

Supporting Information

DFT Calculations for Intermediate and Active States of the Diron Center with Tryptophan or Tyrosine Radical in *Escherichia coli* Ribonucleotide Reductase

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Cartesian coordinates of the $S_{\text{total}} = 0$ state X(di- μ -oxo)-Trp48⁺ geometry (Figure 1):

141 atoms:

Fe	0.030764635	0.320281930	0.533346092
Fe	-1.072988189	-0.030188518	3.073464665
O	0.046248227	-0.852022494	2.011233340
O	-1.401500059	0.968953766	1.664727974
O	-1.242491644	-0.982742244	-0.549052665
H	-2.044404712	-1.145368089	0.020206435
H	-1.524017745	-0.413940416	-1.329378763
C	-0.897854991	2.916134101	-2.930993998
C	-0.952935577	1.636775030	-2.125548126
O	-1.624952879	0.656879595	-2.545032703
O	-0.271010486	1.651789838	-1.037792422
C	3.458116793	3.486378292	1.385599742
C	2.634459464	3.072502385	2.592692002
C	1.550358198	2.020145222	2.377517113
O	1.428048682	1.577950428	1.170365180
O	0.863138396	1.669493340	3.357561939
C	2.757917914	0.207420273	-2.444835814
C	2.637508727	-0.921961778	-1.482642299
N	1.715779185	-0.981793895	-0.448849667
C	3.374112185	-2.085392661	-1.477962514
C	1.905201282	-2.155493118	0.139795515
N	2.892153208	-2.846658380	-0.446991215
C	1.530075650	1.047222855	-9.491492023
C	0.661151165	0.512631172	-8.390901538
C	0.136491078	-0.786905890	-8.450336745
C	0.348100061	1.283334091	-7.268061682
C	-0.673868629	-1.298609411	-7.440905706
C	-0.463448412	0.789683768	-6.250517440
C	-0.981500972	-0.503828878	-6.332488566
O	-1.788823642	-1.032629656	-5.361989091
C	-5.458225939	0.797769926	4.288344110
C	-4.221912404	1.507753075	3.746860445
C	-3.077829608	1.594064300	4.740273767
O	-3.254087262	2.138636961	5.846635547
O	-1.901693619	1.140864711	4.414314051
C	-2.990578646	-4.543499471	2.566862768
C	-3.928148912	-3.336685207	2.602917512
C	-3.219081094	-2.065315346	2.147613117
O	-3.307412860	-1.730003300	0.939251090
O	-2.574217724	-1.448719854	3.064014724
C	-1.935735454	-1.454214708	6.567854964
C	-0.586105238	-1.610913305	5.961801023
N	-0.165192616	-1.103053712	4.740031215
C	0.467993930	-2.291786384	6.522601186
C	1.101107458	-1.476297738	4.593605210
N	1.513662824	-2.187743974	5.647221933
C	8.572612619	-8.883235907	-1.721426365
C	7.322169473	-8.072753497	-1.720470962
C	6.572242552	-7.721965286	-0.588054723
C	6.647082664	-7.455119016	-2.826333731
N	5.524861202	-6.946166755	-0.928714230
C	5.531661615	-6.751599024	-2.297048328
C	6.866480428	-7.428004050	-4.215816042
C	4.656965549	-6.025059898	-3.095512534
C	5.991004070	-6.703968298	-5.023574054
C	4.905124596	-6.009643581	-4.472905384

C	2.025510410	-5.216139447	2.492585468
C	3.309710487	-5.850902792	1.952091196
O	4.011737382	-6.557983403	2.726769981
O	3.612124595	-5.587513169	0.736370659
C	6.422052196	-3.705534397	6.868388024
C	5.233627970	-4.112498355	6.036539584
O	4.093271184	-3.657361529	6.256675335
N	5.475697030	-5.026739798	5.086740001
C	3.985396425	2.035773473	8.104447943
C	2.573459506	2.442064436	7.838368990
C	1.833488825	2.068166193	6.729112251
C	1.686919513	3.249574008	8.634068100
N	0.576142045	2.583148242	6.790711517
C	0.440692537	3.314849865	7.946973332
C	1.803117040	3.926736382	9.863825130
C	-0.659578236	4.017605215	8.433539789
C	0.706073446	4.629571316	10.357540568
C	-0.509434814	4.677282693	9.652542423
O	-4.792767363	1.446040254	8.516113736
H	-1.112266556	3.774601097	-2.285499728
H	0.118917202	3.056128577	-3.319231147
H	-1.605987346	2.897178055	-3.762395674
H	4.018729700	2.642618552	0.967452153
H	2.828697565	3.892837972	0.585861877
H	4.180754799	4.260682575	1.673576548
H	2.125349322	3.942838562	3.029882456
H	3.283130423	2.688590232	3.391971960
H	3.642897543	0.066759080	-3.072993577
H	1.885500665	0.259547979	-3.106919368
H	2.841712534	1.172029699	-1.934304656
H	4.185406612	-2.420657790	-2.112082548
H	1.342958369	-2.526082426	0.982451271
H	3.208459568	-3.767717389	-0.139632249
H	2.198000000	0.260000000	-9.844000000
H	0.935562662	1.381525541	-10.352961162
H	2.135301423	1.895626662	-9.155904687
H	0.372223612	-1.423718598	-9.304422978
H	0.748098418	2.293859325	-7.176003488
H	-1.064333487	-2.314004938	-7.500317377
H	-0.691287276	1.410691371	-5.389846599
H	-1.821696401	-0.412414693	-4.614786166
H	-6.257914721	0.811688021	3.537553218
H	-5.243581682	-0.250304218	4.529788808
H	-5.837526456	1.285002961	5.193278125
H	-4.479835500	2.548827462	3.504916966
H	-3.879842199	1.037857991	2.822507576
H	-2.127108077	-4.391348948	3.225561942
H	-3.518346385	-5.445912255	2.899851494
H	-2.615141168	-4.728107472	1.552050610
H	-4.304807835	-3.191939323	3.622286111
H	-4.784535726	-3.507513654	1.938977092
H	-1.967087825	-1.998032577	7.517191683
H	-2.168267246	-0.404427203	6.766939425
H	-2.721128285	-1.850416691	5.917787216
H	0.552689745	-2.826958915	7.459894605
H	1.733885036	-1.242017262	3.752178979
H	2.431622740	-2.606623663	5.758288380
H	9.468000000	-8.258000000	-1.545000000
H	8.552444053	-9.636276723	-0.925344564

