	-0.61139100	-0.15851100	2.43093500
C	-2.02448200	-1.56073300	-2.23654600
O	-2.43256800	-0.53707400	-1.55738100
O	-0.74829900	-1.85451700	-2.13927800
C	4.78021200	1.58229900	0.08034600
C	4.90058500	0.63540100	-0.95855300
C	4.02692600	-0.43859400	-1.01885700
C	2.98047600	-0.56478800	-0.05799800
H	5.47189700	2.41743100	0.12395400

H	5.68354100	0.74730700	-1.70009300
H	4.11033000	-1.17584500	-1.80969400
O	1.50442500	0.32095500	-1.07902400
O	0.25384200	0.95437100	-2.41868700
H	0.73778500	0.52987500	-3.15877400
Fe	-0.38305700	-0.14545800	-0.91118600
C	-3.62562500	3.89815700	1.43300700
H	-3.42685900	4.29994000	2.43410100
H	-3.85996800	4.74229700	0.77327500
H	-4.51995800	3.27403400	1.49793100
C	-0.63079500	-2.59858300	4.28073500
H	-1.51382100	-3.20766800	4.50834100
H	0.24718100	-3.11788300	4.68335900
H	-0.73332500	-1.65455500	4.82104600
C	-2.93651200	-2.34530200	-3.11748100
H	-2.92451400	-1.91143700	-4.12548700
H	-2.60211700	-3.38163900	-3.19609100
H	-3.96095500	-2.29787000	-2.74371600
C	3.78920600	1.44964700	1.06262300
H	3.72475000	2.17266500	1.86855500
C	2.90579700	0.37170200	1.01133800
H	2.14901700	0.24012800	1.77651500
H	2.43630800	-1.49841900	0.01073900

BNZ-FeIII-O-C1-concerted-INT-model1-GAS (epoxide):

C	-1.56820500	3.51847300	1.09248400
N	-0.16788500	3.55758200	1.07461000
H	0.39777200	4.30310400	1.45153900
C	0.30722600	2.44263200	0.45562900
H	1.34701100	2.20800300	0.31339700
N	-0.72622900	1.68062100	0.07422700
C	-1.89940600	2.34020700	0.46062200
H	-2.86436700	1.91578800	0.24519400
C	-0.01275900	-2.01238000	2.91491400
N	-0.46413600	-3.09999900	2.15677500
H	-0.61170500	-4.03520700	2.50546100
C	-0.68577300	-2.69413800	0.87530300
H	-1.04631900	-3.31456400	0.07409300
N	-0.39746200	-1.39090600	0.77051400
C	0.02822300	-0.96028200	2.03218500
H	0.32397300	0.05736300	2.20973800
C	-2.80480500	-1.37736200	-1.54425300
O	-2.74789500	-0.18359100	-1.01925600
O	-1.67640200	-1.99596000	-1.71371700
C	4.59934600	-0.34973900	0.08607800
C	4.55963300	0.99868000	-0.46395800
C	3.62646900	1.36598000	-1.38032200
C	2.54831400	0.44315700	-1.74989000
H	5.42049900	-0.60751000	0.74687500

H	5.35639000	1.68376300	-0.19239600
H	3.68504700	2.31950300	-1.89444700
O	1.58338800	0.06216600	-0.59249800
O	-0.18450100	0.16232600	-2.69234900
H	-0.60815700	-0.20325300	-3.48989200
Fe	-0.60193600	-0.16072100	-0.93788500
C	-2.38708100	4.60041900	1.71763700
H	-2.16803200	4.71032700	2.78665000
H	-2.21510300	5.57069700	1.23634500
H	-3.45025500	4.36868400	1.62000800
C	0.30617900	-2.10193300	4.36926800
H	-0.57086400	-2.38848500	4.96225600
H	1.09918200	-2.83216800	4.57137400
H	0.64946600	-1.13179200	4.73645400
C	-4.10482600	-1.99570900	-1.95449600
H	-4.51638600	-1.44899400	-2.81103800
H	-3.95960800	-3.03969400	-2.23308300
H	-4.83396400	-1.91752800	-1.14234000
C	3.70703200	-1.29900400	-0.29458200
H	3.81873800	-2.33336900	0.01145700
C	2.58984600	-0.94754700	-1.17727400
H	2.07221600	-1.74068100	-1.70503000
H	1.96160200	0.61542000	-2.64399700

Benzene Model 2 GAS

BNZ-FeIII-RC-model2-GAS:

C	-4.02910000	2.06597800	1.04711800
N	-2.94375500	2.71193200	0.43470200
H	-2.77646200	3.70701800	0.42406900
C	-2.13851400	1.79060400	-0.15208500
H	-1.24091500	2.01448600	-0.70399500
N	-2.65385700	0.57080900	0.05968000
C	-3.83225800	0.72775500	0.79929000
H	-4.43457700	-0.12166400	1.07077700
C	0.96188200	-1.21042400	2.68981600
N	1.80487400	-1.19134800	1.57082100
H	2.82761400	-1.09290500	1.52197400
C	1.05422700	-1.26503400	0.44992500
H	1.44965700	-1.25135700	-0.55016100
N	-0.24829300	-1.33062700	0.78474500
C	-0.31424800	-1.30033200	2.18269000
H	-1.25244100	-1.34325400	2.70874200
C	5.93924800	-0.30626800	-1.18188500
H	5.75461600	0.77509600	-1.13400900
H	5.24037100	-0.69017700	-1.93554900
C	5.47764700	-0.87584600	0.15162400
O	4.27480500	-0.73997200	0.52378900
N	6.38697700	-1.51712400	0.92072500

H	6.10579700	-1.89742500	1.81260600
H	7.34610500	-1.63212900	0.63450800
C	-3.14468900	-3.24885500	-0.79919300
O	-2.00462500	-3.07464100	-1.41647700
O	-3.51853900	-2.26693000	-0.02894300
C	-3.97197300	-4.47095900	-1.00565900
H	-4.66719400	-4.30048000	-1.83775600
H	-3.33836200	-5.32172300	-1.26180400
H	-4.56316700	-4.68550200	-0.11335500
C	1.44303100	-1.13250100	4.10227200
H	2.01301400	-0.21405800	4.28605100
H	0.59188800	-1.14072000	4.78724400
H	2.08654700	-1.98193700	4.36055300
C	-5.10189500	2.80028500	1.78124300
H	-5.63190900	3.50514600	1.12939900
H	-5.83829700	2.09325900	2.17031200
H	-4.70109900	3.36495900	2.63176100
C	7.39143500	-0.57899900	-1.61263100
H	7.57732800	-0.12711900	-2.59107900
H	8.11552400	-0.14100300	-0.91508400
H	7.59496200	-1.65206400	-1.70772000
Fe	-1.75566400	-1.15364900	-0.56847300
C	0.25638900	4.61968200	-0.95204400
C	0.48973200	3.65063500	-1.93915700
C	1.29851900	2.54066100	-1.65516300
C	1.87877200	2.40112000	-0.38575800
H	-0.34556400	5.49408200	-1.18213500
H	0.05650100	3.76589900	-2.92774300
H	1.47308200	1.79103300	-2.41948800
O	-0.64434000	-0.44268400	-1.98007800
O	-1.92385200	-0.55604500	-2.80299000
H	-1.73767200	-1.34536100	-3.36850100
C	0.82916400	4.47563900	0.31966400
H	0.66356900	5.23315900	1.07971500
C	1.64062600	3.36778900	0.60081500
H	2.09667100	3.26690500	1.58079300
H	2.52451100	1.55380300	-0.17222800

BNZ-FeIII-O-C1-concerted-TS-model2-GAS:

C	4.92727300	-2.04584800	1.15494800
N	3.95077400	-3.00766200	0.85644400
H	4.04164800	-3.99954700	1.01702500
C	2.87959800	-2.39727000	0.28145700
H	1.99525800	-2.88625600	-0.08763200
N	3.11974600	-1.08320900	0.20245000
C	4.39072800	-0.85177300	0.73488800
H	4.82656800	0.13169300	0.74039800
C	0.83551100	2.35450600	2.72451400
N	0.50742500	3.25607700	1.70304300

H	0.09477500	4.16703900	1.83847300
C	0.84576200	2.71788400	0.49780500
H	0.70847800	3.18331500	-0.46330900
N	1.37761100	1.50498500	0.69322300
C	1.38223700	1.27203400	2.07448600
H	1.78066600	0.36375400	2.49146100
C	-7.83499700	0.48870200	0.67792800
H	-8.88919600	0.23176700	0.83903200
H	-7.78911600	1.58555100	0.60916000
C	-7.35630800	-0.06683200	-0.65770100
O	-6.14072100	-0.24795600	-0.91354000
N	-8.32574700	-0.33337300	-1.57818700
H	-8.05437200	-0.66394600	-2.49258600
H	-9.30610600	-0.20804400	-1.38309500
C	2.96927400	1.87383600	-2.44802900
O	1.67553300	1.84458200	-2.21932100
O	3.69793900	1.08865200	-1.72215200
C	3.55181100	2.72250300	-3.53203300
H	3.54734500	2.15462100	-4.47099500
H	2.95391400	3.62368700	-3.68167300
H	4.58617000	2.98019900	-3.29780200
C	0.57528200	2.62474500	4.17112500
H	-0.49392300	2.76285600	4.37189700
H	0.91986900	1.78272300	4.77598100
H	1.10133400	3.52121300	4.52036700
C	6.23384700	-2.38378000	1.78913400
H	6.81665600	-3.08012600	1.17415400
H	6.83180400	-1.47816600	1.91555700
H	6.10440700	-2.83786800	2.77919000
Fe	1.88634800	0.19256700	-0.87374100
C	-3.43297700	-1.68234500	-0.55321200
C	-3.04477700	-0.35558100	-0.30746000
C	-1.83164700	-0.09666500	0.32332500
C	-0.97184300	-1.16794800	0.69295200
H	-4.39360700	-1.85531800	-1.02378100
H	-3.72117600	0.44161900	-0.58919900
H	-1.52774600	0.92254400	0.53349200
O	0.32426700	-0.99711800	-0.87376500
O	1.54695100	-1.11084600	-2.32809800
H	0.87035500	-0.90475500	-3.00791600
C	-2.60578500	-2.75735300	-0.17022500
H	-2.92342700	-3.77687000	-0.35996500
C	-1.39957600	-2.50771500	0.46762600
H	-0.76367400	-3.32849900	0.78270100
H	-0.15385300	-0.98145000	1.37785100
C	-6.97564300	0.00940600	1.85688600
H	-7.27422700	0.51404000	2.78104500
H	-7.08113600	-1.07028100	2.00878800
H	-5.91977600	0.21847800	1.66435300

BNZ-FeIII-O-C1-concerted-INT-model2-GAS (epoxide):

C	-4.46298300	2.10771100	0.87426100
N	-3.36420100	2.94851800	0.65430500
H	-3.33790700	3.93617100	0.85714900
C	-2.34632100	2.22929600	0.10964100
H	-1.37877700	2.61884500	-0.14947200
N	-2.73550600	0.95549000	-0.03121100
C	-4.05429300	0.86739300	0.43459600
H	-4.58845800	-0.06592800	0.39908400
C	0.23180200	-1.22669200	3.03962300
N	0.39754300	-2.48602400	2.44816900
H	0.85848100	-3.27584200	2.87353700
C	-0.14945000	-2.47414400	1.20042200
H	-0.16421700	-3.29984100	0.51098600
N	-0.66633100	-1.26387800	0.95861200
C	-0.43256500	-0.48037900	2.09573200
H	-0.74678000	0.54629600	2.14424100
C	6.04563200	0.52970500	-0.66111200
H	5.37930500	1.33916600	-0.34933400
H	6.03846500	0.53093500	-1.76116400
C	5.38455500	-0.76358900	-0.20193600
O	4.14942700	-0.82944700	0.03101700
N	6.18311400	-1.86045000	-0.08916900
H	5.76688300	-2.74020900	0.17722600
H	7.17438200	-1.83097000	-0.26391500
C	-2.69926900	-2.87585700	-1.33019800
O	-1.40474600	-2.80411700	-1.38831300
O	-3.32787900	-1.81578300	-0.90080300
C	-3.43766300	-4.09957000	-1.79508000
H	-3.83781000	-3.91886000	-2.80021600
H	-2.76478500	-4.95699400	-1.83477300
H	-4.28483300	-4.30687600	-1.13643000
C	0.72517400	-0.89150400	4.40995600
H	1.81308600	-1.00559900	4.48985900
H	0.48207900	0.14648400	4.64951800
H	0.26396200	-1.52529300	5.17705600
C	-5.73060200	2.61185400	1.48560300
H	-6.18572700	3.40603000	0.88151900
H	-6.45825400	1.80059900	1.56415500
H	-5.56492100	3.00785100	2.49494900
C	7.47592000	0.78302200	-0.15131800
H	7.81204800	1.77795600	-0.45919800
H	7.52739200	0.73484100	0.94159400
H	8.19921200	0.06647700	-0.55984900
Fe	-1.54746700	-0.59352200	-0.84007000
C	2.17704400	3.04411200	0.22656800
C	1.47725800	3.68139500	-0.88162200
C	0.91142600	2.95272000	-1.87896700
C	0.87624800	1.48706200	-1.79665900

H	2.68117500	3.68261500	0.94532300
H	1.49688300	4.76524500	-0.94301800
H	0.51091100	3.42629100	-2.76896700
O	0.07557800	0.91789400	-0.61437300
O	-1.33058600	-0.28570300	-2.63002100
H	-1.44243100	-0.90590500	-3.37284600
C	2.30178000	1.69447100	0.30650600
H	2.94636900	1.21315300	1.03062900
C	1.61223000	0.82690500	-0.65689500
H	1.96171000	-0.19317000	-0.74912300
H	0.64446700	0.91628700	-2.68641200

Separate reactants

BNZ-GAS:

C	0.77076500	1.16928100	0.00000100
C	1.39800800	-0.08288500	-0.00000800
C	0.62724700	-1.25214200	0.00000900
C	-0.77078500	-1.16926800	-0.00000100
C	-1.39801000	0.08286100	-0.00000700
C	-0.62722500	1.25215300	0.00000600
H	1.36836000	2.07579100	0.00000200
H	2.48187000	-0.14709500	-0.00000900
H	1.11350500	-2.22293000	0.00001000
H	-1.36832400	-2.07581400	-0.00000100
H	-2.48186700	0.14713700	-0.00000600
H	-1.11354300	2.22291100	0.00000800

Asn-GAS:

C	0.69291600	-0.72436500	0.21426700
H	0.59863000	-1.64963200	-0.37013400
H	0.74215700	-1.02928300	1.27055700
C	-0.56200300	0.12696000	0.04225100
O	-0.54199900	1.37505600	0.07699700
N	-1.73046700	-0.57130500	-0.12486500
H	-2.59359200	-0.05539800	-0.20607200
H	-1.75884300	-1.57671300	-0.17310100
C	1.96905000	0.03412200	-0.16770900
H	2.01568500	0.98513600	0.36925400
H	2.85902600	-0.55621300	0.07389300
H	1.98642300	0.26049100	-1.23917000

FeIII+ligands-GAS:

C	-3.32676100	-1.45326300	-0.69608500
N	-3.39348000	-1.51663500	0.70444900
H	-4.13231200	-1.95649800	1.23349100
C	-2.32713900	-0.86735800	1.23824000

H	-2.13345200	-0.73465800	2.28876000
N	-1.56698100	-0.39217800	0.23983400
C	-2.18194400	-0.74409300	-0.96652300
H	-1.77727400	-0.43438800	-1.91399700
C	2.77304400	-2.47137600	-0.16491200
N	3.61858200	-1.35250000	-0.19435300
H	4.62005700	-1.38215200	-0.32011500
C	2.88565900	-0.22287400	-0.02404700
H	3.26977000	0.78278400	-0.00619100
N	1.59458500	-0.56242900	0.11561600
C	1.51399200	-1.95792500	0.02994400
H	0.57541600	-2.47683000	0.11008300
C	0.56714000	2.67380100	-1.10709900
O	1.33219700	2.41230600	-0.07412900
O	-0.44162200	1.86923300	-1.26896100
O	-0.04878300	0.99209900	2.37331000
O	-0.94807800	2.17770200	2.04337700
H	-0.42863900	2.93667100	2.40257800
C	0.81023400	3.83424800	-2.00417300
H	0.26922600	4.70801000	-1.61834400
H	1.87245800	4.08333300	-2.03380400
H	0.43413200	3.62534800	-3.00735300
C	3.26062700	-3.87192600	-0.32534500
H	3.97330400	-4.14673300	0.46127000
H	2.42103500	-4.56839900	-0.26847600
H	3.75291300	-4.02324400	-1.29332100
C	-4.34911500	-2.06432800	-1.59144200
H	-5.34568500	-1.63994000	-1.42059400
H	-4.08754600	-1.87957200	-2.63582800
H	-4.41845100	-3.14997900	-1.45265200
Fe	0.09469200	0.78008800	0.48059800

Naphthalene Model 1

NPY-FeIII-RC:

C	3.4279880	3.4446530	0.2902520
N	2.6686650	3.6305570	-0.8565490
H	2.7045370	4.4462080	-1.4583800
C	1.8687650	2.5661020	-1.0388290
H	1.1674250	2.4558360	-1.8513650
N	2.0712720	1.6848700	-0.0609520
C	3.0375170	2.2248200	0.7740720
H	3.3723440	1.7060140	1.6594040
C	4.5200840	-2.1227840	-1.4887640
N	3.7238130	-3.1818790	-1.0762510
H	3.9572430	-4.1645960	-1.1715860
C	2.5980800	-2.7055370	-0.5214460
H	1.8097100	-3.3131140	-0.1055250
N	2.6160140	-1.3730650	-0.5531590

C	3.8093800	-1.0012890	-1.1563870
H	4.0748740	0.0346340	-1.2989410
C	0.6660990	-1.0863000	2.3952050
O	1.1989170	0.0621920	2.2573260
O	0.3384380	-1.7115070	1.3249680
C	-3.2181230	-1.3877150	0.9745460
C	-3.9348520	-0.6444420	1.9507720
C	-4.9927530	0.1527800	1.5757750
C	-5.3872820	0.2521230	0.2117420
C	-4.6640370	-0.4943040	-0.7769860
C	-3.5756370	-1.3120910	-0.3585570
H	-2.3910180	-2.0229890	1.2797660
H	-3.6477440	-0.7144280	2.9963790
H	-5.5455670	0.7199330	2.3208670
O	-0.2222670	0.0728200	-1.1253430
O	-1.0000600	0.7318470	-0.0953850
H	-1.7083290	0.0669860	0.0820160
H	0.5883690	-2.7530330	3.7330060
H	1.0276580	-1.1918530	4.5047960
H	-0.6471330	-1.5148240	4.0037580
Fe	1.1189310	-0.1428080	0.1629150
C	0.4078170	-1.6747710	3.7466620
C	5.8500500	-2.3089230	-2.1347630
H	6.5344100	-2.8715940	-1.4884680
H	5.7633930	-2.8533270	-3.0828930
H	6.3024570	-1.3356930	-2.3423470
H	5.2179500	4.6108870	0.0431350
H	3.9480280	5.4121740	0.9820550
H	4.8805700	4.0891530	1.7031120
C	4.4202440	4.4437940	0.7771490
C	-5.0580790	-0.3967010	-2.1391070
C	-6.1194070	0.4008830	-2.5085190
C	-6.4763420	1.0662700	-0.2032950
C	-6.8345810	1.1387170	-1.5319460
H	-3.0359570	-1.8882380	-1.1070280
H	-7.6695970	1.7633880	-1.8372480
H	-7.0230600	1.6309690	0.5481020
H	-4.5077000	-0.9646240	-2.8854740
H	-6.4132340	0.4672390	-3.5525430

NPY-FeIII-O-C1-concerted-TS-model1:

C	-2.05200000	-1.27100000	3.20200000
N	-2.35500000	-2.43400000	2.51200000
H	-2.76400000	-3.26900000	2.91800000
C	-2.03600000	-2.27600000	1.21500000
H	-2.17800000	-3.02200000	0.45000000
N	-1.53200000	-1.06000000	1.01700000
C	-1.54000000	-0.42600000	2.25100000
H	-1.19200000	0.58800000	2.37100000

C	-2.93600000	-1.28800000	-2.07400000
O	-2.96500000	-0.06200000	-1.75200000
O	-1.90000000	-1.97200000	-1.74200000
C	3.24700000	-0.23000000	0.50900000
C	4.26800000	-0.74100000	-0.34900000
C	4.08500000	-2.02200000	-0.96000000
C	2.95600000	-2.77200000	-0.73400000
C	1.92800000	-2.26500000	0.09800000
C	2.04700000	-0.99800000	0.68500000
H	4.87600000	-2.40400000	-1.60200000
H	2.84100000	-3.74900000	-1.19200000
H	1.05500000	-2.87100000	0.30700000
H	1.31900000	-0.66900000	1.41800000
C	5.44500000	0.01900000	-0.54700000
C	5.61400000	1.23500000	0.09000000
H	6.52200000	1.80900000	-0.06800000
C	4.61400000	1.72900000	0.95300000
H	4.76300000	2.67800000	1.46200000
C	3.45000000	1.00700000	1.16100000
H	2.68400000	1.38200000	1.83500000
H	6.21800000	-0.37100000	-1.20500000
O	0.90000000	-0.61500000	-1.04700000
O	0.03000000	0.08100000	-2.57000000
H	0.43700000	0.96400000	-2.51700000
Fe	-0.97500000	-0.31000000	-0.90600000
C	-2.30400000	-1.11100000	4.66300000
H	-3.37200000	-1.19700000	4.89800000
H	-1.77200000	-1.87100000	5.24900000
H	-1.96300000	-0.12700000	4.99600000
C	-4.04800000	-1.93200000	-2.84600000
H	-3.75900000	-1.98100000	-3.90400000
H	-4.21200000	-2.95600000	-2.49900000
H	-4.96800000	-1.34900000	-2.76300000
C	-1.80600000	3.83400000	-0.01700000
N	-0.42600000	3.79500000	0.11600000
H	0.17000000	4.59400000	0.30700000
C	0.00200000	2.53000000	-0.06600000
H	1.03600000	2.22400000	-0.03100000
N	-1.03700000	1.73500000	-0.30800000
C	-2.16700000	2.53800000	-0.28100000
H	-3.14900000	2.12900000	-0.46800000
C	-2.60000000	5.09100000	0.11000000
H	-2.48000000	5.54600000	1.10100000
H	-2.29400000	5.83400000	-0.63700000
H	-3.66100000	4.87500000	-0.04000000

Naphthalene Model 1 GAS

NPY-FeIII-RC-model1-GAS:

C	3.3509350	3.4508880	0.4825930
N	2.4623520	3.7395590	-0.5644260
H	2.4009130	4.6218570	-1.0509230
C	1.6762980	2.6566860	-0.8014250
H	0.8908260	2.5980470	-1.5350550
N	2.0242830	1.6771340	0.0446950
C	3.0576960	2.1610860	0.8531520
H	3.4781270	1.5650040	1.6440210
C	4.4759190	-1.9749220	-1.7034090
N	3.7305180	-3.0794310	-1.2669470
H	3.9877690	-4.0464660	-1.4008990
C	2.6071080	-2.6483520	-0.6365500
H	1.8541510	-3.2748070	-0.1901310
N	2.5919380	-1.3071910	-0.6471020
C	3.7478760	-0.8789350	-1.3102050
H	3.9687600	0.1646180	-1.4455920
C	0.7999040	-1.2968110	2.4023420
O	1.3529300	-0.1265870	2.2984530
O	0.4104930	-1.8430090	1.2747150
C	-3.1373480	-1.4845660	0.7825240
C	-3.9533760	-1.0003750	1.8431870
C	-5.0593250	-0.2221180	1.5688300
C	-5.4078070	0.1150090	0.2281270
C	-4.5860500	-0.3702160	-0.8473960
C	-3.4494870	-1.1739270	-0.5336580
H	-2.2822380	-2.1164690	1.0038590
H	-3.7084900	-1.2578810	2.8684370
H	-5.6868120	0.1427320	2.3767100
O	-0.2433760	0.1677200	-1.1391160
O	-0.9778180	0.7523350	0.0625640
H	-1.7839160	0.1599800	0.1312700
H	0.5510660	-3.0441690	3.6026630
H	1.3774130	-1.6734300	4.4171450
H	-0.3674050	-1.6278210	4.1396730
Fe	1.1026040	-0.1522980	0.1779880
C	0.5898340	-1.9595710	3.7173230
C	5.7766960	-2.0930110	-2.4218820
H	6.5316280	-2.6080120	-1.8158060
H	5.6731540	-2.6410960	-3.3659420
H	6.1638350	-1.0992280	-2.6582850
H	5.0725890	4.7186280	0.2149960
H	3.8873280	5.3338620	1.3797470
H	4.9268010	3.9738370	1.8113200
C	4.3586730	4.4223460	0.9930990
C	-4.9358810	-0.0398400	-2.1867890
C	-6.0475470	0.7347070	-2.4532850
C	-6.5455370	0.9124020	-0.0816650
C	-6.8587440	1.2150310	-1.3919390
H	-2.8422930	-1.5611840	-1.3477290
H	-7.7300410	1.8208140	-1.6172800

H	-7.1666460	1.2768800	0.7310960
H	-4.3158350	-0.4112110	-2.9975480
H	-6.3088960	0.9780100	-3.4777640

NPY-FeIII-O-C1-concerted-TS-model1-GAS:

C	-1.3432530	3.9004470	-0.1348450
N	0.0330280	3.6723030	-0.0005890
H	0.7276480	4.3842840	0.1694010
C	0.2880260	2.3438000	-0.1629520
H	1.2648010	1.8917620	-0.1212700
N	-0.8673690	1.7048380	-0.3899390
C	-1.8885680	2.6606180	-0.3789320
H	-2.9085450	2.3796650	-0.5753040
C	-1.8573290	-1.0048210	3.3391170
N	-2.2276680	-2.2138660	2.7381940
H	-2.6119430	-3.0125190	3.2210860
C	-2.0067200	-2.1378820	1.3972320
H	-2.2260400	-2.9089230	0.6790460
N	-1.5032460	-0.9314780	1.1020650
C	-1.4053130	-0.2199240	2.3040190
H	-1.0461480	0.7933200	2.3316740
C	-3.3116350	-1.1199780	-1.8104110
O	-3.1190600	0.1400510	-1.5723790
O	-2.3370800	-1.9283640	-1.4689750
C	3.2060720	-0.4065620	0.4866770
C	4.2081690	-0.7923640	-0.4626320
C	4.0325910	-2.0071480	-1.2046500
C	2.9277850	-2.8056000	-1.0246300
C	1.9135390	-2.4163570	-0.1077320
C	2.0409320	-1.2279830	0.6285900
H	4.8058700	-2.2959170	-1.9101820
H	2.8136560	-3.7251230	-1.5861520
H	1.0643060	-3.0667410	0.0597870
H	1.3163780	-0.9853430	1.3976590
C	5.3583920	0.0215100	-0.6167700
C	5.5224610	1.1689990	0.1443700
H	6.4102050	1.7797620	0.0217440
C	4.5433260	1.5392270	1.0945320
H	4.6944390	2.4249730	1.7028240
C	3.4048220	0.7637420	1.2624430
H	2.6637820	1.0329910	2.0110590
H	6.1169810	-0.2704240	-1.3363810
O	0.7778170	-0.8226220	-1.1325050
O	-0.1789090	-0.1963480	-2.6287670
H	0.4377400	0.5224670	-2.8779160
Fe	-1.0966090	-0.3253420	-0.8832040
C	-1.9560360	5.2562750	-0.0212230
H	-1.7790900	5.7046260	0.9639460
H	-1.5644570	5.9451970	-0.7793170

H	-3.0368690	5.1888770	-0.1649880
C	-1.9945600	-0.7459910	4.8013810
H	-3.0383520	-0.8165590	5.1302320
H	-1.4067280	-1.4529710	5.3991190
H	-1.6419260	0.2605160	5.0387080
C	-4.5470830	-1.6338350	-2.4656950
H	-4.3637790	-1.7369850	-3.5427520
H	-4.8045130	-2.6223870	-2.0791130
H	-5.3746510	-0.9370320	-2.3240450

Oxygen-oxygen bond cleavage

NBZ-OO-cleavage-TS-modell1:

C	-2.11725000	-1.21556300	4.34225200
N	-2.72735100	-0.91393600	3.13255500
H	-3.72504300	-0.94295800	2.95252200
C	-1.78643900	-0.59118900	2.22842400
H	-1.98529400	-0.31687800	1.20407100
N	-0.58301900	-0.66438000	2.79189100
C	-0.77623100	-1.05774200	4.10637000
H	0.05483800	-1.20212800	4.77968600
C	1.33186100	3.51868100	3.60543100
N	2.63725400	3.36487300	3.16072300
H	3.37335100	4.05776600	3.24302200
C	2.77969600	2.15005700	2.60524800
H	3.69118200	1.76987700	2.17269100
N	1.62378700	1.49265900	2.66976700
C	0.71346900	2.33896600	3.28611800
H	-0.30940200	2.04354900	3.45945200
C	3.31256800	-1.45365400	2.49115800
O	2.18308100	-1.62457500	3.07191000
O	3.35686700	-0.60944400	1.53830800
C	4.89772800	-0.52579900	-4.00355100
C	5.92474700	-0.88094300	-4.87347600
C	6.44753900	-2.17842100	-4.85152100
C	5.94503600	-3.13143600	-3.95911900
C	4.91632900	-2.79655000	-3.08274700
C	4.41067900	-1.49422100	-3.12148000
N	3.33339000	-1.12492200	-2.21255000
O	2.87779100	-2.01374600	-1.46728300
O	2.91725100	0.02810600	-2.21457400
H	4.47606100	0.47175100	-4.00377300
H	6.31625900	-0.14532700	-5.56897600
H	7.24930300	-2.44838000	-5.53248500
H	6.35364300	-4.13689100	-3.94557800
H	4.51220500	-3.51914400	-2.38487200
O	0.57671300	0.33904900	0.29257300
O	0.87534300	-1.51725300	0.32558400

H	1.60640200	-1.48572600	-0.35384700
H	5.43468500	-1.71870700	2.63971900
H	4.48585100	-2.49703000	3.95209300
H	4.50365900	-3.19785400	2.32327100
Fe	1.22619900	-0.33569000	1.78231200
C	4.51604600	-2.25594700	2.88653900
C	0.84391200	4.75725100	4.27997300
H	1.37758100	4.93844000	5.22098300
H	0.98032800	5.63995500	3.64391600
H	-0.22131500	4.66288500	4.50647000
H	-3.59155100	-0.82814700	5.86032500
H	-3.46311600	-2.52979400	5.38473400
H	-2.20213900	-1.79408800	6.38881400
C	-2.88737300	-1.61223800	5.55664100

NBZ-OO-cleavage-TS-model2:

C	-2.11481000	-1.22420400	4.34139900
N	-2.72388400	-0.91688000	3.13200700
H	-3.72248100	-0.93527000	2.95422100
C	-1.78362800	-0.60109100	2.22691300
H	-1.98242900	-0.32302400	1.20361600
N	-0.57887100	-0.68531400	2.78962200
C	-0.77299100	-1.07825700	4.10471500
H	0.05758700	-1.22886600	4.77713700
C	1.32497300	3.52256400	3.59346900
N	2.62489300	3.37488000	3.12918100
H	3.35827200	4.07215500	3.20146400
C	2.76635200	2.16340900	2.56999900
H	3.67325600	1.78820700	2.12371100
N	1.61307900	1.50012500	2.65120300
C	0.70645100	2.34129800	3.28158400
H	-0.31235600	2.04118400	3.46987900
C	0.35801700	6.09433100	-3.29417100
H	-0.25224700	5.20859800	-3.07669000
H	0.91814600	5.85610000	-4.20994100
C	1.38025200	6.28729600	-2.17407900
O	1.67801500	7.39243100	-1.72499300
N	1.93592700	5.13391000	-1.70483900
H	2.72928900	5.21338400	-1.08140200
H	1.80557100	4.24238400	-2.17160700
C	3.31467600	-1.45154200	2.49311700
O	2.19120400	-1.59821900	3.09296600
O	3.34689900	-0.62730700	1.52071100
C	1.63703600	-0.31648100	-3.74283600
C	1.69665300	-1.68105200	-4.02350200
C	2.52225100	-2.51951600	-3.26989200
C	3.30289900	-1.99720500	-2.23008600
C	3.26136900	-0.63366400	-1.93854700
C	2.42111100	0.18244300	-2.70274100

N	2.35914100	1.61021000	-2.38988600
O	3.09046500	2.05043500	-1.50306700
O	1.57188000	2.31204900	-3.03652100
H	0.99999300	0.34899000	-4.31204300
H	1.09568800	-2.08741400	-4.83081500
H	2.56317200	-3.58130900	-3.49366100
H	3.95167900	-2.64874000	-1.65267100
H	3.85914700	-0.20878100	-1.14170800
O	0.56875700	0.30552400	0.29159700
O	0.90361600	-1.54652000	0.33187900
H	1.61957600	-1.45272300	-0.33390500
H	5.43516700	-1.73279800	2.61300100
H	4.50035400	-2.47318500	3.95744700
H	4.48507200	-3.21018800	2.34500000
Fe	1.22096800	-0.33128900	1.80518000
C	4.51603700	-2.25594500	2.88653600
C	0.84391100	4.75726300	4.27997500
H	1.39243800	4.93546700	5.21289200
H	0.96859900	5.64188700	3.64443100
H	-0.21739100	4.65910000	4.52228600
C	-0.52136800	7.32213600	-3.52063600
H	-3.58405100	-0.82108200	5.85893600
H	-3.47145600	-2.52459900	5.38572200
H	-2.20326300	-1.79902600	6.38855600
H	0.08773500	8.20455000	-3.73783000
H	-1.20197000	7.15623000	-4.36318300
H	-1.12603200	7.54766000	-2.63508200
C	-2.88736700	-1.61223700	5.55663500

NBZ-OO-cleavage-TS-model3:

C	-2.11443500	-1.20956000	4.34551400
N	-2.72660600	-0.86399100	3.14903400
H	-3.72647300	-0.85779600	2.97954900
C	-1.78481800	-0.54594900	2.24367300
H	-1.98608900	-0.24067700	1.22877900
N	-0.57891800	-0.66478000	2.79303800
C	-0.77139300	-1.08269800	4.10002300
H	0.06172100	-1.26404900	4.76169000
C	1.33753900	3.51776400	3.61131000
N	2.64251400	3.36823500	3.16463700
H	3.37445600	4.06641500	3.23903100
C	2.78896500	2.15279100	2.61153000
H	3.70133200	1.77608300	2.17786800
N	1.63609800	1.49010200	2.68024000
C	0.72381000	2.33440200	3.29655900
H	-0.29773600	2.03620500	3.47197900
C	0.09336700	5.95281300	-3.80824700
H	-0.64345900	5.27987100	-4.26363300
H	0.90675200	6.05535400	-4.54118300

C	0.69212900	5.29669800	-2.56349600
O	1.08363700	5.94575300	-1.59411700
N	0.77688300	3.94037300	-2.61531500
H	1.24935300	3.45359500	-1.86445400
H	0.50104500	3.39848900	-3.42553700
C	3.31541000	-1.45662200	2.47067400
O	2.17578700	-1.64827700	3.02827600
O	3.37453400	-0.58534400	1.54657600
C	-1.06310800	-0.26130700	-6.23445600
C	-1.53720000	-1.42791100	-6.82767400
C	-1.36150300	-2.66173000	-6.19263600
C	-0.70858100	-2.73716000	-4.95777400
C	-0.22314500	-1.58239300	-4.35114400
C	-0.40900800	-0.36004400	-5.00312500
N	0.08014900	0.86105900	-4.37595600
O	0.76747800	0.78080900	-3.34737900
O	-0.21671300	1.94295400	-4.88687700
H	-1.18902900	0.70390100	-6.70880000
H	-2.04359000	-1.37315700	-7.78601700
H	-1.73669900	-3.56710000	-6.66034500
H	-0.57929600	-3.69535900	-4.46464100
H	0.27699200	-1.62648500	-3.39233900
O	0.52561800	0.38889300	0.31706400
O	0.90146500	-1.45435300	0.27755000
H	1.54003500	-1.29522100	-0.49613700
H	5.41167000	-1.91143000	2.36656600
H	4.65601200	-2.17732000	3.96978900
H	4.33944400	-3.31260400	2.65444800
Fe	1.22862300	-0.32592600	1.76699800
C	4.51604600	-2.25594800	2.88653900
C	0.84391200	4.75725300	4.27997300
H	1.38249700	4.95074400	5.21570100
H	0.96829800	5.63545400	3.63533000
H	-0.21897600	4.65564800	4.51421800
C	-0.52137000	7.32215000	-3.52064300
H	-3.57331900	-0.81898300	5.87769000
H	-3.48317300	-2.51421700	5.37103000
H	-2.20276200	-1.82346000	6.38238300
H	0.21153500	7.98298700	-3.04871300
H	-0.86717100	7.79244000	-4.44781900
H	-1.37884900	7.23900100	-2.84291100
C	-2.88737300	-1.61223800	5.55664100
O	2.43599500	-0.99855100	-1.81265100
H	2.69770800	-1.77066500	-2.34260600
H	1.92713300	-0.42073900	-2.41465700

NBZ-OO-cleavage-TS-model4:

