

Supporting Information

A Geometric and Electrostatic Study of the [4Fe-4S] Cluster of Adenosine-5'-Phosphosulfate Reductase from Broken Symmetry Density Functional Calculations and Extended X-ray Absorption Fine Structure Spectroscopy

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Supplementary Figure Legends

Supplementary Fig. 1. Structure-based sequence alignment of APS reductases from *Pseudomonas aeruginosa* and *Mycobacterium tuberculosis*. The ClustalW Multiple Sequence Alignment program was used. Strictly conserved residues are outlined in red, red letters indicate conserved residues and conserved regions are boxed in blue. Residues flanking the active site are outlined in green.

Supplementary Fig. 2. Comparison of XAS spectra for Mt-APSR with and without APS bound. A) XANES spectra; B) k^3 weighted EXAFS; and C) Fourier transforms.

Supplementary Fig. 3. Comparison of the k^3 weighted EXAFS (top) and the Fourier transforms for Mt-APSR, [4Fe-4S] and [3Fe-4S] ferredoxins.

Cartesian coordinates of the optimized Fe1·Fe2·Fe3·Fe4 state wild-type 4Fe-4S quantum cluster in chain-A.

211 atoms

Fe	-0.107163578	0.141433877	-0.071225829
Fe	-0.198227030	0.084430746	2.610912383
Fe	2.183164085	0.143843532	1.371700639
Fe	0.718969659	-2.061308632	1.140269589
S	1.602736596	-1.346877473	3.036453877
S	1.870503940	-0.965415894	-0.539619531
S	-1.451681704	-1.221230441	1.242881426
S	0.537043229	1.778339840	1.252125310
S	-1.211913153	1.221988848	4.348255839
S	4.314827513	0.829183148	1.584941905
S	0.894538389	-4.260319821	0.484547506
S	-1.023752245	0.914816947	-2.007302940
N	2.814945142	-1.131756403	8.352908172
C	2.630658353	-2.528426347	8.028899337
C	3.897498754	-3.218330292	7.493887576
N	4.760798954	-2.437043051	6.824206595
O	4.030531216	-4.441947797	7.651548704
C	1.510596542	-2.683361765	7.002705823
C	0.141270660	-2.201435845	7.471692621
C	-0.833092416	-2.236742036	6.296836826
N	-2.148793914	-1.694652729	6.606272481
C	-3.202752462	-2.359821474	7.066113476

N	-3.144567271	-3.659243998	7.350708690
N	-4.365994470	-1.704665019	7.227461965
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H	1.450288698	-3.741164636	6.749238435
H	1.800509062	-2.148361516	6.091952257
H	0.197073979	-1.173061913	7.844866198
H	-0.219560016	-2.833663836	8.292338539
H	-0.939578601	-3.248711057	5.905642582
H	-0.442379369	-1.617776027	5.489475859
H	-2.269069799	-0.699033027	6.446675358
H	-2.377288059	-4.242500672	7.028988864
H	-4.008651983	-4.144769876	7.567591018
H	-4.330207597	-0.693263267	7.311143786
H	-5.072471442	-2.149914533	7.804807027
H	2.558967275	-0.423287359	7.666953264
C	5.977111000	-2.929906000	6.238907000
H	6.869350000	-2.636805000	6.801957000
C	1.997669812	5.097724892	0.562735770
H	1.743299000	6.022431000	0.036064000
C	2.707613436	5.349097582	1.874270553
O	2.599425940	4.582996234	2.842153837
C	2.788692722	4.158455198	-0.366632709

C	4.171407136	4.562525602	-0.726089756
N	4.493900142	5.599935530	-1.579299724
C	5.813090571	5.684451499	-1.732589854
N	6.349424273	4.723192536	-0.992455757
C	5.364859830	4.013406729	-0.357905298
H	1.056352157	4.596539551	0.795646930
H	2.206420649	4.034656240	-1.283992115
H	2.861429080	3.180403701	0.105529851
H	3.835502010	6.213091144	-2.053261167
H	5.578245489	3.169285533	0.274847642
H	6.343711652	6.396304492	-2.343190209
H	7.349099906	4.554952497	-0.911127970
N	1.851781405	2.441429385	-6.986286499
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H	1.476316000	4.465196000	-7.300786000
C	0.602304989	3.062243297	5.631491151
H	0.982050000	4.110914000	5.606559000
C	1.756295478	2.068372025	5.591746219
N	2.579895950	2.117495110	4.517683197
O	1.946715695	1.271931071	6.524545166
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C	4.649552585	1.385011288	5.642420468

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H	3.455742591	0.217932421	4.357267917
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H	5.668849935	1.347484651	3.455062010
H	5.323203000	2.690085000	6.970951000
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H	-0.269354869	-3.259866189	-1.363657588
H	-1.318440501	-4.369094126	-0.472819566
H	-3.034079000	-5.540736000	-3.483255000
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C	-0.652499495	-0.722114230	-5.791526197
N	-0.973879323	-1.936988002	-6.245323764
O	0.198477658	0.015071503	-6.305377188
C	-0.356135303	-0.077456745	-3.401063682
H	-1.830818095	0.706940452	-4.775303509
H	-0.031269820	-1.059717558	-3.047128378
H	0.514728034	0.422897408	-3.822098570
C	-0.358249000	-2.570636000	-7.389921000
H	-1.111311000	-2.639926000	-8.181831000
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C	-0.384875398	-6.389709039	5.799845004
H	1.466691000	-7.130947000	5.085305000
N	-0.963179494	-7.540668443	5.424603407
O	-0.942734331	-5.591419167	6.571487584
C	1.131519288	-5.429452514	3.942096624
O	0.177215033	-5.994180754	3.030418686
C	2.556222095	-5.597507510	3.434136432
H	1.596924646	-5.666257177	6.033382962
H	0.908070043	-4.366180708	4.084971676
H	0.282656739	-5.482242524	2.184997661
H	2.742078412	-4.976101329	2.557680914
H	2.726874286	-6.647691473	3.164624520
H	3.272466642	-5.320028509	4.209591446
H	-1.938787000	-7.684524000	5.661721000
C	3.080778000	0.711402000	-8.141230000
H	3.027971000	0.637566000	-9.232461000
C	2.900252454	2.169919822	-7.776099284
O	3.679943971	3.049098994	-8.193160390
C	4.468020634	0.178325561	-7.745682969

C	4.663564514	-1.305307100	-8.075127872
C	4.070244442	-2.278220530	-7.058709543
N	4.758434579	-2.248011769	-5.765085018
C	5.882274403	-2.888661125	-5.446714106
N	6.492114473	-2.576179494	-4.282724603
N	6.386241751	-3.836250940	-6.222750176
H	2.282915943	0.102886085	-7.716137729
H	4.658892271	0.366107375	-6.681676941
H	5.216469753	0.752373463	-8.301051296
H	5.735459257	-1.519883670	-8.169724586
H	4.213587556	-1.531705317	-9.051496357
H	4.085046523	-3.301016899	-7.445243215
H	3.024185533	-2.059369455	-6.840047832
H	4.419245054	-1.586246986	-5.076180558
H	6.474154410	-1.595008641	-4.022695565
H	7.393642776	-3.016624988	-4.118710936
H	5.823963652	-4.284156895	-6.936499629
H	7.227176185	-4.322930812	-5.931659799
N	3.516609831	6.419167490	1.929881111
H	4.046672000	6.552932000	2.783092000
C	6.235497073	-2.572263417	4.770871983
C	5.334747867	-3.314926617	3.791081710
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C	6.883712395	-3.610234684	1.791757732
N	7.032691457	-3.320651862	0.328656602
C	2.580952725	4.279902513	-5.443270928
C	2.954932322	3.272894846	-4.397709648
C	2.082111902	2.636321616	-3.551154712
N	2.743904218	1.693858144	-2.808200805
C	4.068334810	1.701915111	-3.140667291
C	4.243531899	2.696525269	-4.141007179
C	5.121997219	0.935099373	-2.646523870
C	6.386890755	1.173154207	-3.161085637
C	6.594239144	2.163542071	-4.139600584
C	5.541712394	2.924976485	-4.622321091
C	0.165471568	-3.973511496	-7.039407791
H	0.736896000	-4.386578000	-7.879897000
O	1.053932726	-3.969267659	-5.919961232
C	-3.748830460	-0.834269085	-4.106473549
O	-4.265410215	0.171240276	-4.602123323
H	-4.321424000	-1.617048000	-3.604721000
C	3.223803242	-0.686823622	9.550738005
O	3.526790657	-1.389571173	10.519820306
H	3.237939000	0.408880000	9.561120000
N	5.756789645	4.764352652	-9.458928009
C	6.867234570	4.052777097	-9.214152532
N	6.950339478	3.384894639	-8.055136326
N	7.891919616	4.092253793	-10.053817752
C	9.146220609	3.357720176	-9.894941087