H	8.718542166	-9.396857011	-2.677389236
H	6.740609061	-7.993457075	0.448738739
H	4.854744475	-6.522055669	-0.261532623
H	7.703213960	-7.964355490	-4.661705162
H	3.803653878	-5.495412572	-2.674587206
H	6.150888704	-6.678658697	-6.100469160
H	4.235659370	-5.450854177	-5.125096644
H	1.606000000	-5.719000000	3.376000000
H	2.259654720	-4.186653325	2.790243762
H	1.260516928	-5.164786120	1.711321463
H	6.513000000	-4.433000000	7.686000000
H	7.356417235	-3.716744617	6.297819825
H	6.253984226	-2.713112458	7.292649185
H	6.412494029	-5.364795189	4.927717850
H	4.739241393	-5.395209108	4.496478783
H	4.382000000	1.434000000	7.275000000
H	4.642696438	2.904923606	8.240604523
H	4.065462093	1.436449310	9.022130647
H	2.137014794	1.462806674	5.885974613
H	-0.151898929	2.414017043	6.111183674
H	2.735212485	3.904472428	10.428010790
H	-1.598960025	4.051661806	7.884009445
H	0.789496725	5.153232921	11.309372208
H	-1.351652519	5.234693804	10.061006864
H	-4.333734275	1.652004473	7.684600371
H	-5.677118071	1.813762891	8.369984751

Cartesian coordinates of the $S_{\text{total}} = 0$ state X(di- μ -oxo)-Tyr122' geometry (Figure 4a):

141 atoms:

Fe	0.188658	-0.006657	0.867403
Fe	-1.030475	-0.235103	3.292877
O	0.204803	-1.111261	2.363614
O	-1.346431	0.668944	1.846036
O	-1.052086	-1.263715	-0.262968
H	-1.856709	-1.532802	0.319978
H	-1.423377	-0.808347	-1.033615
C	-1.529641	3.015957	-2.959588
C	-1.135444	1.832854	-2.131388
O	-1.340752	0.608012	-2.652483
O	-0.610911	1.914819	-1.031332
C	3.329839	3.480128	1.569230
C	2.543168	3.008787	2.779493
C	1.531625	1.885789	2.577330
O	1.400568	1.457131	1.358815
O	0.905869	1.464063	3.566224
C	2.947506	0.711866	-1.928890
C	2.827619	-0.612824	-1.259858
N	1.821550	-0.948323	-0.364485
C	3.628590	-1.716787	-1.444456
C	2.026136	-2.219937	-0.039669
N	3.099418	-2.713759	-0.666720
C	1.338522	0.943006	-9.888474
C	0.411352	0.707707	-8.745623
C	-0.104440	-0.591848	-8.488226

C	0.013677	1.769617	-7.895761
C	-0.951462	-0.830247	-7.436435
C	-0.830584	1.558410	-6.835157
C	-1.345193	0.237654	-6.538577
O	-2.095399	0.022449	-5.539407
C	-5.470320	1.296397	4.085792
C	-4.064738	1.600855	3.582957
C	-3.008141	1.661299	4.672125
O	-3.198184	2.350987	5.694628
O	-1.887983	1.021170	4.523539
C	-3.494172	-4.785531	2.632739
C	-4.113465	-3.395014	2.764986
C	-3.165397	-2.300849	2.287674
O	-3.030632	-2.154337	1.039914
O	-2.587743	-1.632561	3.203390
C	-2.298173	-1.366295	6.677645
C	-0.910202	-1.667067	6.235727
N	-0.329849	-1.259267	5.041951
C	0.025609	-2.390367	6.933580
C	0.911784	-1.729489	5.042335
N	1.159244	-2.410495	6.165459
C	8.596490	-8.926255	-1.483322
C	7.311405	-8.168391	-1.598612
C	6.465588	-7.831526	-0.563441
C	6.719114	-7.601009	-2.780038
N	5.395923	-7.105285	-1.019990
C	5.521004	-6.940559	-2.373629
C	7.071939	-7.578183	-4.144415
C	4.687220	-6.281484	-3.284567
C	6.244974	-6.921919	-5.048943
C	5.062319	-6.282077	-4.623173
C	1.919359	-5.255534	2.431224
C	3.211451	-5.839145	1.852498
O	4.010958	-6.424724	2.638687
O	3.411777	-5.661446	0.604662
C	6.106437	-3.671200	7.007154
C	4.925389	-4.247554	6.263231
O	3.751146	-4.063669	6.641774
N	5.225933	-4.992854	5.189316
C	4.075564	2.133639	8.062380
C	2.648176	2.546527	7.885194
C	1.793916	2.106424	6.900877
C	1.880503	3.469406	8.681085
N	0.561338	2.693848	7.031662
C	0.575829	3.537284	8.111087
C	2.152368	4.247829	9.823208
C	-0.434595	4.348855	8.636399
C	1.148933	5.051143	10.351267
C	-0.130843	5.103448	9.763555
O	-4.615805	1.477379	8.366307
H	-1.683593	3.877956	-2.307383
H	-0.702053	3.249553	-3.642271
H	-2.426261	2.824776	-3.555260
H	3.943506	2.677090	1.146123
H	2.671801	3.849728	0.774795
H	4.002464	4.297948	1.857416
H	1.979547	3.842054	3.221925
H	3.221341	2.667952	3.573217
H	3.896695	0.772996	-2.468921