C	-1.69396700	-5.96491700	-0.90838900
H	-0.94819600	-6.65659000	-1.31846000
H	-2.47219000	-5.88144200	-1.67763400
C	-1.01132000	-4.60288200	-0.84791700
O	-0.47549700	-4.13438400	-1.87063400
N	-1.02805900	-3.94759300	0.32719000
H	-0.54920500	-3.05388800	0.42339000
H	-1.41111600	-4.36831400	1.16198100
C	-2.11264500	-1.13799900	4.37733600
N	-2.71870300	-0.59669300	3.25362500
H	-3.71677100	-0.46834200	3.12732000
C	-1.77236700	-0.26506300	2.35699000
H	-1.96768000	0.17314400	1.39065300
N	-0.57153100	-0.56192600	2.84618100
C	-0.77018300	-1.10885900	4.10162400
H	0.05831400	-1.44349900	4.70722400
C	1.33657800	3.55115000	3.55121400
N	2.58896000	3.47126200	2.95809600
H	3.28597300	4.20809500	2.94886600
C	2.73769200	2.26283500	2.38928300
H	3.61573400	1.93495600	1.85562600
N	1.63736400	1.53890900	2.58625300
C	0.75817200	2.33509200	3.30624900
H	-0.21579500	1.98258300	3.60376700
C	-0.23395300	5.82486900	-3.65279100
H	-1.05657600	5.31102500	-4.16596800
H	0.65603100	5.66734400	-4.27906300
C	0.03033300	5.13856800	-2.31131100
O	0.31160400	5.76236100	-1.28898900
N	-0.06402300	3.77884500	-2.32776300
H	0.22588100	3.27288300	-1.50009800
H	-0.18513100	3.23884100	-3.17759700
C	3.32059500	-1.43451200	2.49763100
O	2.20245300	-1.56272300	3.11314900
O	3.35661700	-0.62403300	1.51650200
C	-1.04884100	-0.13975700	-6.60407900
C	-1.42287500	-1.13200200	-7.50578300
C	-1.64364000	-2.43984800	-7.06121600
C	-1.49125000	-2.76364900	-5.70914300
C	-1.11215500	-1.78653900	-4.79295300
C	-0.89341600	-0.48702800	-5.25886100
N	-0.50447800	0.55147200	-4.31188100
O	-0.17999800	0.22588500	-3.16166000
O	-0.52326200	1.72477100	-4.69405200
H	-0.87356800	0.87869200	-6.92769000
H	-1.54076500	-0.88347000	-8.55578800
H	-1.93713400	-3.20836000	-7.77012300
H	-1.66624400	-3.77756600	-5.36365500

H	-1.00571500	-2.02925300	-3.74345400
O	0.49946900	0.25993900	0.28421600
O	0.75861200	-1.59442900	0.47682200
H	1.12604400	-1.65292900	-0.50191400
H	5.44050600	-1.73642200	2.62356000
H	4.49486400	-2.48731700	3.95429200
H	4.48113300	-3.20050500	2.32882100
Fe	1.23737000	-0.32349600	1.77791800
C	4.51604700	-2.25594800	2.88653900
H	-2.73530900	-7.50757500	0.19654000
H	-1.51784800	-6.66700800	1.16016500
H	-3.07255300	-5.88143200	0.79470900
C	0.84391200	4.75725400	4.27997400
H	1.48970700	5.00281600	5.13184000
H	0.80706900	5.63527000	3.62406900
H	-0.16476400	4.57401500	4.65924600
C	-0.52137000	7.32214800	-3.52064300
H	-3.46928200	-0.80034400	6.00983400
H	-3.58768700	-2.41123000	5.28372200
H	-2.20638800	-2.00500900	6.31645500
C	-2.28518200	-6.52820500	0.38930400
H	-0.64581100	7.77627300	-4.50996000
H	-1.43673700	7.50251400	-2.94616900
H	0.29843300	7.83244700	-3.00649200
C	-2.88737400	-1.61223800	5.55664200
O	1.29005000	-2.03277200	-1.93849000
H	0.66829300	-2.81022700	-1.98321400
H	0.85660300	-1.31779500	-2.44449200

B97D

FeIII-RC-modell¹-B97D:

C	-2.13987100	-1.27209500	4.30834900
N	-2.75414000	-1.16778000	3.06182400
H	-3.74557000	-1.30961700	2.88211100
C	-1.82730500	-0.86837300	2.12836300
H	-2.02846400	-0.74538600	1.07088200
N	-0.62528200	-0.76635500	2.71285200
C	-0.80820200	-1.01744700	4.06557500
H	0.02396700	-1.00771600	4.76026100
C	1.28856400	3.53543800	3.54254800
N	2.55641300	3.41952300	2.97948200
H	3.27951100	4.13456100	3.01036700
C	2.68229900	2.21112200	2.39481200
H	3.56734300	1.85077000	1.88520000
N	1.54222200	1.52369800	2.55010300
C	0.66786000	2.33790300	3.26140700
H	-0.32975500	2.00525100	3.52460200
C	3.25746600	-1.55121800	2.45928600

O	2.14090500	-1.76511600	3.04931800
O	3.26817400	-0.71754200	1.47731500
O	0.68300400	-0.47340200	-0.03016500
O	1.02102400	-1.88884700	-0.06456400
H	1.95483100	-1.85092700	-0.38159800
H	5.31048300	-1.51510400	3.06656100
H	4.34376300	-2.85479600	3.78997400
H	4.85551000	-2.91121800	2.06763000
Fe	1.17868200	-0.35096100	1.78426300
C	4.51604600	-2.25594800	2.88653900
C	0.84391200	4.75725200	4.27997300
H	1.50114500	4.96154300	5.14173000
H	0.85676900	5.64606100	3.62740000
H	-0.18059600	4.61441800	4.65071700
H	-3.67173800	-0.86766800	5.77305100
H	-3.37454900	-2.59806900	5.47224200
H	-2.19067900	-1.64120900	6.40597700
C	-2.88737300	-1.61223800	5.55664100

OO-cleavage-TS-model1'-B97D:

C	-2.13393400	-1.04928200	4.39731400
N	-2.74795500	-0.58132100	3.23639500
H	-3.75205400	-0.48728800	3.10029100
C	-1.80536400	-0.28473100	2.32013600
H	-2.00062400	0.08963500	1.32269100
N	-0.59172300	-0.53662600	2.83455700
C	-0.78375100	-1.01406500	4.12061100
H	0.05248700	-1.30028900	4.74769600
C	1.54911300	3.49753100	3.85737900
N	2.73918400	3.44452000	3.13499800
H	3.44874700	4.17357300	3.11756500
C	2.80230000	2.28128800	2.45689700
H	3.62098600	1.97334800	1.81915500
N	1.69922300	1.56102600	2.70817600
C	0.91303800	2.30831100	3.57488200
H	-0.03903200	1.93990100	3.93840400
C	3.31712300	-1.35488300	2.57700100
O	2.17676100	-1.50850100	3.16285200
O	3.35686400	-0.60944500	1.53830500
O	0.59847300	0.27843300	0.25238100
O	0.87534600	-1.51725200	0.32558800
H	1.66854800	-1.48993700	-0.25941200
H	5.24369200	-1.24322100	3.48433800
H	4.31150300	-2.71561300	3.92356800
H	5.06892600	-2.55183800	2.29443500
Fe	1.21089900	-0.25486100	1.85045400
C	4.55606400	-2.01986300	3.11059800
C	1.17251700	4.66605000	4.70873600

H	1.90751500	4.82998500	5.51433600
H	1.11616100	5.59112800	4.11080700
H	0.18965500	4.48932000	5.16732300
H	-3.51697600	-0.64709600	6.00047300
H	-3.57678600	-2.31444400	5.37340900
H	-2.20213900	-1.79408800	6.38881300
C	-2.90232500	-1.47314800	5.60534100

OO-cleavage-PC-modell1'-B97D:

C	-2.13317500	-1.13331700	4.36055800
N	-2.76082700	-0.63908400	3.22732900
H	-3.76729600	-0.56007300	3.10034700
C	-1.82140800	-0.29124600	2.31523500
H	-2.03583100	0.12467500	1.33781400
N	-0.60113200	-0.53327600	2.80754800
C	-0.77406000	-1.05792700	4.06810900
H	0.07022600	-1.35836300	4.67893500
C	1.30648800	3.55392900	3.53089800
N	2.35249700	3.58831900	2.61857700
H	2.89519600	4.41477000	2.37410400
C	2.53756500	2.35441400	2.10984400
H	3.27416000	2.09076900	1.36188400
N	1.65735800	1.49302900	2.67241100
C	0.89094400	2.21666300	3.53787900
H	0.10033700	1.76304500	4.12452800
C	3.39028900	-1.33605400	2.46349900
O	2.23496900	-1.43522300	3.04435200
O	3.52358500	-0.51487500	1.50395500
O	0.70679500	0.71314700	0.44828200
O	1.02468000	-1.77385200	0.58748600
H	1.10539700	-1.51678600	-0.35638200
H	5.48694900	-1.83672300	2.58980600
H	4.48696200	-2.43716500	3.97074800
H	4.37465400	-3.22265400	2.37433900
Fe	1.24139400	-0.32653000	1.67691700
C	4.51604600	-2.25595100	2.88653900
C	0.84391000	4.75725400	4.27997300
H	1.63699200	5.13484100	4.94836200
H	0.58640500	5.57033500	3.58002800
H	-0.03959600	4.50846100	4.88240400
H	-3.50934200	-0.80702100	5.98328800
H	-3.55745600	-2.44801600	5.29266800
H	-2.18452300	-1.95867800	6.32659000
C	-2.88737100	-1.61223700	5.55664000

NBZ-FeIII-RC-modell1-B97D:

C	-2.12497900	-1.22797900	4.33001500
N	-2.74514400	-0.93501500	3.11781000

H	-3.74857900	-0.95624500	2.95137100
C	-1.80626300	-0.63947400	2.19421600
H	-2.00822700	-0.38926300	1.15976800
N	-0.59124500	-0.72240300	2.75228900
C	-0.77707600	-1.08913800	4.07778500
H	0.06301400	-1.23728900	4.74621700
C	1.23082500	3.59864100	3.41781800
N	2.20275400	3.69218600	2.42540900
H	2.73361400	4.53130100	2.20322400
C	2.33388100	2.50243200	1.80450100
H	3.01432400	2.30408900	0.98312100
N	1.47966200	1.62384300	2.35097400
C	0.78986000	2.29546900	3.35530900
H	0.03631600	1.79754900	3.95519900
C	3.24849000	-1.54615600	2.49526500
O	2.16122200	-1.68912200	3.15228500
O	3.22684800	-0.77620700	1.46143300
C	3.76131200	-1.42994000	-1.62596900
C	3.52434100	-2.71499100	-2.13743600
C	2.50941600	-2.92296100	-3.09072900
C	1.72121700	-1.84591900	-3.53390400
C	1.93257400	-0.55937600	-3.02259000
C	2.95197000	-0.37209700	-2.07580100
N	3.15356300	0.97270500	-1.49974000
O	2.31368600	1.84840600	-1.74776100
O	4.15312400	1.15613200	-0.78662500
H	4.52796400	-1.24740900	-0.87782500
H	4.13391400	-3.55097400	-1.79214300
H	2.33268900	-3.92484500	-3.48461000
H	0.93478900	-2.00791600	-4.27170400
H	1.32010700	0.28304100	-3.33669100
O	0.60324300	-0.55385200	-0.00103000
O	0.84834900	-1.98667100	0.05662000
H	1.72395900	-2.04194500	-0.39689300
H	5.32779500	-1.52072700	3.00103400
H	4.38169200	-2.81989900	3.81841200
H	4.80473400	-2.94304200	2.07434300
Fe	1.19968400	-0.33170800	1.77375000
C	4.51604600	-2.25594900	2.88653900
C	0.84391100	4.75725300	4.27997300
H	1.70986300	5.14638400	4.84087400
H	0.43404300	5.58365900	3.67561900
H	0.07701100	4.44164500	5.00078400
H	-3.59593800	-0.82126300	5.85434000
H	-3.46486700	-2.53762900	5.39353300
H	-2.18833900	-1.78305100	6.38719200
C	-2.88737300	-1.61223800	5.55664100

NBZ-OO-cleavage-TS-model1-B97D:

C	-2.12899200	-1.18839000	4.34087500
N	-2.75760600	-0.88403100	3.13509000
H	-3.76069300	-0.92389500	2.96966200
C	-1.82698300	-0.54944200	2.21772000
H	-2.03569500	-0.27353300	1.19147500
N	-0.60940100	-0.61686500	2.77351800
C	-0.78392000	-1.01460100	4.08960900
H	0.06077000	-1.15560100	4.75423200
C	1.30615800	3.53660300	3.54839900
N	2.56298700	3.44962400	2.95408800
H	3.26547100	4.18540100	2.95474000
C	2.70704400	2.23771200	2.38039200
H	3.58538900	1.90306600	1.84350800
N	1.59467500	1.51662600	2.57755900
C	0.71600700	2.31620900	3.29814900
H	-0.26346000	1.95844200	3.59255600
C	3.31808500	-1.45213900	2.45230000
O	2.17349800	-1.63976800	3.02047400
O	3.38538100	-0.59473900	1.50949000
C	6.23435100	-0.77681300	-1.84179300
C	7.61735700	-0.99115700	-1.84807000
C	8.15321000	-2.17250300	-1.30357100
C	7.30544400	-3.14979700	-0.75090500
C	5.91926300	-2.95569900	-0.73842600
C	5.40529300	-1.76592800	-1.28445700
N	3.95617700	-1.53742200	-1.26624200
O	3.23016200	-2.45459700	-0.81732900
O	3.50797200	-0.46715800	-1.68085200
H	5.79923800	0.12938300	-2.25839700
H	8.27612000	-0.23641200	-2.27885500
H	9.23232200	-2.33304100	-1.31143800
H	7.72328000	-4.06498100	-0.33010400
H	5.24874700	-3.70140300	-0.31765000
O	0.58306900	0.16441600	0.14884000
O	0.85678700	-1.63483000	0.30324700
H	1.67530400	-1.70797800	-0.27324300
H	5.42374400	-1.91246300	2.37407000
H	4.64109000	-2.17716100	3.97759900
H	4.33513600	-3.31707000	2.65033000
Fe	1.19386900	-0.34471000	1.74750800
C	4.51604600	-2.25594700	2.88653900
C	0.84391200	4.75725100	4.27997300
H	1.50869400	4.98725300	5.12951500
H	0.82645300	5.63810400	3.61672700
H	-0.17147200	4.59509200	4.66764300
H	-3.61012100	-0.83931000	5.86770900
H	-3.44890500	-2.54326400	5.37100800
H	-2.18873300	-1.78900000	6.38620900

C -2.88737300 -1.61223800 5.55664100

NBZ-OO-cleavage-PC-model1-B97D:

C -2.11660400 -1.11015300 4.37660500
N -2.73685600 -0.53860500 3.26961300
H -3.74026600 -0.41417400 3.15819200
C -1.79796200 -0.19027800 2.36139100
H -2.00210600 0.28080200 1.40755300
N -0.58635800 -0.50804600 2.82903300
C -0.76816300 -1.08068800 4.07655000
H 0.07163900 -1.44087200 4.65997400
C 1.30511700 3.54857500 3.52774100
N 2.36119000 3.58951700 2.62074900
H 2.91170200 4.41567500 2.39649200
C 2.54621700 2.36403000 2.09332300
H 3.28983900 2.10781700 1.34994900
N 1.65674100 1.50733900 2.63137100
C 0.88010500 2.22791900 3.51255200
H 0.08065100 1.76343900 4.07734100
C 3.39089000 -1.33251800 2.46888200
O 2.24777200 -1.41083100 3.07713400
O 3.50748700 -0.52902200 1.49432700
C 6.18913900 -0.76369900 -1.89184100
C 7.57919000 -0.91986400 -1.93914200
C 8.18307800 -2.05902700 -1.37638400
C 7.39675900 -3.05186400 -0.76400900
C 6.00457300 -2.91599300 -0.71065400
C 5.42180900 -1.76758500 -1.27562000
N 3.96498000 -1.60107800 -1.21797300
O 3.29445800 -2.53677300 -0.72392700
O 3.45807800 -0.56287600 -1.64665400
H 5.70283200 0.10962900 -2.32160000
H 8.19017200 -0.15274000 -2.41612400
H 9.26733300 -2.17401800 -1.41598400
H 7.86681100 -3.93427900 -0.32850700
H 5.38173400 -3.67486200 -0.24281100
O 0.63419200 0.67746300 0.45450000
O 1.00621400 -1.70957300 0.57837500
H 1.76887600 -1.84470800 -0.05708900
H 5.46679700 -1.92242900 2.45071900
H 4.58931900 -2.30189800 3.98335100
H 4.28161500 -3.26917300 2.52129200
Fe 1.22138100 -0.31122500 1.72138100
C 4.51604700 -2.25594900 2.88653900
C 0.84391200 4.75725300 4.27997300
H 1.63662800 5.13747400 4.94632800
H 0.57284000 5.56836700 3.58354900
H -0.03516600 4.50492100 4.88828400
H -3.47460600 -0.80434200 6.02479400

H	-3.58784100	-2.41230400	5.26381300
H	-2.19368500	-2.01719500	6.30669600
C	-2.88737300	-1.61223800	5.55664100

B3LYP-D2

FeIII-RC-modell'-B3LYP-D2:

C	-2.11959800	-1.24179700	4.33469300
N	-2.72092500	-1.04318300	3.10006000
H	-3.71317900	-1.13230800	2.90981600
C	-1.78065700	-0.73523800	2.19162300
H	-1.96587500	-0.54228700	1.14616000
N	-0.58636800	-0.71969400	2.77990600
C	-0.78470700	-1.03625900	4.11380200
H	0.04132200	-1.10498900	4.80558400
C	1.30008700	3.53118900	3.56445600
N	2.56083100	3.42089500	2.99521500
H	3.27506100	4.14103400	3.00836900
C	2.69302900	2.21042400	2.43182100
H	3.57308900	1.84961700	1.92198700
N	1.56845300	1.51690700	2.60638300
C	0.69307500	2.33104900	3.31097200
H	-0.29300300	1.99208900	3.58985400
C	3.25659000	-1.55197100	2.48664500
O	2.15123100	-1.76521200	3.08262200
O	3.25108700	-0.69914000	1.52848800
O	0.63267000	-0.35916300	0.07921400
O	0.91843600	-1.78382800	0.10696700
H	1.80489800	-1.81839300	-0.31358000
H	5.23435700	-1.51644300	3.26311600
H	4.31573700	-3.00324600	3.65787200
H	4.96405500	-2.73044300	2.00539500
Fe	1.20870600	-0.34854800	1.86398400
C	4.51604600	-2.25595000	2.88653900
C	0.84390300	4.75724000	4.27997600
H	1.49820900	4.98408700	5.13190800
H	0.84282900	5.62972700	3.61387200
H	-0.17310800	4.60892900	4.65549800
H	-3.63423100	-0.84754300	5.80737200
H	-3.41503700	-2.56523100	5.41990500
H	-2.20231300	-1.71679600	6.40354900
C	-2.88736400	-1.61222400	5.55663800

OO-cleavage-TS-modell'-B3LYP-D2:

C	-2.09616800	-1.11106300	4.36941500
N	-2.70944200	-0.64705500	3.21353500
H	-3.71028100	-0.54929400	3.08039100
C	-1.77264400	-0.35487100	2.29779900

H	-1.96858600	0.02342000	1.30636300
N	-0.56675000	-0.60690500	2.80437200
C	-0.75483300	-1.08089500	4.09263400
H	0.08175000	-1.36751200	4.71149700
C	1.51243000	3.33522900	3.93046000
N	2.70201500	3.31244300	3.21766500
H	3.40742000	4.04118100	3.22798800
C	2.77719400	2.17349600	2.51104900
H	3.59853300	1.88795600	1.87325100
N	1.68432500	1.44522700	2.73131900
C	0.88760800	2.15940200	3.61260600
H	-0.05877300	1.77362100	3.95837900
C	3.32461200	-1.35873800	2.56547100
O	2.18411200	-1.53320100	3.13246200
O	3.35686700	-0.60944400	1.53830800
O	0.61387900	0.33538300	0.29948200
O	0.87534300	-1.51725300	0.32558400
H	1.62730000	-1.47405300	-0.30371900
H	5.38316300	-1.92849600	2.41266500
H	4.82586400	-1.49415900	4.05581500
H	4.34614300	-3.05171600	3.36164900
Fe	1.22412000	-0.32803200	1.82176900
C	4.55447400	-2.00351400	3.12132700
C	1.12381900	4.47095100	4.81391200
H	1.85345000	4.61729100	5.62088700
H	1.05655600	5.40845700	4.24645100
H	0.14716800	4.27064700	5.26508000
H	-3.53688400	-0.72264200	5.91240900
H	-3.50460000	-2.40358900	5.34548800
H	-2.20213900	-1.79408800	6.38881400
C	-2.87750700	-1.53034900	5.56897000

OO-cleavage-PC-modell'-B3LYP-D2:

C	-3.68117900	-2.43271900	4.31709100
N	-4.33345900	-1.66446000	3.36373500
H	-5.32022500	-1.43025900	3.37468100
C	-3.45388300	-1.28878700	2.41869300
H	-3.69137600	-0.69044600	1.55270300
N	-2.25204100	-1.77618300	2.71629300
C	-2.37984300	-2.49060500	3.89440400
H	-1.53718200	-2.99669200	4.33915500
C	0.37458500	1.85293600	3.55733600
N	1.59536600	1.53101800	2.98249300
H	2.44204400	2.08471900	3.05937400
C	1.48922400	0.37244400	2.31438100
H	2.28055600	-0.11103300	1.76503600
N	0.24498000	-0.08797000	2.44260100
C	-0.46270600	0.82804300	3.20646000
H	-1.50327500	0.67615100	3.44604600

C	1.42717000	-3.06211000	2.01242200
O	1.56151400	-2.30292200	1.01454000
O	0.32829700	-2.97443600	2.68868500
O	-1.17030800	-0.57625800	0.36687100
O	-1.07971100	-2.85603800	0.21913300
H	-0.49837000	-2.79907300	-0.56956800
C	2.45764500	-4.07080100	2.42019100
H	2.04569200	-5.07664600	2.26907800
H	3.36596700	-3.95041500	1.82490900
H	2.68289300	-3.96148800	3.48750500
C	0.16611700	3.09932200	4.35118000
H	0.35298400	3.99035200	3.73776300
H	-0.86541700	3.13902800	4.71372100
H	0.84039700	3.13692600	5.21641600
C	-4.38016500	-3.02223500	5.49444700
H	-3.66388200	-3.57859400	6.10663500
H	-4.83843800	-2.24434100	6.11920100
H	-5.17409900	-3.71214700	5.17972500
Fe	-0.55759900	-1.67840000	1.51332900

NBZ-FeIII-RC-modell1-B3LYP-D2:

C	-2.11540000	-1.24148800	4.33669800
N	-2.71392000	-1.04589700	3.10025800
H	-3.70570700	-1.13529000	2.90807900
C	-1.77136200	-0.73969400	2.19326900
H	-1.95391700	-0.54963300	1.14685000
N	-0.57835900	-0.72243000	2.78369400
C	-0.77983700	-1.03541500	4.11795800
H	0.04502700	-1.10214300	4.81136400
C	1.28954300	3.54030900	3.54314800
N	2.51405100	3.46683700	2.89441300
H	3.19972500	4.21281800	2.84845000
C	2.65323000	2.25672100	2.33294700
H	3.50283600	1.93990200	1.74723800
N	1.56483300	1.52767100	2.58274500
C	0.70829300	2.31907200	3.33581500
H	-0.24467700	1.94791800	3.68129300
C	3.25715300	-1.53675000	2.51441300
O	2.14827600	-1.77139200	3.09351300
O	3.25387300	-0.66774900	1.57171800
C	4.12786600	-1.20095200	-1.29958700
C	3.82053300	-2.38461900	-1.97237500
C	2.77344500	-2.41410400	-2.90335600
C	2.02660000	-1.25977100	-3.16626700
C	2.30892300	-0.07354700	-2.49049700
C	3.35850200	-0.06553700	-1.56974600
N	3.62624900	1.15922800	-0.81556600
O	2.77142500	2.04871700	-0.82734800
O	4.68728500	1.24066100	-0.19180400

H	4.91724600	-1.15300800	-0.56131700
H	4.39453100	-3.28289000	-1.76687300
H	2.53928100	-3.33904500	-3.42216200
H	1.21567700	-1.28565600	-3.88734300
H	1.72908900	0.82528700	-2.65688500
O	0.62267900	-0.38217000	0.08491200
O	0.97025200	-1.79165100	0.08452800
H	1.83185300	-1.78404900	-0.38558200
H	5.34264000	-1.54093700	2.95949500
H	4.39162600	-2.79872200	3.82679600
H	4.76068000	-2.96777800	2.08677300
Fe	1.21485500	-0.34508000	1.85991400
C	4.51604400	-2.25594300	2.88654000
C	0.84391500	4.75724800	4.27997200
H	0.78936300	5.62798800	3.61384700
H	-0.14878900	4.58831600	4.70847000
H	1.53621800	5.00032000	5.09676500
H	-3.63722000	-0.84915200	5.80326200
H	-3.41191400	-2.56684800	5.41898100
H	-2.20557300	-1.71384700	6.40655000
C	-2.88737400	-1.61223800	5.55664100

NBZ-OO-cleavage-TS-model1-B3LYP-D2:

C	-2.10650900	-1.18990700	4.35734300
N	-2.71199800	-0.89015300	3.14555800
H	-3.70821800	-0.93321700	2.96084300
C	-1.76937900	-0.55359400	2.24887000
H	-1.95703400	-0.28196400	1.22149300
N	-0.57043900	-0.61425400	2.82267300
C	-0.76575800	-1.01331000	4.13396300
H	0.06513200	-1.15130500	4.80935000
C	1.32980700	3.50355900	3.63284500
N	2.63611700	3.35060800	3.19281600
H	3.36715100	4.04907600	3.27109500
C	2.78476600	2.13136200	2.65027500
H	3.69602900	1.74697400	2.22097700
N	1.63063100	1.47163800	2.72063500
C	0.71525200	2.31818200	3.32745900
H	-0.30494100	2.01285300	3.50098500
C	3.31052300	-1.45010500	2.50482700
O	2.18410700	-1.63497600	3.08583900
O	3.35455800	-0.57553700	1.58033700
C	6.13888900	-0.16776200	-1.47579600
C	7.52208300	-0.30174600	-1.37879000
C	8.08025100	-1.47696900	-0.86186300
C	7.25756400	-2.52933500	-0.44275100
C	5.87202300	-2.41640600	-0.53798900
C	5.33685000	-1.23151400	-1.05280000
N	3.89121300	-1.08813700	-1.13750200

O	3.19394700	-2.08912500	-0.88134700
O	3.41154900	-0.00388700	-1.44452300
H	5.68338600	0.73164900	-1.87208100
H	8.16357200	0.51008400	-1.70722100
H	9.15943400	-1.57368500	-0.78655000
H	7.69454000	-3.43848400	-0.04165000
H	5.21721200	-3.21692800	-0.21803500
O	0.60127200	0.32822700	0.31071400
O	0.86524500	-1.52837100	0.37811300
H	1.64938000	-1.56189100	-0.24176200
H	5.39223300	-1.93555400	2.31839300
H	4.69891700	-2.15169800	3.96277400
H	4.31001800	-3.31506700	2.68846800
Fe	1.22524600	-0.32865900	1.81890500
C	4.51592200	-2.25579800	2.88658500
C	0.84400300	4.75713100	4.27993900
H	1.39031400	4.96351400	5.20967400
H	0.97322900	5.62061900	3.61461600
H	-0.21967000	4.66201400	4.51876600
H	-3.60464700	-0.83776300	5.85826800
H	-3.44965300	-2.53416600	5.35842300
H	-2.20730600	-1.79769300	6.39374400
C	-2.88734000	-1.61226700	5.55662900

NBZ-OO-cleavage-PC-model1-B3LYP-D2:

C	-2.09411600	-1.12249500	4.39012000
N	-2.69716700	-0.58888100	3.26155100
H	-3.69665700	-0.48836300	3.12361700
C	-1.74777200	-0.23799900	2.37505100
H	-1.93655200	0.20191300	1.40791300
N	-0.54846500	-0.51391300	2.87668900
C	-0.74821100	-1.06752100	4.12830300
H	0.08211600	-1.39086000	4.73804500
C	1.35769000	3.49669800	3.66299500
N	2.68425200	3.32569600	3.29459000
H	3.42138300	4.01170000	3.41618500
C	2.84684100	2.10899100	2.74980900
H	3.77200500	1.71577200	2.36080300
N	1.68079800	1.46643100	2.75752000
C	0.74372600	2.32235700	3.31812000
H	-0.28832800	2.03175700	3.42900400
C	3.38008000	-1.34548100	2.50778800
O	2.25502000	-1.41354700	3.13223400
O	3.46457000	-0.53405400	1.54144600
C	6.06208200	-0.55285900	-1.70721300
C	7.44880400	-0.68408800	-1.70909400
C	8.05003600	-1.80387100	-1.12209800
C	7.26692900	-2.80265800	-0.53108600
C	5.87818800	-2.69207000	-0.52449600

C	5.29981900	-1.56308600	-1.11331800
N	3.85263900	-1.42381100	-1.10026600
O	3.18169300	-2.38077900	-0.66463200
O	3.34212500	-0.38543900	-1.50217700
H	5.57439100	0.30464500	-2.15465000
H	8.05936700	0.08644900	-2.16936500
H	9.13195100	-1.89903900	-1.12574900
H	7.73717800	-3.66910000	-0.07663400
H	5.25397300	-3.45277200	-0.07338900
O	0.63580500	0.65026700	0.54150200
O	0.95351400	-1.61010900	0.64379400
H	1.69535600	-1.74053600	-0.01609100
H	5.42453100	-1.97114400	2.35080100
H	4.68014700	-2.22645700	3.96957500
H	4.23828900	-3.28363300	2.61941700
Fe	1.26027700	-0.27362600	1.82091100
C	4.51603900	-2.25593800	2.88654200
C	0.84391600	4.75724000	4.27997100
H	1.33935900	4.96430800	5.23736400
H	1.01508100	5.61608500	3.61821100
H	-0.23165700	4.66746800	4.45980100
H	-3.49215600	-0.80635700	5.99276900
H	-3.56662200	-2.42277700	5.26162400
H	-2.21233800	-1.99355700	6.32910000
C	-2.88736900	-1.61223600	5.55663900

B3LYP-D3

FeIII-RC-modell'-B3LYP-D3:

C	-2.12017900	-1.25056800	4.33222900
N	-2.72165600	-1.04751200	3.09678800
H	-3.71442900	-1.13031700	2.90646700
C	-1.78026900	-0.74476300	2.18752300
H	-1.96193700	-0.54808300	1.14268100
N	-0.58580200	-0.73742300	2.77552100
C	-0.78403000	-1.05391300	4.10972200
H	0.04401500	-1.12608800	4.79781700
C	1.29783800	3.53296300	3.56115500
N	2.56075700	3.41649600	2.99481800
H	3.27930600	4.13226400	3.01085400
C	2.68827700	2.20600900	2.43000600
H	3.56647900	1.83822300	1.92311000
N	1.55910300	1.51895800	2.60044100
C	0.68522000	2.33659200	3.30334900
H	-0.30323700	2.00192600	3.57651400
C	3.25606600	-1.55475200	2.48768700
O	2.15048100	-1.77137300	3.08188900
O	3.24963200	-0.69962600	1.53136200
O	0.62844200	-0.35431300	0.07820300

O	0.89900000	-1.78171600	0.09041200
H	1.77103700	-1.82512300	-0.35864300
H	5.23633100	-1.51611300	3.25459800
H	4.32034400	-2.99766000	3.66242200
H	4.95996500	-2.73658200	2.00825000
Fe	1.20631800	-0.34953200	1.86245300
C	4.51604600	-2.25595000	2.88653900
C	0.84390300	4.75724000	4.27997600
H	1.49291400	4.97833900	5.13598100
H	0.84893600	5.63332900	3.62055000
H	-0.17448200	4.61486700	4.65079300
H	-3.62470200	-0.84120600	5.81105500
H	-3.42563200	-2.55863400	5.42489300
H	-2.20386900	-1.72405500	6.40244600
C	-2.88736400	-1.61222400	5.55663800

OO-cleavage-TS-model1'-B3LYP-D3:

C	-2.10299000	-1.13713800	4.36086600
N	-2.71757500	-0.68377700	3.19980600
H	-3.71870700	-0.59499200	3.06258500
C	-1.78089400	-0.38668100	2.28525100
H	-1.97500700	-0.01409900	1.29174500
N	-0.57434100	-0.62572600	2.79703300
C	-0.76121100	-1.09647000	4.08724600
H	0.07697900	-1.37160400	4.70823400
C	1.50498900	3.38564400	3.85765100
N	2.69197600	3.34675200	3.13912100
H	3.39719000	4.07571100	3.12833800
C	2.76359700	2.19314300	2.45596700
H	3.58091600	1.89341900	1.82040500
N	1.67193100	1.46953200	2.69841300
C	0.87891000	2.20289200	3.56832800
H	-0.06577400	1.82630800	3.92692100
C	3.32009200	-1.35142000	2.57017800
O	2.17806000	-1.51524900	3.13828700
O	3.35686700	-0.60944400	1.53830800
O	0.59890600	0.33359500	0.29595300
O	0.87534300	-1.51725300	0.32558400
H	1.62908100	-1.46554500	-0.30049000
H	5.37477900	-1.93371400	2.42485100
H	4.81854400	-1.48846400	4.06225400
H	4.33218300	-3.04450800	3.37626400
Fe	1.21419800	-0.32080000	1.82006800
C	4.54501800	-1.99975100	3.13098800
C	1.11832400	4.53962400	4.71745500
H	1.84778200	4.70484000	5.51935100
H	1.04844400	5.46470800	4.13246300
H	0.14402800	4.35210900	5.17646600
H	-3.55498600	-0.75945200	5.89630100

H	-3.48691900	-2.44454600	5.35403000
H	-2.20213900	-1.79408800	6.38881400
C	-2.87880200	-1.55603900	5.56356300

OO-cleavage-PC-modell'-B3LYP-D3:

C	-2.10622900	-1.15877900	4.36866300
N	-2.72050500	-0.65869400	3.22841400
H	-3.72165900	-0.56587400	3.09518600
C	-1.78266900	-0.32372300	2.32654000
H	-1.97856000	0.09457600	1.35202600
N	-0.57672900	-0.58195800	2.82797700
C	-0.76272600	-1.10588300	4.09645800
H	0.07531600	-1.40381000	4.70758400
C	1.34986800	3.50887000	3.63418900
N	2.66430400	3.35247800	3.21058900
H	3.39974100	4.04463700	3.30811200
C	2.82017600	2.14073500	2.65667500
H	3.73060900	1.75247500	2.23021000
N	1.65938500	1.48681200	2.71163600
C	0.73373300	2.33045600	3.31017300
H	-0.28851600	2.02862600	3.46541000
C	3.41738000	-1.32981700	2.44162700
O	2.26660600	-1.37246900	3.04137400
O	3.54935700	-0.54901000	1.46315600
O	0.55378000	0.70841600	0.54925800
O	1.04626000	-1.51939800	0.49656100
H	1.68036700	-1.37520900	-0.23915600
H	5.48591800	-1.86746900	2.56953500
H	4.49021900	-2.39816200	3.96997800
H	4.35150700	-3.23076400	2.41074100
Fe	1.22437900	-0.24917400	1.79241300
C	4.51603700	-2.25593700	2.88654300
C	0.84391600	4.75723700	4.27997100
H	1.36817600	4.96148800	5.22108600
H	0.98226500	5.62401900	3.62303400
H	-0.22275600	4.65626000	4.49585700
H	-3.49063400	-0.79564000	5.97118100
H	-3.56621200	-2.43312400	5.29590900
H	-2.20822300	-1.96623100	6.33670300
C	-2.88736700	-1.61223400	5.55663900

NBZ-FeIII-RC-modell1-B3LYP-D3:

C	-2.11653700	-1.24957200	4.33420100
N	-2.71526200	-1.04742800	3.09728600
H	-3.70763800	-1.12959600	2.90498500
C	-1.77144600	-0.74578500	2.18975200
H	-1.95034600	-0.55065100	1.14416100
N	-0.57828300	-0.73837100	2.77990300

C	-0.77964400	-1.05311100	4.11405500
H	0.04723100	-1.12474100	4.80361300
C	1.29077700	3.54108600	3.54366500
N	2.52169500	3.45906700	2.90496000
H	3.21383900	4.19943300	2.86556800
C	2.65702300	2.24870800	2.34253700
H	3.50750700	1.92412500	1.76316100
N	1.56053000	1.52810100	2.58195700
C	0.70255700	2.32446300	3.32903000
H	-0.25540700	1.95900000	3.66452200
C	3.25412100	-1.54315700	2.51659700
O	2.15052100	-1.76800700	3.10804400
O	3.24344600	-0.68590900	1.56194900
C	4.12340900	-1.18827400	-1.33714000
C	3.81810400	-2.36056000	-2.02906300
C	2.78236200	-2.37210700	-2.97203500
C	2.04360800	-1.21150500	-3.22683200
C	2.32330400	-0.03680300	-2.53138800
C	3.36277100	-0.04636800	-1.60029300
N	3.62917000	1.16754500	-0.82801700
O	2.77956300	2.06223800	-0.83852300
O	4.68337200	1.23445800	-0.19077700
H	4.90528900	-1.15435100	-0.59034600
H	4.38605900	-3.26398500	-1.82994100
H	2.55034100	-3.28847700	-3.50658500
H	1.24097700	-1.22354700	-3.95735300
H	1.74906200	0.86661400	-2.69162000
O	0.61945900	-0.38836500	0.08307800
O	0.92264300	-1.80809500	0.09768700
H	1.77972100	-1.83581600	-0.37958300
H	5.33692200	-1.53674400	2.96495600
H	4.39563500	-2.80361400	3.82275500
H	4.76853600	-2.96020000	2.08440900
Fe	1.21094600	-0.34374000	1.85925200
C	4.51604400	-2.25594300	2.88654000
C	0.84391500	4.75724800	4.27997200
H	0.79887100	5.63083000	3.61875800
H	-0.15262900	4.59449900	4.69895500
H	1.52716900	4.99569900	5.10417300
H	-3.62655600	-0.84221900	5.80869200
H	-3.42383600	-2.55944400	5.42319200
H	-2.20645100	-1.72304300	6.40467300
C	-2.88737400	-1.61223800	5.55664100