C	9.027970000	1.861262000	-10.151452000
H	8.816378000	1.617659000	-11.197833000
H	4.606322935	-1.433329427	6.779211379
H	1.289349613	1.661825885	-6.657338257
H	4.222338319	3.385838804	5.838075662
H	-2.334886945	-6.515185150	-2.219478947
H	-1.742686214	-2.422868962	-5.796025079
H	-0.552603981	-8.129194086	4.709579256
H	3.588649907	7.104680572	1.188648967
H	7.286380968	-2.832625758	4.588721753
H	6.145531238	-1.490834549	4.628996021
H	4.294107104	-3.055639933	3.998732344
H	5.434648259	-4.394895724	3.959400056
H	5.581927526	-1.932679896	2.146261581
H	4.758706422	-3.430807948	1.725904620
H	6.906682387	-4.699439297	1.885797451
H	7.770410690	-3.186817548	2.266908576
H	7.903395296	-3.720121307	-0.044139584
H	7.064663363	-2.308289355	0.158980088
H	6.255233343	-3.724220311	-0.208841311
H	0.552805203	3.692281051	-5.999322601
H	2.161014731	5.188438580	-4.988395253
H	3.477162461	4.586258403	-5.987057630
H	1.020737636	2.779102712	-3.415421949
H	2.325521041	1.109659627	-2.092982607
H	4.956290849	0.202740719	-1.864025746
H	7.236971459	0.608694237	-2.783728876
H	7.601996806	2.339048499	-4.508360745
H	5.729518326	3.711167585	-5.345487333
H	-2.172488533	-1.987523830	-3.605853601
H	0.452021815	-1.925039689	-7.728135736
H	-0.684370702	-4.643658364	-6.849853435
H	0.482359550	-3.930208400	-5.123834966
H	9.986308614	1.393993448	-9.893014236
H	8.255758348	1.392566721	-9.535621969
H	9.848710157	3.815331744	-10.596431199
H	9.537807830	3.551511106	-8.889413542
H	7.742536692	4.591016409	-10.926339732
H	5.640395562	5.139266418	-10.395140818
H	4.897827947	4.424175581	-9.028949725
H	7.715228938	2.743411105	-7.897039453
H	6.082748757	3.172945084	-7.578382102
H	5.940755698	-4.022585404	6.323985157

Cartesian coordinates of the optimized Fe1·Fe2·Fe3·Fe4·state wild-type 4Fe-4S quantum cluster in chain-B.

250 atoms

Fe	19.396986524	67.098967432	56.308529360
Fe	17.491248673	65.134308275	56.458016892
Fe	19.860088525	64.718218139	55.162330743
Fe	17.947835850	66.361463918	54.119847136
S	17.748790882	64.089553997	54.485618459
S	20.186105800	66.821240370	54.263555910
S	17.106275331	67.301134090	55.914209267
S	19.640578559	65.036720377	57.306009251
S	15.705038845	64.723061435	57.835590561
C	15.187628311	66.287429310	58.662006741
S	20.546738678	68.741982740	57.442095716
C	19.950291474	68.964543351	59.169319863
S	21.545425264	63.383797719	54.373596091
C	21.016767824	63.084584721	52.654975810
S	17.185530524	67.155427901	52.149731675
C	18.563313865	67.178537028	50.949742155
H	15.401924271	67.112450703	57.983973318
H	14.097840315	66.226040468	58.774929012
H	20.813394426	69.331817107	59.732089410
H	19.200518618	69.763069450	59.186622107
H	20.543256168	62.098157312	52.610310241
H	20.255748471	63.823295137	52.400140163
H	18.936826763	68.197583141	50.863881769
H	19.390184996	66.555090194	51.298879912
C	24.644002000	76.620997000	48.376996000
C	24.845930179	75.376409984	49.210413132
N	26.269407614	75.163829772	49.449448202
C	26.794123151	74.277507187	50.290095587
N	28.117585890	74.089232722	50.311037580
N	26.020689515	73.572117499	51.119631307
H	25.141612000	76.554791000	47.403845000
C	21.415000000	71.340996000	47.975999000
C	20.194111459	72.135296907	48.397864541
O	20.121338576	73.363447142	48.214689961
C	22.650295227	71.697081896	48.805287323
C	23.944641029	71.070145353	48.285561440
C	24.030438443	69.548299219	48.385920270
N	23.916835743	69.056605444	49.758566157
C	24.880950323	69.126685637	50.681964258
N	24.552019493	68.822580444	51.960672980
N	26.113629246	69.473695689	50.372639712
H	21.618741000	71.609153000	46.934074000
N	19.217146883	71.415462385	48.977583760
C	17.991000000	71.973996000	49.510998000
C	18.151813509	72.662023593	50.876927515
C	18.922565079	71.854839761	51.864350043
C	18.614773893	70.589553441	52.288524132

C	20.177763167	72.187068369	52.464621182
N	19.607035928	70.115101389	53.106398602
C	20.579729877	71.065293386	53.237449935
C	21.001100836	73.321651051	52.447823218
C	21.764522518	71.049843176	53.967609294
C	22.175539535	73.311847512	53.182129798
C	22.556326836	72.185370673	53.932151753
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C	15.701382029	70.892953061	56.288805692
C	16.053536848	70.966667924	57.766042366
O	16.252781943	69.942471805	58.434933890
C	16.950896225	70.820873427	55.391592375
C	17.875906551	71.975016768	55.496220045
N	17.653274222	73.209609703	54.921005235
C	19.070772952	72.086060419	56.143637874
C	18.660865591	74.036265692	55.187964230
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N	19.519478233	63.813261328	62.721583918
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C	18.382648588	61.796282376	60.756924706
C	17.844573193	61.691352764	59.330999065
N	16.534778938	61.058375909	59.226958123
C	16.288781970	59.753229927	59.164526764
N	15.017292526	59.337941490	59.009201601
N	17.266109416	58.854707009	59.229946030
C	19.374936036	63.925411899	64.050326600
O	19.937676049	63.236059925	64.908847909
H	18.677061000	64.732842000	64.291576000
N	22.005157589	64.599352565	61.692091827
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C	23.264095182	66.029566290	60.079461871
C	24.672364252	66.293794464	59.546393651
C	24.690562726	67.205985668	58.314685427
C	24.510292807	68.671315453	58.682927025
N	24.035258723	69.471110984	57.506494364
H	23.715284000	65.719872000	62.186842000
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C	21.387038063	59.245191518	58.382256246
O	20.249697795	59.305704842	58.877241851
C	22.129997260	61.509961392	57.482898780
O	22.213666694	60.895501450	56.185404259
C	23.184562672	62.594564831	57.659369117
H	23.378128000	60.073913000	58.312270000