H	2.140971	0.863116	-2.656381
H	2.900814	1.534421	-1.210882
H	4.506446	-1.871181	-2.059141
H	1.417192	-2.803222	0.633794
H	3.450137	-3.655596	-0.522185
H	2.198001	0.260000	-9.843999
H	0.833208	0.730453	-10.842409
H	1.706600	1.972306	-9.912767
H	0.186317	-1.414860	-9.142221
H	0.392241	2.772826	-8.092419
H	-1.339605	-1.828907	-7.239756
H	-1.136929	2.382534	-6.195005
H	-1.750179	0.660038	-3.536570
H	-6.178779	1.312457	3.248349
H	-5.522252	0.301251	4.545660
H	-5.805223	2.030518	4.826381
H	-4.054139	2.593168	3.107579
H	-3.766357	0.884154	2.816693
H	-2.576410	-4.871485	3.228497
H	-4.197464	-5.548850	2.988266
H	-3.244710	-5.013627	1.589549
H	-4.384885	-3.201664	3.808329
H	-5.026131	-3.338813	2.157373
H	-2.501782	-1.889402	7.616648
H	-2.436505	-0.294083	6.841988
H	-3.036097	-1.683578	5.936204
H	-0.026858	-2.884817	7.895080
H	1.633524	-1.595173	4.251165
H	2.026985	-2.889988	6.380611
H	9.468001	-8.258000	-1.544999
H	8.658059	-9.451702	-0.524182
H	8.705537	-9.672157	-2.280649
H	6.549998	-8.063889	0.493326
H	4.690559	-6.667063	-0.415228
H	7.980973	-8.068827	-4.493575
H	3.770737	-5.789940	-2.958341
H	6.512416	-6.901073	-6.105330
H	4.431841	-5.777105	-5.354173
H	1.606001	-5.719000	3.376000
H	2.092689	-4.192532	2.638496
H	1.102516	-5.315818	1.704296
H	6.513001	-4.433000	7.685999
H	6.911600	-3.372994	6.326937
H	5.782820	-2.813161	7.600786
H	6.184741	-5.109545	4.898329
H	4.510522	-5.420936	4.612574
H	4.382000	1.434001	7.274999
H	4.756756	2.994489	8.026861
H	4.241374	1.640017	9.029777
H	1.972945	1.416064	6.086809
H	-0.227370	2.516167	6.425168
H	3.135935	4.220987	10.293449
H	-1.423293	4.386964	8.178152
H	1.352626	5.652833	11.236725
H	-0.897222	5.744328	10.198313
H	-4.182404	1.751597	7.540459
H	-5.165759	2.242914	8.583976

Cartesian coordinates of the active state model A(O_{br},H₂O₂) (Figure 6a):

142 atoms:

Fe	0.247053299	0.168364897	0.305994504
Fe	-1.060089279	0.112684048	3.172481749
O	-0.085060715	-0.671289371	1.841911670
O	-2.006434851	1.248857094	1.439184896
O	-1.166589999	-1.192256905	-0.721112304
H	-1.886869135	-1.392446101	-0.056414020
H	-1.627043606	-0.719706548	-1.429298981
C	-0.684789897	3.433479789	-2.424162584
C	-0.836815200	2.616272894	-1.167624561
O	-1.486563367	3.100039597	-0.199365580
O	-0.313722297	1.447839092	-1.181856239
C	3.435398329	3.417625523	1.598171672
C	2.506766443	2.944171564	2.703333291
C	1.391452155	1.997788977	2.289676836
O	1.436067855	1.567667496	1.085246949
O	0.517641596	1.710223560	3.153510370
C	2.829723895	0.292559252	-2.406633657
C	2.736189794	-0.896241613	-1.518608754
N	1.818672269	-1.018262646	-0.485891323
C	3.492094483	-2.044290462	-1.549162007
C	2.029336384	-2.206182416	0.074109342
N	3.025180521	-2.847508083	-0.541564142
C	1.510350574	1.027722524	-9.479282865
C	0.646923425	0.484716330	-8.394739836
C	0.151115817	-0.843715281	-8.471803972
C	0.290096883	1.277726882	-7.276060631
C	-0.665635334	-1.359165025	-7.498182536
C	-0.530957374	0.789461134	-6.291013470
C	-1.063730047	-0.556687826	-6.357736165
O	-1.841691658	-1.004128680	-5.466539600
C	-5.601164500	0.880326953	4.526300948
C	-4.364270692	1.528173811	3.921229380
C	-3.184267366	1.694959355	4.870195171
O	-3.355407738	2.228279451	5.986170531
O	-2.009679874	1.328254439	4.466866599
C	-2.924777875	-4.509208821	2.615287582
C	-3.807002382	-3.263480198	2.706233615
C	-3.108753261	-2.012529251	2.187938484
O	-3.132712732	-1.775095297	0.951283747
O	-2.555369624	-1.273954777	3.072801712
C	-1.939659044	-1.370969360	6.595193132
C	-0.586145946	-1.570085271	6.009292087
N	-0.129094004	-1.031791484	4.812747611
C	0.425660098	-2.323409528	6.551553136
C	1.117009119	-1.466220180	4.659342695
N	1.484051191	-2.239818499	5.687619812
C	8.606709063	-8.916213116	-1.732811072
C	7.317540077	-8.153528904	-1.722083214
C	6.564396472	-7.846706889	-0.608030417
C	6.637495397	-7.535177296	-2.828581241
N	5.475276647	-7.088320690	-0.946512740
C	5.489820473	-6.872921864	-2.297381518
C	6.864667678	-7.469358524	-4.218365217
C	4.591627030	-6.164915016	-3.104861955
C	5.972321174	-6.767429534	-5.020221031