NBZ-OO-cleavage-TS-model1-B3LYP-D3:

C	-2.11930600	-1.16621800	4.35890800
N	-2.74214100	-0.69911400	3.20872800
H	-3.74447800	-0.62160700	3.07495400
C	-1.81012600	-0.37776700	2.29639300

H	-2.01033800	0.00489500	1.30809800
N	-0.60059900	-0.61067800	2.80097000
C	-0.77821500	-1.10467800	4.08289300
H	0.06594700	-1.38184200	4.69497200
C	1.30612900	3.53505900	3.55891800
N	2.56150800	3.43635800	2.97352300
H	3.26968400	4.16219400	2.97633000
C	2.69819600	2.22586600	2.40748400
H	3.56896900	1.87565900	1.87751900
N	1.58534400	1.52067000	2.60080600
C	0.70931300	2.32717000	3.31283300
H	-0.27058500	1.97972400	3.59820600
C	3.33700900	-1.41260300	2.49738800
O	2.19583800	-1.58596100	3.06075100
O	3.41798200	-0.55020800	1.56930400
C	6.08490200	0.16011100	-1.39254500
C	7.47376400	0.07484900	-1.34936100
C	8.09423100	-1.14050400	-1.03996800
C	7.32836100	-2.28052300	-0.77223100
C	5.93790900	-2.21581000	-0.81428700
C	5.34026300	-0.99086700	-1.12259600
N	3.88791400	-0.90087000	-1.15522500
O	3.23786500	-1.94963600	-0.97709900
O	3.35779500	0.18650900	-1.34669700
H	5.58268300	1.09010600	-1.62918800
H	8.07131300	0.95637100	-1.55933100
H	9.17816400	-1.19950600	-1.00746200
H	7.81402100	-3.22129300	-0.53294600
H	5.32589000	-3.08541900	-0.61084000
O	0.52298400	0.27827900	0.25218400
O	0.90500000	-1.55770000	0.34472600
H	1.68241800	-1.54040200	-0.28555300
H	4.51757700	-2.43861500	3.96450900
H	4.42247300	-3.22487600	2.38060400
H	5.44844200	-1.78245300	2.57286700
Fe	1.18131900	-0.31903600	1.77019400
C	4.51597800	-2.25589500	2.88656400
C	0.84393300	4.75719400	4.27996500
H	1.49797000	4.98889300	5.12935200
H	0.83203000	5.63097600	3.61753300
H	-0.16918700	4.60374400	4.66085100
H	-3.51059500	-0.80272500	5.95533400
H	-3.54617400	-2.45501100	5.31473500
H	-2.19868100	-1.93263400	6.34282700
C	-2.88732600	-1.61223400	5.55662400

NBZ-OO-cleavage-PC-model1-B3LYP-D3:

C	-2.11038600	-1.14036000	4.37290600
N	-2.72822200	-0.64207700	3.23460900

H	-3.72977700	-0.55998600	3.09936900
C	-1.78991600	-0.29411500	2.33539700
H	-1.98923700	0.12200000	1.36053500
N	-0.58350100	-0.53953200	2.83714100
C	-0.76688100	-1.06998900	4.10252700
H	0.07348100	-1.36353800	4.71269900
C	1.34990400	3.50696900	3.63756400
N	2.66839100	3.34374900	3.23263100
H	3.40613800	4.03149700	3.33993700
C	2.82313300	2.13047000	2.67847600
H	3.73705700	1.73734200	2.26520700
N	1.65938700	1.48333800	2.71348200
C	0.73219300	2.33212800	3.30191400
H	-0.29433000	2.03703200	3.44034200
C	3.40588300	-1.32656700	2.47559800
O	2.26018300	-1.39218300	3.06781600
O	3.53642300	-0.51895700	1.51499000
C	6.10878700	-0.40141400	-1.63334700
C	7.49160000	-0.56218400	-1.62246400
C	8.05704500	-1.75134200	-1.14909700
C	7.24199200	-2.79057100	-0.68698600
C	5.85681000	-2.65020400	-0.69406500
C	5.31449600	-1.45194100	-1.16701600
N	3.87053700	-1.28026400	-1.16021600
O	3.17447200	-2.25132900	-0.80048500
O	3.38828100	-0.20533500	-1.49358000
H	5.64766100	0.50991300	-1.99374600
H	8.12732000	0.24026200	-1.98312100
H	9.13652900	-1.86947400	-1.14153000
H	7.68499500	-3.71124900	-0.32069600
H	5.20770200	-3.44108300	-0.34043700
O	0.58656300	0.68387200	0.50897300
O	0.97501700	-1.57179900	0.57797800
H	1.71068700	-1.66452600	-0.09765200
H	5.48071300	-1.85811400	2.56572400
H	4.50481500	-2.42286600	3.96672800
H	4.34801500	-3.22033600	2.39184200
Fe	1.23078500	-0.25001900	1.77366800
C	4.51603800	-2.25593100	2.88654200
C	0.84391900	4.75723000	4.27997000
H	1.35636000	4.95542600	5.22897100
H	0.99656000	5.62554800	3.62814300
H	-0.22628700	4.66345700	4.48158700
H	-3.50231800	-0.80713300	5.97674200
H	-3.55494800	-2.44057100	5.28998100
H	-2.20463300	-1.96247900	6.33538000
C	-2.88737100	-1.61223400	5.55664000

Fe^{III}-OOH and HO-Fe^V=O attacks Model 1

Nitrobenzene Modell

NBZ-RC-FeIII-modell:

C	-2.11593600	-1.23575200	4.33813500
N	-2.72207100	-0.89143800	3.13828200
H	-3.72178800	-0.86982300	2.96830000
C	-1.77557100	-0.60679000	2.22778100
H	-1.96974000	-0.31991000	1.20584100
N	-0.57140700	-0.74678200	2.77743900
C	-0.77161300	-1.14149800	4.09131400
H	0.05762100	-1.34014400	4.75275800
C	1.13853500	3.63359900	3.34462900
N	1.74139200	3.81972100	2.10778000
H	2.03664400	4.71093600	1.72322000
C	1.87220800	2.63720400	1.48748900
H	2.29130400	2.50140200	0.49918800
N	1.37625800	1.67285800	2.26547800
C	0.91683400	2.28549500	3.42488600
H	0.46016300	1.71910000	4.22207000
C	3.26632200	-1.52389200	2.50592600
O	2.19811400	-1.60504600	3.19536800
O	3.22644800	-0.78982700	1.45663700
C	3.07281100	-0.72547700	-2.88242100
C	3.05754500	-1.83697000	-3.72281200
C	2.04577200	-1.98289000	-4.67805700
C	1.04118400	-1.01729000	-4.79844400
C	1.03647200	0.09738000	-3.96254600
C	2.05704600	0.22417800	-3.01881600
N	2.05677900	1.38642200	-2.13060900
O	1.10484800	2.16447100	-2.17826800
O	3.02313400	1.53419200	-1.37165300
H	3.84874400	-0.58652400	-2.13942600
H	3.83801800	-2.58656300	-3.63420400
H	2.04251900	-2.85015600	-5.33187700
H	0.25951500	-1.13211200	-5.54293500
H	0.26609600	0.85529200	-4.03496300
O	0.60610600	-0.47254500	0.05211400
O	0.87012100	-1.89687100	0.10895200
H	1.72455600	-1.95537400	-0.36963000
H	5.33129400	-1.53776100	3.02707300
H	4.36837800	-2.83309700	3.80073300
H	4.80618600	-2.92431700	2.06815400
Fe	1.22225100	-0.32789000	1.82020500
C	4.51604600	-2.25594800	2.88653900
C	0.84391200	4.75725200	4.27997300
H	1.75756700	5.29218400	4.56565700

H	0.15876700	5.48419400	3.82705500
H	0.37719400	4.37156100	5.19002000
H	-3.55712900	-0.80413700	5.87492900
H	-3.50061200	-2.50493700	5.38378400
H	-2.20069900	-1.82804800	6.37944100
C	-2.88737300	-1.61223800	5.55664100

NBZ-RC-FeV-modell:

C	-2.10642800	-1.18774200	4.35731000
N	-2.71235500	-0.84280300	3.15853500
H	-3.70997000	-0.85654800	2.97716100
C	-1.76591900	-0.50030200	2.26522200
H	-1.96552000	-0.18984900	1.25141600
N	-0.56470200	-0.60118600	2.82530200
C	-0.76257800	-1.03435900	4.12592300
H	0.06609600	-1.20670200	4.79591400
C	1.36149500	3.50951600	3.64074200
N	2.68470900	3.34459800	3.25484300
H	3.42328500	4.03022400	3.37109600
C	2.84439600	2.13159500	2.70073600
H	3.76822100	1.74700500	2.30010600
N	1.68080800	1.48389100	2.71705700
C	0.74817400	2.33562400	3.29270000
H	-0.28306300	2.04850200	3.41706700
C	3.39105300	-1.34883800	2.46840300
O	2.24830100	-1.41859400	3.06585200
O	3.49725700	-0.54637900	1.49963700
C	4.37048500	-0.12779400	-4.18741300
C	5.28564300	-0.36061100	-5.20994400
C	5.80514300	-1.64422100	-5.40930300
C	5.41235400	-2.70504200	-4.58621600
C	4.50045300	-2.49216300	-3.55584100
C	3.99548100	-1.20156400	-3.37503300
N	3.04482200	-0.95611500	-2.29881200
O	2.76062600	-1.91110500	-1.54971000
O	2.56404200	0.16407000	-2.16774300
H	3.95497100	0.85738000	-4.01484300
H	5.59288800	0.45967300	-5.85092300
H	6.51847700	-1.81840700	-6.20945200
H	5.81649400	-3.69968300	-4.74582100
H	4.18444700	-3.29923600	-2.90670700
O	0.59010300	0.68594300	0.54286800
O	1.00984100	-1.54498100	0.52552900
H	1.64285600	-1.49937400	-0.24772600
H	5.47608700	-1.84075600	2.57299500
H	4.50272800	-2.42095000	3.96709400
H	4.37478600	-3.22601600	2.39360300
Fe	1.26360700	-0.26779400	1.77777000
C	4.51604700	-2.25594900	2.88653900

C	0.84391200	4.75725300	4.27997300
H	1.33959200	4.95413000	5.23814100
H	1.00350300	5.62961900	3.63517600
H	-0.22904000	4.66150600	4.46504300
H	-3.58487600	-0.82967900	5.87918800
H	-3.47165700	-2.51830800	5.35493200
H	-2.20927900	-1.82556500	6.38726000
C	-2.88737300	-1.61223800	5.55664100

NBZ-FeIII-O-C2-concerted-TS-model1:

C	-3.72403100	2.22846000	0.18992300
N	-2.64587700	3.10209600	0.21576800
H	-2.70169500	4.09974600	0.38811900
C	-1.51556300	2.41780500	-0.03685400
H	-0.53156100	2.85622100	-0.08655800
N	-1.80175600	1.13217900	-0.22365500
C	-3.17512300	1.00450600	-0.08803900
H	-3.66524900	0.05193100	-0.21470000
C	-0.33632900	-1.73038800	3.25870700
N	0.13004700	-2.83339100	2.56048200
H	0.41251400	-3.71588300	2.97242300
C	0.16272600	-2.54633700	1.24727300
H	0.48645400	-3.22679500	0.47581000
N	-0.25985600	-1.29980700	1.04692500
C	-0.57426200	-0.78465200	2.29594900
H	-0.95600700	0.21704200	2.41670800
C	-1.36012100	-2.41761700	-1.93315200
O	-2.16022500	-1.52153100	-1.52737400
O	-0.10465000	-2.23944600	-1.72976900
C	2.48081300	2.96241000	1.07990900
C	2.68624300	2.41934600	-0.18019500
C	2.88784400	1.01652400	-0.34850100
C	2.97048300	0.23298700	0.83523400
H	2.31451200	4.02934900	1.19088700
H	2.67584300	3.04616500	-1.06544100
H	3.33642300	0.63765200	-1.25584900
O	1.12810400	0.63122800	-1.04082800
O	-0.07854600	0.47221100	-2.59823700
H	0.53529300	-0.12460000	-3.07050800
Fe	-0.45696500	-0.36116200	-0.83589700
C	-5.12953100	2.66656900	0.42898500
H	-5.24882800	3.11429600	1.42333300
H	-5.45079500	3.40895500	-0.31173200
H	-5.80257300	1.80783900	0.36089900
C	-0.49286900	-1.71345200	4.74210000
H	-1.19392900	-2.48505400	5.08257300
H	0.46397000	-1.88702200	5.24968500
H	-0.87687500	-0.74193200	5.06474100
C	-1.84000100	-3.65014300	-2.64359500

H	-1.46410200	-3.64237000	-3.67334700
H	-1.43573100	-4.54291100	-2.15470600
H	-2.93068300	-3.69235900	-2.65585900
C	2.51461700	2.13906100	2.21509000
H	2.36358200	2.56613400	3.20152700
C	2.76156700	0.76337700	2.09560800
H	2.81615600	0.12639700	2.96917600
N	3.30729500	-1.18713500	0.70280600
O	3.52897700	-1.61814100	-0.42889100
O	3.35871600	-1.86656000	1.72962800

NBZ-FeIII-O1-C2-concerted-TS-model1:

Fe	0.91550000	-0.55014500	-0.14643800
O	0.22969500	-0.83040200	-1.74139700
O	-1.36247800	-0.36578600	-0.53105300
H	-1.58647500	-1.21961400	-0.96474200
C	-2.71144200	-0.30148600	0.58835400
N	-4.17903500	-1.52739900	-0.99342500
O	-3.28455200	-2.38402800	-1.06114700
C	-3.85126000	-0.28705000	-0.29655700
O	-5.30112900	-1.65353700	-1.46987200
C	-4.58013700	0.84935700	-0.56087600
C	-4.24380600	2.03168700	0.12281000
C	-3.19907200	2.05911900	1.06294300
C	-2.46864500	0.91674000	1.32233500
H	-4.80981900	2.93513100	-0.08160500
H	-2.98183600	2.97842400	1.59692500
H	-1.66043300	0.90746800	2.04563700
H	-2.50418500	-1.23384000	1.10670200
C	1.95333400	4.94548100	1.18047600
C	1.57512300	3.67733200	0.49135100
C	1.57520800	2.36850300	0.89963400
N	1.11070700	3.63807500	-0.81555000
C	0.85075300	2.35962000	-1.15316200
N	1.12741900	1.55849600	-0.13053800
H	2.26727500	4.73219000	2.20573500
H	1.11262700	5.64903700	1.22221400
H	2.78270000	5.45056500	0.67017500
H	0.98397900	4.44159500	-1.42053500
H	1.85709000	1.95701100	1.85707900
H	0.47559000	2.04198600	-2.11357400
C	6.46181800	-0.57835000	-1.60858600
C	5.12602500	-0.89993700	-1.02485700
C	3.94344500	-0.20811800	-0.99055000
N	4.85845800	-2.08498100	-0.35610300
C	3.57419400	-2.08592500	0.04858000
N	2.98578600	-0.95214300	-0.31932300
H	6.42814600	0.39856400	-2.09806100
H	6.76256800	-1.32258300	-2.35592900

H	7.24155300	-0.54632000	-0.83759300
H	5.52201800	-2.83523300	-0.19888000
H	3.72218400	0.76557300	-1.39942200
H	3.09400600	-2.89252200	0.57957000
C	0.03212800	-2.48520700	3.26856700
C	0.37678100	-1.72044700	2.01834400
O	0.39152800	-0.44970200	1.99766200
O	0.65560600	-2.35136800	0.94099300
H	-0.82532700	-3.13925500	3.07447300
H	-0.19747000	-1.80812500	4.09345700
H	0.87328400	-3.13018700	3.54630900
H	-5.39456200	0.82991400	-1.27526600

NBZ-FeIII-O-C1-TS-modell1:

C	-31.15922200	10.94849400	7.89056300
N	-31.58554200	10.45160900	6.66965200
H	-32.44255600	9.93416200	6.50998000
C	-30.67499600	10.75800500	5.72397900
H	-30.76458600	10.46524600	4.68848200
N	-29.67086500	11.43749300	6.26637700
C	-29.96593700	11.56163300	7.61605800
H	-29.29998400	12.07315100	8.29563000
C	-27.75373800	15.86597400	7.35638700
N	-26.40580000	15.58788900	7.18924400
H	-25.64166700	16.18015500	7.49450900
C	-26.27175700	14.40633600	6.55860100
H	-25.32902000	13.94634900	6.30455200
N	-27.47178000	13.89378500	6.30208500
C	-28.40180600	14.79829500	6.79157800
H	-29.46336000	14.61469900	6.71519200
C	-25.62916800	10.66898800	5.97320900
O	-26.78591000	10.41612800	6.46275900
O	-25.49267000	11.61329400	5.13583700
C	-27.85728300	9.73606000	0.90138100
C	-27.02880900	9.78231400	-0.19890100
C	-27.14543400	10.82169500	-1.14323000
C	-28.13125400	11.81868300	-0.98683300
C	-28.97493900	11.80754400	0.10039600
C	-28.77691200	10.82027500	1.13252400
N	-29.98340400	10.50103900	1.97295400
O	-30.90652200	11.30832000	1.98161500
O	-29.95213000	9.46581900	2.63557400
H	-27.80749800	8.92918500	1.62101800
H	-26.29821100	8.99412300	-0.35159600
H	-26.49284400	10.83966200	-2.01030500
H	-28.24523100	12.58773300	-1.74447500
H	-29.75900300	12.54339700	0.22705000
O	-28.04073000	11.85080400	2.40863500
O	-27.55658300	11.05010500	3.49113600

H	-26.57843700	11.09138000	3.39825600
H	-24.22231500	10.11198900	7.47371800
H	-24.71167200	8.78405100	6.42068900
H	-23.57646900	10.03221400	5.81475600
Fe	-27.76353900	11.96868800	5.53730300
C	-24.45601000	9.84800300	6.43499700
C	-28.24600000	17.09400400	8.04400200
H	-27.89045100	17.14283100	9.08048700
H	-27.91063300	18.00486100	7.53307400
H	-29.33921600	17.09855300	8.06007600
H	-32.92644900	11.18198100	9.09903700
H	-32.01232100	9.69975900	9.41740700
H	-31.39103500	11.26027900	9.98113800
C	-31.91499600	10.76200000	9.16099600

NBZ-FeIII-O-C2-TS-modell1:

C	-31.18364900	11.06046900	7.89743600
N	-31.78611300	11.09447300	6.65015800
H	-32.76939600	10.93030400	6.46603400
C	-30.85213100	11.38155500	5.71852000
H	-31.05880600	11.46242600	4.66246400
N	-29.66724300	11.53758800	6.29475100
C	-29.86538400	11.33980600	7.65183200
H	-29.05036500	11.40376000	8.35823400
C	-27.74497900	15.89804900	7.31058500
N	-26.41336500	15.72828300	6.96369600
H	-25.66732800	16.38896100	7.15079100
C	-26.26578500	14.54692000	6.33638900
H	-25.33114800	14.15276300	5.96983300
N	-27.44158900	13.93201700	6.25358200
C	-28.37005800	14.76781300	6.85492200
H	-29.41285500	14.49735400	6.92677400
C	-25.60622400	10.68949400	5.95391400
O	-26.80702100	10.29989700	6.23165700
O	-25.43290600	11.76393400	5.32394200
C	-30.56024000	12.10366300	1.22093300
C	-30.69431300	10.74962600	0.86657600
C	-29.56700400	9.99074900	0.49754700
C	-28.30867000	10.56379700	0.49897200
C	-28.11921500	11.90882100	0.96434000
C	-29.30314400	12.67308000	1.22213800
N	-29.14984600	14.07916400	1.57593200
O	-28.01702400	14.56383300	1.52222500
O	-30.15773900	14.70591400	1.91442200
H	-31.42711600	12.70478400	1.46767700
H	-31.68127600	10.29855200	0.85549400
H	-29.69396600	8.95835400	0.18634900
H	-27.43488200	9.99670200	0.19551200
H	-27.22111700	12.44451900	0.67805800

O	-27.36612600	11.63370000	2.65281200
O	-28.32532900	11.09573500	3.55248100
H	-28.15393300	10.13026000	3.52575100
H	-23.50347500	10.23813800	6.07095000
H	-24.45080200	9.83914900	7.53154100
H	-24.58399100	8.81183800	6.10409600
Fe	-27.71959500	11.98061700	5.55844300
C	-24.45600500	9.84800300	6.43499900
C	-28.24600000	17.09400100	8.04400100
H	-27.74975300	17.20546800	9.01600900
H	-28.07664300	18.01741100	7.47659300
H	-29.32063900	16.99948000	8.22180500
H	-32.72129800	11.48261500	9.34528300
H	-32.36336400	9.76101100	9.14284900
H	-31.22261700	10.80542600	10.00612600
C	-31.91499900	10.76200000	9.16099800

NBZ-FeV-O-C1-TS-modell1:

C	-31.10365400	11.13534200	7.96296800
N	-31.61168400	11.07928700	6.67539700
H	-32.55652700	10.80843600	6.42734000
C	-30.64678300	11.43823400	5.80397800
H	-30.77526100	11.46253700	4.73366800
N	-29.53324100	11.73666400	6.45896800
C	-29.80382300	11.55027800	7.80434200
H	-29.05231900	11.72229800	8.56063000
C	-27.70482400	15.77963600	7.57115000
N	-26.35334300	15.46126100	7.61661600
H	-25.61850200	16.05938600	7.97803900
C	-26.16284500	14.23641100	7.09750700
H	-25.20334400	13.76059100	6.97717500
N	-27.33229300	13.72211500	6.72349100
C	-28.29900100	14.67813800	7.01251600
H	-29.34077000	14.51118800	6.78953100
C	-25.51897800	10.87086800	6.11558100
O	-26.72043900	10.68948200	6.56422400
O	-25.30312700	11.87007400	5.38439400
C	-29.12261900	12.95299300	1.89995700
C	-29.13156400	11.67437200	1.38853600
C	-27.91840900	10.98590500	1.18669600
C	-26.68022900	11.59777600	1.46503200
C	-26.64062800	12.87421500	1.98007300
C	-27.87243000	13.52963500	2.27300900
N	-27.83151100	15.01020900	2.47229300
O	-26.72924200	15.53338800	2.59351600
O	-28.90366300	15.60536800	2.49691900
H	-30.02996100	13.52485900	2.04682400
H	-30.07194400	11.20055900	1.12643400
H	-27.93704400	9.98043100	0.77741100

H	-25.75615800	11.06580600	1.26424600
H	-25.70931000	13.38405900	2.19074700
O	-27.98811700	13.33554200	4.24209700
O	-27.91914700	10.81271300	4.26698800
H	-27.75293900	9.98709700	4.76357000
H	-23.46876000	10.22282900	6.15862700
H	-24.48024600	9.59040700	7.49828300
H	-24.66769700	8.93398200	5.86719800
Fe	-27.61720600	12.12686100	5.44995500
C	-24.45600800	9.84800700	6.43499900
C	-28.24600000	17.09400000	8.04400100
H	-28.04884600	17.24987400	9.11151700
H	-27.79453400	17.92769400	7.49323600
H	-29.32725600	17.12779200	7.88707200
H	-32.81737400	11.37939800	9.24742100
H	-32.23186800	9.71271200	9.11760200
H	-31.32391000	10.89813400	10.07062000
C	-31.91499500	10.76200000	9.16099500

NBZ-FeV-O-C2-TS-modell1:

C	-2.12422400	-1.14352300	4.36198100
N	-2.74760300	-0.59365800	3.25220400
H	-3.74767800	-0.46894600	3.14160700
C	-1.81358400	-0.25508500	2.34263200
H	-2.02463700	0.19845800	1.38644500
N	-0.60516200	-0.55600300	2.80578500
C	-0.78546500	-1.11461800	4.05988600
H	0.05271200	-1.45584100	4.64824600
C	1.35410100	3.50333100	3.64311400
N	2.66114300	3.35172700	3.19780800
H	3.39601700	4.04654300	3.27532900
C	2.80969200	2.13304900	2.65157200
H	3.72003100	1.75642600	2.21363600
N	1.65682700	1.46964500	2.72503100
C	0.74430900	2.31508600	3.33819000
H	-0.27542300	2.01718300	3.51714000
C	3.36745800	-1.35994000	2.49421000
O	2.26340100	-1.38808900	3.14174600
O	3.44048000	-0.61118800	1.47025700
C	-0.71148000	2.58676100	-2.17279100
C	-1.96342600	1.95242800	-2.04944400
C	-2.04956600	0.60672400	-1.66900200
C	-0.89548300	-0.11400500	-1.38711500
C	0.38168200	0.51410600	-1.44915700
C	0.42970700	1.86002900	-1.90719200
N	1.74047600	2.49360400	-2.05297900
O	2.73657200	1.79710700	-1.84924900
O	1.77510200	3.68252300	-2.37160900
H	-0.63897000	3.62103300	-2.48619700

H	-2.86470200	2.51705400	-2.26583900
H	-3.01993800	0.12431300	-1.60696200
H	-0.94070800	-1.15479600	-1.08792300
H	1.28241200	-0.08038200	-1.48460300
O	0.66849700	0.85461100	0.50596300
O	1.05114000	-1.70779300	0.65730500
H	1.85499400	-1.81310300	0.11190000
H	5.46676500	-1.81184700	2.58287700
H	4.51017000	-2.45284700	3.96140400
H	4.39645200	-3.21203000	2.36164100
Fe	1.23304800	-0.27933500	1.72357100
C	4.51604400	-2.25594500	2.88653900
C	0.84391400	4.75724800	4.27997300
H	1.39198100	4.99557400	5.19938900
H	0.93984100	5.61364900	3.60177300
H	-0.21280500	4.63997700	4.53374600
H	-3.45527200	-0.79440800	6.01676100
H	-3.59715400	-2.40601300	5.29364700
H	-2.19828000	-2.01020100	6.30635000
C	-2.88737300	-1.61223800	5.55664100

NBZ-FeV-O1-C2-TS-modell1:

C	-31.09526800	11.17369800	7.98385400
N	-31.64832300	11.78628300	6.86830100
H	-32.63132600	12.00304900	6.74435100
C	-30.67383700	12.06068700	5.98284400
H	-30.82301400	12.55242100	5.03415700
N	-29.50342600	11.65172900	6.46731700
C	-29.75326100	11.09401300	7.71017100
H	-28.95783500	10.68284100	8.31299100
C	-27.67196200	15.80435400	7.54310800
N	-26.32682100	15.47888800	7.63332300
H	-25.60148000	16.06701800	8.02777100
C	-26.12913100	14.25464800	7.10233600
H	-25.16722000	13.77218700	7.02936200
N	-27.28199800	13.75912100	6.67316100
C	-28.24732900	14.71763900	6.93608100
H	-29.28192600	14.56820600	6.67140500
C	-25.59485100	10.79845300	6.17660900
O	-26.63000800	10.82062700	6.92808400
O	-25.59911400	11.57521400	5.16333300
H	-24.74737200	8.85109000	6.08202300
H	-23.55891800	10.16644200	5.89989200
H	-24.25551600	9.77557900	7.50790400
C	-24.45600700	9.84800700	6.43500100
C	-28.24599800	17.09399600	8.04400000
H	-28.08633300	17.21293400	9.12254500
H	-27.79243300	17.95671100	7.54138700
H	-29.32234900	17.11721700	7.85383700

H	-32.41227600	11.62355800	9.62295700
H	-32.69138100	10.04089800	8.87814500
H	-31.27636700	10.29443400	9.91504500
C	-31.91499800	10.76200100	9.16099800
Fe	-27.64351100	11.98395200	5.57940900
O	-28.26984100	12.83158300	4.34564600
C	-26.94711000	9.89683400	2.73652900
C	-26.99351000	8.47300600	2.80369000
C	-27.79239700	10.53328500	1.78883900
H	-26.12413500	10.44830700	3.17180100
C	-27.90533900	7.75828700	2.04114300
H	-26.32421000	7.96553400	3.48947300
C	-28.71990200	9.83343200	1.04181000
N	-27.63511700	11.97506700	1.55529100
C	-28.77700800	8.43326600	1.17369100
H	-27.94484800	6.67623700	2.11224800
H	-29.36405200	10.35461600	0.34395900
O	-26.57467500	12.48929000	1.90167400
O	-28.55854700	12.56716100	0.99788600
H	-29.49482800	7.87611000	0.58017500
O	-27.93400300	10.10949800	4.59814100
H	-28.84258100	10.11983600	4.23792500

Nitrobenzene FeV attack Model 1 B97D

NBZ-FeV-RC-model1-B97D:

C	-2.11660400	-1.11015300	4.37660500
N	-2.73685600	-0.53860500	3.26961300
H	-3.74026600	-0.41417400	3.15819200
C	-1.79796200	-0.19027800	2.36139100
H	-2.00210600	0.28080200	1.40755300
N	-0.58635800	-0.50804600	2.82903300
C	-0.76816300	-1.08068800	4.07655000
H	0.07163900	-1.44087200	4.65997400
C	1.30511700	3.54857500	3.52774100
N	2.36119000	3.58951700	2.62074900
H	2.91170200	4.41567500	2.39649200
C	2.54621700	2.36403000	2.09332300
H	3.28983900	2.10781700	1.34994900
N	1.65674100	1.50733900	2.63137100
C	0.88010500	2.22791900	3.51255200
H	0.08065100	1.76343900	4.07734100
C	3.39089000	-1.33251800	2.46888200
O	2.24777200	-1.41083100	3.07713400
O	3.50748700	-0.52902200	1.49432700
C	6.18913900	-0.76369900	-1.89184100
C	7.57919000	-0.91986400	-1.93914200
C	8.18307800	-2.05902700	-1.37638400
C	7.39675900	-3.05186400	-0.76400900

C	6.00457300	-2.91599300	-0.71065400
C	5.42180900	-1.76758500	-1.27562000
N	3.96498000	-1.60107800	-1.21797300
O	3.29445800	-2.53677300	-0.72392700
O	3.45807800	-0.56287600	-1.64665400
H	5.70283200	0.10962900	-2.32160000
H	8.19017200	-0.15274000	-2.41612400
H	9.26733300	-2.17401800	-1.41598400
H	7.86681100	-3.93427900	-0.32850700
H	5.38173400	-3.67486200	-0.24281100
O	0.63419200	0.67746300	0.45450000
O	1.00621400	-1.70957300	0.57837500
H	1.76887600	-1.84470800	-0.05708900
H	5.46679700	-1.92242900	2.45071900
H	4.58931900	-2.30189800	3.98335100
H	4.28161500	-3.26917300	2.52129200
Fe	1.22138100	-0.31122500	1.72138100
C	4.51604700	-2.25594900	2.88653900
C	0.84391200	4.75725300	4.27997300
H	1.63662800	5.13747400	4.94632800
H	0.57284000	5.56836700	3.58354900
H	-0.03516600	4.50492100	4.88828400
H	-3.47460600	-0.80434200	6.02479400
H	-3.58784100	-2.41230400	5.26381300
H	-2.19368500	-2.01719500	6.30669600
C	-2.88737300	-1.61223800	5.55664100

NBZ-FeV-O-C1-TS-modell1-B97D:

C	-31.06623900	10.93321500	7.94290900
N	-31.32308700	10.25457300	6.75622100
H	-32.09494600	9.60955000	6.60517900
C	-30.38708800	10.58817300	5.84065600
H	-30.33230800	10.19583900	4.83305600
N	-29.52922000	11.46393300	6.37758900
C	-29.93839100	11.68848600	7.67836300
H	-29.40839000	12.37074000	8.33294400
C	-27.82874100	15.71392100	7.62967000
N	-26.76314000	15.03315700	8.21422100
H	-26.18084500	15.39013500	8.96800400
C	-26.60388600	13.83432700	7.61224000
H	-25.84847200	13.10503000	7.87212000
N	-27.52672500	13.69826700	6.65274200
C	-28.29531200	14.85736200	6.65655700
H	-29.10146900	14.99623300	5.94782200
C	-25.24230200	11.04204500	5.90076700
O	-26.49743400	11.09399200	6.34477800
O	-24.77657000	11.86072600	5.10264800
C	-28.52154700	14.10023700	1.76351100
C	-28.40545700	13.12995300	0.78146000

C	-27.28322000	12.26293900	0.76008600
C	-26.25393400	12.38519600	1.72284400
C	-26.33297900	13.35318900	2.71163300
C	-27.51819300	14.16142000	2.79114700
N	-27.43106500	15.44033800	3.59434400
O	-26.37549100	15.66201700	4.19074700
O	-28.42080700	16.17558100	3.60096700
H	-29.35787200	14.79441300	1.79787300
H	-29.17141500	13.04582700	0.01020900
H	-27.20434400	11.50565500	-0.02103400
H	-25.38744300	11.72553200	1.68498000
H	-25.55877500	13.46658800	3.46459700
O	-28.51491200	13.24416100	4.19858400
O	-27.83152000	10.78925900	4.13118400
H	-27.38532900	10.02756000	4.56140400
H	-23.38125800	10.00578500	6.27225600
H	-24.66251500	9.67999200	7.50269100
H	-24.77450800	8.94500300	5.88715600
Fe	-27.78557700	12.14423400	5.35144400
C	-24.45600800	9.84800700	6.43499900
C	-28.24600000	17.09400000	8.04400100
H	-28.53637400	17.12323300	9.10743400
H	-27.42618800	17.81600300	7.89523200
H	-29.10457600	17.41435300	7.43782600
H	-32.96318800	11.04099200	8.96067500
H	-31.90653800	9.71450900	9.50675400
H	-31.53514700	11.39838400	9.97249400
C	-31.91499500	10.76200000	9.16099500

NBZ-FeV-O-C2-TS-model1-B97D:

C	-2.11967600	-1.09377800	4.38190300
N	-2.72852900	-0.40092600	3.33895500
H	-3.72103900	-0.18766100	3.27638300
C	-1.79317300	-0.06557400	2.42124500
H	-1.98631100	0.47884400	1.50488200
N	-0.59782500	-0.50979300	2.81958200
C	-0.78476900	-1.14941300	4.03353200
H	0.04375400	-1.60413500	4.56442500
C	1.33954800	3.52033800	3.59517400
N	2.54873400	3.47572800	2.90151400
H	3.20643300	4.24722400	2.81476500
C	2.71565600	2.24896800	2.36890600
H	3.55693100	1.93744000	1.76333900
N	1.66681700	1.47590400	2.69543300
C	0.80735700	2.25327000	3.45079500
H	-0.12393300	1.85758700	3.83619500
C	3.37341600	-1.35038000	2.46984400
O	2.25626900	-1.39211800	3.11281300
O	3.46962000	-0.59993900	1.44498800

C	-0.91921200	2.53225300	-2.12532400
C	-2.16527600	1.90190700	-1.90725400
C	-2.22925100	0.56022400	-1.47635000
C	-1.05533200	-0.15855900	-1.24617100
C	0.22069200	0.46863700	-1.40820200
C	0.24644400	1.80732000	-1.90843400
N	1.55835600	2.44702800	-2.11597400
O	2.57124400	1.76034200	-1.91641900
O	1.57671100	3.63348300	-2.47195300
H	-0.86591600	3.56372400	-2.46793000
H	-3.08235900	2.46440200	-2.08479900
H	-3.19880200	0.08178400	-1.33309800
H	-1.07888900	-1.19073100	-0.90205100
H	1.12047400	-0.13372800	-1.47729900
O	0.62519200	0.88531800	0.51935600
O	1.04073800	-1.72987200	0.61062900
H	1.78886700	-1.77409000	-0.02275600
H	5.47844100	-1.81824100	2.58764500
H	4.49501100	-2.44349500	3.96936700
H	4.39130400	-3.22014300	2.36526900
Fe	1.20444800	-0.28841600	1.70096100
C	4.51604400	-2.25594400	2.88653900
C	0.84391400	4.75724700	4.27997300
H	1.56583300	5.11433300	5.03320700
H	0.68542500	5.57173300	3.55311900
H	-0.11040600	4.54646200	4.78206500
H	-3.40847600	-0.79732200	6.08672400
H	-3.64550000	-2.35023900	5.24485800
H	-2.19978300	-2.10010900	6.26149300
C	-2.88737300	-1.61223800	5.55664100

NBZ-FeV-O1-C2-TS-modell1-B97D:

C	-31.10680400	11.17993000	7.97504400
N	-31.67040300	11.82669400	6.87861700
H	-32.65458100	12.06334100	6.77864600
C	-30.70040300	12.10069500	5.97817000
H	-30.85266600	12.61643600	5.03785400
N	-29.52509900	11.65862000	6.43857900
C	-29.76223800	11.08141400	7.67209600
H	-28.95850400	10.64709300	8.25603400
C	-27.77065900	15.71881400	7.68049800
N	-26.94378200	14.95747200	8.50430300
H	-26.55813500	15.26147300	9.39511200
C	-26.71476700	13.75722400	7.92514200
H	-26.11837900	12.96270000	8.35559600
N	-27.35624000	13.69982800	6.75368900
C	-28.00936500	14.91230400	6.58763800
H	-28.60143000	15.11142200	5.70209100
C	-25.57307500	10.82583700	6.15075700