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H	21.170100000	57.394186000	57.563113000
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C	17.268419745	66.551507956	60.236933389
H	15.420306000	67.594068000	60.325163000
O	17.829993240	65.679613919	60.912921138
N	17.959628369	67.587740468	59.698131676
C	19.391255849	67.729973609	59.900144499
C	19.778271831	67.856211768	61.375452974
O	20.854905477	67.404520461	61.783494877
N	18.970037379	68.576270784	62.161668400
H	19.238078000	68.583743000	63.137216000
N	17.906977406	65.286498694	49.557053890
C	18.116917951	66.714469250	49.563900818
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O	19.308887271	68.443360538	48.417378403
N	19.753945808	66.295335142	47.801817296
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O	20.972542621	63.983919272	49.672924569
H	22.652465000	64.135944000	51.642252000
N	21.165454838	61.746403988	49.902273878
H	20.434047000	61.601916000	49.210267000
S	26.544787925	70.950791719	55.146700609
O	26.726606507	71.545774616	56.479295352
O	25.901168095	71.823329495	54.164334480
O	25.983430166	69.581027396	55.191159816
P	28.547583783	70.758736253	53.004917751
O	28.023532330	69.493652753	52.371179532
O	28.284174150	72.106810480	52.394809915
O	28.136794439	70.768161188	54.635858380
O	30.170053174	70.711621912	53.201117709
C	30.911761898	69.485352408	53.369332931
C	31.969981316	69.725471261	54.432471172
O	31.406734743	69.626582660	55.778516284
C	33.140375064	68.758910110	54.415007444
O	34.283600077	69.419688374	54.966319742
C	32.649455837	67.651938499	55.334617488
O	33.726284211	66.892364179	55.845494444
C	31.857351143	68.444452601	56.393549908
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C	29.499822196	66.070766826	57.811560899
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H	15.356828236	65.875885599	60.784356066
H	18.951314708	64.429253705	62.142119536
H	17.461095080	68.302341531	59.175310440
H	19.899958956	66.831975741	59.551252763
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H	23.008073127	63.424926555	56.972053224
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H	24.181738242	62.181183398	57.461473545
H	21.968711641	61.601946812	55.533693151
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H	17.035761064	57.870843876	59.140913759
H	18.240873223	59.103091744	59.082678620
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H	18.551354180	61.170457986	58.682476010
H	17.714592346	62.694138844	58.925173680
H	18.458949104	60.804248182	61.217909919
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H	19.715911835	63.361171199	60.098389412
H	20.456346620	61.772066618	60.227135789
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H	23.956355311	64.320537949	61.179718639
H	22.685461103	65.508508706	59.309435021
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H	25.308663239	66.721027277	60.334274488
H	25.121090787	65.333138877	59.267159221
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H	23.757982330	68.820104042	59.458990847
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H	23.646187853	69.159519311	52.272251711
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H	26.839424909	69.548712962	51.111071418
H	26.425818208	69.409607658	49.411215452
H	23.130777797	68.452301149	49.972623549
H	23.220953037	69.072250304	47.833200861
H	24.961298260	69.190020495	47.931076124
H	24.085129434	71.327487974	47.226257964

H	24.789247107	71.507344509	48.829815815
H	22.765427115	72.785086781	48.780704504
H	22.487689171	71.426479221	49.855951939
H	21.203761866	70.270259632	48.011784871
H	19.341735684	70.411478332	49.043383110
H	17.254408119	71.167319764	49.560648175
H	18.656112687	73.619726567	50.722171629
H	17.140616146	72.893416620	51.241536479
H	20.725284767	74.198549159	51.869187242
H	22.818993571	74.188850014	53.183178092
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H	19.617667752	69.197341719	53.534022542
H	17.756918822	69.971582197	52.074894962
H	20.400753710	73.741304636	56.285022328
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H	16.855589088	73.464094381	54.344319946
H	19.631872289	71.355360378	56.702566178
H	17.515528934	69.923627306	55.635131238
H	16.608711952	70.719047961	54.356331631
H	15.131598887	69.971496378	56.140459758
H	16.080821875	73.038109146	57.754236138
H	33.311004617	66.283923190	56.517684310
H	34.796255456	68.720389754	55.422860755
H	28.093392159	63.445710540	59.264289741
H	27.347105479	64.930556348	58.775030051
H	32.449592476	63.781509095	58.239793493
H	29.040975660	68.987677694	56.637158106
H	30.251577101	68.657959605	53.639567481
H	31.399138217	69.260421163	52.412622769
H	26.484340464	72.976251121	51.807877723
H	25.090212443	73.904096154	51.341727364
H	28.472525127	73.349085849	50.919988038
H	28.657717887	74.318591572	49.486804593
H	26.918920039	75.644053045	48.834413259
H	24.335856646	75.506877489	50.171118487
H	24.427581901	74.502531778	48.700510842
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H	32.479176181	68.684317196	57.265515186
H	32.341042763	70.751559692	54.328395847
H	18.007694338	68.774544391	61.916544553
C	16.838216594	64.670137276	49.021342256
O	15.946914982	65.209684662	48.360524830
H	16.849535000	63.603479000	49.253523000
O	22.483155038	66.155241398	48.716781014
C	22.147720413	65.901909795	47.348931113
H	22.982507000	66.274602000	46.742711000
H	18.555141174	64.704994599	50.082679478

H	21.978260652	65.485264567	49.231225244
H	20.601667000	66.337714000	45.892815000
H	20.989612330	67.688249151	46.959665998
H	22.059246237	64.822055920	47.173568752
H	33.363738234	68.382795240	53.410059769
H	31.945659303	67.018323545	54.774408759
H	23.061204346	69.198900309	57.272926054

Cartesian coordinates of the optimized Fe1·Fe2·Fe3·Fe4 state no-tandem 4Fe-4S quantum cluster model in chain-A.

211 atoms

Fe	-0.054305588	0.187557929	-0.074383955
Fe	-0.233227045	0.069135846	2.597468994
Fe	2.252523730	0.164000675	1.412340746
Fe	0.746584959	-2.039967749	1.144084076
S	1.598885362	-1.324948891	3.062351120
S	1.938094773	-0.929528652	-0.515173723
S	-1.433257776	-1.210288992	1.183730111
S	0.567148204	1.784602845	1.318654212
S	-1.360304293	1.063956262	4.341706409
S	4.441290543	0.775711068	1.577998432
S	0.878305799	-4.242168134	0.499432685
S	-0.975799392	0.960741198	-2.020526024
N	2.800264022	-1.131090654	8.352587838
C	2.605261795	-2.523300186	8.017308721
C	3.864941677	-3.214278324	7.462973284
N	4.760765971	-2.426110808	6.838356325
O	3.957259539	-4.445559496	7.556356601
C	1.473685136	-2.665891924	7.000232026
C	0.103447518	-2.191291774	7.478614305
C	-0.883608505	-2.244268925	6.312794986
N	-2.196354629	-1.697693831	6.625129800
C	-3.251783510	-2.358867188	7.088988779
N	-3.193075815	-3.655219219	7.389087098
N	-4.413754961	-1.701918608	7.243152894
H	2.352590945	-3.059877539	8.937229149
H	1.411829735	-3.721651484	6.739634140
H	1.758572637	-2.130534481	6.086746094
H	0.147418516	-1.161416286	7.852276123
H	-0.243108255	-2.822495497	8.306009588
H	-0.990344754	-3.262435788	5.937776339
H	-0.503861636	-1.637267751	5.491269253
H	-2.324976845	-0.710974308	6.418538100
H	-2.434794512	-4.244023119	7.056186479

H	-4.059262356	-4.135323602	7.610317374
H	-4.382023111	-0.689679241	7.314527410
H	-5.127747885	-2.144382235	7.813132591
H	2.493616736	-0.423185129	7.693025133
C	5.977111000	-2.929905000	6.238906000
H	6.869350000	-2.636804000	6.801956000
C	1.983263985	5.099406029	0.567105016
H	1.743299000	6.022431000	0.036064000
C	2.665096262	5.362945301	1.893812130
O	2.484141005	4.641167620	2.882507578
C	2.781562359	4.160311977	-0.355094907
C	4.155481572	4.581335179	-0.726722725
N	4.456991754	5.632523761	-1.570674723
C	5.773797879	5.735452727	-1.736388270
N	6.328585657	4.771951407	-1.012229410
C	5.358403055	4.041815753	-0.377543282
H	1.036450325	4.603373820	0.787541904
H	2.196993128	4.021123565	-1.269198809
H	2.870340739	3.186970221	0.123525515
H	3.785488240	6.241237752	-2.031955702
H	5.587184232	3.192464417	0.242772236
H	6.290230564	6.463240845	-2.340692498
H	7.330851456	4.616438419	-0.934006958
N	1.856379490	2.444910916	-6.989848484
C	1.539952000	3.763439000	-6.462626000
H	1.476316000	4.465198000	-7.300785000
C	-0.169694739	3.103937559	5.941767704
H	0.090269947	4.171509837	5.993627562
N	2.879477152	1.977430652	4.429586025
C	-0.842322451	2.827025200	4.604188971
H	-0.828418444	2.871841652	6.785436477
H	-1.753725390	3.430185630	4.511967292
H	-0.176058591	3.105140015	3.787277472
C	4.123943506	1.224796361	4.414396097
C	4.959892501	1.514656233	5.676942832
N	4.738762462	2.715986493	6.230416966
O	5.792384059	0.697969768	6.102233149
H	2.831354014	2.664971600	3.679491950
C	4.999731091	1.496334487	3.183248747
H	3.915577662	0.152792081	4.451852178
H	5.092025273	2.582435122	3.057340726
H	6.005014614	1.099014206	3.359471668
H	5.186885107	2.962073568	7.108268522
C	-0.092483957	-5.307275203	-1.930785919
C	-1.131084440	-5.067184910	-2.997561423
H	0.901281896	-5.201978921	-2.376172110
N	-2.233625343	-5.824998279	-2.930413994
O	-1.012035305	-4.154914810	-3.834274992
C	-0.326010410	-4.219279522	-0.878781451

