

Supplementary Material

Computational Study on Redox-Switchable Second-Order Nonlinear Optical Properties of Ferrocene-Tetrathiafulvalene Hybrid

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Compound H

C	-3.21377300	0.16970800	-1.20868000
C	-1.89731200	0.11758900	-0.87744000
C	0.50588100	0.66369400	-0.03697600
C	0.49961900	-0.66483700	-0.22894700
C	2.90816700	-0.10452300	0.49916300
C	4.25704300	-0.12144600	0.55321900
C	6.76434500	0.59263200	0.22505300
C	6.75729400	-0.74926600	0.04060900

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C	7.70170500	2.61449600	-1.44821700
H	7.65443400	1.96011500	-2.32099200
H	8.49306200	3.35586100	-1.58828600
H	6.74776600	3.12605500	-1.30353700
C	9.23214000	-1.73937900	0.91240100
H	9.65729800	-0.74272900	1.04433500
H	10.03117700	-2.44717200	0.67365200
H	8.72198700	-2.06565900	1.82125600
C	-5.28020700	1.65438000	-0.05913400
C	-5.09563000	1.49105200	1.35406600
H	-4.14247600	1.38576900	1.85422500
C	-6.38399000	1.44589900	1.96012600
H	-6.58326800	1.29544300	3.01320000
C	-7.36766700	1.59354500	0.93409600
H	-8.44034900	1.57421300	1.07532500
C	-6.69237400	1.72097300	-0.31413200
H	-7.14701900	1.81799500	-1.29065300
C	-5.27287200	-1.57832400	-0.51421300
C	-5.07407600	-1.80206300	0.88858500
H	-4.11682900	-1.82491400	1.39134200
C	-6.35616000	-1.93718600	1.49459800
H	-6.54573900	-2.07911600	2.55060100
C	-7.34950200	-1.81176400	0.47500300
H	-8.42068500	-1.84374100	0.62507800
C	-6.68690100	-1.58855500	-0.76656900
H	-7.15196200	-1.42243300	-1.72879300
Fe	-6.18235300	-0.08275000	0.55477600
S	-4.02934400	1.75915800	-1.31875300
S	-4.03474900	-1.32025000	-1.76399800
S	-0.94682800	1.57465600	-0.45898500
S	-0.95956100	-1.40628400	-0.89075800
S	1.94400700	1.39039300	0.69593200
S	1.92771500	-1.58365100	0.26833900
S	5.25310600	1.32531300	0.83279000
S	5.23331300	-1.60139200	0.38780500
S	8.16497400	1.65589400	0.04967600
S	8.08795300	-1.77746000	-0.52308500

The one-electron-oxidized species of H

C	3.31362200	0.16678400	1.05254800
C	1.96239900	0.14691700	0.90459600
C	-0.51499000	0.77426000	0.48001300
C	-0.51404200	-0.57794200	0.68158800
C	-2.98156700	0.04228000	0.22158900

C	-4.34917100	0.01227900	0.04539900
C	-6.87660900	0.62615800	-0.37539700
C	-6.87002300	-0.71910200	-0.18036800
C	-9.06923500	1.80040500	0.89142400
H	-9.39815600	0.82237800	1.24568900
H	-9.93868800	2.44355100	0.73172400
H	-8.39506700	2.27451400	1.60719900
C	-8.58942100	-2.01921900	-1.95261300
H	-8.85715800	-1.06406200	-2.40691900
H	-9.43891800	-2.70458300	-2.01351200
H	-7.72760600	-2.46649800	-2.45152000
C	5.41516600	1.62228900	-0.13319800
C	5.27550800	1.46820500	-1.55451800
H	4.34186500	1.37848700	-2.09280300
C	6.58443800	1.42256500	-2.11106400
H	6.82157000	1.27770300	-3.15680200
C	7.53114700	1.56095300	-1.05036400
H	8.60765600	1.53769300	-1.15499600
C	6.81788300	1.68729000	0.17452900
H	7.23996300	1.78581600	1.16530700
C	5.38404000	-1.59447400	0.32356000
C	5.22385200	-1.82781300	-1.08457800
H	4.28409600	-1.85937400	-1.61876400
C	6.52399100	-1.97105200	-1.64536500
H	6.74722200	-2.12045100	-2.69348100
C	7.48476300	-1.84300100	-0.59617100
H	8.55955800	-1.87937500	-0.71374700
C	6.78957000	-1.61255800	0.62397100
H	7.22678700	-1.45150900	1.59992000
Fe	6.31441200	-0.10983900	-0.71054800
S	4.12492000	1.76067000	1.07678900
S	4.11375800	-1.35721500	1.53878300
S	1.00786600	1.63036900	0.60147200
S	1.00850900	-1.36080900	1.04771600
S	-2.04232500	1.53282100	0.12305300
S	-2.03899800	-1.41056500	0.55961300
S	-5.30748000	1.44218500	-0.30025600
S	-5.29752400	-1.46157200	0.14860700
S	-8.27030000	1.65159500	-0.75913000
S	-8.26691300	-1.80934300	-0.15330400