O	-26.62737000	10.85847800	6.89352700
O	-25.53659200	11.59734000	5.13213900
H	-24.66955100	8.91402700	5.88759100
H	-23.49642800	10.24710800	6.07779700
H	-24.40472600	9.61531900	7.50800800
C	-24.45600700	9.84800800	6.43500100
C	-28.24599800	17.09399500	8.04400000
H	-28.82101800	17.08074800	8.98502100
H	-27.40061300	17.79035400	8.17416900
H	-28.89361200	17.48142000	7.24517900
H	-32.39616100	11.63020200	9.64227800
H	-32.71082300	10.05394200	8.87463600
H	-31.26508200	10.27212000	9.89944400
C	-31.91499800	10.76200100	9.16099800
Fe	-27.63555300	12.04526800	5.52943600
O	-28.25318000	12.95947300	4.31133600
C	-26.94298500	9.97510800	2.77965000
C	-27.12350300	8.54712000	2.76816400
C	-27.67376200	10.73959700	1.81192100
H	-26.06602200	10.41835400	3.24390500
C	-28.07790000	7.96155100	1.94316900
H	-26.53173900	7.94748400	3.45869900
C	-28.64851200	10.16381800	1.00700300
N	-27.34373600	12.17109600	1.63545900
C	-28.85427000	8.76605100	1.07771200
H	-28.22928700	6.88216200	1.95920700
H	-29.21240400	10.77711500	0.30662600
O	-26.22857200	12.54234200	2.01619900
O	-28.18458400	12.89091200	1.08470300
H	-29.60940500	8.30838400	0.43804400
O	-27.99706000	10.23311400	4.52569600
H	-28.87807400	10.35197200	4.10849500

2-nitrotoluene Model 1

2NT-FeIII-RC-modell1:

C	-4.3217370	-1.9786490	-1.6292390
N	-3.3836780	-1.7898340	-2.6344900
H	-3.5274550	-1.9867830	-3.6190570
C	-2.2420020	-1.3292800	-2.0960360
H	-1.3437090	-1.1090780	-2.6520140
N	-2.3895120	-1.1999930	-0.7796590
C	-3.6802230	-1.6057760	-0.4775730
H	-4.0459290	-1.6115220	0.5376590
C	-2.6373320	3.4471340	0.0975240
N	-1.2892150	3.7392320	0.2530750
H	-0.8834250	4.6689250	0.2364660
C	-0.5966920	2.6019730	0.4210120
H	0.4774660	2.5458200	0.5406090

N	-1.4362310	1.5651140	0.3848670
C	-2.7098330	2.0830150	0.1836800
H	-3.5759270	1.4426280	0.1119910
C	-0.9037500	-1.1651900	2.8489090
O	-1.8644750	-1.4914410	2.0785210
O	0.0262420	-0.4422040	2.3442530
C	4.0855370	-0.3636880	0.9462620
C	4.9803610	-1.4234920	1.0210330
C	5.7217140	-1.7720190	-0.1114160
C	5.5585400	-1.0651530	-1.3013600
C	4.6541920	0.0014660	-1.4270960
C	3.9247580	0.3265780	-0.2629020
N	2.9449590	1.4138390	-0.2520910
O	2.5381690	1.8714170	-1.3199380
O	2.5568570	1.8299270	0.8493860
H	3.5038950	-0.0585260	1.8070760
H	5.1034280	-1.9646710	1.9539180
H	6.4315570	-2.5931430	-0.0679310
H	6.1492060	-1.3397370	-2.1705870
O	0.5514340	-0.7199260	-0.5982600
O	0.6547970	-2.0575470	-0.0481200
H	1.3835640	-1.9458950	0.5991270
H	-0.8189690	-0.7263920	4.9309570
H	-1.7092110	-2.2266220	4.5309620
H	0.0774560	-2.1690880	4.4494590
Fe	-0.9459430	-0.4293150	0.4972180
C	-0.8472300	-1.6066430	4.2789850
C	-3.6744010	4.4974750	-0.1207940
H	-3.7123750	5.2051540	0.7161470
H	-3.4759210	5.0715330	-1.0339950
H	-4.6592490	4.0333760	-0.2185390
H	-6.2554000	-1.8313440	-2.5593960
H	-5.6676220	-3.4897640	-2.3531360
H	-6.2472200	-2.5757970	-0.9500820
C	-5.6952300	-2.4959330	-1.8903330
C	4.5491780	0.7058740	-2.7563480
H	3.5766080	0.5310120	-3.2273380
H	4.6599100	1.7901200	-2.6579130
H	5.3302890	0.3355110	-3.4265640

2NT-FeIII-O-C1-concerted-TS-modell1:

Fe	-0.6031240	-0.0270110	0.9391880
C	2.6340610	-1.2376610	-1.2646830
C	3.1246210	-2.5446740	-1.1721810
C	3.8391870	-2.9912800	-0.0634830
C	4.0922600	-2.1395100	1.0313220
C	3.6109250	-0.8548030	1.0056140
C	2.8088660	-0.4137620	-0.0953030
N	2.6656830	1.0630700	-0.1748500

O	2.6781690	1.6861220	0.8844850
O	2.5699340	1.5817770	-1.2847080
H	2.9630080	-3.2159170	-2.0098730
H	4.2226950	-4.0073500	-0.0521030
H	4.6756310	-2.4898210	1.8762240
H	3.7927420	-0.1591580	1.8149600
O	1.0779920	-0.8822310	0.6401110
O	-0.2082230	-1.6353540	1.9994130
H	0.4154450	-1.3883440	2.7089500
C	1.9499240	-0.8042250	-2.5267990
H	1.0762140	-0.1787470	-2.3369820
H	2.6340180	-0.2100240	-3.1445740
H	1.6481370	-1.6842250	-3.1025010
C	-5.0883620	-2.4456550	-1.7185780
C	-3.7300720	-2.0931300	-1.2086910
C	-3.2356510	-0.9850770	-0.5693150
N	-2.6466480	-2.9545630	-1.3082110
C	-1.5684930	-2.3767270	-0.7478530
N	-1.8910550	-1.1714300	-0.2896500
H	-5.7813760	-1.6210660	-1.5315760
H	-5.4820100	-3.3394350	-1.2192900
H	-5.0763750	-2.6431240	-2.7975150
H	-2.6662250	-3.8784280	-1.7253110
H	-3.7517020	-0.0815450	-0.2819280
H	-0.5968780	-2.8375900	-0.6654910
C	-0.6754850	3.5215230	-3.5993360
C	-0.5948400	2.9344170	-2.2254910
C	-0.8431220	1.6777240	-1.7352660
N	-0.1740930	3.6612660	-1.1212690
C	-0.1688150	2.8645250	-0.0380990
N	-0.5684680	1.6404960	-0.3737460
H	-1.0440050	2.7717220	-4.3044120
H	0.3094160	3.8597260	-3.9436250
H	-1.3553320	4.3814410	-3.6307070
H	0.1025660	4.6368620	-1.1287900
H	-1.2016550	0.8063190	-2.2616520
H	0.1400690	3.1691590	0.9491940
C	-1.8948290	1.5612350	4.3652030
C	-1.4921460	1.0837430	2.9948600
O	-2.3142430	0.5287760	2.2074570
O	-0.2652870	1.1728200	2.6172770
H	-1.3271710	2.4527000	4.6450020
H	-1.6611600	0.7695020	5.0882160
H	-2.9676720	1.7625030	4.4051890

2NT-FeIII-O-C2-concerted-TS-modell1:

O	-0.3158220	0.6303350	-1.6227110
O	0.9756040	2.1094830	-1.7295460
H	1.5115770	1.6582130	-2.4086890

Fe	0.7830840	0.9469400	-0.1231760
C	-3.3082480	-1.1813040	-0.4872410
C	-2.7620570	-2.3850080	-1.0042490
C	-1.8957980	-2.4154520	-2.0964560
C	-1.5575070	-1.2338420	-2.7453360
C	-2.0481370	0.0073330	-2.2592290
C	-2.9301150	-0.0099380	-1.1387680
N	-3.4318080	1.3028900	-0.7168740
O	-3.4578370	2.2009910	-1.5591340
O	-3.7860940	1.4420560	0.4546130
H	-3.0470440	-3.3168970	-0.5243880
H	-1.5163720	-3.3665270	-2.4566450
H	-0.9242400	-1.2352360	-3.6255800
H	-2.0743640	0.8733110	-2.9045650
C	-4.2697860	-1.2698410	0.6705380
H	-3.8083800	-0.9187460	1.5989330
H	-5.1615310	-0.6576030	0.5101770
H	-4.5808500	-2.3088920	0.8091710
C	5.9319730	-1.6107170	-0.3607780
C	4.5286060	-1.1751040	-0.6275530
C	3.6730610	-0.3372380	0.0425210
N	3.8074070	-1.6050930	-1.7309780
C	2.5845020	-1.0417130	-1.7077760
N	2.4673310	-0.2625720	-0.6356450
H	6.3093370	-1.1155160	0.5378050
H	6.5958290	-1.3541500	-1.1949790
H	5.9946910	-2.6944590	-0.2038400
H	4.1488900	-2.2344800	-2.4488520
H	3.8411660	0.2208150	0.9509440
H	1.8237630	-1.1997420	-2.4564160
C	-0.6408360	-3.7145920	2.9543220
C	-0.4264930	-2.3211990	2.4590400
C	0.2115880	-1.8194450	1.3540110
N	-0.9056260	-1.2012440	3.1236350
C	-0.5600920	-0.0956390	2.4379330
N	0.1191110	-0.4353390	1.3451540
H	-0.2041430	-4.4305090	2.2529720
H	-1.7085890	-3.9435030	3.0559800
H	-0.1722050	-3.8700760	3.9337410
H	-1.4129660	-1.2086020	4.0019060
H	0.7272740	-2.3569950	0.5735600
H	-0.8206230	0.9108240	2.7244480
C	1.1593920	4.3175910	1.9509110
C	1.0750330	2.9671070	1.2960380
O	2.1034130	2.2749940	1.0334100
O	-0.0684420	2.5003830	0.9325850
H	0.2979820	4.4830330	2.6034030
H	1.1372160	5.0824080	1.1640450
H	2.0914160	4.4204750	2.5110910

2NT-FeIII-O1-C2-concerted-TS-model1:

Fe	0.9337980	-0.5506180	-0.1208220
O	0.2729670	-0.8109190	-1.7492230
O	-1.3137250	-0.4266010	-0.5558430
H	-1.5718000	-1.3268680	-0.8548110
C	-2.7033020	-0.2918300	0.6514130
N	-4.1251790	-1.7650110	-0.6887520
O	-3.1466330	-2.5263820	-0.7936540
C	-3.8688510	-0.4228960	-0.1868500
O	-5.2729690	-2.0922830	-0.9740970
C	-4.6590000	0.6566050	-0.5677850
C	-4.3029140	1.9112500	-0.0109840
C	-3.2469260	2.0695950	0.8972130
C	-2.4718300	0.9850720	1.2588220
C	-5.8280060	0.5889140	-1.5154040
H	-4.8908740	2.7774800	-0.2998350
H	-3.0530860	3.0486570	1.3240930
H	-1.6527370	1.0724300	1.9632810
H	-2.4033110	-1.1715950	1.2113820
H	-6.0834380	1.5959740	-1.8555900
H	-5.6161150	-0.0344350	-2.3886840
H	-6.7077340	0.1607310	-1.0231280
C	1.9533340	4.9454810	1.1804760
C	1.5764880	3.6707860	0.5028730
C	1.5952940	2.3639300	0.9160350
N	1.0934610	3.6224430	-0.7973550
C	0.8401140	2.3422100	-1.1280130
N	1.1401180	1.5469130	-0.1058220
H	2.2800600	4.7404000	2.2033540
H	1.1077270	5.6426490	1.2272010
H	2.7732860	5.4530280	0.6576480
H	0.9486790	4.4232560	-1.4021220
H	1.8950130	1.9583770	1.8704770
H	0.4531360	2.0173350	-2.0812340
C	6.4618190	-0.5783500	-1.6085860
C	5.1310840	-0.8969390	-1.0111630
C	3.9508740	-0.2022120	-0.9635890
N	4.8670450	-2.0835840	-0.3434530
C	3.5878070	-2.0846670	0.0733440
N	2.9981370	-0.9475490	-0.2850050
H	6.4274950	0.4019900	-2.0910060
H	6.7490820	-1.3194330	-2.3641980
H	7.2502120	-0.5556590	-0.8462820
H	5.5307410	-2.8355590	-0.1942260
H	3.7276230	0.7731420	-1.3670680
H	3.1114450	-2.8929230	0.6050360
C	0.0321280	-2.4852070	3.2685670
C	0.3956010	-1.7214130	2.0256140
O	0.4233330	-0.4513680	2.0019650

O	0.6784650	-2.3488740	0.9445310
H	-0.8248800	-3.1358110	3.0618260
H	-0.2055950	-1.8068540	4.0899070
H	0.8674510	-3.1332950	3.5567150

2NT-FeV-RC-modell1:

C	-4.8730080	-2.3187430	-0.6453820
N	-4.2230510	-2.3881570	-1.8684060
H	-4.5747680	-2.8592720	-2.6945730
C	-3.0486920	-1.7358010	-1.7852310
H	-2.3456440	-1.6403270	-2.5977960
N	-2.8973470	-1.2402260	-0.5611470
C	-4.0239400	-1.6017070	0.1597650
H	-4.1422190	-1.3273550	1.1971420
C	-3.3353690	3.3405950	-0.1876730
N	-2.3543120	3.6931970	0.7285180
H	-2.2304810	4.6149490	1.1332810
C	-1.5862710	2.6250040	0.9995030
H	-0.7371280	2.6218110	1.6633830
N	-2.0331780	1.5763000	0.3105280
C	-3.1162940	2.0126590	-0.4397250
H	-3.6537850	1.3494920	-1.0975740
C	-0.4053370	-0.3127040	2.4888810
O	-1.4829900	-0.8152170	1.9858510
O	0.3108800	0.4076310	1.7388300
C	5.5580940	0.5021790	-1.1353820
C	6.9143270	0.5660820	-0.7802030
C	7.4480760	-0.1705910	0.2753910
C	6.6290110	-1.0146290	1.0306990
C	5.2808790	-1.1087770	0.7183590
C	4.7590230	-0.3606570	-0.3477930
N	3.3334660	-0.5149480	-0.6055670
O	2.6890930	-1.2832300	0.1401530
O	2.8023040	0.0967380	-1.5271960
H	7.5631270	1.2180430	-1.3573760
H	8.5056110	-0.0852960	0.5082170
H	7.0356690	-1.5929800	1.8540350
H	4.6224920	-1.7533050	1.2857160
O	-0.6188200	0.3121740	-1.4104400
O	0.0123850	-1.5666020	-0.2927320
H	0.9816940	-1.3180430	-0.2328920
H	0.7240690	0.0744500	4.2707780
H	-0.8910460	-0.6572100	4.5539780
H	0.4302510	-1.6457300	3.9132900
Fe	-1.1323100	-0.2331760	0.1156240
C	-0.0127120	-0.6421620	3.9026350
C	-4.3408010	4.3086470	-0.7199570
H	-4.9546950	4.7337170	0.0830730
H	-3.8523140	5.1386870	-1.2444220

H	-5.0049020	3.8036780	-1.4262640
H	-6.9727210	-2.5054460	-1.0764100
H	-6.1890230	-4.0205020	-0.5971340
H	-6.5273990	-2.7755820	0.6182440
C	-6.2119390	-2.9390470	-0.4157370
C	5.0808850	1.3374170	-2.2963560
H	4.6485110	0.7211300	-3.0907740
H	4.3040470	2.0475840	-1.9952650
H	5.9232680	1.8983770	-2.7108630

2NT-FeV-O-C1-TS-modell:

Fe	-0.6072900	-0.7420830	0.4838240
C	3.4652540	1.5632270	0.1005230
C	3.1893140	2.3301100	-1.0365430
C	2.7252770	1.7265640	-2.2175830
C	2.5624220	0.3591000	-2.2555450
C	2.7934490	-0.4162040	-1.0818070
C	3.3002250	0.1785210	0.1257230
H	3.3498420	3.4037030	-1.0059920
H	2.5191140	2.3241500	-3.0992950
H	2.2439430	-0.1505440	-3.1556040
O	0.8689130	-0.7148620	-0.5979970
O	-0.2117450	-2.5170680	-0.2149420
H	0.6506610	-2.8248940	0.1306310
N	2.9601280	-1.8795300	-1.3111370
O	2.8488800	-2.6474470	-0.3558470
O	3.2150010	-2.2352890	-2.4580440
C	3.6249870	-0.5923360	1.3712960
H	2.7205790	-1.0407030	1.7979590
H	4.3254060	-1.4114420	1.1792930
H	4.0665050	0.0787360	2.1128510
H	3.8389760	2.0529890	0.9945860
C	-5.6884760	0.1051010	-2.0134310
H	-6.1543410	0.5405380	-1.1253620
H	-6.2504400	-0.7975800	-2.2825090
H	-5.7927450	0.8210910	-2.8379480
C	-4.2572800	-0.2074440	-1.7341920
N	-3.4161830	-0.7884100	-2.6723510
H	-3.6778480	-1.0564820	-3.6145670
C	-2.1957800	-0.9529830	-2.1296390
H	-1.3553540	-1.4022380	-2.6348250
N	-2.1961530	-0.5034410	-0.8795610
C	-3.4750460	-0.0382480	-0.6216560
H	-3.7445390	0.3737690	0.3390090
C	-0.5764380	4.9741550	0.1602930
H	-0.8120780	4.9844090	-0.9072920
H	0.3795000	5.4927180	0.3028120
H	-1.3491610	5.5501310	0.6839220
C	-0.5142060	3.5651830	0.6518880

N	-0.2057970	3.2328310	1.9628210
H	-0.0022660	3.8917960	2.7062700
C	-0.2241360	1.8927210	2.0969140
H	-0.0047420	1.3654500	3.0119300
N	-0.5379130	1.3287120	0.9356090
C	-0.7193970	2.3611700	0.0289590
H	-0.9828620	2.1686930	-0.9997930
C	-1.2336200	-2.2477660	4.1160480
H	-0.5363680	-1.8545860	4.8606690
H	-1.0286620	-3.3191260	3.9951410
H	-2.2648310	-2.1294900	4.4563960
C	-1.0298540	-1.5723060	2.7900300
O	-1.9959010	-1.3751250	1.9884810
O	0.1426650	-1.2188890	2.4079700

2NT-FeV-O-C2-TS-modell1:

C	-3.7854470	2.5623130	0.3352660
N	-2.5975850	3.2742490	0.4067060
H	-2.5154670	4.2573180	0.6405640
C	-1.5718650	2.4530470	0.1093540
H	-0.5355610	2.7515970	0.0885310
N	-2.0312980	1.2342340	-0.1497280
C	-3.4086260	1.2904280	-0.0177020
H	-4.0250240	0.4210180	-0.1894210
C	-0.7506090	-1.4503300	3.3334470
N	-0.2780910	-2.6081190	2.7291760
H	0.0724680	-3.4268760	3.2145920
C	-0.3481070	-2.4767590	1.3932730
H	-0.0310310	-3.2218470	0.6810570
N	-0.8577850	-1.2844140	1.0894580
C	-1.1112640	-0.6382180	2.2900320
H	-1.5307360	0.3535750	2.3220000
C	-1.8546520	-2.4603430	-1.8486950
O	-2.5173670	-1.4910850	-1.3392050
O	-0.5951380	-2.4774040	-1.6810510
C	3.9679090	1.4664260	0.2557020
C	3.5230820	2.7938510	0.0002070
C	2.5202420	3.0959640	-0.9234250
C	1.9068410	2.0758370	-1.6373220
C	2.2931280	0.7288720	-1.4043820
C	3.3494110	0.4642440	-0.4872590
N	3.7045280	-0.9493000	-0.3381270
O	3.3933500	-1.7152050	-1.2532230
O	4.2785560	-1.3067670	0.6914750
H	3.9994270	3.5992560	0.5506500
H	2.2342070	4.1304970	-1.0859060
H	1.1224120	2.2718870	-2.3590550
H	2.0318530	-0.0391360	-2.1159280
O	0.7432070	0.1372790	-0.2423910

O	-0.5831440	0.1575310	-2.4675500
H	-0.1532030	-0.5448980	-2.9931860
H	-1.9773980	-4.4380340	-2.6829540
H	-3.5674420	-3.6685530	-2.3582330
H	-2.5775900	-3.1332790	-3.7291540
Fe	-0.8215640	-0.4272920	-0.7885250
C	-2.5414720	-3.5027020	-2.6967070
C	-0.7790160	-1.2539470	4.8164730
H	-1.4057360	-2.0058160	5.3108740
H	0.2283210	-1.3238380	5.2441650
H	-1.1822880	-0.2657240	5.0519370
H	-5.1580290	3.5864270	1.6391170
H	-5.3234510	4.0125220	-0.0724390
H	-5.9060610	2.4437520	0.5098820
C	-5.1119570	3.1873390	0.6184590
C	5.0665870	1.2656970	1.2654450
H	4.6831030	0.7786750	2.1681900
H	5.8660880	0.6265590	0.8801960
H	5.4925820	2.2328580	1.5463240

2NT-FeV-O1-C2-TS-modell1:

C	-4.5135730	-3.8389890	0.6804990
C	-3.5008750	-2.8912570	0.1317930
C	-2.5920130	-2.0580420	0.7330330
N	-3.3141400	-2.6941100	-1.2288210
C	-2.3376060	-1.7845370	-1.4125670
N	-1.8804920	-1.3747620	-0.2366310
H	-4.4870990	-3.8214640	1.7733980
H	-4.3204330	-4.8683480	0.3539780
H	-5.5289640	-3.5735470	0.3612220
H	-3.8277280	-3.1602930	-1.9682780
H	-2.4006530	-1.9047210	1.7842920
H	-1.9889850	-1.4420220	-2.3741690
C	-4.4765400	3.7393020	-1.2713350
C	-3.4582860	2.9434950	-0.5101130
C	-2.4065360	2.1630770	-0.9172180
N	-3.4506500	2.8387020	0.8749770
C	-2.4474160	2.0231230	1.2557410
N	-1.7894730	1.5910410	0.1854970
H	-4.2524820	3.6988330	-2.3405440
H	-4.4778890	4.7914480	-0.9627740
H	-5.4878350	3.3433720	-1.1187600
H	-4.0965440	3.3004680	1.5055710
H	-2.0562370	1.9610400	-1.9173830
H	-2.2311260	1.7561800	2.2783970
C	1.4374550	0.5157490	3.5657210
C	0.7343550	0.4824850	2.2328160
O	-0.3370370	-0.2120000	2.0684540
O	1.2037910	1.0728470	1.2121490

H	1.9201960	1.4852280	3.7148170
H	2.2163990	-0.2557110	3.5642320
H	0.7392720	0.3066500	4.3796280
Fe	-0.3648540	0.0629380	0.0463460
O	-0.1630690	0.4033870	-1.5304500
O	0.9150610	-1.5539450	-0.0479890
H	1.4548410	-1.6227890	0.7702210
C	2.8632830	-1.5220040	-1.0863520
N	3.8573960	-0.5749840	0.9251240
O	3.2549800	-1.4500250	1.5762100
C	3.4698360	-0.3966360	-0.4686000
O	4.7488280	0.1191490	1.3984110
C	3.6413280	0.8243760	-1.1226360
C	3.2015750	0.8666170	-2.4691740
C	2.6392080	-0.2359220	-3.1202520
C	2.4766300	-1.4341860	-2.4418600
C	4.2092840	2.0703370	-0.5003760
H	3.3089190	1.8038470	-3.0071730
H	2.3383810	-0.1475910	-4.1593090
H	2.0608110	-2.3086810	-2.9301630
H	2.9531080	-2.4930620	-0.6188160
H	4.0181450	2.9275030	-1.1513280
H	3.7619490	2.2654040	0.4786590
H	5.2905790	1.9834410	-0.3507020

Fe^{III}-OOH and HO-Fe^V=O attacks Model 2

Nitrobenzene Model 2

NBZ-FeIII-RC-model2:

C	-2.12962700	-1.26313600	4.32162200
N	-2.73799400	-1.05846200	3.09057400
H	-3.73246200	-1.13470400	2.90612800
C	-1.80126300	-0.75898800	2.17516000
H	-1.99977400	-0.55994500	1.13368100
N	-0.60081800	-0.75564500	2.75175500
C	-0.79432600	-1.07308700	4.08744700
H	0.03314200	-1.14959600	4.77629800
C	1.29899000	3.54574000	3.54124000
N	2.55007900	3.44462900	2.94852500
H	3.26126200	4.16823400	2.94814200
C	2.67767000	2.23831500	2.37549400
H	3.55331400	1.89202000	1.84895500
N	1.55982200	1.53635900	2.56468600
C	0.69420000	2.34452800	3.28896400
H	-0.28718300	2.00661400	3.58296100
C	-0.36525000	5.89828200	-2.99099000
H	-1.19820500	5.64100600	-2.32224400
H	-0.40918500	5.17146100	-3.81323800

C	0.93942600	5.68123600	-2.22297400
O	1.72324700	6.59285100	-1.96460000
N	1.15563600	4.39773300	-1.81936500
H	2.04632400	4.17969400	-1.39155200
H	0.57990500	3.62234600	-2.13167000
C	3.25770300	-1.56287700	2.46492900
O	2.14521200	-1.78263500	3.04614500
O	3.25758800	-0.70584900	1.51124700
C	-3.31140000	0.24704900	-2.17133400
C	-4.07572900	-0.84156800	-2.58404200
C	-3.59716900	-1.69896900	-3.58052900
C	-2.35173300	-1.46945800	-4.17403700
C	-1.57554900	-0.38271500	-3.77748800
C	-2.07001900	0.45586600	-2.77680400
N	-1.26546900	1.59891200	-2.34911500
O	-0.21798500	1.83574600	-2.96412500
O	-1.66624000	2.28043400	-1.40513600
H	-3.66388000	0.92938800	-1.40752100
H	-5.04645700	-1.01754800	-2.13083300
H	-4.19796200	-2.54662500	-3.89694700
H	-1.98423600	-2.13594300	-4.94798600
H	-0.60987200	-0.18437600	-4.22554000
O	0.64602700	-0.32959200	0.04325400
O	0.89981800	-1.75781100	0.00836600
H	1.76859100	-1.79387200	-0.44643400
H	5.18024400	-1.52761900	3.36738000
H	4.30002500	-3.06540600	3.58578300
H	5.03902000	-2.64484200	2.00704100
Fe	1.20599400	-0.34766400	1.83333400
C	4.51604300	-2.25594700	2.88654000
C	0.84391200	4.75725100	4.27997400
H	1.50261100	4.97763500	5.12881500
H	0.82765200	5.64115600	3.63121800
H	-0.16686700	4.60038400	4.66532900
C	-0.52137000	7.32214800	-3.52064200
H	-3.61315100	-0.83263400	5.81809100
H	-3.43748300	-2.55353100	5.43773400
H	-2.19569400	-1.72769300	6.39521600
H	-0.49338200	8.05234800	-2.70563400
H	0.28321800	7.57653300	-4.21857700
H	-1.47625600	7.43164100	-4.04710400
C	-2.88737100	-1.61223800	5.55663900

NBZ-RC-FeV-model2:

C	-0.00224100	0.00653000	-0.00289400
N	-0.00250000	-0.09991700	1.38070600
H	0.82263700	-0.18891300	1.96385300
C	-1.26929500	-0.08003300	1.82900700
H	-1.55079500	-0.14808400	2.86831100

N	-2.10565800	0.03646600	0.79985200
C	-1.32793100	0.08616600	-0.34679900
H	-1.77194300	0.17318800	-1.32674600
C	-3.98377800	4.23915100	0.91163900
N	-5.34609800	4.01951400	0.75332600
H	-6.05778900	4.74183600	0.71520200
C	-5.58509300	2.70312000	0.66668900
H	-6.55836900	2.25265100	0.55772600
N	-4.42732100	2.04274900	0.74573000
C	-3.42496400	2.98935100	0.90632500
H	-2.38840600	2.71041500	0.99944000
C	-6.07182800	3.37313000	8.47402900
H	-5.63780400	2.60459200	9.12523800
H	-7.15804200	3.20272600	8.48839700
C	-5.59784500	3.14776800	7.03691900
O	-5.36718400	4.07313900	6.25859400
N	-5.46001800	1.84190800	6.68231100
H	-5.25083900	1.62372300	5.71624100
H	-5.73495400	1.07755500	7.29051200
C	-5.72313500	-0.54856000	-0.90286200
O	-4.43678800	-0.41164800	-0.93510700
O	-6.31291200	-0.22618300	0.16603800
C	-7.14489100	-2.73319800	9.85002100
C	-7.48409900	-3.95134400	10.43355400
C	-7.21198000	-5.15083100	9.76742100
C	-6.59705800	-5.14049100	8.51100700
C	-6.25022800	-3.93240700	7.91174800
C	-6.53052100	-2.74701300	8.59554400
N	-6.16718900	-1.47696100	7.97214800
O	-5.62574800	-1.49435500	6.86592700
O	-6.42174100	-0.43210700	8.58642300
H	-7.34667700	-1.79316000	10.34852300
H	-7.96130600	-3.96337300	11.40840700
H	-7.47919400	-6.09666100	10.22968300
H	-6.38760900	-6.07324700	7.99661400
H	-5.77269700	-3.89909500	6.94030800
O	-4.30546500	0.37036000	2.64588800
O	-4.37845000	-1.65650700	1.61525900
H	-5.26955700	-1.79802800	1.99960700
H	-7.51592200	-0.92199600	-2.01660000
H	-6.03526000	-0.74475200	-3.01841800
H	-6.29590000	-2.22051200	-2.07588600
Fe	-4.21569800	0.04588700	0.97307100
C	-6.44723200	-1.13389100	-2.08313800
C	-3.38653500	5.60065900	1.06156500
H	-3.60381400	6.23254300	0.19226500
H	-3.77741900	6.10727900	1.95193100
H	-2.30152500	5.51968600	1.16408600
C	-5.75653100	4.77319000	8.99823400
H	1.89077800	0.88092400	-0.53413800

H	1.84482700	-0.88687500	-0.64909600
H	1.02293200	0.10121200	-1.86902700
H	-6.18536300	5.53904200	8.34506700
H	-6.16602100	4.90825200	10.00543500
H	-4.67539000	4.94645400	9.04603300
C	1.25805800	0.02659300	-0.80399600

NBZ-FeIII-O-C1-TS-model2:

C	-31.18661100	11.06679200	7.89610900
N	-31.79487400	11.12003100	6.65211500
H	-32.78065000	10.96758200	6.47093800
C	-30.86372000	11.40934800	5.71849500
H	-31.07725300	11.50766500	4.66503900
N	-29.67406000	11.54934200	6.29003900
C	-29.86720800	11.33750100	7.64618000
H	-29.04807700	11.38608400	8.34907300
C	-27.74306700	15.89993300	7.30984700
N	-26.40526700	15.71374200	6.99767700
H	-25.65573200	16.36261700	7.21075500
C	-26.25668600	14.53351000	6.36824900
H	-25.31803700	14.12843700	6.02427600
N	-27.43825400	13.93549400	6.25058400
C	-28.37153300	14.78098800	6.83042300
H	-29.41883300	14.52250900	6.87639100
C	-29.44450900	18.31017200	0.76126700
H	-30.31863900	17.75537500	0.39028300
H	-28.56355000	17.76678800	0.39739700
C	-29.48644300	18.24770100	2.28854400
O	-29.90320500	19.17389300	2.98151200
N	-29.03290600	17.08232800	2.82974800
H	-29.14773900	16.94186500	3.82560100
H	-28.78019700	16.27597200	2.26994200
C	-25.60582400	10.69151800	5.95361300
O	-26.80683100	10.30390300	6.23207800
O	-25.43255900	11.76573800	5.32211300
C	-29.30139000	11.24441600	0.82126800
C	-29.13147400	10.25079900	-0.11806500
C	-27.96737500	10.20327400	-0.91162400
C	-26.96937100	11.19007500	-0.77262300
C	-27.10426300	12.19909000	0.15359500
C	-28.22902500	12.17651400	1.05683500
N	-28.63822300	13.50124900	1.63722200
O	-27.90613000	14.46785000	1.42292800
O	-29.66721800	13.54138400	2.30274600
H	-30.20536600	11.32553900	1.41087500
H	-29.91708600	9.51713100	-0.26938500
H	-27.85274600	9.42110500	-1.65528000
H	-26.09815400	11.17194400	-1.41970200
H	-26.36332400	12.98127100	0.25955000

O	-27.38291700	11.63836400	2.55264400
O	-28.31661800	11.18109300	3.53882500
H	-28.25717300	10.20518300	3.46648900
H	-23.50280600	10.23843500	6.07306000
H	-24.45272200	9.83666600	7.53147000
H	-24.58449100	8.81291600	6.10102300
Fe	-27.72001400	11.98203300	5.55606300
C	-24.45601300	9.84800200	6.43499700
C	-28.24600000	17.09400900	8.04400600
H	-27.77577400	17.18444400	9.03096000
H	-28.04627600	18.02222100	7.49463200
H	-29.32653100	17.01457000	8.19049500
C	-29.46900000	19.74098900	0.22200200
H	-32.71056900	11.49095500	9.35841900
H	-32.37672200	9.76741000	9.13259200
H	-31.21711400	10.78591400	10.00234400
H	-28.57714400	20.29790500	0.53101000
H	-29.50422100	19.73853500	-0.87313400
H	-30.34337800	20.28128800	0.59624800
C	-31.91499200	10.76200000	9.16099200

NBZ-FeIII-O-C2-TS-model2:

C	-31.18389500	11.06320600	7.89720800
N	-31.78819600	11.10298500	6.65089200
H	-32.77219100	10.94147100	6.46801300
C	-30.85542200	11.39136800	5.71852700
H	-31.06420900	11.47701400	4.66309200
N	-29.66889600	11.54299900	6.29314400
C	-29.86533100	11.34074400	7.65008600
H	-29.04886200	11.40055300	8.35520000
C	-27.74312100	15.89764500	7.31381900
N	-26.40735900	15.71823200	6.98905800
H	-25.65904000	16.37053200	7.19587500
C	-26.25870000	14.53861000	6.35885500
H	-25.32119100	14.13681500	6.00822500
N	-27.43857200	13.93468000	6.25230500
C	-28.37016100	14.77536700	6.84171700
H	-29.41622700	14.51341900	6.89485300
C	-28.63881000	18.47166800	0.40929500
H	-29.27652200	17.60984400	0.64110500
H	-28.11986100	18.22256600	-0.52785300
C	-27.56507400	18.61577600	1.48795400
O	-27.11975200	19.70545100	1.84407600
N	-27.12541700	17.44068400	2.01724200
H	-26.33051200	17.46661200	2.64294500
H	-27.43252200	16.53523700	1.67861300
C	-25.60108400	10.69401700	5.94920400
O	-26.80556800	10.30134400	6.20958500
O	-25.42112700	11.77528200	5.33363700

C	-30.45352200	12.33258300	1.14642500
C	-30.75710900	10.98063600	0.91531100
C	-29.73671900	10.05816100	0.61047300
C	-28.41661100	10.46570200	0.56414200
C	-28.05640100	11.80961800	0.91500200
C	-29.13345800	12.73734500	1.09545500
N	-28.80721700	14.13775500	1.30103400
O	-27.61576500	14.46796800	1.22371300
O	-29.72245100	14.92828400	1.53946200
H	-31.23784500	13.05518100	1.33723100
H	-31.79238300	10.65674900	0.94410600
H	-29.99609300	9.02800800	0.38632200
H	-27.62383000	9.77003800	0.31015100
H	-27.09715100	12.19850900	0.59229300
O	-27.34686200	11.59910500	2.63539200
O	-28.33647400	11.13101300	3.53820600
H	-28.21816900	10.15692900	3.53014200
H	-23.50068200	10.23529800	6.07532100
H	-24.45538400	9.83978800	7.53162100
H	-24.58613100	8.81225600	6.10391500
Fe	-27.71820300	11.98496000	5.55794300
C	-24.45600500	9.84800300	6.43499900
C	-28.24600000	17.09400100	8.04400100
H	-27.76097700	17.19998900	9.02221200
H	-28.06438900	18.01790200	7.48119700
H	-29.32325000	17.00547700	8.20847600
C	-29.46900000	19.74099700	0.22200100
H	-32.71876600	11.48451200	9.34861900
H	-32.36636500	9.76248800	9.13911500
H	-31.22147000	10.80007500	10.00541100
H	-30.17704800	19.61999500	-0.60544700
H	-30.04227600	19.97896600	1.12539700
H	-28.82428200	20.59727200	0.00350200
C	-31.91499900	10.76200000	9.16099800

NBZ-FeV-O-C1-TS-model2:

C	-31.10562500	11.14635800	7.96530200
N	-31.63104300	11.15018400	6.68357300
H	-32.58676100	10.91705800	6.43868600
C	-30.66673700	11.50900000	5.81176600
H	-30.80970900	11.57528900	4.74503200
N	-29.53597500	11.75018200	6.46150800
C	-29.79532600	11.52585800	7.80349500
H	-29.02964400	11.64861500	8.55522700
C	-27.70431600	15.78479900	7.55619100
N	-26.35173700	15.46833100	7.59191700
H	-25.61659300	16.06383900	7.95731400
C	-26.16145400	14.24769200	7.06362000
H	-25.20220000	13.77254900	6.93878100