H	-0.184907014	-6.306000568	-1.492576735
H	-0.258713340	-3.249554942	-1.372668268
H	-1.335104447	-4.317166675	-0.463725511
H	-3.034078000	-5.540736000	-3.483256000
N	-2.442820433	-1.116899780	-4.084999374
C	-1.387261474	-0.239873411	-4.527390682
C	-0.670922629	-0.710182532	-5.802881582
N	-0.975702459	-1.935081649	-6.242808980
O	0.160289872	0.036638998	-6.334700589
C	-0.350215916	-0.058854586	-3.415463146
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H	-0.034948465	-1.042094907	-3.055348923
H	0.522381101	0.425052359	-3.851816115
C	-0.358249000	-2.570636000	-7.389921000
H	-1.111310000	-2.639926000	-8.181831000
C	1.001816669	-6.171714610	5.264340215
C	-0.390449592	-6.385474176	5.799349139
H	1.466690000	-7.130947000	5.085306000
N	-0.966124065	-7.538634200	5.428219567
O	-0.950638867	-5.580500281	6.562494761
C	1.111689642	-5.429915583	3.935748650
O	0.139375143	-5.984605754	3.036609199
C	2.527117964	-5.609862914	3.408145408
H	1.592709080	-5.659187648	6.023774534
H	0.896947096	-4.365276385	4.082443178
H	0.238152666	-5.469377808	2.192563083
H	2.707884080	-4.988002190	2.531365550
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H	-1.938788000	-7.684524000	5.661722000
C	3.080778000	0.711404000	-8.141230000
H	3.027971000	0.637569000	-9.232461000
C	2.910753663	2.171416163	-7.770561531
O	3.703910707	3.046463313	-8.173942581
C	4.463336007	0.172338378	-7.742061871
C	4.667614770	-1.306865921	-8.086138982
C	4.080541286	-2.297048351	-7.082890464
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C	5.892582456	-2.916874443	-5.473571011
N	6.516861987	-2.588197876	-4.323185835
N	6.382229487	-3.880183800	-6.239277799
H	2.278288409	0.107688748	-7.717228601
H	4.646909220	0.350457159	-6.675032616
H	5.215519080	0.751889046	-8.286070327
H	5.741321934	-1.513205031	-8.179448589
H	4.222330816	-1.525550372	-9.066381426
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H	6.506485156	-1.604552792	-4.073254015
H	7.410957834	-3.040174926	-4.151842549
H	5.808798227	-4.341745508	-6.935070565
H	7.235088097	-4.353364278	-5.960898886
N	3.506989762	6.412083899	1.935009596
H	4.046672000	6.552931000	2.783093000
C	6.213249472	-2.566414694	4.772534741
C	5.312443095	-3.323447256	3.803558074
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C	6.874198354	-3.631393488	1.819833899
N	7.039142806	-3.346703534	0.357322321
C	2.575211531	4.284372928	-5.441427451
C	2.964231093	3.273883379	-4.405191006
C	2.102590481	2.628879446	-3.553969355
N	2.776333914	1.687638206	-2.820537996
C	4.097644078	1.704098238	-3.165089167
C	4.258270387	2.703438266	-4.163454790
C	5.159701851	0.940451204	-2.684313814
C	6.418000523	1.187062228	-3.210858547
C	6.610305499	2.180862560	-4.189036079
C	5.549543361	2.938106589	-4.660031642
C	0.156488114	-3.975671414	-7.041520453
H	0.736896000	-4.386578000	-7.879897000
O	1.030898201	-3.981667103	-5.911460272
C	-3.755649323	-0.825623575	-4.102669684
O	-4.277123230	0.176697755	-4.598652146
H	-4.321424000	-1.617049000	-3.604721000
C	3.217636837	-0.684748171	9.552516474
O	3.546011118	-1.388947740	10.508668972
H	3.237939000	0.408881000	9.561120000
N	5.710472249	4.793739343	-9.601616052
C	6.798316424	4.065509779	-9.309430110
N	6.813878952	3.399646174	-8.145294241
N	7.857025494	4.086939684	-10.106308754
C	9.109012949	3.360773319	-9.889356273
C	9.027971000	1.861263000	-10.151451000
H	8.816379000	1.617661000	-11.197832000
H	4.659694433	-1.417762731	6.900014619
H	1.285725365	1.665828090	-6.674772885
H	3.897611597	3.209829694	5.944268955
H	-2.376460773	-6.496188550	-2.184397395
H	-1.735717362	-2.427358766	-5.785691864
H	-0.554065312	-8.128515625	4.715323569
H	3.661730968	7.024748032	1.144876878
H	7.265667518	-2.811486471	4.579080900
H	6.110801146	-1.485115746	4.637200150
H	4.270874043	-3.064078886	4.006965574
H	5.414047568	-4.400556877	3.988030482
H	5.548222310	-1.965355165	2.137863756

H	4.746779806	-3.479796176	1.737786036
H	6.906484726	-4.719847418	1.920285881
H	7.751541081	-3.198450684	2.303599634
H	7.925166101	-3.726670093	-0.000191396
H	7.049456479	-2.334834731	0.181357525
H	6.281037058	-3.770537822	-0.192134324
H	0.550921920	3.688359502	-6.002791220
H	2.143952725	5.183054892	-4.977848634
H	3.466774344	4.607474650	-5.983133155
H	1.041786695	2.764565926	-3.407352935
H	2.366531188	1.095026669	-2.107216664
H	5.005112216	0.203402874	-1.903974239
H	7.274351047	0.624830526	-2.844609610
H	7.613240190	2.361582755	-4.568373773
H	5.725721241	3.720188463	-5.390602650
H	-2.173323516	-1.964064780	-3.591123245
H	0.451754322	-1.925026171	-7.726906889
H	-0.698267513	-4.643861903	-6.867091615
H	0.451554033	-3.958306640	-5.119466007
H	9.998577632	1.419762272	-9.897226239
H	8.268654482	1.371700425	-9.534406515
H	9.835978643	3.826751686	-10.559834336
H	9.455173570	3.558951340	-8.867987605
H	7.768548159	4.627674356	-10.962250495
H	5.619723858	5.152148882	-10.546743854
H	4.837998545	4.502964206	-9.164508343
H	7.565385544	2.751708154	-7.953068903
H	5.908642553	3.166250331	-7.748524232
H	5.927193536	-4.020124188	6.325910432
H	0.757080428	2.534928354	6.043702636
H	2.091114258	1.351279616	4.305134025

Cartesian coordinates of the optimized Fe1·Fe2·Fe3·Fe4 state no-tandem 4Fe-4S quantum cluster model in chain-B.