Two-electron-oxidized species of H

C	3.31045300	0.04776800	1.08501600
C	1.96137300	0.02568900	0.88854900

C	-0.52594500	0.65754000	0.48922900
C	-0.51259400	-0.69301900	0.56172800
C	-2.99080700	-0.06094900	0.21016800
C	-4.37013300	-0.08943300	0.06423900
C	-6.89674200	0.57342900	-0.16049100
C	-6.88289400	-0.80421600	-0.08923900
C	-7.82536900	3.21259500	-0.36323600
H	-7.28767100	3.51099600	0.54058700
H	-8.74604500	3.79745000	-0.43182100
H	-7.22788100	3.39119200	-1.26104400
C	-8.74838600	-1.99667900	-1.81015400
H	-8.98434800	-1.02024400	-2.23582400
H	-9.64489400	-2.62213200	-1.82223300
H	-7.95359100	-2.49153300	-2.37087600
C	5.33238300	1.66409600	0.04377400
C	5.12296600	1.61363800	-1.38016800
H	4.16604400	1.51836400	-1.87591800
C	6.39478100	1.72890100	-2.01530300
H	6.57508800	1.70751100	-3.08290500
C	7.38918900	1.85081000	-1.00443500
H	8.45753600	1.91652200	-1.17005800
C	6.74760100	1.80208700	0.26185200
H	7.23222400	1.83935300	1.22946600
C	5.35818400	-1.63169700	0.20646400
C	5.14912900	-1.72524400	-1.21538200
H	4.19180500	-1.69479700	-1.71855100
C	6.42317900	-1.88251000	-1.83686000
H	6.60405200	-1.96412300	-2.90149600
C	7.41856400	-1.88869800	-0.81966600
H	8.48795500	-1.95380800	-0.97873300
C	6.77512300	-1.72582800	0.43603400
H	7.25868500	-1.66078700	1.40272000
Fe	6.26328300	-0.02032800	-0.75790800
S	4.13746400	1.61403400	1.35332800
S	4.16346600	-1.47021600	1.50740500
S	0.99830900	1.51627600	0.69650100
S	1.02742300	-1.49495100	0.85651800
S	-2.07055100	1.44259600	0.23433900
S	-2.03896500	-1.53356100	0.39299100
S	-5.32977600	1.37065900	-0.11907200
S	-5.30768200	-1.55386500	0.05993100
S	-8.38934900	1.47545000	-0.26355800
S	-8.30000600	-1.85486600	-0.02653500

Compound R

N	-7.68258100	0.10408300	-0.01629500
C	-8.35077300	1.35404700	0.17758000
C	-8.02761700	2.18047400	1.25807100
C	-9.36735100	1.75906000	-0.70264700
C	-8.68413500	3.39683700	1.45448600
H	-7.25144800	1.87343400	1.95258900
C	-10.03798400	2.95709800	-0.50358700
H	-9.63001600	1.12336400	-1.54255600
C	-9.69934600	3.79056700	0.57395600
H	-8.40660200	4.01499600	2.30035000
H	-10.82513600	3.27684700	-1.17902500
C	-8.48925600	-1.06499600	-0.18138000
C	-8.28744300	-1.93288100	-1.25894000
C	-9.52227500	-1.34572800	0.72808400
C	-9.08111200	-3.06990300	-1.42488100
H	-7.50000400	-1.72010000	-1.97569100
C	-10.32746400	-2.46238200	0.55961900
H	-9.69095400	-0.67687200	1.56629900
C	-10.11166800	-3.33841200	-0.51574900
H	-8.89679400	-3.72305300	-2.27006500
H	-11.12868900	-2.68543600	1.25702300
C	-6.28670100	0.02906100	-0.03242700
C	-5.49928900	1.14240200	-0.39758200
C	-5.61624300	-1.16532900	0.32462400
C	-4.11742300	1.05779000	-0.39910900
H	-5.98276900	2.06845500	-0.68704500
C	-4.23577200	-1.23622300	0.31465900
H	-6.19560900	-2.03118900	0.62465600
C	-3.43655500	-0.12794900	-0.04744300
H	-3.53827700	1.92987600	-0.69411600
H	-3.76554100	-2.16870100	0.61344100
C	-1.99052700	-0.14509300	-0.06991700
H	-1.52999500	0.80663400	-0.33727800
C	-1.16514400	-1.19416700	0.19802800
H	-1.58755700	-2.16327900	0.45625900
C	0.26709900	-1.16617300	0.17338500
C	1.11105600	-2.25258400	0.42884000
S	1.21588700	0.25681000	-0.18563900
C	2.47231800	-1.95247500	0.33612600
H	0.72268800	-3.23567600	0.67309700
C	2.73403500	-0.62014600	0.00703700
H	3.25729800	-2.68258100	0.50051900
C	3.96782400	0.05838700	-0.17729600