C	4.846670788	-6.120475236	-4.469827147
C	2.025512802	-5.236495077	2.485549835
C	3.295626850	-5.904188413	1.953146605
O	3.991447913	-6.599513221	2.746426602
O	3.587887691	-5.676598974	0.731326080
C	6.376850454	-3.698792955	6.882097056
C	5.183232856	-4.126792492	6.067549199
O	4.036649991	-3.699398807	6.310731418
N	5.429833209	-5.022526508	5.101761668
C	4.011519643	2.037233173	8.113679293
C	2.594087304	2.451476491	7.874116899
C	1.829872883	2.088508570	6.789515949
C	1.738481258	3.271025903	8.693651836
N	0.572692136	2.627397540	6.877239567
C	0.477448676	3.353502504	8.033753058
C	1.892004784	3.940694355	9.924513872
C	-0.603253777	4.070790219	8.555511874
C	0.817883127	4.652194905	10.447837236
C	-0.416473594	4.718229574	9.770370991
O	-4.592418259	1.391567955	8.625760930
H	-0.872457291	4.491353546	-2.224770450
H	0.307214293	3.292963227	-2.863640415
H	-1.427395641	3.080782108	-3.151350245
H	3.989677799	2.585644078	1.149938969
H	2.883210318	3.918282579	0.794591428
H	4.164215108	4.130228526	2.003267238
H	2.028746685	3.792175293	3.210645137
H	3.075501939	2.421619007	3.485712956
H	3.666871866	0.174181989	-3.099884803
H	1.913329048	0.424803697	-2.992751393
H	2.984749274	1.211394312	-1.830318549
H	4.311505407	-2.343591215	-2.190371966
H	1.472249929	-2.612528574	0.903659640
H	3.356802144	-3.770553507	-0.267504640
H	2.198000000	0.260000000	-9.843999000
H	0.891616603	1.329429920	-10.338982307
H	2.078764330	1.904699460	-9.156885189
H	0.431572894	-1.461383564	-9.325854758
H	0.681795245	2.292635253	-7.203259861
H	-1.043711277	-2.378795970	-7.559623656
H	-0.806172389	1.399269500	-5.432464758
H	-1.791456678	2.024338177	0.795612103
H	-6.402591014	0.840705796	3.777291692
H	-5.395101448	-0.149453505	4.844692403
H	-5.975557020	1.437452894	5.391459494
H	-4.611995580	2.545183536	3.581253339
H	-4.045616487	0.973936320	3.039798822
H	-2.016892787	-4.403774740	3.222035170
H	-3.475619424	-5.384170317	2.982734738
H	-2.622464445	-4.713727931	1.580721291
H	-4.107768818	-3.099177375	3.746845914
H	-4.713429339	-3.414441591	2.106665416
H	-2.014237280	-1.931227846	7.532328564
H	-2.137560807	-0.316377679	6.808015535
H	-2.726363096	-1.724468578	5.922074182
H	0.474679571	-2.901200210	7.466100233
H	1.769255516	-1.238809466	3.829071331
H	2.381590078	-2.703756570	5.797933816
H	9.467999000	-8.258002000	-1.545000000

H	8.618568649	-9.686663621	-0.953296406
H	8.777168955	-9.413534700	-2.693989675
H	6.732395594	-8.116826918	0.429651903
H	4.8144440039	-6.669924526	-0.277264666
H	7.726899899	-7.962230990	-4.667804114
H	3.714902492	-5.675793614	-2.681229124
H	6.141213220	-6.715927598	-6.095629857
H	4.162868379	-5.579201099	-5.123026571
H	1.606001000	-5.719000000	3.376000000
H	2.282348118	-4.208611812	2.769857943
H	1.257909082	-5.183137073	1.707305545
H	6.513002000	-4.433000000	7.686000000
H	7.297198004	-3.670942971	6.289718819
H	6.188220505	-2.719144222	7.326810872
H	6.370193042	-5.342755690	4.927593105
H	4.690884738	-5.409079027	4.525851209
H	4.382000000	1.434001000	7.275000000
H	4.679354763	2.901563325	8.227081655
H	4.111716567	1.438176637	9.029279867
H	2.098945456	1.471531281	5.942270486
H	-0.179740600	2.456054316	6.225385451
H	2.836208578	3.899385045	10.467917182
H	-1.555346822	4.116358498	8.028580431
H	0.926756213	5.166144695	11.402497247
H	-1.241809478	5.280393394	10.206272893
H	-4.223727542	1.652375919	7.763709182
H	-5.455669391	1.828571278	8.632725967
H	-2.648478011	0.683042034	0.988790799

Cartesian coordinates of the active state model A(O_{br},H₂O_{tl}) (Figure 6b):

142 atoms:

Fe	0.178184598	0.199571674	0.295002609
Fe	-0.930788825	0.021271589	3.217960682
O	-0.030280715	-0.719027907	1.822993809
O	-1.788640247	1.253613664	1.211835762
O	-1.255623564	-1.116801377	-0.722552153
H	-1.953133298	-1.360622173	-0.041049763
H	-1.735981384	-0.615936754	-1.396566632
C	-0.608380541	3.424702186	-2.618582482
C	-0.790326823	2.628282043	-1.350034163
O	-1.498830187	3.133834857	-0.429002217
O	-0.245521412	1.474852422	-1.305446912
C	3.397940141	3.390354390	1.639513275
C	2.477844395	2.907285901	2.746456614
C	1.347610940	1.978622497	2.336380267
O	1.267898317	1.678821176	1.100018901
O	0.562263166	1.589409564	3.249229730
C	2.827596442	0.368035708	-2.443383751
C	2.730697355	-0.816062121	-1.548950171
N	1.803939505	-0.949012117	-0.523690800
C	3.508117847	-1.949952608	-1.568424271
C	2.032260100	-2.132319529	0.040171514
N	3.047064665	-2.757826398	-0.561933954
C	1.484927246	1.013721226	-9.495299344
C	0.629680777	0.469622561	-8.404062476

C	0.129590280	-0.857674358	-8.477463699
C	0.275547273	1.265217642	-7.286051381
C	-0.695444780	-1.365013053	-7.506394160
C	-0.552333510	0.785007098	-6.303320831
C	-1.099330981	-0.555183137	-6.372606665
O	-1.898828116	-0.989301483	-5.494285504
C	-5.571693278	0.932948156	4.462549884
C	-4.326005897	1.556360734	3.849245466
C	-3.136425160	1.675745056	4.793508695
O	-3.286579027	2.177118126	5.926609587
O	-1.973282751	1.306833101	4.363032855
C	-2.898157512	-4.522189443	2.645061144
C	-3.755652773	-3.264188357	2.784298052
C	-3.069409721	-2.031475932	2.211609791
O	-3.107462617	-1.855847733	0.965996711
O	-2.516393474	-1.247492156	3.057873455
C	-1.911730319	-1.386510319	6.595467734
C	-0.555022648	-1.620205915	6.031942701
N	-0.069903201	-1.098325848	4.839382513
C	0.441028878	-2.377620214	6.595948983
C	1.177659767	-1.540594608	4.711986694
N	1.515994597	-2.308826348	5.751463584
C	8.603852890	-8.918947225	-1.719933039
C	7.310957953	-8.161628563	-1.700238749
C	6.556886607	-7.868024676	-0.582742490
C	6.625195679	-7.539521845	-2.801653564
N	5.459739669	-7.117568241	-0.915353805
C	5.474058533	-6.889009121	-2.264018288
C	6.849817895	-7.463406174	-4.191478154
C	4.569958877	-6.181598958	-3.065281854
C	5.952469945	-6.760630930	-4.986832521
C	4.823217622	-6.125576720	-4.430274048
C	2.021212175	-5.228687518	2.486946469
C	3.306954025	-5.874649565	1.964900315
O	3.996312697	-6.575777630	2.760204071
O	3.616086388	-5.626222204	0.752157621
C	6.339037533	-3.687702490	6.902109615
C	5.140650229	-4.147730527	6.115955750
O	3.983451594	-3.802656986	6.430413568
N	5.395044830	-4.980299417	5.098655607
C	4.013279593	2.048196221	8.107066061
C	2.595062851	2.464890685	7.872979309
C	1.818071177	2.099597641	6.798481011
C	1.751545626	3.294655373	8.694737504
N	0.564373092	2.646979286	6.894510853
C	0.484205184	3.380239508	8.048190621
C	1.922093604	3.969602733	9.919611732
C	-0.588062339	4.102201922	8.580687719
C	0.858298243	4.689464751	10.451943343
C	-0.384441477	4.754899829	9.789973444
O	-4.578786501	1.266118753	8.566928271
H	-0.703921125	4.495513253	-2.418422144
H	0.351446396	3.204118413	-3.091853629
H	-1.408796225	3.139861254	-3.313735117
H	3.928615554	2.559311956	1.161816978
H	2.845156876	3.923982727	0.858413512
H	4.147278922	4.076279489	2.053285826
H	2.006625655	3.754476676	3.263490798
H	3.048413967	2.378309118	3.521921074

H	3.667096802	0.241893597	-3.132774277
H	1.913734081	0.501081316	-3.031543832
H	2.984018560	1.290105625	-1.872791368
H	4.337279845	-2.238430504	-2.202326999
H	1.477664113	-2.546070552	0.867698007
H	3.392508278	-3.673829001	-0.285000083
H	2.198000000	0.260000000	-9.843999000
H	0.862549800	1.276169836	-10.365126973
H	2.024315435	1.914224952	-9.189081212
H	0.409110198	-1.479734639	-9.328667215
H	0.668481862	2.279963915	-7.216235588
H	-1.079731170	-2.382438772	-7.566643738
H	-0.831690158	1.400604025	-5.450344884
H	-1.713357228	2.076189635	0.591988248
H	-6.383058053	0.910708291	3.723920713
H	-5.383768716	-0.100643013	4.779912445
H	-5.923002250	1.497088591	5.332779884
H	-4.551323737	2.584199785	3.526317115
H	-4.026605081	1.005777290	2.956858222
H	-1.954142586	-4.426967180	3.196218771
H	-3.436503326	-5.389600828	3.046871129
H	-2.660477286	-4.731009665	1.594915729
H	-3.993498496	-3.088866753	3.838740072
H	-4.697758422	-3.403120328	-2.238689641
H	-2.017582518	-1.948989391	7.528030700
H	-2.080725543	-0.327392133	6.811827329
H	-2.697791085	-1.711427119	5.907989159
H	0.469643091	-2.947992726	7.515821036
H	1.846730265	-1.318715637	3.893189247
H	2.408490091	-2.779593984	5.883458672
H	9.467999000	-8.258002000	-1.545000000
H	8.626400759	-9.685701138	-0.936980534
H	8.766315288	-9.421345382	-2.680078747
H	6.726602414	-8.147832768	0.452112092
H	4.812099961	-6.683770061	-0.243653753
H	7.713761812	-7.948984422	-4.645767542
H	3.689929231	-5.702271368	-2.637075006
H	6.119609483	-6.700168763	-6.062032705
H	4.134519701	-5.584718628	-5.078625554
H	1.606001000	-5.719000000	3.376000000
H	2.254747443	-4.194178622	2.767265272
H	1.258541877	-5.191711862	1.702610827
H	6.513002000	-4.433000000	7.686000000
H	7.245363698	-3.620811128	6.292593986
H	6.128529169	-2.725942097	7.374781094
H	6.342065902	-5.256863060	4.889121080
H	4.654647887	-5.402084107	4.549715991
H	4.382000000	1.434001000	7.275000000
H	4.683269455	2.912588593	8.206965196
H	4.117763296	1.459515037	9.028816048
H	2.074474402	1.475198966	5.953135468
H	-0.193073258	2.482346494	6.246604677
H	2.873136156	3.928500375	10.450880883
H	-1.547610286	4.146639241	8.067262989
H	0.981693241	5.209399886	11.401283513
H	-1.203196207	5.320436359	10.233758744
H	-4.193751554	1.549287173	7.720253976
H	-5.348527618	1.844700310	8.655833842
H	-2.565409534	0.774453434	0.893663993