N	-27.33249500	13.73397600	6.69183000
C	-28.29944600	14.68628600	6.99245800
H	-29.34216300	14.51899900	6.77505700
C	-28.38048800	18.79277600	0.72173100
H	-28.81730100	17.88247700	1.14917000
H	-27.75428600	18.46658800	-0.12154600
C	-27.44777500	19.44542400	1.74151300
O	-27.25186400	20.65839600	1.78195400
N	-26.83725200	18.57864100	2.59682200
H	-26.11355300	18.93799000	3.20634100
H	-26.93153000	17.57302100	2.51149600
C	-25.52268000	10.86850200	6.12168700
O	-26.71778600	10.69701100	6.58990900
O	-25.31696700	11.85761800	5.37273600
C	-29.18278200	12.83069700	1.92171600
C	-29.20628900	11.53582100	1.45452800
C	-27.99974800	10.83703700	1.24787600
C	-26.75389500	11.45506000	1.47279900
C	-26.69830700	12.74827900	1.94136600
C	-27.92218300	13.41463700	2.24867700
N	-27.87911200	14.89995700	2.37856500
O	-26.77028000	15.43478400	2.38847800
O	-28.94457700	15.49813200	2.46103600
H	-30.08592500	13.40936700	2.06799600
H	-30.15352200	11.05663000	1.22970300
H	-28.03063400	9.81812900	0.87430900
H	-25.83602300	10.91428600	1.26756800
H	-25.75977800	13.26012100	2.11032900
O	-27.97455800	13.30996000	4.21153400
O	-27.92711100	10.78193200	4.29484300
H	-27.79033400	9.96401200	4.81303500
H	-23.47097000	10.22588100	6.15490300
H	-24.47533100	9.58707000	7.49741200
H	-24.66800900	8.93563000	5.86452100
Fe	-27.61772300	12.11714600	5.44991500
C	-24.45600800	9.84800600	6.43499900
C	-28.24600000	17.09400200	8.04400100
H	-28.04327000	17.23971300	9.11184300
H	-27.79970900	17.93411400	7.49892700
H	-29.32811800	17.12645500	7.89322800
C	-29.46899900	19.74099300	0.22200300
H	-32.78271200	11.42022300	9.29052000
H	-32.28593000	9.73303200	9.07855100
H	-31.30289400	10.82833500	10.06449100
H	-30.06719300	19.26284000	-0.56173900
H	-30.14576600	20.03245700	1.03352300
H	-29.02921200	20.65514800	-0.18731000
C	-31.91499500	10.76200000	9.16099400

NBZ-FeV-O-C2-TS-model2:

C	-2.12056000	-1.14415300	4.36558900
N	-2.74166300	-0.58995700	3.25701200
H	-3.74115900	-0.45926500	3.14759300
C	-1.80679500	-0.25425500	2.34822200
H	-2.01752200	0.19995000	1.39292200
N	-0.59955200	-0.56115400	2.81100400
C	-0.78165800	-1.12067700	4.06439100
H	0.05488200	-1.46600800	4.65266400
C	1.33013000	3.52261700	3.58329500
N	2.59905700	3.41667300	3.02751900
H	3.31428100	4.13563500	3.04822300
C	2.74342700	2.20550200	2.46445200
H	3.62933400	1.86216200	1.95441200
N	1.62449300	1.50092200	2.63074300
C	0.73814500	2.31312300	3.32421400
H	-0.25063600	1.97774400	3.59021400
C	0.76559700	6.63229600	-3.98169500
H	0.63434400	5.54620500	-4.01121600
H	1.00393200	6.95044400	-5.00587500
C	1.96543300	7.01310700	-3.11521200
O	2.19458300	8.17828500	-2.79445400
N	2.78006000	5.98247200	-2.75829900
H	3.57504900	6.18384800	-2.16474400
H	2.51881300	5.01292800	-2.89549200
C	3.38079500	-1.34314300	2.49042200
O	2.29154300	-1.32360200	3.16485400
O	3.44251400	-0.63883400	1.43552600
C	-1.08271000	2.04469400	-2.36482700
C	-2.24129400	1.27925200	-2.13361100
C	-2.14631600	-0.01930700	-1.61690000
C	-0.90530300	-0.55628300	-1.29807700
C	0.28343400	0.21481200	-1.45969600
C	0.14764200	1.49873300	-2.05961000
N	1.35639700	2.27014400	-2.31935500
O	2.43315800	1.81127700	-1.94520500
O	1.22880600	3.35184700	-2.90706300
H	-1.15057600	3.03858600	-2.78917700
H	-3.21078800	1.70330400	-2.37427900
H	-3.04554900	-0.61009100	-1.47329100
H	-0.81331000	-1.55519200	-0.88935700
H	1.24904500	-0.26912300	-1.47988100
O	0.60847700	0.74086200	0.44067900
O	1.07386800	-1.79582100	0.73466500
H	1.89413100	-1.92517200	0.21945600
H	5.47247200	-1.83514700	2.56767700
H	4.51660100	-2.43777300	3.96390100
H	4.37248800	-3.21586200	2.37477400
Fe	1.22530500	-0.30243100	1.71511900
C	4.51604500	-2.25594700	2.88653900

C	0.84391200	4.75725200	4.27997400
H	1.47680400	5.00600100	5.14020500
H	0.84188600	5.62025800	3.60363100
H	-0.17646500	4.60286100	4.64006200
C	-0.52137000	7.32215000	-3.52064200
H	-3.45405300	-0.79353900	6.01673300
H	-3.59902300	-2.40324900	5.29035200
H	-2.20188500	-2.01376600	6.30775300
H	-0.82441600	6.97664300	-2.52453800
H	-0.37647500	8.40549100	-3.47062700
H	-1.34367100	7.11460800	-4.21448700
C	-2.88737300	-1.61223800	5.55664100

NBZ-FeV-O1-C2-TS-model2:

C	-31.10569600	11.16609500	7.97271200
N	-31.66653700	11.78066900	6.86217500
H	-32.65023700	11.99582400	6.74319200
C	-30.69555800	12.05849400	5.97243000
H	-30.85254800	12.55486700	5.02778000
N	-29.52264100	11.65142800	6.44563900
C	-29.76540200	11.08840400	7.68674300
H	-28.96543900	10.67742000	8.28400900
C	-27.75139200	15.72193900	7.70753000
N	-26.90436700	14.98027900	8.52177000
H	-26.50324200	15.29348100	9.39904000
C	-26.67644800	13.78031400	7.95339200
H	-26.05789600	13.00712300	8.38204000
N	-27.33546800	13.70038400	6.80173300
C	-28.00002900	14.90595300	6.63686300
H	-28.60675000	15.09393700	5.76561700
C	-29.14572700	18.24921000	0.32215100
H	-30.05038800	17.66643600	0.54013300
H	-28.77406700	17.87642800	-0.64298800
C	-28.08531000	17.93213300	1.37848800
O	-27.41586200	18.80255600	1.93086600
N	-27.93768500	16.60822100	1.67133900
H	-27.16698900	16.32875400	2.26492500
H	-28.39053800	15.87048800	1.14695000
C	-25.56172700	10.83136900	6.11543500
O	-26.68940200	10.76058900	6.74012500
O	-25.44985200	11.69526000	5.20071900
H	-23.49362500	10.22875300	6.08653800
H	-24.42087300	9.64611800	7.50912100
H	-24.66668000	8.90058500	5.92337100
Fe	-27.65474100	12.09881500	5.54853300
C	-24.45600400	9.84800300	6.43500000
C	-28.24600000	17.09400100	8.04400000
H	-28.81301400	17.09602200	8.98272700
H	-27.41942300	17.80704100	8.15008100

H	-28.90243600	17.45248300	7.24696600
C	-29.46900000	19.74099900	0.22200000
H	-32.39703200	11.62883600	9.62955800
H	-32.70339900	10.04971300	8.88894400
H	-31.27215200	10.28711400	9.90699500
H	-30.19683400	19.92145000	-0.57695400
H	-29.89075100	20.12021600	1.15914600
H	-28.56816800	20.32316800	0.00595700
C	-31.91499900	10.76200000	9.16099800
C	-26.75971300	10.75710800	2.47184000
C	-26.61606600	9.34749600	2.29893800
C	-27.44222100	8.65657500	1.42380600
C	-28.39495900	9.35150000	0.66692000
C	-28.49898900	10.75639600	0.74775900
C	-27.66341200	11.43487000	1.60690400
N	-27.66728900	12.90072100	1.59505100
O	-28.64458300	13.46792700	1.09968100
O	-26.67911000	13.47624200	2.04332500
H	-26.01368900	11.32008300	3.01736500
H	-25.87025100	8.82585400	2.89062800
H	-27.34535400	7.58127800	1.31565100
H	-29.04630500	8.81457500	-0.01511100
H	-29.19674100	11.29678000	0.11932100
O	-28.28519700	13.11145700	4.44404900
O	-27.93878800	10.55958300	4.22092600
H	-27.54808900	9.75448000	4.61828600

Fe^{III}-OOH and HO-Fe^V=O attacks Model 3

Nitrobenzene Model 3

NBZ-FeIII-RC-model3:

C	-2.12518600	-1.23741800	4.33091300
N	-2.74039400	-0.92144500	3.12755000
H	-3.74048900	-0.92278100	2.95917400
C	-1.80105400	-0.62366300	2.21291100
H	-2.00300000	-0.34392400	1.19068700
N	-0.59332100	-0.72792500	2.76250200
C	-0.78398400	-1.11426100	4.08001200
H	0.04899400	-1.28294800	4.74538900
C	1.30527100	3.53579000	3.56477400
N	2.59759200	3.38654900	3.08348600
H	3.33534600	4.07891200	3.15408100
C	2.72221800	2.17861900	2.51046400
H	3.62404200	1.79495400	2.06050100
N	1.56480000	1.52449400	2.59255100
C	0.67439100	2.36414500	3.24483100

H	-0.34471600	2.06978200	3.44239700
C	0.07272500	5.91914700	-3.63701700
H	-0.42665800	5.36064100	-4.44144300
H	1.13253400	5.96576900	-3.92007500
C	-0.05804900	5.09764200	-2.35318900
O	-0.73218800	5.46312800	-1.39167400
N	0.63611400	3.92500000	-2.35188300
H	0.49245700	3.28510000	-1.58102700
H	1.10474000	3.56343500	-3.17498200
C	3.24831600	-1.59410200	2.43633800
O	2.10940200	-1.95585400	2.87199800
O	3.27862300	-0.62075800	1.60233500
C	3.40642800	1.07570500	-6.68958100
C	3.87579600	0.22982800	-7.69072900
C	3.51414600	-1.12144500	-7.69719000
C	2.68096700	-1.63861700	-6.69923200
C	2.21261400	-0.81193200	-5.68195300
C	2.58806600	0.53456100	-5.69450400
N	2.09578200	1.41198400	-4.64236100
O	1.61811200	0.90741600	-3.61412400
O	2.16100200	2.63046500	-4.81637100
H	3.67177000	2.12554200	-6.66618800
H	4.52260500	0.62648300	-8.46673700
H	3.87908700	-1.77331000	-8.48533000
H	2.39114800	-2.68440000	-6.71668000
H	1.55001600	-1.19020100	-4.91289300
O	0.51568000	-0.07198100	0.07377800
O	0.77808900	-1.48800900	-0.10065000
H	1.52645800	-1.46048400	-0.78091900
H	5.15679000	-1.51604100	3.37949000
H	4.30577500	-3.07765000	3.57312200
H	5.06269000	-2.63117400	2.01448600
Fe	1.21203500	-0.35945300	1.78941100
C	4.51604600	-2.25594800	2.88653900
C	0.84391200	4.75725200	4.27997300
H	1.40940000	4.91611800	5.20656800
H	0.95964500	5.65476600	3.66065800
H	-0.21333500	4.66019500	4.54031500
C	-0.52137000	7.32215000	-3.52064300
H	-3.57070400	-0.81216000	5.86623900
H	-3.48488200	-2.51805700	5.39731900
H	-2.19488700	-1.80475100	6.38038800
H	-0.42831400	7.85601600	-4.47310100
H	-1.58148800	7.27925800	-3.25222900
H	-0.00918700	7.90861000	-2.75025700
C	-2.88737300	-1.61223800	5.55664100
O	2.61954400	-1.29265800	-1.98985300
H	2.64686600	-2.07717300	-2.56358600
H	2.32029900	-0.56211200	-2.56744900

NBZ-FeV-RC-model3:

C	-2.10492700	-1.16622400	4.36462700
N	-2.71409800	-0.68033900	3.21760400
H	-3.71409000	-0.59097100	3.07546400
C	-1.76820500	-0.34508100	2.32032000
H	-1.97148300	0.06599000	1.34386900
N	-0.56367700	-0.58743600	2.82705200
C	-0.75985800	-1.10477700	4.09693900
H	0.07130700	-1.39480800	4.72176400
C	1.36917500	3.51108700	3.64612200
N	2.68421400	3.36404000	3.22676000
H	3.41412700	4.06269100	3.31704900
C	2.84785900	2.15026900	2.67625500
H	3.76635700	1.77661300	2.25415000
N	1.69490100	1.48460100	2.72736200
C	0.76540000	2.32600000	3.32259200
H	-0.25725400	2.02530600	3.47833600
C	0.00119500	5.89190400	-3.65362900
H	-0.64197800	5.29974900	-4.31632700
H	0.99572700	5.89939800	-4.12280300
C	0.14552700	5.17856300	-2.30821500
O	0.26668800	5.78432200	-1.24408500
N	0.14339200	3.81953500	-2.37746500
H	0.33925500	3.29183600	-1.53636000
H	0.12496600	3.31211300	-3.25443400
C	3.39692800	-1.34469500	2.45425500
O	2.23653400	-1.44042000	3.01615300
O	3.52913100	-0.51470700	1.51550500
C	0.58352800	0.11222400	-6.88803400
C	0.69950700	-0.93034700	-7.80296800
C	0.67002200	-2.25819200	-7.36420200
C	0.52431600	-2.55349900	-6.00433200
C	0.41299500	-1.52486500	-5.07327600
C	0.44917800	-0.20495100	-5.53321900
N	0.33433300	0.88207000	-4.57167100
O	0.39835900	0.62326100	-3.35915100
O	0.16768800	2.02695000	-4.99541800
H	0.60465600	1.14686000	-7.20701500
H	0.81211300	-0.70521600	-8.85871400
H	0.75749900	-3.06586300	-8.08489600
H	0.49152000	-3.58535400	-5.66947100
H	0.28640800	-1.73682800	-4.01862700
O	0.57840100	0.75247000	0.56722400
O	1.03787400	-1.46735800	0.46534400
H	1.54469300	-1.26789300	-0.39774400
H	5.47918300	-1.85211600	2.56828700
H	4.50024900	-2.40154200	3.97018100
H	4.36744300	-3.23431500	2.41284500
Fe	1.26638800	-0.24938200	1.76077500

C	4.51604600	-2.25594800	2.88653900
C	0.84391200	4.75725200	4.27997300
H	1.37258500	4.99095900	5.21182900
H	0.95066100	5.61782100	3.60888000
H	-0.21749800	4.63583300	4.51091200
C	-0.52137000	7.32215000	-3.52064300
H	-3.49589400	-0.79598300	5.96441100
H	-3.56198300	-2.44014800	5.30664500
H	-2.20850300	-1.95454300	6.34227300
H	-0.53711900	7.81854700	-4.49726600
H	-1.54002800	7.33763600	-3.11651900
H	0.11223900	7.90523000	-2.84581800
C	-2.88737300	-1.61223800	5.55664100
O	2.25081200	-0.94074000	-1.80354200
H	2.48400500	-1.73722900	-2.31026500
H	1.64975200	-0.42717300	-2.37963300

NBZ-FeIII-O-C1-TS-model3:

C	-31.18671500	11.11155200	7.90648800
N	-31.81955900	11.49853600	6.73522500
H	-32.82220200	11.57560800	6.60513600
C	-30.88971100	11.75927500	5.79366900
H	-31.11446000	12.08192800	4.78832700
N	-29.67471900	11.55906100	6.29216900
C	-29.85046700	11.15177600	7.60599200
H	-29.01010700	10.91248800	8.24094100
C	-27.74170400	15.91924000	7.28338500
N	-26.41083200	15.75855300	6.93422500
H	-25.66616500	16.41711200	7.13376000
C	-26.26247100	14.58396200	6.29162800
H	-25.32375700	14.19485500	5.93135500
N	-27.43546800	13.96823600	6.19948700
C	-28.36427900	14.79391300	6.81155100
H	-29.40675200	14.52245200	6.88466900
C	-29.43657400	18.34796000	0.84921100
H	-30.30732800	17.76031700	0.52718700
H	-28.55585200	17.78858800	0.50524300
C	-29.42359600	18.37446800	2.37864100
O	-29.49132700	19.41475200	3.02978800
N	-29.36101300	17.14751300	2.97167700
H	-29.26377300	17.10987000	3.97851300
H	-29.16757100	16.29746100	2.45344900
C	-25.71583300	10.53806900	5.99554000
O	-26.84610000	9.94937500	6.05833400
O	-25.66980200	11.75304000	5.61501800
C	-29.60163000	11.19761800	1.00599700
C	-29.46278600	10.24612000	0.01901700
C	-28.38918800	10.30483400	-0.89166500
C	-27.45676500	11.36062300	-0.82393700
C	-27.56430100	12.33082900	0.14595300

C	-28.57869300	12.19922600	1.16417000
N	-29.01857300	13.47763000	1.81935000
O	-28.36359500	14.49333900	1.58231500
O	-29.99061100	13.43796000	2.56727600
H	-30.43684600	11.18898700	1.69388100
H	-30.20509200	9.45927400	-0.07367700
H	-28.29719200	9.55195200	-1.66803900
H	-26.65986900	11.42519100	-1.55825100
H	-26.87427400	13.16321200	0.20135100
O	-27.55590000	11.70347700	2.54934200
O	-28.34309700	11.15034600	3.59759300
H	-28.17782100	10.14368500	3.54691400
H	-23.59392400	10.22491500	5.87900900
H	-24.29358300	10.06554300	7.49862500
H	-24.53893100	8.76468700	6.31900300
Fe	-27.75993200	11.98069200	5.52937400
C	-24.45600900	9.84800100	6.43499700
C	-28.24600000	17.09401000	8.04400300
H	-27.74911700	17.18411300	9.01801000
H	-28.08171500	18.03282900	7.50067700
H	-29.31999800	16.99127300	8.22166600
C	-29.46900000	19.74099100	0.22200200
H	-32.50105700	11.60971800	9.53643800
H	-32.60455000	9.92286500	9.00841700
H	-31.19937200	10.47567200	9.93620700
H	-30.35548200	20.29761700	0.54198000
H	-28.58975500	20.32660800	0.51020400
H	-29.48642600	19.66661000	-0.87119100
C	-31.91499700	10.76200000	9.16099500
O	-27.81915000	8.63208000	3.89583600
H	-27.37531600	8.84565800	4.75280100
H	-28.61224200	8.12353900	4.13949800

NBZ-FeIII-O-C2-TS1-model3:

C	-2.13830900	-1.48770000	4.27612700
N	-2.44362700	-2.22285600	3.14263300
H	-3.19334000	-2.90099100	3.06517700
C	-1.57483400	-1.90489400	2.16255600
H	-1.58503800	-2.35128200	1.17995200
N	-0.71676800	-0.98888400	2.59757300
C	-1.05965700	-0.72505400	3.91479900
H	-0.50535700	-0.01572500	4.51126100
C	1.27800100	3.52788400	3.55967000
N	2.59785500	3.29081900	3.21122700
H	3.37561200	3.91568200	3.39304100
C	2.68701600	2.10038900	2.59155700
H	3.60066600	1.66191400	2.22232300
N	1.48258800	1.53961600	2.51661400
C	0.59767900	2.42409200	3.11621000

H	-0.45670600	2.20363900	3.19268500
C	0.49318500	6.18902400	-3.36736800
H	0.35794900	5.66702200	-2.41332300
H	0.33327300	5.43942000	-4.15581700
C	1.93861500	6.67030900	-3.50221700
O	2.25310500	7.61801800	-4.21962200
N	2.85409000	5.95438200	-2.79445200
H	3.83361400	6.19045600	-2.88865000
H	2.59939200	5.18017500	-2.19251100
C	3.34745000	-1.52364500	2.29047500
O	2.16572700	-1.83184400	2.68834100
O	3.49339300	-0.58594200	1.45283400
H	4.31377600	-3.33064400	2.91958500
H	5.43187500	-2.06187000	2.32426700
H	4.65366000	-1.91514800	3.92032300
Fe	1.11548300	-0.37993100	1.76875900
C	4.51604600	-2.25594800	2.88653900
C	0.84391200	4.75725200	4.27997300
H	1.35153400	4.85378100	5.24758800
H	1.06068300	5.66252400	3.69963700
H	-0.23308900	4.72330900	4.46509700
C	-0.52137000	7.32215000	-3.52064300
H	-3.95415200	-1.39211000	5.42710200
H	-2.80572000	-2.62395700	5.97275400
H	-2.48403000	-0.91174800	6.29288500
H	-0.36087900	7.85577300	-4.46192400
H	-1.54493900	6.93112500	-3.51320300
H	-0.43166900	8.05071000	-2.70633000
C	-2.88737400	-1.61223800	5.55664100
C	-0.90021400	2.75684200	-0.48272000
C	-2.15855200	2.14011000	-0.38668000
C	-2.36767200	0.85605600	-0.92743700
C	-1.33049000	0.16911100	-1.52604000
C	0.00411600	0.71957600	-1.55817200
C	0.13765000	2.07906600	-1.09695600
N	1.41627200	2.72711700	-1.26193700
O	2.33992000	2.09311400	-1.78958800
O	1.53515100	3.89970800	-0.87803500
H	-0.74481900	3.76013400	-0.10550500
H	-2.97653500	2.67349000	0.08588500
H	-3.35859100	0.41441500	-0.88853200
H	-1.48366600	-0.81393200	-1.95796200
H	0.66644800	0.39505400	-2.35200000
O	0.90387500	-0.22216800	-0.29430500
O	1.21804200	-1.51447100	-0.79610500
H	2.15778700	-1.32625300	-1.12956900
O	3.64461400	-0.65280000	-1.31544400
H	3.40171400	0.26674600	-1.52879200
H	3.84437500	-0.62746600	-0.35229800

NBZ-FeIII-O-C2-INT1-model3:

C	-2.99513000	-2.87621700	3.60285300
N	-3.21630200	-3.69272500	2.50668300
H	-3.93732400	-4.40193400	2.43755700
C	-2.31287200	-3.40106500	1.54968800
H	-2.26222100	-3.90561400	0.59692300
N	-1.50911300	-2.42902300	1.96462100
C	-1.92624500	-2.09715300	3.24457600
H	-1.42890900	-1.32913000	3.81857700
C	0.38660000	2.21664300	2.86289900
N	1.71669100	1.97533200	2.55765300
H	2.48859900	2.60196600	2.75698300
C	1.82402500	0.77865400	1.95196000
H	2.74865600	0.33869600	1.61284400
N	0.62287400	0.21773400	1.84228400
C	-0.27917100	1.10751400	2.40885900
H	-1.33624200	0.89018200	2.45170000
C	-0.35477500	4.86809900	-3.94700500
H	-0.67602500	4.33287100	-3.04642700
H	-0.36991100	4.13423300	-4.76595900
C	1.09475000	5.33087800	-3.79270200
O	1.55729300	6.27327700	-4.43320300
N	1.84117800	4.60498300	-2.91706200
H	2.82173400	4.83176700	-2.81186900
H	1.45887200	3.84062000	-2.37170900
C	2.54843100	-2.92127700	1.45387200
O	1.41584800	-3.28084500	1.92792600
O	2.60193400	-1.90036700	0.69862800
H	3.58870900	-4.76087700	1.81457700
H	4.62647500	-3.43237900	1.20327900
H	4.03710000	-3.42851700	2.88356000
Fe	0.31621100	-1.74466400	1.14546400
C	3.78176700	-3.68463700	1.84767100
C	-0.06885700	3.45983400	3.54979400
H	0.41369000	3.57695800	4.52778700
H	0.16018200	4.35368700	2.95669500
H	-1.15013200	3.42621000	3.70805700
C	-1.30847700	6.01844300	-4.26964200
H	-4.87535100	-2.71481900	4.63621500
H	-3.77537100	-3.92834400	5.30846000
H	-3.45641300	-2.20606600	5.56762500
H	-0.97646600	6.55305900	-5.16427600
H	-2.32275300	5.64323700	-4.44646200
H	-1.35322400	6.74131900	-3.44659100
C	-3.82077100	-2.93722100	4.84096400
C	-2.22325800	1.30358200	-1.30346300
C	-3.44250100	0.60393700	-1.36767500
C	-3.48015100	-0.74939900	-1.79703400
C	-2.33190300	-1.40990700	-2.12710200

C	-0.98165400	-0.76853000	-2.03013800
C	-1.04631900	0.67124100	-1.63440000
N	0.17328200	1.42104200	-1.67647600
O	1.19455900	0.87152100	-2.12097300
O	0.16158800	2.60052400	-1.28502500
H	-2.20757300	2.35002900	-1.02352800
H	-4.36084800	1.11791100	-1.10470500
H	-4.43763400	-1.25682800	-1.86469800
H	-2.34580200	-2.44552000	-2.45019500
H	-0.41742400	-0.89505700	-2.96115100
O	-0.17569200	-1.45616400	-1.00063200
O	0.25578700	-2.74488900	-1.51028500
H	1.19389500	-2.48381800	-1.80780200
O	2.63967900	-1.78012400	-2.03186900
H	2.36952600	-0.85420400	-2.17227900
H	2.90188600	-1.81001200	-1.08275600

NBZ-FeIII-O-C2-TS2-model3:

C	-2.14859400	-1.26720600	4.31159800
N	-2.76128300	-1.09449900	3.07847400
H	-3.75432800	-1.18975800	2.89611700
C	-1.82788700	-0.79161200	2.15779400
H	-2.02129600	-0.61487900	1.11007600
N	-0.63073900	-0.75498400	2.73587300
C	-0.81801600	-1.05381000	4.07494000
H	0.00961900	-1.10400700	4.76665600
C	1.25726600	3.60702300	3.42666300
N	2.44306100	3.58159000	2.70812600
H	3.12913200	4.32796300	2.67507400
C	2.54693200	2.40750500	2.06168800
H	3.38866100	2.11750500	1.45326900
N	1.47757200	1.65818300	2.31761800
C	0.66635900	2.40004000	3.16525500
H	-0.27123900	2.01467900	3.53526900
C	-0.07427700	5.86241300	-3.49956300
H	-0.49031500	5.35148200	-2.61921200
H	-0.46320600	5.32197500	-4.37105600
C	1.44654400	5.70391500	-3.44652800
O	2.20172900	6.62325400	-3.13309500
N	1.89773800	4.46079500	-3.76409200
H	2.88729200	4.26974500	-3.67541600
H	1.27088400	3.68160300	-3.93916900
C	3.31192000	-1.50516300	2.40888300
O	2.15367400	-1.81763600	2.85881900
O	3.39528100	-0.53704600	1.58689700
H	4.32329500	-3.33247800	2.85323600
H	5.39581400	-2.01133700	2.28815400
H	4.70828600	-1.98910800	3.93301600
C	4.51604600	-2.25594800	2.88653900
C	0.84391200	4.75725200	4.27997300

H	1.56771600	4.94258100	5.08277600
H	0.75157400	5.68048100	3.69508000
H	-0.12585800	4.54915200	4.73968100
C	-0.52137000	7.32215000	-3.52064300
H	-2.18558900	-1.69930400	6.39034900
H	-3.62786800	-0.84499400	5.81402700
H	-3.41894600	-2.56674900	5.45936800
H	-0.16219700	7.83482600	-4.41976100
H	-1.61501300	7.38971300	-3.50651300
H	-0.13037200	7.86400600	-2.65414600
C	-2.88737300	-1.61223800	5.55664100
C	-2.13755100	0.36160500	-3.76490500
C	-3.04115400	-0.69135900	-3.56235700
C	-2.69498800	-1.80869100	-2.74987700
C	-1.48154300	-1.87147600	-2.13082500
C	-0.47544200	-0.75728100	-2.20878700
C	-0.89211500	0.31348200	-3.17303200
N	0.06600000	1.34563600	-3.44172900
O	1.20481100	1.23531100	-2.96460500
O	-0.27564300	2.30465700	-4.15920900
H	-2.39933600	1.20107700	-4.39791600
H	-4.01555600	-0.65035700	-4.03789900
H	-3.41444300	-2.61328600	-2.62846000
H	-1.21333100	-2.71607100	-1.50269900
H	0.52565700	-1.13478500	-2.45267300
O	-0.42862800	-0.04502200	-0.96617600
O	0.88713300	-0.82725200	0.06767900
H	1.65719200	-0.63558000	-0.55930800
O	3.13326300	-0.44418600	-1.23409400
H	3.14465400	0.44973600	-1.61662700
H	3.62775600	-0.39390000	-0.39087000
Fe	1.17873300	-0.33552200	1.82883200

NBZ-FeIII-O1-C2-TS-model3:

C	-4.90349200	2.30807300	2.97727500
N	-5.53740900	1.61879100	1.95691300
H	-6.04737800	0.74903900	2.06260600
C	-5.36839200	2.28871100	0.79805300
H	-5.77449100	1.96938600	-0.14949400
N	-4.64538400	3.38112300	1.00968000
C	-4.34771800	3.40007200	2.36363800
H	-3.75902000	4.19219900	2.80390400
C	-7.88530800	7.12364300	1.22948800
N	-8.06312200	7.20633700	-0.14285900
H	-8.83705100	7.64946300	-0.62724000
C	-7.04629100	6.56511200	-0.75404500
H	-6.93907700	6.48846400	-1.82495500
N	-6.21117900	6.06595500	0.14681500
C	-6.72576600	6.40900800	1.38560700

H	-6.23291500	6.12468300	2.30419800
C	-11.45727700	6.30558700	-3.86157500
H	-12.01362700	6.08336000	-2.94053500
H	-10.75422800	5.47950400	-4.01347700
C	-10.70913500	7.61569300	-3.62404400
O	-11.27877300	8.70263800	-3.61331400
N	-9.36630700	7.49136100	-3.36958600
H	-8.82662100	8.34989100	-3.39726100
H	-8.87427300	6.64783400	-3.64941100
C	-2.11545100	6.29072600	-0.10658400
O	-2.08832900	5.02385300	-0.30230100
O	-3.23651400	6.86056500	0.05600800
C	-6.48937500	2.75136500	-5.24192500
C	-5.63663800	1.76116000	-5.76651100
C	-4.23824700	1.96311600	-5.80612100
C	-3.67806800	3.09984400	-5.27239000
C	-4.50491400	4.07313900	-4.56547800
C	-5.94188200	3.90231200	-4.72134900
N	-6.80868400	4.97893300	-4.29967700
O	-6.32022400	6.10324100	-4.15154900
O	-8.01083600	4.72890800	-4.13067300
H	-7.56560500	2.63512200	-5.28858000
H	-6.06813700	0.85846900	-6.18548400
H	-3.60761300	1.22339600	-6.28941900
H	-2.60867700	3.27708800	-5.31665600
H	-4.14721600	5.09685800	-4.52017600
O	-4.90654600	4.60769600	-2.04701100
O	-4.22884000	3.64339200	-2.89896800
H	-3.18798600	3.79831500	-2.77961400
H	-1.02466400	8.14515600	-0.01709900
H	-0.27513800	6.77840600	0.85021400
H	-0.20466600	6.82937700	-0.91223000
Fe	-4.36086800	5.07790900	-0.21757500
C	-0.83214900	7.07124200	-0.04796700
C	-8.81359200	7.73673200	2.22240700
H	-8.87885500	8.82429800	2.09478700
H	-9.82969000	7.33225800	2.13524900
H	-8.45583800	7.53709900	3.23621800
C	-12.43658200	6.41063000	-5.03547900
H	-5.94139100	1.82086600	4.79606700
H	-4.47478000	0.86815000	4.51980800
H	-4.34763600	2.56488500	5.01365900
H	-13.02506100	5.49158200	-5.13075500
H	-13.12402100	7.24842600	-4.88616200
H	-11.90711300	6.57230300	-5.98191200
C	-4.91942600	1.86375100	4.39989200
O	-1.73187000	3.97546900	-2.66329700
H	-1.65940900	4.41060200	-1.76408500
H	-1.30311500	3.10581600	-2.56666700

NBZ-FeV-O-C1-TS-model3:

C	-31.11716600	11.20621100	7.97874400
N	-31.70411000	11.57099100	6.77907300
H	-32.69990900	11.57800900	6.58812200
C	-30.73892900	11.91394800	5.90041700
H	-30.92970100	12.23301500	4.88773800
N	-29.54669600	11.79738200	6.46947900
C	-29.76767100	11.35598600	7.76441000
H	-28.95132300	11.18543100	8.45065600
C	-27.70233300	15.79563300	7.53025200
N	-26.34899000	15.48138500	7.54790800
H	-25.61099800	16.07334700	7.91319100
C	-26.16279100	14.26747800	7.00114100
H	-25.20459600	13.79370400	6.86381700
N	-27.33652500	13.75813500	6.63363300
C	-28.30075500	14.70431200	6.95636200
H	-29.34534700	14.53928100	6.74735000
C	-28.41401300	18.75513300	0.71942800
H	-28.87888000	17.83326500	1.08860000
H	-27.75926400	18.45722800	-0.11254000
C	-27.51517000	19.34713900	1.80478000
O	-27.32190000	20.55540000	1.92345100
N	-26.93445100	18.42912500	2.62666200
H	-26.22856100	18.74751500	3.27839200
H	-27.02241000	17.43162900	2.46808000
C	-25.53559900	10.86814800	6.16652000
O	-26.69167000	10.74376900	6.73558600
O	-25.37799200	11.81312600	5.35087000
C	-29.38040500	12.71844300	2.04647600
C	-29.43933600	11.39663800	1.66752000
C	-28.25133500	10.67842300	1.41957500
C	-26.99341700	11.30760700	1.49686800
C	-26.90336000	12.62574500	1.88111100
C	-28.09951400	13.31164400	2.25740600
N	-28.04807000	14.80378700	2.28478700
O	-26.94167400	15.33311600	2.17710700
O	-29.10379100	15.41202000	2.41140200
H	-30.26948200	13.31278200	2.21370300
H	-30.40082300	10.90951300	1.54156000
H	-28.31040200	9.63676600	1.11926800
H	-26.09393500	10.75241500	1.25252200
H	-25.95515500	13.14365600	1.94406100
O	-27.96644600	13.32243300	4.18429000
O	-27.93396900	10.75981900	4.34040600
H	-28.16563800	9.93838900	4.87143100
H	-23.48159200	10.22927500	6.12366400
H	-24.43745000	9.57288900	7.49337300
H	-24.68493700	8.94482400	5.85543400
Fe	-27.63066300	12.11072200	5.43077000

C	-24.45601100	9.84801100	6.43499700
C	-28.24600000	17.09400100	8.04400200
H	-28.03371000	17.22425100	9.11197400
H	-27.81070600	17.94576200	7.50817000
H	-29.32975300	17.12207600	7.90441500
C	-29.46899800	19.74098900	0.22200400
H	-32.61007400	11.54291100	9.49233300
H	-32.50454500	9.86548400	8.93329800
H	-31.24837700	10.52662800	9.99498200
H	-30.03964000	19.30974600	-0.60807600
H	-30.17542900	20.00306100	1.01809600
H	-29.00100600	20.66740300	-0.12328200
C	-31.91499300	10.76200100	9.16099200
O	-28.27792000	8.63968900	5.98092000
H	-27.63618800	9.12486100	6.54383300
H	-29.12217000	8.72544400	6.45665800

NBZ-FeV-O-C2-TS-model3:

C	-2.11715000	-1.11446900	4.37909000
N	-2.72575700	-0.43936900	3.33297500
H	-3.71501700	-0.22760100	3.26544200
C	-1.79401700	-0.11037600	2.41831800
H	-1.99835700	0.42333100	1.50394300
N	-0.60055000	-0.53673500	2.81668600
C	-0.78850400	-1.16636200	4.03547900
H	0.03641900	-1.60952800	4.57218300
C	1.32900000	3.51604800	3.59706400
N	2.64672900	3.34010100	3.19638600
H	3.39603700	4.01231100	3.32099900
C	2.78321300	2.13452500	2.61919300
H	3.70182400	1.74213600	2.21459200
N	1.61111900	1.50112300	2.62611400
C	0.69859500	2.35586500	3.22906600
H	-0.33552400	2.08223300	3.35758000
C	0.56855200	6.25395900	-3.56796200
H	0.31512200	5.40426200	-2.92268400
H	0.65396400	5.84507600	-4.58501700
C	1.94844200	6.78308900	-3.17602300
O	2.22496100	7.97976400	-3.16234900
N	2.85411800	5.82030800	-2.83510100
H	3.82141600	6.09762600	-2.72351500
H	2.66292200	4.83634200	-2.98172200
C	3.38872400	-1.32868200	2.50538200
O	2.27868700	-1.34572600	3.13237700
O	3.49644700	-0.55302200	1.49815300
C	-0.96134400	2.15694400	-2.42087200
C	-2.22603900	1.63046300	-2.09792900
C	-2.34295900	0.37362300	-1.48765900
C	-1.20605600	-0.35552200	-1.16715900
C	0.09303600	0.18297400	-1.40877900