H	3.90291700	1.11076600	-0.43565400
C	5.21132800	-0.52234300	-0.05074800
H	5.25827100	-1.57497600	0.20509500
C	6.46446400	0.11419600	-0.25305100
C	6.79691300	1.39595500	-0.67452600
C	7.78586900	-0.63051900	-0.05297300
O	8.79008300	0.29333600	-0.53374700
C	7.88689200	-1.85265300	-1.00576900
C	5.87632100	2.43787900	-0.94937800
N	5.06257200	3.24663600	-1.15219900
C	8.22691800	1.48368700	-0.83746700
C	9.05057200	2.51574200	-1.22957700
C	8.56018800	3.81016300	-1.56566300
C	10.45952700	2.30209900	-1.30445600
N	8.20628800	4.88370200	-1.84622000
N	11.61049400	2.13595700	-1.36494700
F	7.07199200	-2.84479600	-0.58380300
F	7.52341800	-1.51751100	-2.25460800
F	9.13371700	-2.34223200	-1.05678300
C	8.14643300	-1.00545800	1.38923000
C	9.48625500	-1.30949600	1.67894100
C	7.20507500	-1.02497500	2.42357700
C	9.86673500	-1.64279300	2.97650200
H	10.23161300	-1.26979100	0.89354100
C	7.59113100	-1.36210300	3.72247300
H	6.17063200	-0.76491600	2.23184200
C	8.91988400	-1.67512300	4.00236500
H	10.90789900	-1.87110200	3.18564600
H	6.84819800	-1.36892400	4.51510500
H	9.21935000	-1.93337400	5.01431600
O	-10.95272400	-4.40930700	-0.58456900
C	-10.79214400	-5.32387900	-1.65795800
H	-11.55920700	-6.08732400	-1.51745500
H	-10.94076400	-4.83506800	-2.62982400
H	-9.80165900	-5.79759400	-1.63977000
O	-10.41165100	4.94831400	0.67489600
C	-10.11503800	5.82982100	1.74743300
H	-10.79109800	6.67864100	1.63203000
H	-10.29278400	5.35423200	2.72099600
H	-9.07683600	6.18431000	1.70267300

Compound 1

C	-12.94089438	2.00953082	3.54756460
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C	-11.79052359	1.60313862	2.95143559
C	-9.96185067	0.26068408	1.67594739
C	-9.47687382	1.50905594	1.76397194
C	-7.63232063	0.15577213	0.56705029
C	-6.41430428	-0.28796804	0.18818265
C	-4.32467421	-1.82984563	-0.13606039
C	-3.81425153	-0.52134559	-0.04162901
C	-15.58064379	1.32377289	2.95580809
C	-15.65915195	1.41209345	1.52614191
H	-14.85697489	1.18279906	0.83785260
C	-16.95611716	1.89550249	1.18977466
H	-17.31447050	2.10386682	0.19009711
C	-17.68788054	2.09619212	2.40068879
H	-18.69620845	2.48143162	2.47669993
C	-16.84370841	1.74638845	3.49387535
H	-17.08427585	1.81279325	4.54615808
C	-14.39095183	4.35870442	3.15405893
C	-14.43878725	4.50072261	1.72759540
H	-13.66123814	4.19715594	1.03986167
C	-15.70108787	5.06655748	1.38778166
H	-16.05601120	5.26575651	0.38502959
C	-16.43231725	5.28892818	2.59514732
H	-17.43633426	5.68633927	2.66563257
C	-15.62926910	4.85287257	3.68823787
H	-15.90159586	4.85790859	4.73489149
Fe	-15.95733453	3.26424808	2.40769511
S	-14.19771635	0.79804364	3.94251037
S	-13.06975672	3.69322004	4.14031445
S	-11.50465296	-0.09386987	2.45859618
S	-10.41475335	2.70976297	2.65607460
S	-9.05488174	-0.91768694	0.71801121
S	-7.96899920	1.87718369	0.91592478
S	-6.08307808	-1.99260716	-0.20308147
S	-5.01139355	0.78847604	-0.01403509
C	-2.44456961	-0.29628652	-0.01431537
C	-1.54349166	-1.37932545	-0.08952738
C	-2.07384330	-2.68181322	-0.18839657
C	-3.44579147	-2.91214804	-0.20799625
H	-2.07469629	0.72080035	0.06570047
H	-1.39404300	-3.52752130	-0.24331650
H	-3.82834155	-3.92611337	-0.27497764
C	-0.09590883	-1.21484968	-0.06398062
H	0.46623015	-2.14431460	-0.15140373
C	0.59829695	-0.05632418	0.05840461