Cartesian coordinates of the active state model A(O_{br},OH⁻_{br})-Asp84H (Figure 6d):

142 atoms:

Fe	0.233433178	0.038297677	0.774703049
Fe	-1.070126075	-0.158313306	3.335950243
O	0.125015152	-1.008498290	2.211505476
O	-1.495271867	0.898624196	1.558928038
O	-1.048054956	-1.148790245	-0.441924377
H	-1.794180859	-1.452614780	0.173704676
H	-1.476650167	-0.633734197	-1.140043362
C	-1.560016147	3.196718273	-3.108404418
C	-1.027854866	2.067821920	-2.280556645
O	-1.235841175	0.814924733	-2.734998986
O	-0.399705069	2.209730459	-1.244133139
C	3.302270519	3.505425976	1.768677853
C	2.454115325	2.988805061	2.917792757
C	1.426773619	1.912232216	2.595906659
O	1.340164995	1.568218803	1.353467235
O	0.734694208	1.452700959	3.530630539
C	3.062760374	0.720464756	-1.869199111
C	2.916824496	-0.601702454	-1.201519408
N	1.896277404	-0.919186023	-0.315748764
C	3.710336558	-1.714368965	-1.360476327
C	2.086919658	-2.189115254	0.029657566
N	3.162069479	-2.697804886	-0.578969125
C	1.269622703	0.835761637	-9.969905175
C	0.357559762	0.630502968	-8.807963839
C	-0.115278941	-0.667747776	-8.478920497
C	-0.060393756	1.719611269	-8.005437133
C	-0.943697076	-0.878222289	-7.405463970
C	-0.887818568	1.536775031	-6.924542198
C	-1.362379519	0.220062386	-6.558504346
O	-2.104705859	0.035796873	-5.545503379
C	-5.637037401	1.489153981	4.335477905
C	-4.226566391	1.656821675	3.793640031
C	-3.114933386	1.724657878	4.834303612
O	-3.297312582	2.314911612	5.922282639
O	-1.972826584	1.212444400	4.518433809
C	-3.550749069	-4.719105789	2.572691825
C	-4.090315399	-3.300413776	2.744062711
C	-3.115683726	-2.236851346	2.253315167
O	-2.926932642	-2.148948902	1.012995579
O	-2.580404698	-1.505923575	3.156850354
C	-2.272962632	-1.355923608	6.793199592
C	-0.904081916	-1.699763053	6.321713702
N	-0.326255201	-1.247065098	5.144162689
C	0.003597848	-2.504377880	6.967081415
C	0.889834659	-1.776596823	5.099480034
N	1.124231564	-2.534706578	6.179567535
C	8.605420357	-8.928850091	-1.417773999
C	7.316039193	-8.183542141	-1.552041694
C	6.473184970	-7.811961778	-0.524647742
C	6.722213129	-7.651128632	-2.748497133
N	5.407707691	-7.095249772	-0.999868947
C	5.528772562	-6.972646953	-2.359247210
C	7.072273819	-7.672450120	-4.113012294
C	4.697774385	-6.334876163	-3.286625676
C	6.246483447	-7.038977682	-5.034687321