250 atoms

Fe	19.456112321	67.170510792	56.435488094
Fe	17.468860469	65.170955277	56.453879129
Fe	19.901278452	64.776935263	55.267920603
Fe	18.041597871	66.417142105	54.187823400
S	17.832380510	64.137391636	54.497964333
S	20.280209298	66.880441540	54.396663481
S	17.185539923	67.373512771	55.973542990
S	19.563126340	65.092297317	57.428882544
S	15.669434913	64.523085737	57.696080082

C	14.835102764	65.899928761	58.606509228
S	20.637231300	68.830715680	57.551842384
C	20.250436524	69.064739264	59.344382839
S	21.535699484	63.421780399	54.400667331
C	20.997922644	63.125223015	52.679741971
S	17.249937591	67.131883171	52.198271664
C	18.587456729	67.159436798	50.946768512
H	15.227685202	66.849105855	58.236299600
H	13.777163766	65.844245299	58.323611989
H	21.200302947	69.275315237	59.845345863
H	19.627147836	69.963948759	59.437102114
H	20.511607934	62.144058098	52.643037734
H	20.247385072	63.873524158	52.424014663
H	18.973037052	68.175663917	50.866733990
H	19.416044698	66.516878290	51.257608774
C	24.644002000	76.620996000	48.376995000
C	24.830976692	75.368758120	49.200860005
N	26.253059585	75.145968850	49.436612080
C	26.769430877	74.226759700	50.246813202
N	28.086889616	74.014741892	50.252915487
N	25.984422689	73.504573794	51.055271542
H	25.141612000	76.554789000	47.403844000
C	21.415000000	71.340996000	47.975999000
C	20.197436723	72.138310005	48.400217860
O	20.127545323	73.367684123	48.220180856
C	22.651803670	71.684202558	48.807855657
C	23.937421076	71.032259295	48.297336416
C	23.997283298	69.511342881	48.425813852
N	23.881224712	69.049501357	49.807753478
C	24.852334917	69.105841972	50.723577372
N	24.525425630	68.823866651	52.008227691
N	26.090556857	69.417034819	50.401997061
H	21.618741000	71.609153000	46.934074000
N	19.219848889	71.417870003	48.978510811
C	17.991000000	71.973996000	49.510998000
C	18.144828081	72.655003789	50.880881235
C	18.913574235	71.840508854	51.863403306
C	18.600512122	70.573108725	52.276941519
C	20.173472544	72.159414687	52.461036344
N	19.594624635	70.084770066	53.084246569
C	20.572358690	71.028194911	53.221605886
C	21.002905597	73.289923324	52.453557621
C	21.759217479	70.998398579	53.948078390
C	22.179840443	73.266318869	53.183712833
C	22.558401295	72.129614896	53.920267100
H	17.633684000	72.744706000	48.820090000
C	15.680715526	70.883580470	56.291553002
C	16.011006914	70.961807766	57.773698082
O	16.122887853	69.938520940	58.460325539

C	16.922812190	70.791275159	55.388877122
C	17.867745637	71.928103608	55.484096195
N	17.662168484	73.165533081	54.909420323
C	19.071227405	72.014960155	56.118597449
C	18.688701733	73.972148749	55.163555699
N	19.547010980	73.281252995	55.903165035
H	15.078911000	71.721456000	55.939197000
N	16.187320837	72.193249810	58.298261584
H	16.562673000	72.275889000	59.244499000
N	19.510963601	63.809786437	62.711777051
C	20.335021542	62.824880605	62.045714884
C	21.789038131	63.275193136	61.811248669
O	22.657822854	62.408756452	61.648451451
C	19.730649297	62.461540855	60.688383016
C	18.369065780	61.771678861	60.727794938
C	17.853040544	61.623383493	59.295989123
N	16.553572645	60.971898739	59.191611262
C	16.321841927	59.662388560	59.130198975
N	15.054973608	59.239838428	58.982386565
N	17.308052040	58.773934746	59.194461661
C	19.387833385	63.936287005	64.047902263
O	19.993002141	63.275100933	64.893506487
H	18.677061000	64.732841000	64.291576000
N	22.003092543	64.599790284	61.705077013
C	23.289001000	65.171998000	61.339999000
C	23.253766529	66.027649626	60.080806267
C	24.662386901	66.258762308	59.529034068
C	24.692253983	67.158561528	58.288835681
C	24.557158354	68.629494646	58.651069370
N	24.056991213	69.438544304	57.493566386
H	23.715284000	65.719872000	62.186842000
C	22.357872828	60.395068119	58.482014704
C	21.387531451	59.243686462	58.369914389
O	20.246800815	59.306856939	58.857804701
C	22.129794648	61.505057089	57.465500368
O	22.205572742	60.889861080	56.168169228
C	23.189493988	62.585112485	57.638472904
H	23.378129000	60.073913000	58.312270000
N	21.829276909	58.146914452	57.736100646
H	21.170101000	57.394186000	57.563113000
C	14.967872766	65.827169920	60.122778369
H	14.342282492	66.610732638	60.575214208
N	18.126729919	67.799583738	59.745536044
C	19.546015423	67.904579323	60.056926733
C	19.779441266	68.040816533	61.577582677
O	20.895900943	67.827795796	62.075882272
N	18.699626597	68.411072054	62.278971658
H	18.739084701	68.468973379	63.291823715
N	17.877069479	65.299951869	49.540549861

C	18.099288330	66.725811363	49.560577269
C	19.102047874	67.230829851	48.512053116
O	19.278157625	68.450716972	48.391819023
N	19.750132907	66.301114827	47.801645686
C	20.853000000	66.606999000	46.924000000
C	22.118341495	63.173598248	51.626585547
C	21.387619647	63.015059003	50.313587506
O	20.916440085	63.992668518	49.706838173
H	22.652465000	64.135944000	51.642252000
N	21.160900645	61.756692791	49.904883312
H	20.434046000	61.601916000	49.210267000
S	26.573594656	70.992773130	55.222100805
O	26.872958723	71.379830714	56.610938025
O	25.963577534	72.050988013	54.411627674
O	25.888174877	69.680606054	55.117769936
P	28.496817793	70.699555285	52.976510893
O	27.989254872	69.406357423	52.387730903
O	28.189844362	72.019260697	52.329455069
O	28.113610466	70.745339438	54.613738417
O	30.120181113	70.682599503	53.159638568
C	30.873890045	69.467895125	53.358486133
C	31.917000008	69.724714341	54.433940646
O	31.350126332	69.614149736	55.777374381
C	33.099627987	68.772705076	54.419919706
O	34.225225188	69.450860817	54.983468680
C	32.615389095	67.654950354	55.331632884
O	33.696063759	66.899907971	55.841778713
C	31.813249769	68.434849042	56.391012672
N	30.665695764	67.645117964	56.886543873
C	29.342858298	67.999688817	56.981773468
N	28.584971559	67.060316220	57.513881893
C	29.468702394	66.038902686	57.793092997
C	29.304798581	64.752682694	58.339036767
N	28.099659040	64.249730320	58.668194564
N	30.395316119	63.973071911	58.493790827
C	31.584935121	64.439728720	58.096770102
N	31.861406444	65.624630893	57.543889148
C	30.762901496	66.385964949	57.419241473
H	15.998900201	66.001017221	60.441270803
H	18.875384018	64.368131256	62.150847692
H	17.796242151	68.569901127	59.166930017
H	20.059068434	66.979047653	59.781949995
H	17.150372977	67.216536069	49.324954094
H	19.520210166	65.326548637	47.964201332
H	22.838277513	62.364478166	51.788096137
H	21.448412749	60.962804717	50.466662725
H	23.013539421	63.417926757	56.954529043
H	23.176132138	62.971692423	58.660278388
H	24.183281257	62.167506953	57.433072827