C	0.16518300	1.42266100	-2.10753700
N	1.47727300	1.93763200	-2.46741100
O	2.47900000	1.30164600	-2.12283500
O	1.52778100	2.99421100	-3.10231800
H	-0.87212000	3.11063200	-2.92566000
H	-3.11450000	2.20188100	-2.34606100
H	-3.32692500	-0.03698000	-1.28390500
H	-1.27562800	-1.33475600	-0.70783600
H	0.93933200	-0.48235300	-1.44534400
O	0.59030600	0.75595200	0.41403100
O	1.09809200	-1.74571600	0.69814400
H	1.78105300	-1.74652800	-0.03601200
H	5.47988800	-1.76196900	2.73854300
H	4.41489900	-2.59675500	3.91906900
H	4.47442300	-3.12875000	2.22286900
Fe	1.21255600	-0.29228300	1.68691600
C	4.51604400	-2.25594700	2.88654000
C	0.84391200	4.75725200	4.27997200
H	1.35602500	4.91256500	5.23720100
H	1.01550700	5.64545000	3.66037400
H	-0.22856100	4.67929100	4.47624000
C	-0.52137000	7.32215000	-3.52064300
H	-3.39702500	-0.79295700	6.07815600
H	-3.64864400	-2.34311300	5.25787100
H	-2.21294700	-2.09787800	6.26684600
H	-0.65991700	7.70575500	-2.50350400
H	-0.26459100	8.17132900	-4.16069200
H	-1.47827700	6.91119200	-3.86180000
C	-2.88737200	-1.61223800	5.55664000
O	3.16728700	-1.46190900	-1.05818300
H	3.05807800	-0.65548800	-1.59403200
H	3.63909900	-1.14662800	-0.25646900

NBZ-FeV-O1-C2-TS-model3:

C	-31.10020000	11.15033900	7.96770600
N	-31.68266300	11.67118400	6.82223300
H	-32.67612500	11.82061300	6.68537700
C	-30.72066800	11.96074400	5.92688700
H	-30.89682700	12.40239900	4.95950100
N	-29.53032000	11.64969600	6.42815800
C	-29.75271800	11.13779500	7.69723800
H	-28.93699300	10.80467100	8.32135700
C	-27.67662400	15.80333300	7.53827000
N	-26.32669900	15.48278900	7.59239200
H	-25.59464900	16.07152300	7.97370600
C	-26.13158500	14.26998600	7.03798700
H	-25.17143600	13.79501700	6.91791900
N	-27.29407500	13.77417500	6.63005700
C	-28.26079700	14.72229000	6.93312100

H	-29.29901600	14.56934500	6.68703300
C	-29.25367800	18.41049700	0.94493500
H	-29.91760700	18.34961100	1.81947600
H	-29.52059800	17.56388100	0.30054200
C	-27.82159600	18.23958900	1.45419400
O	-27.08749700	19.19708300	1.69451900
N	-27.42252600	16.95201400	1.63871700
H	-26.51120200	16.78424300	2.04557500
H	-28.03065400	16.15258800	1.50059800
C	-25.48283300	10.91401400	6.08835500
O	-26.67929300	10.81378100	6.54960100
O	-25.20437900	11.85415100	5.29109600
C	-30.36103800	11.88723800	1.74104500
C	-30.90360300	10.58455600	1.77346000
C	-30.06876000	9.46214000	1.87246100
C	-28.69747100	9.62788400	1.97739900
C	-28.11782500	10.93775000	2.03762600
C	-28.99617300	12.04274800	1.84630300
N	-28.41496900	13.37660800	1.69711900
O	-27.19090700	13.47759800	1.69992900
O	-29.18973100	14.32813100	1.55250800
H	-30.99990100	12.75042200	1.60020500
H	-31.97821500	10.45906400	1.68902200
H	-30.49757300	8.46572900	1.85506500
H	-28.03748700	8.77004500	2.04700400
H	-27.06602200	11.06997900	1.81624900
O	-28.50261100	13.16831500	4.44460600
O	-27.62640000	10.75742600	4.01180900
H	-26.69877400	10.50173000	3.75492200
H	-23.44408400	10.23844600	6.30728300
H	-24.59846900	9.48411500	7.45598400
H	-24.59837100	8.99932300	5.75398000
Fe	-27.71309000	12.14040700	5.43687300
C	-24.45600400	9.84800300	6.43500000
C	-28.24600000	17.09400100	8.04400000
H	-28.06436800	17.22205500	9.11795000
H	-27.80607400	17.95370200	7.52464000
H	-29.32592000	17.11041000	7.87518600
C	-29.46900000	19.74099900	0.22200000
H	-32.44872600	11.62513700	9.57686100
H	-32.65937600	9.99791700	8.90670300
H	-31.26623800	10.35611900	9.94183100
H	-30.52226100	19.86437200	-0.05377700
H	-29.17669000	20.57905000	0.86121200
H	-28.87029700	19.79726600	-0.69438500
C	-31.91499900	10.76200000	9.16099800
O	-25.11811000	10.43581800	2.97466200
H	-24.57178700	9.63692300	3.06383300
H	-24.77649800	11.06556200	3.64665800

Fe^{III}-OOH and HO-Fe^V=O attacks Model 4

Nitrobenzene Model 4

NBZ-FeIII-RC-model4:

C	-1.77938900	-6.06738600	-0.98289900
H	-1.00203500	-6.74561700	-1.35208400
H	-2.59016800	-6.11433600	-1.72218100
C	-1.19003200	-4.66529700	-1.08186400
O	-0.57361900	-4.32208500	-2.10847200
N	-1.39250300	-3.83134500	-0.04432100
H	-0.95444400	-2.91257200	-0.03271400
H	-1.81810000	-4.15544200	0.81268300
C	-2.11946800	-1.16908100	4.36101300
N	-2.72673300	-0.65455400	3.22489100
H	-3.72474100	-0.52666900	3.09747200
C	-1.78154800	-0.34852000	2.31814300
H	-1.97573600	0.06468900	1.34052600
N	-0.57976000	-0.63811100	2.81074100
C	-0.77866400	-1.15171700	4.08097500
H	0.04860900	-1.47718100	4.69299300
C	1.32750600	3.55313300	3.55205800
N	2.58480600	3.46011100	2.97243700
H	3.29002800	4.18920900	2.97250500
C	2.72399200	2.25161500	2.40377400
H	3.60522400	1.90995600	1.88353000
N	1.61040500	1.54357800	2.58567500
C	0.73483900	2.34734000	3.29919100
H	-0.24724600	2.00556000	3.58429500
C	-0.67096500	5.80632100	-3.67054200
H	-1.73543600	5.53524900	-3.72169800
H	-0.22834000	5.46181800	-4.61400000
C	-0.05265800	5.01900900	-2.51296800
O	0.27851000	5.54599400	-1.45147800
N	0.09935500	3.68412000	-2.73614300
H	0.43882600	3.10511600	-1.97867600
H	-0.22599200	3.20844600	-3.56960500
C	3.24772800	-1.58851100	2.44794300
O	2.12200500	-1.87964000	2.96506000
O	3.25975300	-0.68273900	1.53838500
C	-1.79511100	-0.35490600	-6.61765200
C	-2.35728800	-1.36461000	-7.39388800
C	-2.50064400	-2.65517400	-6.87357900
C	-2.08207600	-2.94373100	-5.57073300
C	-1.51078500	-1.94901600	-4.78174300
C	-1.37329900	-0.66795200	-5.32261600
N	-0.77572700	0.38678400	-4.51032200
O	-0.19102000	0.07886400	-3.46367100

O	-0.88489900	1.55235000	-4.90094300
H	-1.67179700	0.64995100	-7.00213000
H	-2.68071500	-1.14364300	-8.40614400
H	-2.94080400	-3.43761900	-7.48470700
H	-2.19657000	-3.94342900	-5.16424700
H	-1.19785700	-2.16333300	-3.76805400
O	0.45752900	-0.09888600	0.12462100
O	0.47965200	-1.54735200	0.09124000
H	0.94273200	-1.75660100	-0.80699200
H	5.22891000	-1.49696200	3.22710900
H	4.32303000	-2.97093200	3.68794100
H	4.97089700	-2.77078000	2.03267200
Fe	1.23117800	-0.33304700	1.81339000
C	4.51604600	-2.25594800	2.88653900
H	-2.64466300	-7.56042700	0.32389500
H	-1.48990200	-6.50349100	1.14357900
H	-3.12303000	-5.91697000	0.74637400
C	0.84391200	4.75725200	4.27997300
H	1.48487200	4.99232100	5.13863800
H	0.82153100	5.64025600	3.62989500
H	-0.16978500	4.58417700	4.65070900
C	-0.52137000	7.32215000	-3.52064300
H	-3.46502900	-0.78844200	5.99344200
H	-3.59068400	-2.41657800	5.30836400
H	-2.20157600	-1.98747500	6.32088200
C	-2.28518200	-6.52820600	0.38930400
H	-1.02409400	7.83854600	-4.34589400
H	-0.95873800	7.66758100	-2.57908900
H	0.53285300	7.61983000	-3.52523500
C	-2.88737300	-1.61223800	5.55664100
O	1.23261900	-2.24827600	-2.24214300
H	0.60399100	-3.01709500	-2.28209600
H	0.84357900	-1.56029500	-2.81515700

NBZ-FeV-RC-model4:

C	-1.85466900	-5.78898500	-0.88214600
H	-1.25716300	-6.44887900	-1.52278500
H	-2.73321500	-5.51473700	-1.47980300
C	-1.03925100	-4.51085800	-0.72728000
O	-0.65178700	-3.90499300	-1.74638800
N	-0.77248000	-4.07823500	0.51742500
H	-0.22972900	-3.22843300	0.66243400
H	-1.06093000	-4.59982200	1.33357700
C	-2.11006200	-1.12932200	4.38102800
N	-2.71793700	-0.60122800	3.25362300
H	-3.71716600	-0.49285200	3.11982900
C	-1.76897500	-0.24681800	2.36557100
H	-1.96877600	0.19690500	1.40258400
N	-0.56724600	-0.51611800	2.86321700

C	-0.76519900	-1.07035200	4.11479500
H	0.06400700	-1.38595500	4.73001400
C	1.36270700	3.52848900	3.60407700
N	2.67604600	3.38568400	3.17420700
H	3.40714900	4.08277300	3.26873800
C	2.83609300	2.18046900	2.60571100
H	3.75347500	1.81098800	2.17700800
N	1.68155900	1.51481300	2.65388300
C	0.75580300	2.34983000	3.26435000
H	-0.26571300	2.04762400	3.42130700
C	-0.80410900	5.82016400	-3.45165200
H	-1.88585400	5.64681000	-3.35580000
H	-0.49995600	5.32092300	-4.38010300
C	-0.12948500	5.13487800	-2.26142500
O	0.25504300	5.75341100	-1.26939500
N	0.00042800	3.78477900	-2.37119800
H	0.36681200	3.26955500	-1.58089100
H	-0.36266800	3.24692900	-3.14997400
C	3.40137500	-1.33310900	2.46802500
O	2.26313800	-1.38068100	3.07935300
O	3.51044300	-0.54383800	1.49083800
C	-1.93159600	-0.26047000	-6.14278400
C	-2.43396100	-1.32515700	-6.88554700
C	-2.54539500	-2.59525800	-6.30902800
C	-2.15673000	-2.80767900	-4.98257400
C	-1.64877800	-1.75655400	-4.22476600
C	-1.53926500	-0.49815800	-4.82210900
N	-1.00058600	0.61033900	-4.04463300
O	-0.46175200	0.37494900	-2.95368700
O	-1.10902300	1.75135100	-4.50174700
H	-1.83132800	0.72888400	-6.57165000
H	-2.73488500	-1.16397400	-7.91585400
H	-2.93658500	-3.42116300	-6.89579700
H	-2.24188400	-3.79047400	-4.53085800
H	-1.36242700	-1.91487100	-3.19378000
O	0.59629500	0.70310700	0.52783200
O	0.94819900	-1.58479500	0.64045200
H	1.16077700	-1.57600900	-0.38864700
H	5.48152500	-1.84967100	2.57776500
H	4.49770100	-2.42564400	3.96620800
H	4.36700300	-3.22115800	2.38649000
Fe	1.27303800	-0.26056400	1.76856600
C	4.51604600	-2.25594800	2.88653900
H	-2.85625000	-7.42309500	0.12138000
H	-1.42267800	-6.85584500	0.98127900
H	-2.92866100	-5.90808500	1.02497700
C	0.84391200	4.75725200	4.27997300
H	1.36495600	4.94523800	5.22642700
H	0.97003900	5.64257200	3.64574700
H	-0.22139800	4.63914500	4.49370400

C	-0.52137000	7.32215000	-3.52064300
H	-3.48310000	-0.80698000	6.00373000
H	-3.57505200	-2.42124500	5.28097500
H	-2.20707900	-1.99406700	6.32274000
C	-2.28518200	-6.52820600	0.38930400
H	-1.07936900	7.78010900	-4.34483700
H	-0.81249400	7.81536700	-2.58854800
H	0.54444400	7.51902000	-3.68209400
C	-2.88737300	-1.61223800	5.55664100
O	1.14740800	-1.84970700	-1.85074400
H	0.52153900	-2.62516900	-1.87420000
H	0.67713800	-1.11874800	-2.29745000

NBZ-FeIII-O-C1-TS-model4:

C	-30.29114000	6.19611900	5.43997100
H	-30.82474900	6.47784700	6.35612000
H	-29.70778200	5.29921000	5.69215700
C	-29.28776600	7.28991200	5.08869200
O	-29.04920600	7.58222700	3.90314400
N	-28.67235200	7.88556100	6.12807100
H	-27.96363200	8.60881200	6.00081500
H	-28.89599700	7.62195600	7.07868500
C	-31.18565900	11.04197500	7.89188700
N	-31.78532500	11.05599700	6.64257000
H	-32.76732900	10.88487000	6.45778400
C	-30.85145100	11.34216800	5.70967300
H	-31.05563100	11.41302800	4.65208500
N	-29.67012200	11.51441400	6.28720900
C	-29.86929700	11.32890100	7.64564800
H	-29.05795600	11.41319600	8.35438100
C	-27.74785200	15.89598100	7.31250100
N	-26.41270400	15.71375500	6.98682700
H	-25.66349600	16.36642200	7.18892600
C	-26.26665200	14.53397000	6.35638400
H	-25.32998900	14.13209600	6.00363900
N	-27.44741500	13.93189300	6.25047800
C	-28.37710900	14.77452200	6.84075000
H	-29.42371300	14.51389900	6.89331400
C	-29.08290300	18.85379800	1.40616700
H	-29.74279700	19.06819900	2.25891700
H	-29.22384100	17.79411200	1.16464900
C	-27.65056800	19.10642700	1.87705000
O	-27.14059700	20.22527400	1.86148900
N	-27.00000300	18.01224300	2.36047500
H	-26.02720200	18.11247700	2.62227300
H	-27.36165200	17.07404700	2.23631900
C	-25.61483300	10.67490300	5.95193100
O	-26.82099800	10.27388000	6.21798400
O	-25.45083600	11.76065500	5.34663800

C	-29.58727400	12.82207200	1.41215700
C	-30.16411200	11.81263800	0.67889500
C	-29.40437400	11.06520800	-0.24963300
C	-28.04408100	11.36489600	-0.45714800
C	-27.43413100	12.37633000	0.25346700
C	-28.16984700	13.05649300	1.29598100
N	-27.71958300	14.46628000	1.58618900
O	-26.55452300	14.75063100	1.33935600
O	-28.53785900	15.24318900	2.08039500
H	-30.16086400	13.42590400	2.10344700
H	-31.22388800	11.60555100	0.79348600
H	-29.88115300	10.27994100	-0.82774000
H	-27.47593900	10.81720900	-1.20271800
H	-26.39884800	12.64855900	0.09009600
O	-27.35345900	12.48293700	2.76297200
O	-28.17813300	11.56058100	3.46180000
H	-27.79479600	10.63988500	3.18133700
H	-23.50912300	10.25888900	6.08001300
H	-24.45826500	9.83168700	7.53159300
H	-24.56199200	8.81254000	6.09390700
Fe	-27.72980200	11.98851600	5.55692200
C	-24.45600800	9.84800200	6.43499800
H	-31.93519600	5.05489300	4.61202300
H	-31.89998700	6.74228300	4.06868700
H	-30.74571400	5.57809800	3.40344600
C	-28.24600000	17.09400300	8.04400100
H	-27.76176500	17.19623600	9.02303200
H	-28.05874500	18.01757800	7.48250400
H	-29.32395200	17.01100000	8.20693000
C	-29.46900000	19.74099600	0.22200100
H	-32.71973400	11.48651100	9.33646300
H	-32.36603900	9.76199300	9.15932400
H	-31.22077600	10.81750900	10.00395700
C	-31.27499800	5.87600100	4.31300100
H	-30.52412200	19.60189300	-0.03862000
H	-29.30726700	20.79538600	0.46407600
H	-28.86804800	19.50571500	-0.66436100
C	-31.91499800	10.76200000	9.16099700
O	-27.23083400	9.25592200	2.90029600
H	-27.86624800	8.60361900	3.31589900
H	-27.25680900	9.06936700	1.94644000

NBZ-FeIII-O-C2-TS-model4:

C	-30.36027100	6.17333800	5.50608000
H	-30.93783800	6.55839900	6.35459500
H	-29.89045500	5.24120700	5.85042600
C	-29.22328500	7.13449800	5.17863500
O	-28.71204800	7.15185700	4.04433100
N	-28.79698300	7.92266200	6.18467200

H	-28.01827700	8.57304600	6.07613200
H	-29.24317200	7.89024500	7.09161900
C	-31.19749500	11.04275200	7.88352100
N	-31.82226800	11.10556800	6.64804500
H	-32.81386700	10.97552000	6.48165800
C	-30.89938900	11.38114200	5.70130500
H	-31.12833500	11.48470100	4.65173600
N	-29.70003900	11.50075000	6.25438300
C	-29.87708700	11.29136100	7.61375500
H	-29.04787100	11.33165400	8.30533700
C	-27.77169500	15.88874100	7.30609400
N	-26.44296900	15.69717500	6.96117200
H	-25.68724500	16.34700000	7.14771200
C	-26.31340400	14.51276300	6.33591800
H	-25.38438400	14.10433100	5.97042500
N	-27.49835500	13.91533200	6.25155000
C	-28.41450600	14.76687500	6.85028700
H	-29.46115100	14.51144900	6.92391700
C	-29.13894300	18.42719100	0.92892500
H	-29.78754600	17.61683400	0.57450900
H	-28.11026800	18.12130400	0.68870600
C	-29.23367800	18.52983100	2.45178600
O	-29.13199400	19.59736000	3.05407900
N	-29.43344800	17.34515100	3.09299700
H	-29.37810100	17.33574200	4.10366800
H	-29.39695000	16.45268800	2.61084100
C	-25.63106500	10.66454300	5.96857200
O	-26.82751500	10.27165500	6.27550500
O	-25.48193300	11.73294300	5.32452200
C	-30.60579300	11.57168100	1.37459900
C	-30.38957800	10.27131300	0.89501900
C	-29.12886100	9.89554000	0.39001800
C	-28.08075900	10.79574000	0.38372300
C	-28.22743500	12.09539600	0.97860300
C	-29.55586200	12.47191100	1.36634800
N	-29.76874500	13.81867700	1.85295200
O	-28.82092000	14.61582100	1.77643900
O	-30.86970100	14.11513600	2.32499100
H	-31.58353400	11.88129900	1.72366600
H	-31.21027200	9.56126500	0.89120400
H	-28.99416800	8.89924600	-0.02015700
H	-27.11299500	10.52580500	-0.02608700
H	-27.54391300	12.88324900	0.68343500
O	-27.30751700	11.92575400	2.56855800
O	-27.97902400	11.07567100	3.47125700
H	-27.48395400	10.17802700	3.36859900
H	-23.51564800	10.29761100	6.11105000
H	-24.47342200	9.77574600	7.52857900
H	-24.53234800	8.82922900	6.03916500
Fe	-27.74795900	11.95844700	5.51026100

C	-24.45600500	9.84800300	6.43499900
H	-32.02449200	5.12751800	4.59022900
H	-31.80248900	6.77740700	3.97983100
H	-30.69758800	5.49125600	3.46773800
C	-28.24600000	17.09400100	8.04400100
H	-27.74808800	17.18817300	9.01694800
H	-28.05250800	18.01557300	7.48144000
H	-29.32286200	17.02576900	8.22050300
C	-29.46900000	19.74099700	0.22200100
H	-32.67041400	11.52720300	9.37825200
H	-32.42625700	9.79190400	9.13584500
H	-31.20118000	10.74795000	9.98912300
C	-31.27500000	5.87600000	4.31300000
H	-29.31769200	19.64573500	-0.85902100
H	-30.51075500	20.03489400	0.39383400
H	-28.83154700	20.54993100	0.59073600
C	-31.91499900	10.76200000	9.16099800
O	-26.76138500	8.81597000	3.30224600
H	-27.44485700	8.14875700	3.60209300
H	-26.55813500	8.58332500	2.38070700

NBZ-FeIII-O1-C2-TS-model4:

C	-0.08015300	-0.02242800	0.12986400
H	-0.24294500	-0.05281400	1.21323100
H	1.00816900	-0.02316300	-0.02331200
C	-0.59180400	1.29940600	-0.43062300
O	-0.81598300	1.42871800	-1.65116900
N	-0.74699700	2.30480600	0.44745700
H	-1.06921300	3.23268000	0.16498600
H	-0.56505200	2.15924600	1.43155700
C	-4.96211700	2.37608900	3.00081400
N	-5.71446200	1.77801300	2.00318600
H	-6.28256600	0.94600500	2.11579200
C	-5.56879000	2.47831200	0.86010400
H	-6.05241900	2.22664600	-0.07087300
N	-4.75382600	3.50583100	1.06020100
C	-4.36631700	3.44897800	2.38930500
H	-3.68923200	4.17682100	2.81248200
C	-7.88260000	7.15557400	1.21277700
N	-8.06704100	7.27514200	-0.15531400
H	-8.83784100	7.75010800	-0.61167600
C	-7.05729600	6.64508800	-0.79106700
H	-6.96550200	6.58401100	-1.86439700
N	-6.21975300	6.12033800	0.09236900
C	-6.72423800	6.43433400	1.34327900
H	-6.22907600	6.11929700	2.25044500
C	-11.18453900	6.23728700	-4.17451100
H	-11.46550900	6.22564900	-3.11145900
H	-10.70071400	5.27444300	-4.37511400

C	-10.18450700	7.37858400	-4.36210900
O	-10.53646000	8.52901700	-4.61270500
N	-8.87534400	7.03982900	-4.17215000
H	-8.17720500	7.73681500	-4.40304900
H	-8.57240800	6.07082800	-4.15824800
C	-2.07600000	6.21834000	-0.08276100
O	-2.05122600	4.96201900	0.06309000
O	-3.20564100	6.80243400	-0.26507700
C	-6.92540800	1.59977400	-3.50355900
C	-6.26235000	0.36251300	-3.43597600
C	-4.88256500	0.27230200	-3.73354700
C	-4.15017500	1.39811200	-4.02284000
C	-4.75341400	2.72823300	-3.92174700
C	-6.20697000	2.73851100	-3.80618700
N	-6.89964900	3.98262000	-4.03063600
O	-6.28732200	4.91507100	-4.55784700
O	-8.09815800	4.05037300	-3.70850600
H	-7.99912700	1.66040500	-3.37075000
H	-6.82981700	-0.53359000	-3.20798400
H	-4.40684400	-0.70316800	-3.76186600
H	-3.09658700	1.33046800	-4.27130000
H	-4.33561300	3.51094400	-4.54865100
O	-4.81047300	4.51965900	-2.02082500
O	-4.18164600	3.24411700	-2.40330000
H	-3.14873700	3.47098400	-2.58562600
H	-0.93486600	7.83781300	0.72779100
H	0.05797800	6.46856200	0.14385400
H	-0.72321700	7.59039500	-1.00680000
Fe	-4.35752800	5.11488900	-0.24486300
C	-0.83214800	7.07124100	-0.04796700
H	-0.23132700	-2.16861700	-0.14134200
H	-1.77025400	-1.31658300	-0.36453800
H	-0.52385200	-1.23595700	-1.62298400
C	-8.81359200	7.73673200	2.22240700
H	-8.88266300	8.82733900	2.12700700
H	-9.82775700	7.33067800	2.12173800
H	-8.45663600	7.50872800	3.23049900
C	-12.43658200	6.41063000	-5.03547900
H	-5.91526600	1.86913700	4.85972400
H	-4.53903800	0.83576100	4.44413400
H	-4.26418000	2.49320100	5.00814400
C	-0.69009900	-1.25885500	-0.54210100
H	-13.16649800	5.62303500	-4.81823900
H	-12.90452900	7.38064100	-4.84412300
H	-12.19447900	6.36261300	-6.10350200
C	-4.91942600	1.86375100	4.39989200
O	-1.74101500	3.62290800	-2.78023600
H	-1.31822700	2.82193000	-2.33022400
H	-1.45782900	3.59930300	-3.71101300

NBZ-FeV-O-C1-TS-model4:

C	-30.41444100	6.18041100	5.54563900
H	-31.03176100	6.57074300	6.36311800
H	-29.96350900	5.24889500	5.91570500
C	-29.25821300	7.13656300	5.27135000
O	-28.65144900	7.11854400	4.18651400
N	-28.91897400	7.96456700	6.28171600
H	-28.14559800	8.61977400	6.20124100
H	-29.42309800	7.95498300	7.15799200
C	-31.12597200	11.13725600	7.94874300
N	-31.67648100	11.16167000	6.67717900
H	-32.64145700	10.95185600	6.44839900
C	-30.72128900	11.51095500	5.79039500
H	-30.88161500	11.58246500	4.72631200
N	-29.57442200	11.72527500	6.41936900
C	-29.81246800	11.49419700	7.76350300
H	-29.03088200	11.59914400	8.50127100
C	-27.72231700	15.76984200	7.57068600
N	-26.37670700	15.42747300	7.62323000
H	-25.63457500	16.00891400	7.99642700
C	-26.20569700	14.19916300	7.09981700
H	-25.25356900	13.70645100	6.98497000
N	-27.37984100	13.70583700	6.71660000
C	-28.32983300	14.67903000	7.00312900
H	-29.37298200	14.53299400	6.77192700
C	-28.38255500	18.84576700	0.81466800
H	-28.82360400	17.99859400	1.35311600
H	-27.77201100	18.41446300	0.00797900
C	-27.43029800	19.60153700	1.74172100
O	-27.23257300	20.81143900	1.65070600
N	-26.80900400	18.82619100	2.67342100
H	-26.07234100	19.24120700	3.22967000
H	-26.90169300	17.81661700	2.68101500
C	-25.63246700	10.74982000	6.14289700
O	-26.79486900	10.50531400	6.61689400
O	-25.50648400	11.75799700	5.37625600
C	-29.44523700	13.25220100	2.20367700
C	-29.61052600	11.98148100	1.69990800
C	-28.48655400	11.22664900	1.31346100
C	-27.19087100	11.77905100	1.35508500
C	-26.99734800	13.04860500	1.85098400
C	-28.11934600	13.74732200	2.38432600
N	-27.97402700	15.21429500	2.59686800
O	-26.84782500	15.69798500	2.47391200
O	-28.97930900	15.85515100	2.88081400
H	-30.28284700	13.87192300	2.49737600
H	-30.60610400	11.56311800	1.59410200
H	-28.62680500	10.22335400	0.92268300
H	-26.34467900	11.20593200	0.99066700

H	-26.01847900	13.50877800	1.88939300
O	-27.88556000	13.45935900	4.26854600
O	-28.06026800	10.88639600	4.13802300
H	-27.37076300	10.15869300	4.00003600
H	-23.51525000	10.38328300	6.28966700
H	-24.51659100	9.44881600	7.45102700
H	-24.50248000	9.00873300	5.73094100
Fe	-27.66788800	12.07435500	5.39776700
C	-24.45600700	9.84800700	6.43499900
H	-32.03597200	5.12921100	4.56157400
H	-31.78657100	6.77533600	3.95084200
H	-30.65985200	5.48543800	3.49731700
C	-28.24599900	17.09400000	8.04400000
H	-28.05407100	17.24424200	9.11325000
H	-27.77730800	17.92163600	7.49848500
H	-29.32539400	17.14575900	7.87928100
C	-29.46899900	19.74099400	0.22200200
H	-32.75464000	11.44815600	9.32655300
H	-32.32639800	9.74870000	9.07513600
H	-31.27515400	10.79287200	10.04715600
C	-31.27500000	5.87600000	4.31300000
H	-30.08577000	19.18098700	-0.48989000
H	-30.12871200	20.13577400	1.00331100
H	-29.02655700	20.59427800	-0.30041100
C	-31.91499600	10.76200000	9.16099600
O	-26.52592400	8.75326900	3.85821900
H	-27.26848400	8.09278600	3.95638200
H	-26.17387600	8.61976100	2.96239100

NBZ-FeV-O-C2-TS-model4:

C	-1.55564900	-5.96214900	-0.83075600
H	-0.86468100	-6.70970400	-1.24144900
H	-2.26496200	-5.74320500	-1.63753400
C	-0.73513100	-4.69429600	-0.63799100
O	-0.23452000	-4.13324100	-1.63348600
N	-0.58028800	-4.22277700	0.61120100
H	-0.02696400	-3.37997100	0.77749300
H	-0.95977600	-4.70942600	1.41130200
C	-2.12147200	-1.13803800	4.36848200
N	-2.74145500	-0.60803000	3.24831300
H	-3.74163400	-0.49343300	3.12913000
C	-1.80076200	-0.26349200	2.34600600
H	-2.00731900	0.17427300	1.38190400
N	-0.59470700	-0.54159600	2.82523100
C	-0.77992000	-1.09028300	4.08139300
H	0.05690900	-1.41126400	4.68322900
C	1.34399100	3.51014100	3.61960800
N	2.65515000	3.35206100	3.18930700
H	3.39463300	4.03974800	3.28366600

C	2.80029300	2.13755400	2.63213000
H	3.71430700	1.75555600	2.20711400
N	1.64145300	1.48274200	2.68150200
C	0.72830000	2.33052600	3.29115800
H	-0.29559700	2.03857900	3.45510600
C	0.70907100	6.62461300	-4.11729200
H	0.63111400	5.54030400	-3.98878200
H	0.75695400	6.82781200	-5.19386300
C	2.00233200	7.15756700	-3.50473900
O	2.36658200	8.32041700	-3.67025900
N	2.72256000	6.25746300	-2.77793700
H	3.52768900	6.60013400	-2.26785900
H	2.32272000	5.37156300	-2.48801800
C	3.38252400	-1.33583700	2.50714400
O	2.27668600	-1.36704200	3.15606300
O	3.46404500	-0.57035000	1.50001200
C	-1.30903700	2.34001900	-1.89792300
C	-2.36987900	1.41676800	-1.84321400
C	-2.11812500	0.05366800	-1.63555200
C	-0.81737100	-0.40045100	-1.45800200
C	0.27612800	0.51451200	-1.44555400
C	-0.01885800	1.87863800	-1.73999000
N	1.09143700	2.81823400	-1.81180200
O	2.23654500	2.37245800	-1.79694700
O	0.81888600	4.02421300	-1.88507800
H	-1.49543900	3.39134200	-2.07876800
H	-3.38654400	1.77064300	-1.98046900
H	-2.94198500	-0.65333400	-1.63283100
H	-0.61404100	-1.45576100	-1.31953400
H	1.28402000	0.15422000	-1.59866100
O	0.65663600	0.79102700	0.46865100
O	1.04175300	-1.76920900	0.76083100
H	1.55834700	-1.90002000	-0.09425300
H	5.47441200	-1.82805100	2.58356800
H	4.51079600	-2.46311100	3.95963500
H	4.37588600	-3.20385200	2.35201300
Fe	1.24974800	-0.30164900	1.71605500
C	4.51604300	-2.25594600	2.88653900
H	-2.84959300	-7.42219700	0.10402200
H	-1.58738900	-6.82543000	1.18168500
H	-2.99824800	-5.80822300	0.80825700
C	0.84391200	4.75725100	4.27997300
H	1.36955000	4.95129900	5.22274700
H	0.98208700	5.63237300	3.63391800
H	-0.22260200	4.65926900	4.49864600
C	-0.52137000	7.32215000	-3.52064300
H	-3.47090300	-0.80142000	6.00975500
H	-3.58450700	-2.41688000	5.29219000
H	-2.19963700	-1.99737500	6.31438300
C	-2.28518200	-6.52820600	0.38930400

H	-0.44536400	8.40716000	-3.64570900
H	-1.43759300	6.98398900	-4.01770600
H	-0.61865800	7.10938300	-2.44928200
C	-2.88737100	-1.61223800	5.55664000
O	2.03200800	-2.64495200	-1.49258200
H	1.23200000	-3.22246800	-1.61977800
H	2.14622000	-2.15801100	-2.32498400

NBZ-FeV-O1-C2-TS-model4:

C	-30.56562000	6.29053700	5.60704200
H	-31.24155300	6.85972100	6.25566500
H	-30.27695400	5.39260100	6.17117200
C	-29.28421700	7.08158100	5.37276600
O	-28.52720400	6.81327400	4.42343800
N	-29.00929700	8.04777300	6.27331100
H	-28.17353700	8.62077900	6.20412700
H	-29.66247600	8.28044600	7.00861300
C	-31.11050500	11.17629100	7.97188300
N	-31.69115600	11.68863500	6.82184000
H	-32.68488300	11.82831100	6.67693300
C	-30.72247500	11.99010000	5.93401400
H	-30.89535700	12.42245200	4.96099100
N	-29.53455700	11.69493800	6.44580600
C	-29.76107200	11.18469800	7.71301000
H	-28.94597100	10.87266500	8.34884700
C	-27.67866700	15.77846000	7.59348400
N	-26.33421300	15.44620900	7.69589400
H	-25.60640500	16.03763500	8.08060300
C	-26.13889400	14.21282900	7.18369900
H	-25.17819000	13.72884200	7.10876800
N	-27.29218700	13.71264600	6.75965500
C	-28.25509400	14.68099900	7.00724000
H	-29.28707100	14.53095700	6.73386600
C	-29.15125200	18.44505600	0.97032400
H	-29.81872600	18.34268800	1.83835800
H	-29.33950600	17.56926500	0.33719800
C	-27.71642400	18.40038500	1.49881900
O	-27.06253500	19.41892000	1.71889400
N	-27.21952900	17.15385000	1.72519600
H	-26.30416500	17.07299000	2.14946600
H	-27.75742700	16.30244400	1.60414700
C	-25.58188700	10.80235600	6.08705800
O	-26.77173000	10.60657700	6.55813400
O	-25.41805800	11.78235600	5.30922500
C	-29.80965000	11.95395200	1.25316600
C	-30.31664500	10.65397600	1.05311800
C	-29.50568100	9.53243900	1.26328600
C	-28.20365100	9.69419000	1.71403300
C	-27.68952900	10.99156800	2.02070100

C	-28.51130600	12.10512600	1.69282400
N	-27.93931300	13.45131400	1.75148400
O	-26.73194600	13.56056800	1.93954700
O	-28.70495400	14.40393800	1.56767200
H	-30.41284700	12.82456300	1.02764400
H	-31.33684800	10.53437700	0.70282900
H	-29.89146900	8.53759000	1.06651800
H	-27.57283100	8.83294700	1.89597500
H	-26.62650000	11.14836400	2.14925600
O	-28.33684100	13.16667600	4.44807300
O	-27.87234000	10.65703600	4.07871200
H	-27.19981200	9.91838300	4.10144200
H	-23.49817600	10.25047800	6.09957500
H	-24.43283700	9.66633200	7.51438600
H	-24.65580100	8.89524300	5.93392100
Fe	-27.67620800	12.08135000	5.46515300
C	-24.45600400	9.84800300	6.43500000
H	-32.14898600	5.25801700	4.54309200
H	-31.61678500	6.75117600	3.74813300
H	-30.60349500	5.29900800	3.67067500
C	-28.24600000	17.09400000	8.04400000
H	-28.08744400	17.25568100	9.11707500
H	-27.78378100	17.93069300	7.50668700
H	-29.32159100	17.11676500	7.84980300
C	-29.46900000	19.74099900	0.22200000
H	-32.47815500	11.60601600	9.57734300
H	-32.63517900	9.97476900	8.90649800
H	-31.25489800	10.37802100	9.94354600
C	-31.27500000	5.87600000	4.31300000
H	-30.52497900	19.76854600	-0.06921700
H	-29.25852200	20.61122400	0.85024400
H	-28.86412900	19.83346900	-0.68733600
C	-31.91499900	10.76200000	9.16099800
O	-26.37171500	8.40329500	4.15729000
H	-27.10919300	7.73404400	4.22354200
H	-25.76493600	8.08153800	3.47073700

FeV-O1-C2 pathway (radical cis-dihydroxylation pathway)

Nitrobenzene Model 1

NBZ-FeV-O1-C2-TS1-modell1:

C	-31.09526800	11.17369800	7.98385400
N	-31.64832300	11.78628300	6.86830100
H	-32.63132600	12.00304900	6.74435100
C	-30.67383700	12.06068700	5.98284400
H	-30.82301400	12.55242100	5.03415700
N	-29.50342600	11.65172900	6.46731700
C	-29.75326100	11.09401300	7.71017100