C	5.070348374	-6.378749405	-4.625992084
C	1.937814184	-5.247827596	2.442411932
C	3.229376537	-5.840897322	1.873493167
O	4.023453110	-6.426518262	2.664031638
O	3.431614766	-5.671251342	0.624447997
C	5.948244078	-3.663586810	7.140278004
C	4.842701915	-4.312679500	6.340633551
O	3.657106569	-4.324690313	6.732879051
N	5.219953471	-4.888348371	5.189673361
C	4.103113530	2.164733950	8.043789597
C	2.667934929	2.564895702	7.908030684
C	1.777384897	2.089463539	6.973606713
C	1.928813776	3.513385080	8.701004420
N	0.549081736	2.678855629	7.129638750
C	0.603420550	3.560134164	8.177291361
C	2.243757082	4.335270146	9.801037865
C	-0.387807060	4.390861972	8.709378787
C	1.259760530	5.159937226	10.334474321
C	-0.042072095	5.189706453	9.793277884
O	-4.792373211	1.272520968	8.410549461
H	-1.710439940	4.070498577	-2.471508438
H	-0.808130308	3.451206314	-3.866307482
H	-2.491705616	2.933959675	-3.618200440
H	3.916143409	2.711471363	1.329160840
H	2.685598695	3.929051309	0.968006340
H	3.978099206	4.292386692	2.126335315
H	1.894554611	3.810618297	3.385670390
H	3.088743749	2.582586919	3.716527627
H	4.012228802	0.761722826	-2.410768778
H	2.256608296	0.892712361	-2.592012140
H	3.037445255	1.541714477	-1.147849367
H	4.599784053	-1.880532825	-1.954690855
H	1.465844944	-2.753309240	0.707686145
H	3.500254405	-3.642705559	-0.422812824
H	2.198000000	0.259999000	-9.844000000
H	0.808070766	0.465074401	-10.895867644
H	1.531762637	1.888553323	-10.103768952
H	0.192437886	-1.513505447	-9.095080916
H	0.289666752	2.722237585	-8.251973883
H	-1.299726704	-1.876746531	-7.155402239
H	-1.207750322	2.383077549	-6.320571154
H	-1.716430916	0.818667299	-3.584087414
H	-6.360823946	1.504689484	3.510759244
H	-5.751199558	0.531058276	4.858601404
H	-5.902578311	2.289412364	5.034126710
H	-4.156054189	2.603319917	3.234335165
H	-3.990062106	0.865758105	3.077692010
H	-2.631311331	-4.870651902	3.152633542
H	-4.291269957	-5.449942371	2.920951309
H	-3.329552183	-4.938056091	1.521320531
H	-4.333691888	-3.109589177	3.794554205
H	-5.013072071	-3.190134740	2.157717924
H	-2.481993422	-1.882192016	7.729579761
H	-2.372087402	-0.281432576	6.971644219
H	-3.036369779	-1.638813827	6.061973747
H	-0.055422790	-3.046050801	7.902765021
H	1.608388062	-1.634186912	4.305514331
H	1.973490812	-3.057652451	6.367042941
H	9.468001000	-8.258000000	-1.544997000

H	8.693413400	-9.390246957	-0.428208407
H	8.702289927	-9.722889064	-2.168940339
H	6.561006371	-8.010575598	0.538655283
H	4.698738025	-6.648396644	-0.403289738
H	7.976937054	-8.179866714	-4.449402396
H	3.785886158	-5.826246805	-2.973659852
H	6.510716169	-7.053360340	-6.091882504
H	4.441927823	-5.891564372	-5.370703616
H	1.606001000	-5.719000000	3.376000000
H	2.122104112	-4.190189118	2.667239501
H	1.130230394	-5.288547852	1.704145915
H	6.513002000	-4.432998000	7.685998000
H	6.657573885	-3.136591581	6.491755659
H	5.518621042	-2.965119997	7.862222636
H	6.185774237	-4.872026564	4.897902623
H	4.559071316	-5.375192209	4.593973717
H	4.382000000	1.434002000	7.274999000
H	4.777144947	3.026449220	7.943738326
H	4.309958370	1.714928323	9.024271269
H	1.929460132	1.366586086	6.182502383
H	-0.257612632	2.493483900	6.549342513
H	3.245171766	4.329595571	10.231963682
H	-1.392884354	4.412005313	8.287228458
H	1.496062192	5.798890878	11.184961360
H	-0.791783807	5.848878532	10.229614904
H	-4.352924947	1.602447151	7.608327541
H	-5.325853503	2.031253787	8.689513565
H	-1.366819192	1.840935889	1.731063184

Cartesian coordinates of the met Fe(III)Fe(III) state model M(O_{br},H₂O₁₂) (Figure 7a):

143 atoms:

Fe	0.232077134	0.237084785	0.250158929
Fe	-1.065824926	0.099668457	3.162940605
O	-0.112235018	-0.612702448	1.782913506
O	-2.100929972	1.315248284	1.409135727
O	-1.187622433	-1.132073659	-0.734197670
H	-1.878112813	-1.379183417	-0.048522256
H	-1.693057694	-0.671115677	-1.417898552
C	-0.660649302	3.492560953	-2.510405320
C	-0.855085754	2.646716376	-1.277739739
O	-1.526225627	3.112549901	-0.321675881
O	-0.335683911	1.471135418	-1.303830818
C	3.391126948	3.410217079	1.695106118
C	2.438052880	2.922625111	2.771290207
C	1.283336801	2.048462442	2.316322353
O	1.258714903	1.727421403	1.077419684
O	0.435170746	1.714779400	3.188759498
C	2.931374637	0.352598530	-2.372302924
C	2.786245381	-0.833394887	-1.487684631
N	1.842486479	-0.934370484	-0.475602246
C	3.517176455	-1.997518299	-1.500135090
C	2.017351622	-2.126205385	0.091248855
N	3.013558360	-2.788499691	-0.500326870
C	1.532041286	1.068992105	-9.524729448
C	0.866600541	0.727858937	-8.221115325
C	0.216391550	-0.502145468	-8.038279259