H	21.968315487	61.602504452	55.519777385
H	21.131969104	61.937337108	57.601858798
H	22.296855490	60.795129546	59.496155816
H	22.722076751	58.131059396	57.257012792
H	17.082953432	57.785993039	59.138408489
H	18.282017393	59.025203081	59.043784049
H	14.868800464	58.248012699	59.093224125
H	14.307699057	59.853375033	59.292390774
H	15.756641593	61.578805649	59.025958828
H	18.577844926	61.095949826	58.673980870
H	17.715448533	62.610984277	58.856813160
H	18.465668086	60.789531756	61.206178498
H	17.638623195	62.347497390	61.309153851
H	19.675020664	63.373264519	60.081173738
H	20.438092463	61.798797440	60.191079583
H	20.393642805	61.937595698	62.683958141
H	21.258464040	65.240064158	61.958549044
H	23.949323417	64.315194841	61.176876079
H	22.654038070	65.517012236	59.319658057
H	22.756984483	66.974647772	60.301847310
H	25.315458395	66.676675936	60.308207885
H	25.083730343	65.283842544	59.256091802
H	25.631185421	67.013634780	57.741359541
H	23.876057967	66.861150556	57.617618344
H	23.836308899	68.794999805	59.452949068
H	25.512952902	69.064367468	58.955468168
H	24.044135726	70.434230245	57.746427888
H	24.662265224	69.353992058	56.652416298
H	23.628966561	69.183465429	52.320928831
H	25.260894383	68.929436100	52.704181431
H	26.826523514	69.472344048	51.134218323
H	26.391188990	69.359755110	49.436127251
H	23.070920085	68.487768591	50.044464627
H	23.177509128	69.039467402	47.885330299
H	24.917726624	69.123359355	47.973451844
H	24.080724919	71.268758390	47.233746171
H	24.788142556	71.466440065	48.834874611
H	22.783667692	72.770105456	48.778246017
H	22.480222370	71.421983490	49.859002137
H	21.196159411	70.271666429	48.008129625
H	19.337595456	70.412064169	49.031099258
H	17.256381060	71.164883224	49.554712318
H	18.645779260	73.615872636	50.735060352
H	17.130714794	72.878810833	51.242437692
H	20.728196778	74.175166211	51.886631026
H	22.825998702	74.141134293	53.193090413
H	23.498938391	72.133306725	54.456931725
H	22.034406235	70.125065802	54.529059470
H	19.597235084	69.167195454	53.512509581

H	17.738530380	69.961903943	52.060429574
H	20.433586958	73.647113439	56.239485666
H	18.800967263	74.989926405	54.829002318
H	16.863184238	73.431723793	54.339924407
H	19.621625356	71.273026520	56.675394756
H	17.475894857	69.886292957	55.628192895
H	16.571239873	70.691868482	54.356615530
H	15.091491693	69.974205057	56.144882179
H	16.172506076	73.028655595	57.725259067
H	33.282068591	66.279289411	56.502594167
H	34.802820063	68.747351870	55.348241684
H	28.071674953	63.405097418	59.231385823
H	27.325964922	64.892373289	58.763133537
H	32.429577629	63.771489822	58.243298616
H	28.995785747	68.957914186	56.629129742
H	30.218345634	68.637714107	53.628388092
H	31.374677395	69.237613067	52.411725890
H	26.456225200	72.902622354	51.734094430
H	25.089760187	73.887203658	51.332326799
H	28.444449460	73.270837863	50.853856644
H	28.642564227	74.295870087	49.453074111
H	26.903359730	75.623471940	48.820241178
H	24.321793751	75.494384484	50.162781418
H	24.406149374	74.501887421	48.684225925
H	23.573840831	76.778246752	48.198869323
H	25.033228782	77.493915021	48.912966881
H	32.431853802	68.678582249	57.264046977
H	32.273908652	70.756243646	54.334798895
H	17.805069567	68.397856411	61.795300008
C	16.799331941	64.674444356	49.033949350
O	15.871046960	65.200724700	48.413368754
H	16.849535000	63.603478000	49.253524000
O	22.479645970	66.129784626	48.714302841
C	22.145641407	65.894565812	47.343233169
H	22.982507000	66.274601000	46.742711000
H	18.548727025	64.715109587	50.030492470
H	21.957957800	65.468877866	49.223331701
H	20.601667000	66.337713000	45.892815000
H	20.992916612	67.688065055	46.958714262
H	22.055332129	64.817006549	47.153192080
H	33.334852547	68.404237196	53.414193530
H	31.919450028	67.018993720	54.764747228
H	23.073901009	69.169245698	57.280881859
H	14.634821341	64.859006964	60.513068393
H	17.945662409	66.948779314	59.223140218

Cartesian coordinates of the optimized Fe1·Fe2·Fe3·Fe4 state K144A 4Fe-4S quantum cluster model in chain-A.

199 atoms

Fe	-0.144539720	0.196975706	-0.081662473
Fe	-0.245547735	0.093471428	2.608586257
Fe	2.157733280	0.128683596	1.357114349
Fe	0.656450272	-2.058096363	1.144667721
S	1.549709570	-1.346762810	3.028719584
S	1.828131163	-0.958191792	-0.555516387
S	-1.510088508	-1.179246970	1.231168536
S	0.538766374	1.792018095	1.274793729
S	-1.213728320	1.210444745	4.387821635
S	4.310417364	0.743907225	1.617286379
S	0.871519588	-4.257752479	0.497020769
S	-1.026377570	0.973455188	-2.039924457
N	2.812448972	-1.144235117	8.372553786
C	2.637610287	-2.544295466	8.058889141
C	3.905498942	-3.231916668	7.521788363
N	4.779311669	-2.443796413	6.879809248
O	4.026239451	-4.460180023	7.657665862
C	1.514590873	-2.708143239	7.036775623
C	0.145776715	-2.228411752	7.510617751
C	-0.834718271	-2.255721559	6.340420228
N	-2.146327437	-1.707827787	6.658423801
C	-3.194582402	-2.364724204	7.142315038
N	-3.138723046	-3.663138384	7.434378422
N	-4.351057333	-1.702824618	7.321199643
H	2.384682756	-3.071675198	8.984167769
H	1.457685146	-3.766530257	6.787462466
H	1.800434369	-2.176120872	6.122352578
H	0.203181950	-1.202523485	7.890415999
H	-0.211348637	-2.865253741	8.329337480
H	-0.949835090	-3.266219306	5.948266559
H	-0.445716832	-1.636691219	5.531832822
H	-2.260023283	-0.709360962	6.511711330
H	-2.384065790	-4.251659661	7.093097071
H	-4.006171862	-4.142618411	7.651859486
H	-4.312719592	-0.690154037	7.382939658
H	-5.047549491	-2.136519163	7.918862695
H	2.538318941	-0.441901919	7.687048409
C	5.977111000	-2.929906000	6.238907000
H	6.869350000	-2.636805000	6.801957000
C	2.007541964	5.096863435	0.558304007
H	1.743299000	6.022431000	0.036064000
C	2.693467027	5.355877522	1.881632020
O	2.561421422	4.601486240	2.855244407
C	2.826115350	4.170938441	-0.361236480

C	4.201817764	4.604468308	-0.714376983
N	4.503115478	5.650132570	-1.565363840
C	5.820323090	5.763195191	-1.718525440
N	6.376502281	4.814275844	-0.976881696
C	5.406405184	4.080900984	-0.346048050
H	1.071523408	4.580277634	0.777154490
H	2.255141145	4.026576917	-1.282882422
H	2.917631749	3.196429434	0.116167138
H	3.831413838	6.246312474	-2.042071826
H	5.643312777	3.242209284	0.285402693
H	6.335950163	6.486869947	-2.328285207
H	7.379278827	4.663004000	-0.894333609
N	1.856169819	2.444883833	-6.992414952
C	1.539951000	3.763438000	-6.462627000
H	1.476316000	4.465197000	-7.300786000
C	0.600139221	3.064758941	5.650834713
H	0.982050000	4.110914000	5.606559000
C	1.749542100	2.065825801	5.613363571
N	2.568122038	2.101465341	4.534639949
O	1.941730204	1.276341840	6.551524102
C	-0.458234231	2.896883357	4.552823618
H	0.137540461	2.935474359	6.633947941
H	-1.283220901	3.583046328	4.778175521
H	-0.050034124	3.177450482	3.582130960
C	3.741267468	1.243701718	4.437453430
C	4.634344640	1.377105116	5.664618920
N	4.848478381	2.629101260	6.087704335
O	5.222167206	0.405332353	6.152798605
H	2.428199248	2.814222611	3.823682266
C	4.622262421	1.590073606	3.220573579
H	3.441021090	0.196938488	4.397922236
H	4.597010178	2.672489178	3.058796929
H	5.655146174	1.330713512	3.473321348
H	5.323203000	2.690085000	6.970952000
H	0.913280561	-5.169970008	-2.390702619
C	-0.076931442	-5.323146549	-1.951690960
C	-1.121015034	-5.077908007	-3.012873410
N	-2.225150430	-5.834260580	-2.943215550
O	-1.005769704	-4.160725881	-3.844589613
C	-0.351988884	-4.278101468	-0.865378165
H	-0.137435575	-6.338515473	-1.547109648
H	-0.347090072	-3.293242921	-1.333853327
H	-1.346357534	-4.443590117	-0.437128310
H	-3.034079000	-5.540736000	-3.483254000
N	-2.441811576	-1.116416310	-4.092100095
C	-1.392344028	-0.233881081	-4.539824077
C	-0.674636879	-0.705064787	-5.813125889
N	-0.971267746	-1.935288262	-6.242354397
O	0.146511327	0.045820480	-6.355420715