H	-28.95783500	10.68284100	8.31299100
C	-27.67196200	15.80435400	7.54310800
N	-26.32682100	15.47888800	7.63332300
H	-25.60148000	16.06701800	8.02777100
C	-26.12913100	14.25464800	7.10233600
H	-25.16722000	13.77218700	7.02936200
N	-27.28199800	13.75912100	6.67316100
C	-28.24732900	14.71763900	6.93608100
H	-29.28192600	14.56820600	6.67140500
C	-25.59485100	10.79845300	6.17660900
O	-26.63000800	10.82062700	6.92808400
O	-25.59911400	11.57521400	5.16333300
H	-24.74737200	8.85109000	6.08202300
H	-23.55891800	10.16644200	5.89989200
H	-24.25551600	9.77557900	7.50790400
C	-24.45600700	9.84800700	6.43500100
C	-28.24599800	17.09399600	8.04400000
H	-28.08633300	17.21293400	9.12254500
H	-27.79243300	17.95671100	7.54138700
H	-29.32234900	17.11721700	7.85383700
H	-32.41227600	11.62355800	9.62295700
H	-32.69138100	10.04089800	8.87814500
H	-31.27636700	10.29443400	9.91504500
C	-31.91499800	10.76200100	9.16099800
Fe	-27.64351100	11.98395200	5.57940900
O	-28.26984100	12.83158300	4.34564600
C	-26.94711000	9.89683400	2.73652900
C	-26.99351000	8.47300600	2.80369000
C	-27.79239700	10.53328500	1.78883900
H	-26.12413500	10.44830700	3.17180100
C	-27.90533900	7.75828700	2.04114300
H	-26.32421000	7.96553400	3.48947300
C	-28.71990200	9.83343200	1.04181000
N	-27.63511700	11.97506700	1.55529100
C	-28.77700800	8.43326600	1.17369100
H	-27.94484800	6.67623700	2.11224800
H	-29.36405200	10.35461600	0.34395900
O	-26.57467500	12.48929000	1.90167400
O	-28.55854700	12.56716100	0.99788600
H	-29.49482800	7.87611000	0.58017500
O	-27.93400300	10.10949800	4.59814100
H	-28.84258100	10.11983600	4.23792500

NBZ-FeV-O1-C2-INT1-modell (radical intermediate):

C	-31.08487100	11.15129000	7.98530300
N	-31.60474100	11.83791300	6.89696300
H	-32.57269400	12.12184900	6.79032500
C	-30.62458300	12.08132600	6.01248300
H	-30.74845000	12.60870500	5.08002200

N	-29.48200700	11.57475000	6.46910200
C	-29.75484200	10.99160400	7.69738400
H	-28.98251600	10.51412500	8.28048700
C	-27.76751300	15.71363600	7.72637000
N	-26.94377400	14.98274900	8.57114900
H	-26.55698100	15.31228100	9.44883800
C	-26.71802900	13.76965800	8.03181800
H	-26.11950700	12.99807600	8.49025600
N	-27.35454100	13.67050200	6.86962800
C	-28.00401000	14.87762900	6.66579800
H	-28.59025100	15.05742000	5.77771700
C	-25.63545100	10.74548000	6.22625800
O	-26.62863700	10.77245900	7.03318500
O	-25.73319400	11.49359500	5.18911000
H	-24.62376900	8.92776000	5.86101200
H	-23.54490300	10.32100500	6.05948100
H	-24.34990500	9.58753000	7.49045500
C	-24.45600500	9.84800500	6.43500000
C	-28.24599900	17.09399900	8.04400000
H	-28.81947800	17.11201800	8.97870100
H	-27.41085500	17.79696100	8.15058300
H	-28.89246800	17.45617100	7.24027100
H	-32.33762500	11.64305000	9.65912100
H	-32.74848200	10.11172100	8.86957500
H	-31.30215700	10.22282200	9.88816100
C	-31.91499900	10.76200000	9.16099800
Fe	-27.65304400	11.93676600	5.71022400
O	-28.21161200	12.76620300	4.43242100
C	-28.59194200	9.06584800	3.62961400
C	-29.52423900	8.33994300	4.54910400
C	-29.32390400	9.86002700	2.58072300
H	-27.98164600	8.30401100	3.10988500
C	-30.86852400	8.28212600	4.33003400
H	-29.05998100	7.81836200	5.38073000
C	-30.68642900	9.78982700	2.39770000
N	-28.51977800	10.62276400	1.67616100
C	-31.46748500	8.99326000	3.25085100
H	-31.50082600	7.70053300	4.99431700
H	-31.14380400	10.34731700	1.58802900
O	-27.27840400	10.57078200	1.83453100
O	-29.05936400	11.28675700	0.78611100
H	-32.53893200	8.93504400	3.09105800
O	-27.66306900	9.85641500	4.40548100
H	-27.02268900	10.19261500	3.74343200

NBZ-FeV-O1-C2-TS2-modell1:

C	-31.10222300	11.12389100	7.96360300
N	-31.64401800	11.76990100	6.86125700
H	-32.61770800	12.03279400	6.75468100

C	-30.67486500	12.00068000	5.96043300
H	-30.81484300	12.50374500	5.01718000
N	-29.51860500	11.52791300	6.41722300
C	-29.77277000	10.97568300	7.66427800
H	-28.98888400	10.52142500	8.25062100
C	-27.77925600	15.71938500	7.69802200
N	-26.93974800	14.97496100	8.51444400
H	-26.53497600	15.29045800	9.38924700
C	-26.72823600	13.77044800	7.95358300
H	-26.12042400	12.99168100	8.38726500
N	-27.39053900	13.69102200	6.80353100
C	-28.04225300	14.90149500	6.63078500
H	-28.64722400	15.09435000	5.75822000
C	-25.65858700	10.70857400	6.18626400
O	-26.69639000	10.66256000	6.92762600
O	-25.70058700	11.50364400	5.18212400
H	-23.54025600	10.42131700	6.26380800
H	-24.47047800	9.44243100	7.44870100
H	-24.46676200	9.01674500	5.71908900
C	-24.45600600	9.84800600	6.43500100
C	-28.24599900	17.09399700	8.04399900
H	-28.80812100	17.10006700	8.98574600
H	-27.40640200	17.79145600	8.15176500
H	-28.90059000	17.47273200	7.25462100
H	-32.34002100	11.65352400	9.63816000
H	-32.74549100	10.09552300	8.89902600
H	-31.28870100	10.24980200	9.89621600
C	-31.91499800	10.76200000	9.16099800
C	-29.56788100	12.19160800	1.48249200
C	-30.74213300	11.43630700	1.54379500
C	-30.76533400	10.15437900	2.17001600
C	-29.62875600	9.61526100	2.68910000
C	-28.29229800	10.27368800	2.54546500
C	-28.40129100	11.69239600	2.03065300
N	-27.15920300	12.39069200	1.80107300
O	-26.11449500	11.78275100	2.10091300
O	-27.17941900	13.52156900	1.31257600
H	-29.55906300	13.16782600	1.01178400
H	-31.65412600	11.84140100	1.11723600
H	-31.70614500	9.61703000	2.23940900
H	-29.62820700	8.64830800	3.18321700
H	-27.75863200	9.71326600	1.74943200
O	-28.25395600	12.73872300	4.27899900
O	-27.55480600	10.10701600	3.75811300
H	-26.66521800	10.47907700	3.58240400
Fe	-27.67736100	11.99361300	5.64038900

NBZ-FeV-O1-C2-PC-modell (diol):

C	-31.11441200	11.14095700	7.96088000
---	--------------	-------------	------------

N	-31.67248800	11.78142100	6.86339000
H	-32.65144700	12.02545400	6.75985800
C	-30.71194400	12.02818600	5.95760000
H	-30.87262000	12.51761400	5.01011300
N	-29.54334200	11.57425100	6.40660900
C	-29.78473000	11.01516600	7.65290700
H	-28.99055600	10.57174300	8.23378600
C	-27.77992600	15.72082900	7.68976100
N	-26.93525800	14.97259700	8.49805600
H	-26.52853400	15.28324200	9.37386100
C	-26.72181800	13.77329600	7.92921500
H	-26.10957800	12.99361000	8.35574200
N	-27.38861700	13.69848100	6.78052700
C	-28.04577500	14.90935900	6.61873700
H	-28.65238600	15.10866600	5.74879600
C	-25.65736700	10.70656200	6.16533100
O	-26.74243400	10.58036600	6.82272800
O	-25.64640900	11.57178900	5.21966900
H	-23.53684800	10.41915800	6.28036900
H	-24.49047400	9.43964100	7.44723200
H	-24.45802300	9.01430300	5.72135100
C	-24.45600600	9.84800600	6.43500100
C	-28.24599900	17.09399700	8.04399900
H	-28.80397900	17.09474300	8.98810400
H	-27.40576200	17.79058600	8.15147200
H	-28.90403500	17.47569500	7.25904600
H	-32.35039200	11.64487600	9.64493200
H	-32.73741300	10.08519300	8.90006700
H	-31.27750100	10.25510300	9.89019300
C	-31.91499800	10.76200000	9.16099800
C	-29.48266700	13.16887300	2.02665400
C	-30.65185200	12.53439500	1.83048000
C	-30.87928400	11.16096900	2.28578300
C	-29.87484900	10.42528700	2.78731100
C	-28.46582100	10.93928400	2.76128700
C	-28.37233100	12.48750100	2.77772700
N	-26.98279400	12.86896600	2.09785800
O	-26.10103500	12.00884700	2.09930600
O	-26.84439200	14.01225500	1.69414700
H	-29.33007300	14.20800200	1.75865900
H	-31.47437600	13.06000100	1.35246200
H	-31.88244400	10.75110600	2.21264300
H	-30.01077700	9.40243000	3.12682300
H	-27.99106800	10.56423000	1.84565300
O	-28.25360500	12.97361900	4.05699000
O	-27.72965500	10.42977100	3.89079000
H	-26.78193800	10.50478700	3.65312400
Fe	-27.68456600	12.02614200	5.56905000

Nitrobenzene Model 2

NBZ-FeV-O1-C2-TS1-model2:

C	-31.10569600	11.16609500	7.97271200
N	-31.66653700	11.78066900	6.86217500
H	-32.65023700	11.99582400	6.74319200
C	-30.69555800	12.05849400	5.97243000
H	-30.85254800	12.55486700	5.02778000
N	-29.52264100	11.65142800	6.44563900
C	-29.76540200	11.08840400	7.68674300
H	-28.96543900	10.67742000	8.28400900
C	-27.75139200	15.72193900	7.70753000
N	-26.90436700	14.98027900	8.52177000
H	-26.50324200	15.29348100	9.39904000
C	-26.67644800	13.78031400	7.95339200
H	-26.05789600	13.00712300	8.38204000
N	-27.33546800	13.70038400	6.80173300
C	-28.00002900	14.90595300	6.63686300
H	-28.60675000	15.09393700	5.76561700
C	-29.14572700	18.24921000	0.32215100
H	-30.05038800	17.66643600	0.54013300
H	-28.77406700	17.87642800	-0.64298800
C	-28.08531000	17.93213300	1.37848800
O	-27.41586200	18.80255600	1.93086600
N	-27.93768500	16.60822100	1.67133900
H	-27.16698900	16.32875400	2.26492500
H	-28.39053800	15.87048800	1.14695000
C	-25.56172700	10.83136900	6.11543500
O	-26.68940200	10.76058900	6.74012500
O	-25.44985200	11.69526000	5.20071900
H	-23.49362500	10.22875300	6.08653800
H	-24.42087300	9.64611800	7.50912100
H	-24.66668000	8.90058500	5.92337100
Fe	-27.65474100	12.09881500	5.54853300
C	-24.45600400	9.84800300	6.43500000
C	-28.24600000	17.09400100	8.04400000
H	-28.81301400	17.09602200	8.98272700
H	-27.41942300	17.80704100	8.15008100
H	-28.90243600	17.45248300	7.24696600
C	-29.46900000	19.74099900	0.22200000
H	-32.39703200	11.62883600	9.62955800
H	-32.70339900	10.04971300	8.88894400
H	-31.27215200	10.28711400	9.90699500
H	-30.19683400	19.92145000	-0.57695400
H	-29.89075100	20.12021600	1.15914600
H	-28.56816800	20.32316800	0.00595700
C	-31.91499900	10.76200000	9.16099800

C	-26.75971300	10.75710800	2.47184000
C	-26.61606600	9.34749600	2.29893800
C	-27.44222100	8.65657500	1.42380600
C	-28.39495900	9.35150000	0.66692000
C	-28.49898900	10.75639600	0.74775900
C	-27.66341200	11.43487000	1.60690400
N	-27.66728900	12.90072100	1.59505100
O	-28.64458300	13.46792700	1.09968100
O	-26.67911000	13.47624200	2.04332500
H	-26.01368900	11.32008300	3.01736500
H	-25.87025100	8.82585400	2.89062800
H	-27.34535400	7.58127800	1.31565100
H	-29.04630500	8.81457500	-0.01511100
H	-29.19674100	11.29678000	0.11932100
O	-28.28519700	13.11145700	4.44404900
O	-27.93878800	10.55958300	4.22092600
H	-27.54808900	9.75448000	4.61828600

NBZ-FeV-O1-C2-INT1-model2 (radical intermediate):

C	-2.76695600	-1.84189700	3.42410600
N	-3.35875500	-1.12550900	2.39174200
H	-4.33988100	-0.87293900	2.33673800
C	-2.42935600	-0.80799500	1.47710400
H	-2.61401700	-0.24371300	0.57671600
N	-1.24942400	-1.29238000	1.86082800
C	-1.44712200	-1.94013900	3.07181400
H	-0.63341300	-2.41836500	3.59369100
C	0.71229000	2.87207200	3.06653600
N	2.04653400	2.50290000	3.12352200
H	2.80109100	3.07086300	3.49194300
C	2.18840700	1.27263400	2.59217600
H	3.13191500	0.76194200	2.48672900
N	1.00561200	0.81784400	2.19900300
C	0.08056400	1.80622600	2.48373400
H	-0.96494400	1.69410500	2.24340400
C	-0.28680800	5.56854000	-4.60245200
H	-0.30547600	5.33067500	-5.67360500
H	0.75071400	5.85205100	-4.37334800
C	-0.59514700	4.30489300	-3.79472200
O	-1.22098400	4.32575200	-2.73650400
N	-0.10975500	3.15243600	-4.33519500
H	-0.16941500	2.28401000	-3.81576700
H	0.46885100	3.16053800	-5.16394700
C	2.58031300	-2.04300400	1.67758900
O	1.47120200	-2.15704000	2.30599600
O	2.59947500	-1.22032700	0.69869700
H	4.69826900	-2.33409500	1.79440700
H	3.75663400	-3.11365000	3.11260800
H	3.74824100	-3.79781200	1.47439500

Fe	0.54555900	-0.87926000	1.04764000
C	3.77657400	-2.86317300	2.04918900
C	0.20130800	4.18340900	3.55562200
H	0.38281500	4.31421000	4.62960800
H	0.68082500	5.01987700	3.03276700
H	-0.87599600	4.25008500	3.38215100
C	-1.22576900	6.73409800	-4.28838100
H	-3.98224800	-1.48809100	5.16068900
H	-4.33023100	-3.01236400	4.32799900
H	-2.85431200	-2.84884700	5.29649900
H	-2.25927100	6.49848400	-4.56645200
H	-1.21438300	6.96468700	-3.21897600
H	-0.92180000	7.63053800	-4.83989800
C	-3.52702200	-2.32278400	4.61428300
C	-2.10123800	-1.88734000	-2.70418600
C	-2.98624000	-2.85026700	-2.19326800
C	-2.51542400	-3.88773800	-1.33848500
C	-1.19534500	-3.98379000	-1.01240300
C	-0.15642500	-3.07616800	-1.59431200
C	-0.75875900	-1.96046400	-2.40755400
N	0.14817800	-1.01160000	-2.97198700
O	1.36600300	-1.18542200	-2.75429300
O	-0.29246700	-0.07414100	-3.65039800
H	-2.46235100	-1.08536300	-3.33798900
H	-4.04039800	-2.78910600	-2.44210600
H	-3.22670300	-4.60003900	-0.93112600
H	-0.82911300	-4.76005900	-0.34728900
H	0.47799800	-3.68260100	-2.26574000
O	-0.05783100	0.05873900	-0.13307700
O	0.72558500	-2.62299100	-0.53527200
H	1.47700200	-2.19877400	-1.00035200

NBZ-FeV-O1-C2-TS2-model2:

C	-31.05632000	11.15410100	8.01834500
N	-31.61597800	11.78109700	6.91290900
H	-32.59696600	12.01555000	6.80485200
C	-30.65538700	12.03849900	6.01092600
H	-30.81073300	12.53188300	5.06491200
N	-29.48454600	11.60369500	6.47215600
C	-29.72185400	11.04759800	7.72176300
H	-28.92439500	10.61843000	8.30859100
C	-27.67147200	15.86559000	7.48436100
N	-26.31575300	15.65178900	7.28710700
H	-25.57677300	16.31508900	7.49273700
C	-26.13024000	14.42115400	6.77192100
H	-25.17070300	14.00716400	6.50423700
N	-27.30350000	13.81535200	6.63019600
C	-28.27006600	14.70682600	7.06552900
H	-29.32070500	14.46338300	7.04575900

C	-28.47086400	18.61024600	-0.03861600
H	-28.47619000	18.30634300	-1.09280800
H	-27.45243100	18.96992900	0.16887200
C	-28.69962700	17.38534000	0.84787400
O	-29.30140300	17.43861100	1.91831300
N	-28.18234700	16.22115300	0.35914800
H	-28.12954200	15.41309300	0.96828800
H	-27.56675200	16.22611800	-0.44346500
C	-25.63907700	10.75927500	6.19540700
O	-26.69477800	10.66233100	6.90036400
O	-25.67099100	11.59806600	5.22166600
H	-23.51568600	10.49302500	6.27663600
H	-24.44117200	9.48616000	7.44211700
H	-24.42810000	9.08749000	5.70655800
Fe	-27.67007800	12.01529200	5.63152100
C	-24.42600100	9.90800000	6.43500000
C	-28.23600000	17.13400100	8.03400100
H	-27.87008100	17.33339300	9.04853100
H	-27.97087500	17.99449600	7.40799400
H	-29.32638900	17.06714000	8.07288600
C	-29.47900000	19.73099900	0.21200000
H	-32.32816300	11.63708400	9.68275800
H	-32.66638900	10.06383000	8.94143700
H	-31.22513800	10.27549000	9.95177900
H	-29.23140900	20.61271200	-0.38925300
H	-30.49608300	19.41750900	-0.04982300
H	-29.48240000	20.02067100	1.26701500
C	-31.86499900	10.76200000	9.21099900
C	-29.63089300	11.98061300	1.51200100
C	-30.78665300	11.21056900	1.66205400
C	-30.76028100	9.96623000	2.36030500
C	-29.59492000	9.47575100	2.86331000
C	-28.27669600	10.14657300	2.63085900
C	-28.43401800	11.53221300	2.04098500
N	-27.22113500	12.24434200	1.74520600
O	-26.15145100	11.68958600	2.06006600
O	-27.27353600	13.34467200	1.18374600
H	-29.66181900	12.93054100	0.99101600
H	-31.72251200	11.57617800	1.25216400
H	-31.68760600	9.41871800	2.49850000
H	-29.55843300	8.53812800	3.40999700
H	-27.75914200	9.54862100	1.85186100
O	-28.27332400	12.67652700	4.24409400
O	-27.49338300	10.06683900	3.82496000
H	-26.62433200	10.45618600	3.59419600

NBZ-FeV-O1-C2-PC-model2 (diol):

C	-2.79814200	-1.76574200	3.49015800
N	-3.37883600	-1.16543900	2.38037900

H	-4.36810400	-0.97157900	2.26695400
C	-2.42673900	-0.88165800	1.47703700
H	-2.60631400	-0.41628100	0.52079700
N	-1.23880100	-1.26979600	1.94170000
C	-1.46081100	-1.82484000	3.19421600
H	-0.64893900	-2.22279500	3.78334800
C	0.60473600	2.95244000	2.88981700
N	1.91487300	2.82847700	2.44841400
H	2.63005200	3.54449000	2.51627300
C	2.09382500	1.60596800	1.91881200
H	3.01881700	1.24798200	1.49425300
N	0.95846400	0.91458500	1.99300700
C	0.02637800	1.74520400	2.59945600
H	-0.98671900	1.42430500	2.78235600
C	-0.24486500	5.61915200	-4.14252100
H	-0.29808600	4.93419400	-4.99766500
H	0.79097800	5.98742800	-4.11179100
C	-0.47789700	4.83844300	-2.84946300
O	-1.03018600	5.32119100	-1.86430100
N	-0.02221500	3.54999500	-2.86844900
H	0.01703000	3.03967900	-1.99487200
H	0.56523700	3.21281400	-3.61895000
C	2.62419500	-2.17668200	1.66813800
O	1.53276200	-2.35435000	2.29097200
O	2.62956300	-1.27902900	0.74435200
H	4.74849700	-2.39701800	1.86908800
H	3.78021600	-3.51161100	2.89252800
H	3.91440900	-3.77591700	1.13733500
Fe	0.58544100	-0.89569200	1.01267700
C	3.84693000	-3.01328100	1.92342400
C	0.05866000	4.20058700	3.50395900
H	0.61399300	4.48512300	4.40557900
H	0.10480400	5.04154700	2.80166500
H	-0.98741100	4.04807100	3.78199900
C	-1.20852800	6.79227200	-4.32038200
H	-4.10000600	-1.33543100	5.14730000
H	-4.36103400	-2.92440000	4.40849700
H	-2.93649100	-2.64419500	5.42578600
H	-0.95596300	7.36348500	-5.22037900
H	-2.24364300	6.44562700	-4.41822000
H	-1.16379900	7.46564500	-3.45934100
C	-3.59416400	-2.18930600	4.68056300
C	-1.31035200	-0.20682100	-2.60078900
C	-2.47083000	-0.88134900	-2.68583600
C	-2.65999800	-2.19240400	-2.06059000
C	-1.62850300	-2.84292400	-1.49969600
C	-0.23133300	-2.31368900	-1.63699900
C	-0.16894200	-0.77439500	-1.80282700
N	1.19947900	-0.45694000	-2.55899200
O	2.10594600	-1.28361900	-2.45209400

O	1.30677900	0.62211100	-3.12169200
H	-1.19272600	0.79812500	-2.99042600
H	-3.31625300	-0.42949200	-3.19806300
H	-3.65693200	-2.62332300	-2.05355800
H	-1.73397000	-3.81789300	-1.03271100
H	0.21708500	-2.78677200	-2.52005000
O	-0.02167500	-0.13724000	-0.59622500
O	0.55525500	-2.67310700	-0.48490000
H	1.48931600	-2.61012000	-0.77266500

2-nitrotoluene Model 1

2NT-FeV-O1-C2-TS1-modell:

C	-4.5135730	-3.8389890	0.6804990
C	-3.5008750	-2.8912570	0.1317930
C	-2.5920130	-2.0580420	0.7330330
N	-3.3141400	-2.6941100	-1.2288210
C	-2.3376060	-1.7845370	-1.4125670
N	-1.8804920	-1.3747620	-0.2366310
H	-4.4870990	-3.8214640	1.7733980
H	-4.3204330	-4.8683480	0.3539780
H	-5.5289640	-3.5735470	0.3612220
H	-3.8277280	-3.1602930	-1.9682780
H	-2.4006530	-1.9047210	1.7842920
H	-1.9889850	-1.4420220	-2.3741690
C	-4.4765400	3.7393020	-1.2713350
C	-3.4582860	2.9434950	-0.5101130
C	-2.4065360	2.1630770	-0.9172180
N	-3.4506500	2.8387020	0.8749770
C	-2.4474160	2.0231230	1.2557410
N	-1.7894730	1.5910410	0.1854970
H	-4.2524820	3.6988330	-2.3405440
H	-4.4778890	4.7914480	-0.9627740
H	-5.4878350	3.3433720	-1.1187600
H	-4.0965440	3.3004680	1.5055710
H	-2.0562370	1.9610400	-1.9173830
H	-2.2311260	1.7561800	2.2783970
C	1.4374550	0.5157490	3.5657210
C	0.7343550	0.4824850	2.2328160
O	-0.3370370	-0.2120000	2.0684540
O	1.2037910	1.0728470	1.2121490
H	1.9201960	1.4852280	3.7148170
H	2.2163990	-0.2557110	3.5642320
H	0.7392720	0.3066500	4.3796280
Fe	-0.3648540	0.0629380	0.0463460
O	-0.1630690	0.4033870	-1.5304500
O	0.9150610	-1.5539450	-0.0479890
H	1.4548410	-1.6227890	0.7702210
C	2.8632830	-1.5220040	-1.0863520

N	3.8573960	-0.5749840	0.9251240
O	3.2549800	-1.4500250	1.5762100
C	3.4698360	-0.3966360	-0.4686000
O	4.7488280	0.1191490	1.3984110
C	3.6413280	0.8243760	-1.1226360
C	3.2015750	0.8666170	-2.4691740
C	2.6392080	-0.2359220	-3.1202520
C	2.4766300	-1.4341860	-2.4418600
C	4.2092840	2.0703370	-0.5003760
H	3.3089190	1.8038470	-3.0071730
H	2.3383810	-0.1475910	-4.1593090
H	2.0608110	-2.3086810	-2.9301630
H	2.9531080	-2.4930620	-0.6188160
H	4.0181450	2.9275030	-1.1513280
H	3.7619490	2.2654040	0.4786590
H	5.2905790	1.9834410	-0.3507020

2NT-FeV-O1-C2-INT1-model1 (radical intermediate):

C	-1.6866830	4.6145820	-1.7944890
C	-1.1970900	3.3946710	-1.0890240
C	-1.1408280	2.0736600	-1.4506020
N	-0.6971900	3.4305050	0.2055540
C	-0.3674030	2.1868600	0.5904100
N	-0.6246200	1.3344180	-0.3970930
H	-2.0036090	4.3576510	-2.8086510
H	-0.9051300	5.3805860	-1.8652370
H	-2.5428460	5.0588620	-1.2722820
H	-0.5969290	4.2636310	0.7753100
H	-1.4370030	1.6046090	-2.3763230
H	0.0396850	1.9251240	1.5538820
C	-5.1574060	-0.0887590	3.1502780
C	-4.2662640	-0.4021780	1.9910450
C	-2.9030870	-0.4871270	1.8739450
N	-4.7434810	-0.6585070	0.7130760
C	-3.7039760	-0.8733700	-0.1153690
N	-2.5642570	-0.7725600	0.5605970
H	-4.5550040	0.0664770	4.0491310
H	-5.8612280	-0.9057130	3.3501760
H	-5.7433790	0.8207630	2.9704710
H	-5.7203160	-0.6835020	0.4415800
H	-2.1468190	-0.3617170	2.6333240
H	-3.7940670	-1.0847630	-1.1692620
C	-0.8354320	-3.1634920	-3.2239150
C	-0.8638610	-2.2512920	-2.0357790
O	-1.2752440	-1.0401610	-2.1137380
O	-0.4170280	-2.6224020	-0.8950800
H	-0.9097000	-4.2067030	-2.9081040
H	0.1249180	-3.0247600	-3.7370710
H	-1.6377250	-2.9125450	-3.9220540

Fe	-0.6124180	-0.6817980	-0.2203020
O	0.0483130	-0.6836720	1.2622050
O	1.5356960	-0.8553560	-1.2214410
H	1.6811210	-1.7969030	-0.9795140
C	2.8261860	-0.2390740	-0.9761610
N	3.2867010	-1.6857310	0.9677610
O	2.9527860	-2.5981970	0.1710730
C	3.2777460	-0.3482540	0.4644190
O	3.6176780	-1.9227570	2.1340190
C	3.7488680	0.7319710	1.2042190
C	3.7665410	1.9955390	0.5607060
C	3.2948490	2.1969050	-0.7614960
C	2.8037700	1.1591150	-1.4937140
C	4.2493620	0.6667990	2.6253010
H	4.1499310	2.8439660	1.1186420
H	3.3167280	3.1989500	-1.1797910
H	2.4174660	1.2940610	-2.4990540
H	3.5442730	-0.8102100	-1.5915680
H	4.5680130	1.6614000	2.9491010
H	3.4727840	0.3049630	3.3060160
H	5.0922800	-0.0233340	2.7249200

2NT-FeV-O1-C2-TS2-modell1:

C	-3.0177050	4.4964370	-1.1742510
C	-2.1223100	3.3898680	-0.7273490
C	-1.8183290	2.1640950	-1.2619510
N	-1.3922850	3.4538180	0.4504640
C	-0.6969770	2.3137210	0.6040260
N	-0.9324810	1.5036120	-0.4236600
H	-3.4762260	4.2414080	-2.1333210
H	-2.4643370	5.4348970	-1.3012620
H	-3.8219000	4.6786160	-0.4510950
H	-1.3842210	4.2354540	1.0963480
H	-2.1729510	1.7103690	-2.1747500
H	-0.0499080	2.0940760	1.4377530
C	-4.2096560	-1.3169530	3.6632880
C	-3.5122890	-1.3129490	2.3430990
C	-2.2134290	-1.0582350	1.9893730
N	-4.1614830	-1.5610790	1.1422670
C	-3.2819910	-1.4498830	0.1291940
N	-2.0831580	-1.1381930	0.6122920
H	-3.4916200	-1.1163720	4.4628210
H	-4.6840810	-2.2842230	3.8680290
H	-4.9901620	-0.5472930	3.7044930
H	-5.1417910	-1.8007190	1.0425460
H	-1.3689320	-0.8203320	2.6173550
H	-3.5278480	-1.5774920	-0.9136730
C	-0.7708330	-2.6829220	-3.7577890
C	-0.7073500	-1.8884440	-2.4854620

O	-1.3262750	-0.7802410	-2.3455790
O	0.0169020	-2.2789280	-1.5056380
H	0.1183310	-2.4496960	-4.3574090
H	-1.6599800	-2.4221490	-4.3362970
H	-0.7553940	-3.7537390	-3.5379390
Fe	-0.4204390	-0.4995430	-0.4700370
O	0.6367780	-0.4499950	0.8089500
O	1.7208170	-0.1793700	-1.6765720
H	1.8673820	-1.1494050	-1.7079510
C	2.8544600	0.3479590	-0.9717000
N	3.1146730	-1.6229070	0.5148630
O	3.0398420	-2.2419740	-0.5676080
C	3.0440120	-0.1831540	0.4410140
O	3.2524520	-2.1882750	1.6004970
C	3.4606860	0.6302170	1.4987640
C	3.5404330	2.0149340	1.2443930
C	3.2061930	2.6080710	-0.0026730
C	2.8196900	1.8361280	-1.0527450
C	3.8088120	0.1451970	2.8836800
H	3.8580650	2.6591850	2.0584660
H	3.2485350	3.6886920	-0.0988620
H	2.5397120	2.2587210	-2.0125480
H	3.7581770	0.0307800	-1.5304230
H	4.1185440	0.9919870	3.5024630
H	2.9527050	-0.3448020	3.3574410
H	4.6178210	-0.5908570	2.8653350

2NT-FeV-O1-C2-PC-model1 (diol):

C	3.8832700	4.1225780	-0.0470390
C	2.7047420	3.2079620	-0.0643360
C	2.3679500	2.1077250	0.6807820
N	1.6696090	3.3458750	-0.9780830
C	0.7736360	2.3638640	-0.7865320
N	1.1681890	1.5864750	0.2198520
H	4.5664460	3.8365040	0.7568820
H	3.5817870	5.1641280	0.1177220
H	4.4338740	4.0793810	-0.9946080
H	1.5974400	4.0741060	-1.6801110
H	2.8976150	1.6521340	1.5031230
H	-0.1274600	2.2343490	-1.3644520
C	3.1229550	-2.5929250	-3.6445390
C	2.7022180	-2.1662120	-2.2773650
C	1.5502620	-1.5948040	-1.8058120
N	3.5161280	-2.2922340	-1.1599260
C	2.8733300	-1.8090870	-0.0828040
N	1.6695010	-1.3705220	-0.4422290
H	2.3196550	-2.3928060	-4.3583470
H	3.3489500	-3.6655810	-3.6784350
H	4.0177550	-2.0523420	-3.9758930

H	4.4466510	-2.6957340	-1.1521730
H	0.6514570	-1.3282060	-2.3395990
H	3.2860420	-1.7754060	0.9133820
C	0.9292130	-1.8355780	4.3164720
C	0.7574700	-1.2708770	2.9363760
O	1.4478090	-0.2868690	2.5151430
O	-0.1390190	-1.7356050	2.1454190
H	0.2279070	-1.3259270	4.9895160
H	1.9436430	-1.6603890	4.6819320
H	0.6942780	-2.9026220	4.3260970
Fe	0.3199120	-0.2646080	0.6870230
O	-1.0406740	-0.2507930	-0.5979410
O	-1.5269180	0.5264150	1.8196200
H	-1.6945670	-0.2708460	2.3587340
C	-2.6444370	0.7296400	0.9231470
N	-3.0086840	-1.5263270	-0.1362100
O	-4.2046720	-1.5492640	0.1438470
C	-2.3699260	-0.0811540	-0.3869430
O	-2.2899660	-2.5035710	-0.2657330
C	-3.0597770	0.4693240	-1.6327580
C	-3.4325690	1.7639100	-1.6408470
C	-3.2578540	2.6555310	-0.4953970
C	-2.8322550	2.1978340	0.6914970
C	-3.1498330	-0.4293010	-2.8331880
H	-3.8476030	2.1855720	-2.5532430
H	-3.4778550	3.7107740	-0.6311960
H	-2.6971710	2.8446100	1.5535930
H	-3.5491250	0.3353700	1.4008740
H	-3.5025810	0.1286970	-3.7053350
H	-2.1751110	-0.8697990	-3.0760880
H	-3.8458000	-1.2621030	-2.6659330

2-nitrotoluene Model 2

2NT-FeV-O1-C2-TS1-model2:

C	5.1414490	0.2966620	3.6447110
C	3.9282400	0.2014340	2.7766490
C	3.7485320	0.0119020	1.4281830
N	2.6450580	0.3230780	3.2884600
C	1.7555190	0.2123020	2.2848200
N	2.3934450	0.0202010	1.1358210
H	6.0444490	0.1709440	3.0413780
H	5.1417990	-0.4785550	4.4207080
H	5.1994610	1.2709390	4.1450620
H	2.4131730	0.4749620	4.2637260
H	4.4895690	-0.1206860	0.6544740
H	0.6857640	0.2818010	2.4018700
C	-0.0603930	5.3427290	0.6898550
C	0.6386090	4.1797280	0.0547040

C	0.3036920	2.8547790	-0.0423360
N	1.8769310	4.2716200	-0.5681690
C	2.2510050	3.0516650	-1.0012050
N	1.3137300	2.1618460	-0.6918520
H	-1.0206650	5.0161560	1.0974730
H	-0.2521470	6.1436540	-0.0342380
H	0.5328550	5.7672970	1.5087840
H	2.4164090	5.1220570	-0.6861580
H	-0.5798690	2.3485910	0.3134080
H	3.1781130	2.8370340	-1.5091350
C	3.5730180	-0.3795480	-4.0874140
C	2.6815890	-0.0529230	-2.9078740
O	3.1899960	0.1313280	-1.7376240
O	1.4220370	-0.0125220	-3.0192880
H	3.0787240	-0.1102510	-5.0234810
H	3.7603490	-1.4605720	-4.0877970
H	4.5355380	0.1316820	-4.0006420
Fe	1.4215540	0.0902270	-0.7393760
O	-0.0853180	0.0283220	-0.1167860
O	1.3951560	-1.9178560	-1.2066640
H	0.8119090	-1.8811660	-1.9955860
C	0.1533630	-3.4310730	-0.4476720
N	-1.8717890	-2.3482420	-1.2587630
O	-1.2873570	-2.2209280	-2.3423850
C	-1.0883280	-2.8135590	-0.1216820
O	-3.0710300	-2.1146490	-1.1014950
C	-1.5155430	-2.6273540	1.1926490
C	-0.6490170	-3.1338690	2.2014410
C	0.5612990	-3.7739310	1.9190940
C	0.9654510	-3.9363720	0.6038620
C	-2.7902480	-1.9570160	1.6243070
H	-0.9569270	-3.0131430	3.2355340
H	1.1714890	-4.1532050	2.7325580
H	1.8867370	-4.4506880	0.3534630
H	0.2773600	-3.8437480	-1.4400640
H	-2.7666740	-1.7841070	2.7040190
H	-2.9673250	-1.0031860	1.1204560
H	-3.6576240	-2.5875010	1.3983420
C	-7.6161940	1.8915290	1.2806370
H	-8.3932770	2.6627410	1.2464190
H	-8.1050840	0.9250480	1.4504150
H	-6.9640650	2.0932400	2.1358050
C	-6.8068970	1.8841810	-0.0198630
H	-7.4499770	1.6521390	-0.8766570
H	-6.3958470	2.8874880	-0.2006590
C	-5.6171680	0.9245040	0.0230510
O	-4.9206640	0.7843850	1.0301190
N	-5.3654950	0.2619730	-1.1357430
H	-4.5670200	-0.3593150	-1.1992420
H	-5.9411760	0.3818690	-1.9572270

2NT-FeV-O1-C2-INT1-model2 (radical intermediate):