C	0.864677699	1.621253711	-7.146232391
C	-0.414485454	-0.827912238	-6.842087479
C	0.235874716	1.314747246	-5.940366937
C	-0.409554892	0.087566073	-5.786220723
O	-1.050621883	-0.271459332	-4.626597537
C	-5.651515873	0.934178373	4.682556101
C	-4.416872071	1.515608466	4.009398683
C	-3.195133294	1.671666990	4.904794980
O	-3.309883499	2.190968277	6.034531542
O	-2.042538734	1.316658605	4.437086946
C	-2.900725239	-4.523925386	2.630304211
C	-3.776748344	-3.276099926	2.739784913
C	-3.087654498	-2.045117701	2.169673548
O	-3.065006729	-1.901940788	0.920731351
O	-2.591790115	-1.230203508	3.024628249
C	-1.920255573	-1.349668359	6.575359218
C	-0.578405236	-1.570013405	5.972141668
N	-0.126991195	-1.040144003	4.768910930
C	0.434256182	-2.324735696	6.510058947
C	1.117908288	-1.479595100	4.609807884
N	1.487289650	-2.249158925	5.639357478
C	8.612702126	-8.931114628	-1.715676294
C	7.314273676	-8.184279008	-1.707605098
C	6.549197133	-7.892267868	-0.597588440
C	6.634986436	-7.569326797	-2.816528602
N	5.449958493	-7.149624932	-0.942029498
C	5.475746102	-6.923794847	-2.291487183
C	6.874645537	-7.494104946	-4.203686553
C	4.576291276	-6.223170684	-3.103927736
C	5.981451734	-6.800276615	-5.010669955
C	4.843011779	-6.170124537	-4.466649724
C	2.014984414	-5.230372611	2.483087801
C	3.293468277	-5.883429223	1.952085826
O	3.981962419	-6.590301048	2.742576775
O	3.598303897	-5.635173679	0.738001424
C	6.334707557	-3.690143614	6.899397526
C	5.140587866	-4.139591032	6.097147289
O	3.986148944	-3.747376229	6.362851612
N	5.396162792	-5.011332850	5.112129022
C	4.008001768	2.012732761	8.128804111
C	2.592003475	2.438786996	7.902464090
C	1.803712468	2.080840619	6.833306118
C	1.764413131	3.277435661	8.730503946
N	0.557428527	2.642618547	6.938551563
C	0.494140073	3.379111557	8.090500217
C	1.952600964	3.952093379	9.952667253
C	-0.562722931	4.119949945	8.628210056
C	0.904282118	4.688842559	10.490155660
C	-0.340628826	4.773676051	9.834499383
O	-4.598264618	1.257380783	8.652563191
H	-0.840539605	4.546704626	-2.287161749
H	0.343558518	3.357883425	-2.921347395
H	-1.388807991	3.174883814	-3.267657147
H	3.901912422	2.577629466	1.198983731
H	2.867986916	3.987107094	0.924334194
H	4.155306225	4.056779019	2.143284758
H	1.996292353	3.763030511	3.322231409
H	2.979213285	2.337332543	3.528389341
H	3.779463826	0.212295799	-3.047785449

H	2.035025371	0.507010698	-2.981368327
H	3.097167360	1.268534487	-1.794568618
H	4.343270273	-2.315540973	-2.123822413
H	1.432633731	-2.517647007	0.909460774
H	3.323212743	-3.718564417	-0.222224614
H	2.198001000	0.260000000	-9.843999000
H	0.793476722	1.211001983	-10.325866006
H	2.120502082	1.988579916	-9.446431457
H	0.198622399	-1.230191989	-8.850638397
H	1.365042813	2.585312176	-7.241854597
H	-0.916512533	-1.786732622	-6.718435991
H	0.254199581	2.036359779	-5.125662833
H	-1.861889022	2.039048697	0.734356407
H	-6.479119267	0.888578559	3.963034026
H	-5.467392846	-0.087245619	5.039461316
H	-5.978113917	1.539559979	5.534655439
H	-4.639888753	2.530026593	3.645254444
H	-4.148873744	0.923982494	3.135032427
H	-1.968596898	-4.409190768	3.197800313
H	-3.434086942	-5.394902004	3.030723155
H	-2.640486169	-4.737585974	1.586463525
H	-4.041451461	-3.092653230	3.786481044
H	-4.704059934	-3.430474725	2.173109451
H	-1.999174336	-1.927765065	7.501106817
H	-2.085238767	-0.295436785	6.814550579
H	-2.723911293	-1.665786357	5.904042290
H	0.487086419	-2.897226333	7.427707841
H	1.768937583	-1.254241258	3.777910244
H	2.384530607	-2.714338095	5.752151642
H	9.467999000	-8.258002000	-1.545000000
H	8.639272698	-9.691055009	-0.926094407
H	8.784760125	-9.438972316	-2.671199384
H	6.712427265	-8.165932616	0.439988826
H	4.799839213	-6.713305355	-0.276039088
H	7.748003844	-7.973632100	-4.646574540
H	3.690093897	-5.746643600	-2.685512344
H	6.160536040	-6.741037481	-6.084142723
H	4.158739687	-5.634563598	-5.123709835
H	1.606002000	-5.719000000	3.376000000
H	2.256251126	-4.197726747	2.764031072
H	1.246771181	-5.189165480	1.704236713
H	6.513002000	-4.433001000	7.686001000
H	7.243997597	-3.624196787	6.293539961
H	6.124948744	-2.727493399	7.370150279
H	6.340102496	-5.314521636	4.927098500
H	4.658184729	-5.408584010	4.542344141
H	4.382000000	1.434001000	7.274999000
H	4.676475288	2.872718526	8.267106255
H	4.107765520	1.387002646	9.026568542
H	2.045445656	1.452409512	5.986022855
H	-0.207339362	2.484794714	6.297563885
H	2.905876208	3.895962238	10.478641151
H	-1.524825738	4.179494881	8.121085643
H	1.041531016	5.207442954	11.438711693
H	-1.146509324	5.354447665	10.282305864
H	-4.228312941	1.560519199	7.805598087
H	-5.385801994	1.811771989	8.752144727
H	-2.738123987	0.743287857	0.963099043
H	-0.984462809	0.467215461	-4.005699321