C	-0.362604066	-0.033679726	-3.425707863
H	-1.853385630	0.723224959	-4.798060133
H	-0.027892634	-1.008527346	-3.060397943
H	0.502485696	0.467601396	-3.857322660
C	-0.358250000	-2.570636000	-7.389921000
H	-1.111312000	-2.639925000	-8.181831000
C	1.024796395	-6.172020935	5.297517751
C	-0.381202231	-6.384679047	5.806496618
H	1.466691000	-7.130947000	5.085305000
N	-0.964802344	-7.529615461	5.418589463
O	-0.942383583	-5.587328642	6.576674390
C	1.172779600	-5.394337274	3.994759458
O	0.291614764	-6.012699886	3.044233304
C	2.627036458	-5.457299971	3.537865294
H	1.609254699	-5.700846682	6.088111931
H	0.875399507	-4.349926529	4.139264043
H	0.373810455	-5.486204988	2.205674506
H	2.784264283	-4.852928015	2.641734438
H	2.895701862	-6.496951344	3.310488239
H	3.297886321	-5.087420075	4.319697343
H	-1.938787000	-7.684525000	5.661722000
C	3.080778000	0.711402000	-8.141230000
H	3.027971000	0.637566000	-9.232461000
C	2.910362646	2.171393095	-7.772868584
O	3.701720338	3.048051651	-8.178335673
C	4.469375333	0.177051292	-7.745356388
C	4.686497028	-1.299821229	-8.093367596
C	4.127174020	-2.300370970	-7.084140384
N	4.835645746	-2.284549859	-5.801788745
C	5.963889004	-2.932761345	-5.503817007
N	6.605076718	-2.623032971	-4.368911530
N	6.446010429	-3.884251711	-6.297016668
H	2.282101537	0.105254636	-7.713198256
H	4.654404854	0.354928890	-6.678917772
H	5.215880609	0.762458782	-8.290637508
H	5.761408753	-1.493052406	-8.199733207
H	4.231874553	-1.522736934	-9.068309010
H	4.153753723	-3.313616872	-7.494236335
H	3.080407287	-2.104153084	-6.845440963
H	4.516033838	-1.619542197	-5.106593289
H	6.524375933	-1.680822787	-4.004502512
H	7.481669190	-3.092495367	-4.165003039
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H	5.273395434	-2.908031213	4.188356485
C	2.585915467	4.280238845	-5.444914452

C	2.992717679	3.267220451	-4.416426348
C	2.144371628	2.612553461	-3.559210914
N	2.832423922	1.675128546	-2.833554458
C	4.151366219	1.703362000	-3.189666080
C	4.294876313	2.708085452	-4.185933042
C	5.222000959	0.941404091	-2.724136617
C	6.473313804	1.198596663	-3.262841848
C	6.649582049	2.200888091	-4.235542875
C	5.580074897	2.954390434	-4.693699016
C	0.158347059	-3.976985130	-7.040865947
H	0.736894000	-4.386578000	-7.879897000
O	1.034559585	-3.981657081	-5.913029688
C	-3.756400938	-0.834810256	-4.116946768
O	-4.283111423	0.154115613	-4.634513775
H	-4.321425000	-1.617047000	-3.604721000
C	3.248216378	-0.686214639	9.555140726
O	3.610123990	-1.372738534	10.517978776
H	3.237939000	0.408880000	9.561120000
N	5.685215154	4.785242694	-9.711400030
C	6.766777249	4.063506617	-9.381649429
N	6.750749884	3.408908253	-8.211676521
N	7.846940163	4.081347616	-10.149707634
C	9.095943897	3.361601094	-9.894271082
C	9.027971000	1.861262000	-10.151451000
H	8.816379000	1.617659000	-11.197832000
H	4.612130844	-1.442774718	6.827446266
H	1.284083682	1.665761139	-6.680593046
H	4.233718334	3.389650067	5.834880350
H	-2.365183072	-6.506084481	-2.197062774
H	-1.720322792	-2.433186065	-5.773464770
H	-0.549770154	-8.118290737	4.706218661
H	3.643926842	7.058266068	1.161887032
H	7.039823407	-2.979067182	4.380254406
H	6.174983520	-1.451312262	4.653060197
H	0.554755741	3.687474532	-5.996679592
H	2.156375963	5.175167392	-4.972401173
H	3.470308856	4.609072661	-5.994986280
H	1.084382694	2.741203564	-3.402638150
H	2.431871601	1.074051860	-2.121947347
H	5.085466136	0.189464251	-1.953212533
H	7.333526225	0.631511831	-2.913523220
H	7.648087699	2.389255499	-4.623704406
H	5.744352492	3.737599132	-5.425912713
H	-2.167188410	-1.950774367	-3.579479008
H	0.455217907	-1.929121790	-7.727853337
H	-0.695761942	-4.645683488	-6.865104064
H	0.456937801	-3.963778429	-5.119533083
H	10.002674909	1.427178222	-9.898667945
H	8.272462401	1.365597725	-9.535628347

H	9.837803924	3.826521280	-10.548967810
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H	7.786238656	4.629070670	-11.003459183
H	5.609690109	5.121476157	-10.665836917
H	4.805411933	4.514698268	-9.276445254
H	7.504958602	2.774477414	-7.988398224
H	5.832743423	3.164225281	-7.848882242
H	5.939707193	-4.023057639	6.306787206

Cartesian coordinates of the optimized Fe1·Fe2·Fe3·Fe4 state K144A 4Fe-4S quantum cluster model in chain-B.

238 atoms

Fe	19.268335560	67.144381298	56.343164714
Fe	17.376200400	65.191752674	56.405553394
Fe	19.766953580	64.805121281	55.143483781
Fe	17.883098382	66.469388509	54.085820800
S	17.673193087	64.184435227	54.414749976
S	20.118713271	66.940447334	54.315918322
S	17.008582048	67.378250176	55.889465724
S	19.513948877	65.059175055	57.288876755
S	15.588360345	64.768911827	57.785182040
C	15.122855075	66.335184712	58.635127693
S	20.388074653	68.751871693	57.490744061
C	19.905033813	68.895320328	59.250410433
S	21.488302176	63.502554556	54.398534654
C	20.971145355	63.178838350	52.674317423
S	17.122956274	67.241353475	52.084506078
C	18.474698112	67.264269791	50.851460825
H	15.379391155	67.164073946	57.976575049
H	14.030627707	66.318570800	58.735843029
H	20.815330046	69.190783935	59.780768421
H	19.190256431	69.718486442	59.362621245
H	20.462644676	62.208875257	52.649730366
H	20.241797878	63.939205804	52.392206277
H	18.832152294	68.288094812	50.740240193
H	19.318835026	66.660318402	51.197157226
C	24.644002000	76.620997000	48.376996000
C	24.906773378	75.402352710	49.235949019
N	26.343827156	75.240257367	49.451219081
C	26.910555091	74.297229615	50.203496348
N	28.226394238	74.091161872	50.131487156
N	26.177129048	73.547221170	51.034642944
H	25.141613000	76.554792000	47.403845000
C	21.415000000	71.340995000	47.975998000