C	4.6242880	0.5679890	3.8121850
C	3.4902880	0.3908080	2.8558430
C	3.4277750	0.2913810	1.4892720
N	2.1697630	0.3139280	3.2768120
C	1.3672990	0.1811840	2.2087570
N	2.1019640	0.1625300	1.0994660
H	5.5718090	0.5959260	3.2678280
H	4.6709410	-0.2540400	4.5365670
H	4.5265270	1.5044500	4.3744140
H	1.8552680	0.3512490	4.2404980
H	4.2281270	0.3119420	0.7654140
H	0.2920770	0.1124550	2.2494310
C	-0.5349310	5.4403350	0.9356710
C	0.2645740	4.3735360	0.2606470
C	0.0227620	3.0401930	0.0634120
N	1.5186940	4.5887130	-0.2946130
C	1.9922240	3.4279840	-0.7877260
N	1.1041120	2.4611250	-0.5809200
H	-1.4931930	5.0301550	1.2648130
H	-0.7382440	6.2811140	0.2614760
H	-0.0119790	5.8358710	1.8150100
H	1.9998010	5.4806360	-0.3349400
H	-0.8408490	2.4568060	0.3421170
H	2.9524800	3.3112960	-1.2651320
C	-8.0154300	1.7478300	0.9235320
H	-7.4073180	2.4184180	1.5380300
H	-8.9024930	2.2942870	0.5852710
H	-8.3490230	0.9219500	1.5622630
C	-7.2128360	1.2349840	-0.2738110
H	-6.9542510	2.0752600	-0.9344200
H	-7.8133130	0.5450880	-0.8793990
C	-5.8961140	0.5624730	0.1216180
N	-5.4298660	-0.3524140	-0.7744590
O	-5.2951620	0.8333590	1.1595830
H	-5.8834510	-0.4987230	-1.6658370
H	-4.5042620	-0.7458990	-0.6513470
C	3.4839130	0.1717410	-4.0498640
C	2.6410330	0.3646080	-2.8218530
O	3.1594090	0.5683240	-1.6661490
O	1.3662310	0.2791170	-2.8600200
H	2.9461270	0.5115790	-4.9383550
H	3.6879940	-0.9009810	-4.1603420
H	4.4369510	0.6967190	-3.9502640
Fe	1.3424760	0.3926520	-0.7755840
O	-0.2008010	0.1528180	-0.3316880
O	1.4741570	-1.8890130	-1.3527640

H	0.8992790	-1.7924230	-2.1428310
C	0.9892580	-3.0980320	-0.7113130
N	-1.3710810	-2.5930370	-1.2219170
O	-0.9228940	-2.4140340	-2.3796440
C	-0.4392600	-2.9964410	-0.2181800
O	-2.5694040	-2.4401880	-0.9500470
C	-0.8347720	-3.3799980	1.0602970
C	0.1775550	-3.8485820	1.9363830
C	1.5486300	-3.9017540	1.5779690
C	1.9622680	-3.5061240	0.3424440
C	-2.2490980	-3.3496940	1.5835400
H	-0.1193120	-4.1663530	2.9307500
H	2.2701250	-4.2485000	2.3119240
H	3.0084710	-3.5183300	0.0525250
H	1.0117830	-3.8720540	-1.4991840
H	-2.2707830	-3.7251160	2.6102210
H	-2.6598550	-2.3354530	1.5701120
H	-2.9177380	-3.9617980	0.9708920

2NT-FeV-O1-C2-TS2-model2:

C	5.0288050	0.9142850	3.8078360
C	3.8764260	0.5756600	2.9178030
C	3.7252990	0.5461290	1.5546180
N	2.6340370	0.2090470	3.4183280
C	1.7907660	-0.0198550	2.3978280
N	2.4239070	0.1764160	1.2434050
H	5.9025800	1.1735860	3.2043140
H	5.2989880	0.0697590	4.4531650
H	4.7949230	1.7689350	4.4540490
H	2.3953170	0.1311990	4.4010530
H	4.4470690	0.7608080	0.7818270
H	0.7592890	-0.3168350	2.5020120
C	-0.4802450	5.3324370	0.8477910
C	0.1064540	4.1929700	0.0817200
C	0.6165230	2.9861610	0.4818510
N	0.2037490	4.1740600	-1.3010370
C	0.7417900	3.0024990	-1.6925890
N	1.0104910	2.2563380	-0.6275670
H	-0.4587370	5.1102680	1.9179750
H	-1.5231390	5.5115690	0.5591060
H	0.0763320	6.2629170	0.6819910
H	-0.0903370	4.9189820	-1.9227510
H	0.7153530	2.5980390	1.4834810
H	0.9018080	2.7128710	-2.7194810
C	-7.7505900	1.2721570	1.3466050
H	-7.2479770	1.3098720	2.3177160
H	-8.5466660	2.0245200	1.3377470
H	-8.2161220	0.2847380	1.2469070
C	-6.7532750	1.5343990	0.2149380

H	-6.3643230	2.5594310	0.2982770
H	-7.2485510	1.4706320	-0.7612300
C	-5.5413860	0.6022100	0.2507590
N	-5.0296600	0.2725850	-0.9639710
O	-5.0456240	0.2023960	1.3056270
H	-4.1899940	-0.2918610	-1.0199230
H	-5.4373090	0.6072920	-1.8256850
C	3.6313360	-0.0233190	-3.9662990
C	2.8338090	0.1543520	-2.7026260
O	3.3884410	0.3103210	-1.5664400
O	1.5520020	0.1066020	-2.7235260
H	3.7184110	-1.0972220	-4.1745970
H	4.6350520	0.3925730	-3.8532680
H	3.1150910	0.4426160	-4.8097820
Fe	1.5210410	0.2192090	-0.6071890
O	0.0329240	-0.2780980	-0.0788430
O	1.5811410	-2.1561560	-1.2184300
H	1.1500120	-1.9838700	-2.0830070
C	0.7198690	-3.0903110	-0.5491230
N	-1.3724820	-2.1728690	-1.5190410
O	-0.7236080	-2.2451690	-2.5845610
C	-0.7115590	-2.6211460	-0.3242360
O	-2.5328750	-1.7493670	-1.4785940
C	-1.4225920	-2.9212860	0.8431200
C	-0.6944830	-3.5143990	1.8963980
C	0.6961860	-3.7971770	1.8326650
C	1.3992570	-3.5518200	0.6955410
C	-2.8919510	-2.6674920	1.0669080
H	-1.2317010	-3.7466010	2.8108130
H	1.1907760	-4.2042050	2.7094500
H	2.4639770	-3.7485720	0.6170860
H	0.6414720	-3.9790850	-1.2066230
H	-3.1904340	-3.0935160	2.0288430
H	-3.1363620	-1.5999010	1.0743000
H	-3.5040120	-3.1203660	0.2814070

2NT-FeV-O1-C2-PC-model2 (diol):

C	-0.06000000	5.15700000	-0.97300000
C	-0.75800000	4.01100000	-0.31700000
C	-0.44000000	2.68400000	-0.19300000
N	-1.98200000	4.14100000	0.32400000
C	-2.36800000	2.94400000	0.79700000
N	-1.45000000	2.02800000	0.49500000
H	0.89000000	4.82000000	-1.39600000
H	0.15200000	5.96100000	-0.25700000
H	-0.66300000	5.58200000	-1.78400000
H	-2.50400000	5.00500000	0.42500000
H	0.43500000	2.15600000	-0.54000000
H	-3.29000000	2.76400000	1.32800000

C	-3.63700000	-0.30100000	4.14300000
C	-2.86300000	-0.13200000	2.86700000
O	-3.44400000	-0.11800000	1.73100000
O	-1.58500000	-0.04800000	2.87100000
H	-3.70200000	-1.37300000	4.36900000
H	-4.65300000	0.08600000	4.03200000
H	-3.12500000	0.19200000	4.97300000
Fe	-1.59500000	-0.03900000	0.70900000
O	0.10400000	-0.41800000	0.04000000
O	-1.16700000	-2.19200000	1.36500000
H	-1.01100000	-1.97800000	2.30600000
C	0.04800000	-2.73400000	0.79100000
N	2.09800000	-1.25900000	1.03700000
O	2.83300000	-2.20600000	1.28800000
C	0.83700000	-1.55500000	0.09300000
O	2.27600000	-0.10500000	1.41000000
C	1.45000000	-1.87300000	-1.27000000
C	1.12700000	-3.02400000	-1.89000000
C	0.22500000	-4.02200000	-1.32400000
C	-0.32000000	-3.87300000	-0.10800000
C	2.30800000	-0.80800000	-1.89400000
H	1.52800000	-3.21300000	-2.88300000
H	-0.01300000	-4.89400000	-1.92700000
H	-1.00600000	-4.60300000	0.31300000
H	0.65900000	-3.12900000	1.61000000
H	2.54800000	-1.07500000	-2.92800000
H	1.79300000	0.16000000	-1.90100000
H	3.25700000	-0.66600000	-1.35900000
C	-5.24700000	0.21600000	-3.62700000
C	-4.08900000	-0.08600000	-2.74000000
C	-3.91500000	-0.02700000	-1.38100000
N	-2.85700000	-0.48700000	-3.23700000
C	-1.99700000	-0.64600000	-2.21800000
N	-2.60800000	-0.36900000	-1.06800000
H	-6.11600000	0.49900000	-3.02500000
H	-5.52400000	-0.65400000	-4.23400000
H	-5.02100000	1.04200000	-4.31000000
H	-2.64000000	-0.63900000	-4.21700000
H	-4.62600000	0.24100000	-0.61500000
H	-0.96900000	-0.95600000	-2.32600000
C	7.47300000	1.65200000	-1.49400000
H	8.47700000	2.07800000	-1.60300000
H	7.39500000	0.77900000	-2.14900000
H	6.75100000	2.39800000	-1.84400000
C	7.20900000	1.26100000	-0.04000000
H	7.26800000	2.13500000	0.61900000
H	7.98400000	0.56200000	0.30500000
C	5.86100000	0.56300000	0.13700000
N	5.29600000	0.68200000	1.36400000
O	5.34000000	-0.08400000	-0.77300000

H	4.40100000	0.23900000	1.55100000
H	5.72000000	1.23500000	2.09600000

HO-Fe^{IV}=O attacks Model 1 (including O-C2 pathway)

NBZ-FeIV-RC-model1:

C	-2.15154700	-1.20674200	4.32176200
N	-2.75665000	-1.12974700	3.07783100
H	-3.72714600	-1.34083500	2.87954800
C	-1.83207400	-0.74405500	2.16596000
H	-2.02701400	-0.62874400	1.10952100
N	-0.66187200	-0.56098200	2.75368900
C	-0.84545300	-0.84756800	4.09199200
H	-0.02945400	-0.78362800	4.79693400
C	1.35696600	3.46434700	3.73514300
N	2.69999300	3.12359500	3.73522700
H	3.45567200	3.69711100	4.08951000
C	2.84204900	1.90644700	3.16223000
H	3.78507100	1.41088900	2.99849600
N	1.66118700	1.43475300	2.79611500
C	0.73048700	2.39621000	3.14398800
H	-0.31992200	2.25892100	2.93980900
C	3.40516000	-1.33217900	2.42816200
O	2.25232700	-1.44683000	2.96968200
O	3.60418600	-0.49434000	1.50620800
C	-1.98993700	1.78526200	-3.14225000
C	-1.84388800	2.77602900	-4.11040400
C	-0.71346500	2.79378300	-4.93400700
C	0.28001200	1.81959200	-4.79294700
C	0.14867400	0.81901100	-3.83270100
C	-0.98705000	0.82132000	-3.02071000
N	-1.13476100	-0.22773600	-2.01193500
O	-0.28640000	-1.12415700	-1.98339900
O	-2.10632700	-0.17502800	-1.25669500
H	-2.85571200	1.75286400	-2.49254100
H	-2.61311100	3.53412200	-4.22172900
H	-0.60551900	3.56983500	-5.68635800
H	1.15851500	1.83695000	-5.43053900
H	0.90520400	0.05506700	-3.70366900
O	0.63945600	0.70065500	0.41989500
O	1.05839200	-1.78881500	0.62148000
H	0.62457300	-1.54700700	-0.21708000
H	5.49500800	-1.85880500	2.60632700
H	4.46979400	-2.41657700	3.96809000
H	4.38464600	-3.23067500	2.40002800
Fe	1.24209200	-0.27929700	1.58645000
C	4.51604800	-2.25595000	2.88653900
C	0.84391200	4.75725400	4.27997300
H	1.06351900	4.86583200	5.34974200

H	1.28597900	5.61775000	3.76213700
H	-0.24095200	4.80935900	4.15217600
H	-3.71829000	-0.93018600	5.77866800
H	-3.30396700	-2.62364300	5.46698200
H	-2.20812400	-1.60486700	6.41392600
C	-2.88737300	-1.61223800	5.55664100

NBZ-FeIV-O-C1-TS-modell:

C	-31.12054700	11.14017100	7.95193400
N	-31.71961900	11.47108100	6.74793300
H	-32.71615500	11.48113000	6.56731000
C	-30.75414400	11.77806200	5.85083500
H	-30.93940600	12.09571200	4.83683500
N	-29.55681600	11.66558700	6.40333900
C	-29.77199800	11.26474400	7.70967100
H	-28.94925400	11.09558000	8.38983900
C	-27.70452100	15.82373200	7.46915200
N	-26.41354400	15.37168600	7.70595500
H	-25.71780900	15.84151600	8.27283400
C	-26.22468400	14.20773100	7.04777600
H	-25.30121200	13.65182800	7.01860200
N	-27.32985000	13.87611600	6.39398200
C	-28.25541300	14.87598100	6.64601800
H	-29.23524200	14.85107200	6.19862100
C	-25.23054900	11.10329800	6.03259800
O	-26.51253300	11.06303800	6.28067700
O	-24.65035800	12.05024200	5.48718200
C	-28.50147400	13.23755900	1.65318700
C	-27.37584300	12.77477300	1.00118100
C	-26.09922000	13.24674600	1.35066500
C	-25.96368500	14.22087200	2.35541500
C	-27.07374200	14.71230400	3.01737000
C	-28.36197500	14.14085500	2.75707200
N	-29.54247600	15.04836900	3.00012700
O	-29.35175400	16.09145100	3.62204000
O	-30.63378600	14.69705600	2.55990500
H	-29.49498700	12.90512500	1.38077500
H	-27.48398100	12.04992000	0.19929900
H	-25.22110600	12.88231900	0.82588700
H	-24.98059300	14.61361700	2.59920800
H	-26.99326700	15.49520500	3.75986400
O	-28.82493500	13.17492700	4.21563900
O	-27.63883900	10.89445500	3.95558000
H	-27.13145800	10.19832600	4.40822900
H	-23.38344300	10.05406700	6.46196300
H	-24.79117200	9.46838800	7.40567700
H	-24.64423400	9.06118900	5.69315600
Fe	-27.70736900	12.21075300	5.18352300
C	-24.45600800	9.84800700	6.43499900

C	-28.24600000	17.09400000	8.04400100
H	-28.25277300	17.07275200	9.14114700
H	-27.65467800	17.96390000	7.73198400
H	-29.27361400	17.24518300	7.70230000
H	-32.59559900	11.56677500	9.46649300
H	-32.52127000	9.86448100	8.98447600
H	-31.24440200	10.55311400	9.99956900
C	-31.91499500	10.76200000	9.16099500

NBZ-FeIV-O-C2-TS1-modell1:

C	-2.17431800	-1.13163000	4.33638500
N	-2.83558500	-0.62185200	3.23082400
H	-3.83939700	-0.52630000	3.13510700
C	-1.91960100	-0.27867000	2.29510800
H	-2.16318900	0.14221100	1.33177000
N	-0.69984800	-0.53393600	2.73850800
C	-0.84334800	-1.06750800	4.00448200
H	0.01756900	-1.37533100	4.57872400
C	1.33954900	3.47012700	3.70359600
N	2.68327100	3.18637300	3.52588100
H	3.45376800	3.80172600	3.75674300
C	2.79815000	1.95598400	2.97153500
H	3.73394300	1.49328400	2.70115400
N	1.60307100	1.42152200	2.78205200
C	0.68943400	2.35602800	3.23299100
H	-0.37276500	2.17077700	3.18923000
C	3.29721700	-1.43871400	2.51324800
O	2.20956700	-1.58592500	3.14796400
O	3.35650500	-0.63957600	1.52258700
C	-0.69998800	3.39279100	-1.07447500
C	-1.83492800	2.73700400	-1.55225300
C	-1.73854400	1.41441200	-2.03431100
C	-0.53329700	0.74027300	-2.00308000
C	0.63106100	1.33327600	-1.40512700
C	0.51683100	2.71985600	-1.06989800
N	1.71745200	3.43386700	-0.68207600
O	2.80974800	2.88841100	-0.87767000
O	1.59726800	4.56542900	-0.19461900
H	-0.74342800	4.42271400	-0.74177500
H	-2.78597500	3.25990500	-1.57993800
H	-2.61730200	0.93215500	-2.45384700
H	-0.45534700	-0.27404300	-2.38215200
H	1.60942700	0.96249800	-1.67859300
O	0.63249300	0.52212200	0.22404200
O	0.90548100	-2.07844200	0.73193100
H	0.61328300	-1.87225700	-0.17064500
H	5.43647200	-1.71229100	2.65551200
H	4.49484000	-2.52952200	3.94503200
H	4.51070700	-3.18011600	2.29464600

Fe	1.16373000	-0.44462600	1.57592700
C	4.51604300	-2.25594400	2.88653900
C	0.84391400	4.75724700	4.27997300
H	1.22074500	4.92229000	5.29733500
H	1.14802900	5.61754300	3.67038800
H	-0.24895800	4.74732100	4.32400100
H	-3.47449800	-0.81298400	6.02658600
H	-3.57359000	-2.43718600	5.32694400
H	-2.16258500	-1.97388500	6.29143200
C	-2.88737300	-1.61223800	5.55664100

NBZ-FeIV-O-C2-INT1-modell1:

C	-2.90050000	-1.94545600	2.73604900
N	-3.56112000	-1.38066000	1.65693300
H	-4.56085600	-1.23361300	1.58565800
C	-2.65161400	-1.05929300	0.70844500
H	-2.89575800	-0.60163900	-0.23802900
N	-1.43626500	-1.38363400	1.11908600
C	-1.57634000	-1.93819000	2.37659400
H	-0.71844300	-2.29784000	2.92425400
C	0.61450400	2.66919200	2.08316800
N	1.92005100	2.47463000	1.66456400
H	2.66798500	3.15441000	1.72654000
C	2.02717800	1.22566000	1.14750700
H	2.93516100	0.81283900	0.73626500
N	0.86675100	0.59468400	1.20796700
C	-0.01688700	1.48501900	1.78950400
H	-1.05150800	1.22546300	1.95509500
C	2.54478900	-2.29720700	0.92771500
O	1.47412700	-2.47541600	1.57610800
O	2.55762100	-1.51315000	-0.08244300
C	-1.69299000	0.49174600	-4.33525600
C	-1.49164500	-0.76350900	-4.93381300
C	-0.38373900	-1.57470300	-4.55866300
C	0.47759600	-1.17009000	-3.57935100
C	0.27440900	0.08828600	-2.77032400
C	-0.82302200	0.93473200	-3.36464700
N	-0.98823600	2.26064600	-2.82968500
O	-0.08273600	2.71249400	-2.11403900
O	-2.01242600	2.90199800	-3.11938000
H	-2.51198800	1.12854900	-4.64946300
H	-2.17609600	-1.10273600	-5.70492600
H	-0.22540100	-2.52052200	-5.07053800
H	1.32492000	-1.78732300	-3.29456400
H	1.20961500	0.66862400	-2.75194100
O	-0.08783000	-0.23817600	-1.44178300
O	0.11220400	-3.00177300	-0.86775100
H	-0.23703300	-2.83907900	-1.75950500
H	4.69486600	-2.47145700	1.07072800

H	3.78895400	-3.33914100	2.35249400
H	3.83896400	-3.97720400	0.69699400
Fe	0.40010000	-1.35386800	-0.03047100
C	3.79988200	-3.05843500	1.29606700
C	0.12900800	3.94811000	2.68727700
H	0.67257600	4.20006600	3.60690600
H	0.24276000	4.79136700	1.99418300
H	-0.93227000	3.86141400	2.93725400
H	-4.15124300	-1.60808400	4.45817200
H	-4.32164000	-3.21709700	3.73828800
H	-2.87414800	-2.81642400	4.67653400
C	-3.60236100	-2.41956700	3.96367000

NBZ-FeIV-O-C2-TS2-modell1:

C	-2.84323300	-2.04564100	2.87908200
N	-3.15490100	-2.71726500	1.70944600
H	-3.90652600	-3.38648900	1.59722700
C	-2.27361800	-2.34878900	0.74880400
H	-2.25128800	-2.74354400	-0.25488800
N	-1.41397800	-1.46564800	1.22859100
C	-1.75737800	-1.26991000	2.55233400
H	-1.19884300	-0.59678900	3.18640500
C	0.59970100	2.83206700	2.33181100
N	1.93426500	2.46252500	2.29417200
H	2.71038300	3.01886200	2.63138800
C	2.03463600	1.25170200	1.69972700
H	2.96215900	0.73647900	1.50755800
N	0.83652000	0.80567800	1.35475900
C	-0.06346000	1.78393100	1.74308800
H	-1.12207000	1.67605300	1.55981500
C	2.55894200	-2.13323200	0.98034000
O	1.41805300	-2.48170900	1.41491800
O	2.67594100	-1.19287200	0.13344500
O	0.07842200	-2.26661000	-1.27241800
H	0.46870800	-3.11025900	-0.99247700
H	4.67352500	-2.60137200	0.90056900
H	3.97857800	-2.53596300	2.53896000
H	3.63194800	-3.92533700	1.50634900
Fe	0.44049800	-0.99348700	0.06376900
C	3.79352600	-2.84248800	1.50173400
C	0.13468200	4.13340000	2.89867300
H	0.38881500	4.23149700	3.96183100
H	0.58187000	4.98593400	2.37199600
H	-0.95205400	4.21333200	2.80480200
H	-4.65777500	-2.01862600	4.04644600
H	-3.51440700	-3.29112700	4.50228300
H	-3.18235600	-1.60655700	4.93581600
C	-3.59093500	-2.25311800	4.15380500
C	-1.06437900	2.76964300	-2.32563600

C	-2.38866900	2.61335600	-2.61805500
C	-2.94547900	1.31911400	-2.95247200
C	-2.18376400	0.20143400	-2.93194600
C	-0.77028000	0.25236200	-2.46569400
C	-0.22154400	1.61720600	-2.31155800
N	1.21091900	1.78525500	-2.25527900
O	1.91860000	0.77476200	-2.35838200
O	1.65529800	2.93519600	-2.09565900
H	-0.62940700	3.73864700	-2.11673000
H	-3.03927200	3.48293700	-2.63627300
H	-3.98397000	1.27151100	-3.26963800
H	-2.57187800	-0.75730000	-3.26369400
H	-0.11843000	-0.51584300	-2.87236300
O	-0.58333300	0.40550800	-1.03536200

NBZ-FeIV-O-C2-INT2-modell1:

C	-2.88886600	-1.81263200	2.73947800
N	-3.55683400	-1.21593600	1.68378100
H	-4.55309700	-1.03947600	1.63820100
C	-2.65923300	-0.91217900	0.71402000
H	-2.91751400	-0.42023200	-0.21291300
N	-1.44307400	-1.28251300	1.08477500
C	-1.57556500	-1.84863700	2.33988500
H	-0.71826100	-2.24344700	2.86567700
C	0.61880800	2.93285800	1.98365400
N	1.90576200	2.79339100	1.48925500
H	2.64920800	3.47578100	1.57657000
C	2.00536300	1.59666000	0.86723600
H	2.90339200	1.21581600	0.40576500
N	0.85083600	0.94920200	0.93014000
C	-0.01708200	1.77281800	1.62327800
H	-1.03748000	1.48008400	1.81862000
C	2.68127500	-2.11346500	0.76089700
O	1.51920200	-2.36725500	1.24070100
O	2.84394500	-1.26238800	-0.15385600
O	-0.04115800	-1.13965600	-1.77536500
H	0.72404800	-1.12062700	-2.37080600
H	4.77821300	-2.65668000	0.77158500
H	4.02239100	-2.54708900	2.38303300
H	3.66872300	-3.93448300	1.35235900
Fe	0.48440800	-0.99369700	0.03155500
C	3.86844600	-2.85749000	1.34219900
C	0.15944600	4.13301200	2.74017000
H	0.73632100	4.27657100	3.66296700
H	0.25275900	5.05058100	2.14549000
H	-0.89256200	4.01793400	3.01600400
H	-4.05953300	-1.40795100	4.50303200
H	-4.34362600	-3.00563300	3.79660600

H	-2.84406700	-2.68381200	4.68210500
C	-3.57313200	-2.24899300	3.99237600
C	-4.09644400	1.20523000	-4.59495300
C	-4.31785000	0.27279400	-5.54949200
C	-3.67248600	-1.02697500	-5.52196800
C	-2.80313700	-1.37236700	-4.54187000
C	-2.60226900	-0.51451800	-3.36891100
C	-3.32622200	0.81644700	-3.40530100
N	-2.68311200	1.95716000	-2.66280900
O	-2.48592300	1.83677800	-1.46008600
O	-2.38238500	2.93685300	-3.34152800
H	-4.46235000	2.22185000	-4.67858900
H	-4.92821000	0.52448800	-6.41240000
H	-3.82488300	-1.68883000	-6.37024300
H	-2.19453100	-2.26915800	-4.61680500
H	-1.69539100	-0.62549200	-2.76251900
O	-3.79227500	-0.20004500	-2.57549100

NBZ-FeIV-O-C2-TS3-modell1:

C	-21.34157800	32.04631800	-0.10801400
H	-20.77409500	31.11555400	-0.19615400
H	-21.39174100	32.30994500	0.95614900
C	-22.70085000	31.86807300	-0.69995600
N	-23.64121800	32.88461000	-0.74481000
H	-23.51002000	33.82561800	-0.39420600
C	-24.76204200	32.41335700	-1.34096600
H	-25.65767900	32.99442400	-1.49952400
N	-24.60273600	31.14610900	-1.68350100
C	-23.32507800	30.79528800	-1.28856800
H	-22.94628200	29.79664700	-1.45182000
C	-24.18516500	32.22570400	-7.49335000
H	-23.13904600	32.28717000	-7.17991700
H	-24.53093000	33.24358700	-7.71537300
C	-25.00163600	31.58588600	-6.41847000
N	-26.36560800	31.37147400	-6.53729300
H	-26.93319600	31.60487800	-7.34279100
C	-26.81364400	30.78755500	-5.40043600
H	-27.84364800	30.52343100	-5.21564800
N	-25.81840700	30.61127100	-4.54801700
C	-24.68607800	31.10099700	-5.17248200
H	-23.72062200	31.07755600	-4.68775000
C	-25.41724200	25.96338100	-3.87731400
H	-25.32756500	25.33968800	-2.97859700
H	-24.46842500	25.89685900	-4.41927600
C	-25.69759200	27.39862600	-3.45838100
O	-26.88398900	27.84004400	-3.50550600
O	-24.73240000	28.10922500	-3.02921000
Fe	-26.10934600	29.75080200	-2.49419200
C	-29.84362800	32.57166700	-2.62472400

C	-29.98148000	33.65806100	-1.83211400
C	-29.38317800	33.70487000	-0.51747800
C	-28.67807400	32.64026000	-0.00611500
C	-28.56758100	31.44702000	-0.75413400
C	-29.00473700	31.41638700	-2.15671500
N	-29.73282900	30.10287000	-2.57733500
O	-30.31698600	29.46259800	-1.71125200
O	-29.71320900	29.83085900	-3.77448100
H	-30.29654700	32.51430800	-3.61001400
H	-30.55041600	34.51762600	-2.17455800
H	-29.50553600	34.60862200	0.07330300
H	-28.23599400	32.68794300	0.98438700
H	-28.06011200	30.53877900	-0.41288400
O	-27.69276800	31.43359300	-2.53105100
O	-26.84314700	29.10524500	-0.84884900
H	-27.34861100	28.30485900	-1.06345000
H	-26.22786900	25.56704800	-4.49425600
H	-24.22226000	31.65311400	-8.42895800
H	-20.77521200	32.83590800	-0.61818100

NBZ-FeIV-O-C2-INT3-modell1: (from TS3-IRC)

C	5.11100000	1.38500000	2.62400000
H	5.71000000	0.47600000	2.52200000
H	5.03200000	1.61900000	3.69300000
C	3.76700000	1.17600000	2.00600000
N	2.78900000	2.15900000	1.98600000
H	2.87800000	3.09000000	2.37400000
C	1.69000000	1.67000000	1.37300000
H	0.77400000	2.22300000	1.23000000
N	1.90100000	0.41900000	0.99000000
C	3.18900000	0.10000000	1.37900000
H	3.60300000	-0.87900000	1.18900000
C	2.27800000	1.56100000	-4.74900000
H	3.34400000	1.43600000	-4.53700000
H	2.07500000	2.63600000	-4.83500000
C	1.46400000	0.93300000	-3.66200000
N	0.07800000	0.95900000	-3.66200000
H	-0.50400000	1.36600000	-4.38400000
C	-0.36900000	0.34700000	-2.54100000
H	-1.41100000	0.24300000	-2.28100000
N	0.64700000	-0.08300000	-1.81100000
C	1.79200000	0.27100000	-2.50300000
H	2.77500000	0.03600000	-2.12100000
C	1.04500000	-4.66000000	-1.13900000
H	0.80400000	-5.31100000	-0.28900000
H	2.06800000	-4.86500000	-1.46100000
C	0.88800000	-3.21700000	-0.70900000
O	-0.29900000	-2.75300000	-0.55200000
O	1.88700000	-2.49200000	-0.45400000

Fe	0.36300000	-0.94300000	0.31200000
C	-3.06000000	1.58200000	0.70100000
C	-4.16300000	1.92900000	1.48200000
C	-4.44200000	1.23300000	2.66100000
C	-3.59500000	0.18700000	3.05400000
C	-2.48700000	-0.16700000	2.29000000
C	-2.19200000	0.52900000	1.09200000
N	-4.25700000	-0.65400000	-0.82600000
O	-5.29700000	-1.08600000	-0.39600000
O	-3.84100000	-0.56500000	-1.95900000
H	-2.83400000	2.12200000	-0.21500000
H	-4.80900000	2.74300000	1.16400000
H	-5.30400000	1.49900000	3.26700000
H	-3.80300000	-0.35900000	3.97200000
H	-1.81200000	-0.95800000	2.59800000
O	-1.14700000	0.24600000	0.32600000
O	0.27500000	-1.74400000	1.99900000
H	-0.16500000	-2.60700000	1.91600000
H	0.34300000	-4.89800000	-1.94500000
H	2.07400000	1.10600000	-5.72700000
H	5.65700000	2.20500000	2.14200000

NBZ-FeIV-O-C2-TS4-model1:

C	-3.11792400	-2.66485300	3.27716200
N	-3.53968300	-3.16369100	2.05533700
H	-4.38701800	-3.69472900	1.89445100
C	-2.62371800	-2.83599100	1.11315700
H	-2.68996300	-3.12221300	0.07474300
N	-1.63540900	-2.14419800	1.65571600
C	-1.93180500	-2.03373800	3.00097700
H	-1.27202900	-1.51759400	3.68284600
C	0.27656300	2.12546400	2.87986400
N	1.62862300	1.83693700	2.78440600
H	2.38299400	2.42977100	3.10854500
C	1.77513900	0.64139100	2.16566900
H	2.72526500	0.18133400	1.94063900
N	0.59278500	0.13398900	1.85758900
C	-0.34592400	1.05081700	2.29590600
H	-1.40380800	0.88146600	2.15923700
C	2.41686300	-2.84129200	1.38112900
O	1.26397400	-2.99988200	1.90989300
O	2.60586600	-2.00653200	0.45441500
H	4.47074900	-3.53575200	1.32752300
H	3.75111300	-3.44808100	2.95781600
H	3.27903200	-4.75353700	1.87039200
C	3.55800200	-3.69471900	1.90684400
C	-0.25290500	3.37816900	3.49753900
H	0.05977400	3.48251900	4.54425900

H	0.08921900	4.27156900	2.95978800
H	-1.34630300	3.37003600	3.47245900
H	-4.88589300	-2.46143700	4.49684700
H	-3.94914900	-3.93061600	4.80815400
H	-3.34761400	-2.36270500	5.37014000
C	-3.86744300	-2.86683800	4.55047100
C	-1.90897800	-0.47818000	-2.58880800
C	-2.22900500	-1.07813300	-3.78183600
C	-1.30813900	-1.93964300	-4.44670900
C	-0.05538300	-2.16754800	-3.91682600
C	0.31917900	-1.54690800	-2.70557600
C	-0.62532900	-0.70733000	-1.97810400
N	0.78111600	0.71400000	-3.78807300
O	0.36780800	0.91339800	-4.91412300
O	1.58774400	1.37327100	-3.15854400
H	-2.61350100	0.16134600	-2.06439500
H	-3.20313200	-0.90284200	-4.23154200
H	-1.59735200	-2.39964800	-5.38735000
H	0.66170200	-2.79484800	-4.43883900
H	1.33781600	-1.58742000	-2.34574100
O	-0.33584400	-0.24578900	-0.82708400
O	-0.00393300	-2.90841500	-0.87339200
H	0.81355200	-3.42890800	-0.96291600
Fe	0.24898900	-1.64181500	0.64389300

NBZ-FeIV-O-C2-PC-modell1:

C	-3.16944000	-1.26973200	2.85817400
N	-3.46989400	-1.84665400	1.63606900
H	-4.30993600	-2.37052600	1.42225900
C	-2.45270000	-1.60049700	0.77714200
H	-2.42437400	-1.94903300	-0.24367300
N	-1.50817800	-0.88888600	1.37119900
C	-1.94383000	-0.68053800	2.66782800
H	-1.34968400	-0.12559100	3.37928500
C	0.53466400	3.50706600	2.67766100
N	1.86180300	3.25997100	2.36760100
H	2.63905800	3.87878000	2.56478400
C	1.94740200	2.06538500	1.73907400
H	2.86112000	1.62670400	1.36808400
N	0.74740800	1.51555400	1.62951500
C	-0.13881900	2.40674400	2.20872500
H	-1.19932500	2.20383100	2.24471600
C	2.63825100	-1.43327400	1.01487700
O	1.47656700	-1.77794300	1.43559000
O	2.78071600	-0.48924100	0.19486500
H	4.73566000	-1.97087500	0.96164900
H	4.02983500	-1.86020600	2.59153300
H	3.65084900	-3.25554900	1.57958000
C	3.84368900	-2.17807400	1.55779300

C	0.08181600	4.74766100	3.37244500
H	0.55471000	4.85823900	4.35673400
H	0.31683900	5.64740800	2.78969500
H	-1.00129300	4.71822500	3.52128100
H	-5.04569300	-0.86088200	3.83771500
H	-4.28629500	-2.38393900	4.32637600
H	-3.62428400	-0.84212700	4.89467500
C	-4.08130200	-1.34526500	4.03778600
C	-1.62296200	0.20830200	-3.02065200
C	-2.05590700	-0.72360500	-3.88691100
C	-1.21048700	-1.85449000	-4.27664100
C	-0.04843400	-2.10922600	-3.65116200
C	0.42549900	-1.26018100	-2.50307400
C	-0.25193700	0.13718100	-2.40595400
N	0.70131600	1.09313000	-3.42386200
O	0.13077400	1.95393900	-4.08851600
O	1.92302700	0.98058200	-3.35395300
H	-2.23995100	1.04622800	-2.71173700
H	-3.05275700	-0.65692600	-4.31697400
H	-1.55929600	-2.50359300	-5.07669300
H	0.55731600	-2.97233700	-3.91895800
H	1.50314900	-1.08553600	-2.55269800
O	-0.16093800	0.69737900	-1.20575800
O	0.12630000	-1.92024700	-1.23997800
H	0.84153100	-2.54779500	-1.03934800
Fe	0.38762500	-0.27561300	0.41825000

NBZ-FeIV-O1-C2-TS-modell1:

C	-31.14848900	11.14218600	7.93706500
N	-31.75689400	11.39199300	6.71736400
H	-32.75163800	11.34203200	6.53188000
C	-30.80722300	11.70829700	5.80864200
H	-31.01328800	11.92614900	4.77073800
N	-29.60935300	11.67575700	6.37491100
C	-29.80893500	11.32401300	7.69793700
H	-28.97968300	11.22284500	8.38233700
C	-27.70923200	15.78859300	7.54650700
N	-26.36309500	15.45867100	7.58256800
H	-25.61926900	16.04704800	7.93820600
C	-26.19926100	14.22708200	7.04821700
H	-25.24718900	13.73668900	6.92107200
N	-27.36852400	13.73253400	6.67296300
C	-28.31417900	14.69671600	6.97561600
H	-29.35993700	14.54830500	6.75501700
C	-25.61871600	10.77526100	6.14970900
O	-26.76162100	10.53796000	6.66652900
O	-25.48169600	11.75209800	5.35118500
H	-24.47087400	9.03447500	5.69852500
H	-23.50427200	10.37659800	6.33714700

H	-24.54468100	9.40615000	7.43113100
C	-24.45600700	9.84800800	6.43500100
C	-28.24599800	17.09399500	8.04400000
H	-28.04838700	17.23347000	9.11435600
H	-27.79983600	17.94218200	7.51012600
H	-29.32819200	17.13160300	7.89170200
H	-32.63155300	11.54113100	9.45008600
H	-32.47837200	9.83201300	9.01364600
H	-31.22801100	10.60936400	9.99814100
C	-31.91499800	10.76200100	9.16099800
Fe	-27.69033800	12.01754300	5.36929400
O	-28.16808200	12.96439500	4.09282500
C	-28.29817800	9.73139500	2.81140400
C	-27.93675700	8.30413000	2.84203300
C	-29.73645500	9.95924200	2.63546400
H	-27.67378600	10.36580700	2.18997600
C	-28.88602400	7.34116000	3.07799700
H	-26.88656600	8.04540500	2.74275200
C	-30.68133100	8.96978600	2.90801000
N	-30.16460100	11.24566300	2.20203200
C	-30.26732100	7.66535100	3.15604900
H	-28.58196800	6.30091900	3.16967800
H	-31.73436100	9.22426200	2.86559000
O	-29.34020700	11.99626500	1.65574900
O	-31.36448700	11.56842200	2.36431500
H	-31.00048600	6.88714400	3.34276000
O	-27.86128800	10.28508100	4.25758400
H	-27.84577200	9.52494600	4.87192700