C	20.195200684	72.132028118	48.405828949
O	20.134925473	73.365842520	48.257903534
C	22.655200874	71.705696386	48.796479825
C	23.955855826	71.123590637	48.241108684
C	24.073049617	69.600463261	48.282420309
N	23.976558624	69.054357099	49.635245442
C	24.943080068	69.120638496	50.558977740
N	24.635967322	68.767933963	51.827044291
N	26.162204993	69.518660224	50.248430335
H	21.618741000	71.609153000	46.934073000
N	19.205745792	71.406310231	48.957418529
C	17.991000000	71.973996000	49.510997000
C	18.201255198	72.681850965	50.869631264
C	19.048099105	71.930432239	51.844791298
C	18.797272579	70.673230403	52.328770369
C	20.309476231	72.327415386	52.398977908
N	19.824245946	70.266305960	53.140327275
C	20.770104581	71.250873887	53.205110481
C	21.103967204	73.480574133	52.312357545
C	21.981723051	71.288630968	53.890733725
C	22.308051888	73.524526717	52.998319992
C	22.749403703	72.436695803	53.773885820
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C	15.749467719	70.922586945	56.272169046
C	16.058147820	70.978330202	57.759283375
O	16.212321585	69.951399732	58.433895127
C	17.019617362	70.939399277	55.400362695
C	17.888570603	72.134051644	55.533036591
N	17.583671332	73.384454557	55.032655396
C	19.107303824	72.268424239	56.129599903
C	18.564434418	74.243715034	55.297738991
N	19.493116306	73.572769573	55.967180366
H	15.078911000	71.721456000	55.939196000
N	16.174890324	72.206081455	58.306100022
H	16.562673000	72.275889000	59.244498000
N	19.506560802	63.814494152	62.711775634
C	20.331197463	62.828089263	62.047332983
C	21.790682546	63.270866326	61.814169512
O	22.667427377	62.398969587	61.709296399
C	19.705806352	62.451606552	60.701279607
C	18.336027276	61.780271805	60.789273386
C	17.752337249	61.635318546	59.383474448
N	16.440764388	60.997339363	59.349718513
C	16.193717194	59.693403073	59.291891770
N	14.921931571	59.271464958	59.182193757
N	17.176354473	58.791865381	59.329195539
C	19.406011179	63.955346110	64.042509365
O	20.028400718	63.315114803	64.899383125
H	18.677061000	64.732842000	64.291576000

N	22.004058865	64.589300681	61.677818634
C	23.289001000	65.171998000	61.339999000
C	23.268299359	66.057575456	60.101251259
H	24.296234680	66.364725173	59.870110298
H	23.715284000	65.719872000	62.186842000
C	22.355536709	60.399580072	58.484156247
C	21.371833341	59.258929395	58.348229550
O	20.212604975	59.340567636	58.786883207
C	22.118574690	61.537823250	57.499826623
O	22.171369774	60.958557862	56.183195250
C	23.175892396	62.617795101	57.682854593
H	23.378128000	60.073913000	58.312272000
N	21.824966527	58.148889074	57.743975864
H	21.170100000	57.394184000	57.563116000
C	15.698730475	66.570481558	60.035213486
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H	15.420306000	67.594069000	60.325163000
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N	17.914856235	67.513152822	59.712642473
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O	20.766501577	67.262236805	61.836530079
N	18.930604769	68.509635210	62.179107174
H	19.238077000	68.583743000	63.137216000
N	17.829743130	65.335658273	49.499633081
C	18.020176558	66.766434205	49.474825360
C	19.033561741	67.251511232	48.429659970
O	19.167880633	68.469537292	48.247890594
N	19.744212900	66.309584508	47.800102992
C	20.853000000	66.607000000	46.924000000
C	22.100927472	63.185044188	51.632789425
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O	20.913448522	64.003482695	49.704706734
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S	26.848492709	70.856337703	54.854352391
O	27.133824506	70.999789126	56.291598851
O	26.313124623	72.067043438	54.218868309
O	26.141831903	69.611478354	54.508872411
P	28.821577553	70.594041234	52.641765229
O	28.251156993	69.337871672	52.032641458
O	28.605117437	71.928872769	51.981937562
O	28.417664995	70.678661125	54.259597199
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C	32.085008011	69.522445452	54.349889858
O	31.471411385	69.492339227	55.677956878
C	33.246374087	68.545846845	54.426850199

O	34.370824593	69.234223939	54.982787387
C	32.710342265	67.492421303	55.386625224
O	33.755303064	66.732957232	55.959428305
C	31.915223798	68.356571305	56.381511586
N	30.749311724	67.633418974	56.936252344
C	29.458935478	68.079537586	57.082655916
N	28.682183480	67.235003499	57.733404410
C	29.519276995	66.184311844	58.046562771
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C	31.553324337	64.485727067	58.365948920
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H	21.442229109	60.975211288	50.476369262
H	22.989346948	63.462004920	57.014787963
H	23.167501596	62.987378814	58.710974317
H	24.171280105	62.210733999	57.463938061
H	21.929257150	61.687692977	55.556423177
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H	22.296375008	60.777167237	59.507728762
H	22.737206260	58.112428854	57.304575525
H	16.944061514	57.826593137	59.117846150
H	18.139311965	59.055868579	59.140506702
H	14.727908974	58.300714133	59.407843451
H	14.182796801	59.918935688	59.438748277
H	15.632785631	61.612180485	59.338315107
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H	17.609289757	62.623777688	58.946813785
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H	17.641838776	62.375566582	61.393177072
H	19.636504263	63.356397424	60.088309657
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H	20.394489565	61.945643153	62.691973931
H	21.235569153	65.241866955	61.803947762
H	23.963453291	64.327469683	61.169681073
H	22.866337384	65.519499122	59.238377227
H	22.668868541	66.954401264	60.260547800
H	23.697165375	69.004449828	52.133418529
H	25.336658970	68.946697681	52.548448499
H	26.920942469	69.513677088	50.960107399
H	26.456651422	69.486978738	49.278801539

H	23.203204918	68.427163074	49.831085559
H	23.270554952	69.131315438	47.713078880
H	25.007186601	69.276099497	47.806962717
H	24.081255158	71.423931635	47.191178557
H	24.796256626	71.557754140	48.794414483
H	22.744256398	72.796784960	48.796339852
H	22.515944292	71.408632299	49.842905215
H	21.209118403	70.269473611	48.013922386
H	19.307063665	70.397836413	48.977617033
H	17.251498549	71.173740436	49.585479288
H	18.662864923	73.653430961	50.674376909
H	17.202409904	72.886914875	51.281171850
H	20.788748700	74.328282499	51.710128786
H	22.927669554	74.416594788	52.937618583
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H	22.311841051	70.452915042	54.502282576
H	19.877178967	69.362267098	53.595387110
H	17.955430142	70.018823830	52.166420092
H	20.366156165	73.974746600	56.299370960
H	18.596630837	75.284332741	55.020442349
H	16.744559461	73.632437283	54.514300863
H	19.720913372	71.542807499	56.636765742
H	17.628504317	70.071018872	55.643988506
H	16.705030145	70.833144714	54.356913738
H	15.239003232	69.974353359	56.086542819
H	16.159769854	73.047043112	57.741976754
H	33.307165372	66.156114308	56.638239849
H	34.930766392	68.540948926	55.391979798
H	28.082794811	63.780241061	59.814290102
H	27.368959821	65.254732917	59.259090212
H	32.363837443	63.776381768	58.514240442
H	29.143331855	69.030700268	56.683944532
H	30.331038610	68.505894801	53.581991329
H	31.589874952	68.845058814	52.366663014
H	26.684752216	72.928318938	51.668008408
H	25.294870032	73.909402143	51.372095923
H	28.615237590	73.322328691	50.684336823
H	28.731722530	74.388581146	49.303544660
H	26.960514644	75.728652991	48.808997206
H	24.410774482	75.533860872	50.204072105
H	24.509833133	74.502784224	48.754032075
H	23.566870552	76.714097620	48.203735255
H	24.989981441	77.528429719	48.884949239
H	32.537888604	68.654802716	57.235180427
H	32.471662490	70.538585925	54.211441406
H	18.010977058	68.833429606	61.908446685
C	16.761835559	64.671117343	49.022724195
O	15.808328421	65.159833194	48.410500693
H	16.849534000	63.603479000	49.253524000

O	22.487007801	66.156084924	48.716479416
C	22.145156163	65.901954774	47.349428065
H	22.982507000	66.274601000	46.742710000
H	18.516693810	64.779521484	50.000993534
H	21.963534595	65.506167916	49.237252647
H	20.601666000	66.337713000	45.892815000
H	20.992600996	67.688935123	46.954401222
H	22.059073998	64.821562755	47.175536770
H	33.502150657	68.115238447	53.451532269
H	32.005326545	66.850504179	54.837810281