H	0.06617720	0.88795648	0.15595595
C	2.03100358	0.07742967	0.07965806
C	2.73510230	1.27311015	0.22312104
S	3.14018842	-1.26029721	-0.07330272
C	4.12794841	1.11872568	0.21243524
H	2.23274463	2.22829557	0.33336683
C	4.54064128	-0.20380205	0.05862909
H	4.82212600	1.94557991	0.31277386
C	5.85107732	-0.76441402	-0.00309589
H	5.90493887	-1.84063134	-0.13549599
C	7.01757135	-0.04748799	0.09525581
H	6.95643320	1.02686522	0.23489040
C	8.33552394	-0.57779272	0.02722535
C	8.81961927	-1.85092921	-0.22477010
C	9.55606377	0.32494623	0.23350219
C	8.02741899	-2.99648565	-0.49037037
N	7.31072166	-3.88988295	-0.70225763
C	10.26448721	-1.81472961	-0.20814571
C	11.20969160	-2.79823718	-0.38336055
C	10.86665633	-4.16269086	-0.61154757
C	12.59714306	-2.46479638	-0.33777097
N	10.63332750	-5.28788665	-0.79915730
N	13.73162221	-2.20554688	-0.30825779
O	10.68226517	-0.54291937	-0.00631015
C	9.69848732	0.71991142	1.73047497
F	8.61354989	1.40590504	2.16529129
F	10.77841886	1.48224141	1.93098987
F	9.80545749	-0.38009493	2.49044733
C	9.61206403	1.50549835	-0.73581314
C	9.20284083	2.79871026	-0.38414925
C	10.04829684	1.26018830	-2.04544774
C	9.23296218	3.82551231	-1.33010899
H	8.87154160	3.02134339	0.62233244
C	10.07720446	2.28861645	-2.98502148
H	10.38172622	0.26775476	-2.32839354
C	9.66780696	3.57576167	-2.63097396
H	8.92169843	4.82505129	-1.03998291
H	10.42522277	2.08250788	-3.99300920
H	9.69335450	4.37823402	-3.36267005

Compound 2

C	-2.80134800	-0.45082400	0.23241100
C	-3.81567000	-0.43284600	-0.67260100
C	-5.61628400	-1.06157100	-2.44904200

C	-5.70705000	0.27166500	-2.32201000
C	-7.35434400	-0.33637500	-4.21268200
C	-8.06192700	-0.27614800	-5.36119400
C	-8.80381100	-0.77586800	-7.82659900
C	-8.89810800	0.57100400	-7.69831800
C	-0.44305600	-1.94032500	0.15093300
C	0.71489500	-1.94945500	0.99936900
H	0.70447500	-2.00460500	2.07887900
C	1.86878200	-1.81094200	0.16650100
C	1.42423100	-1.72396100	-1.19558300
H	2.06472500	-1.58026600	-2.05557900
C	0.00316500	-1.82030100	-1.20657300
H	-0.63704400	-1.76389500	-2.07653000
C	-0.66283700	1.32594700	0.46478900
C	0.49516200	1.32935800	1.31368600
H	0.49235500	1.17788600	2.38390600
C	1.64586400	1.50481600	0.48351900
C	1.19818700	1.61884500	-0.87558500
H	1.84029100	1.72669800	-1.73960000
C	-0.22289500	1.52537100	-0.88532300
H	-0.86124000	1.54915400	-1.75819000
Fe	0.60777200	-0.19253400	-0.07066100
S	-2.11705600	-2.02244700	0.74968600
S	-2.32508700	1.07032700	1.04728400
S	-4.42616900	-1.91538600	-1.46348800
S	-4.62971300	1.07648900	-1.17794400
S	-6.76730000	-1.87706800	-3.51656400
S	-6.97046700	1.11115800	-3.23260400
S	-8.50519900	-1.70129700	-6.32557800
S	-8.70901400	1.23019000	-6.04675300
C	3.79134200	0.95456700	6.07363100
H	3.79841000	2.04269600	6.01606400
C	3.83899000	0.37240000	7.29599500
H	3.80692200	-0.71227800	7.37933500
C	3.92080200	1.05130100	8.56374600
C	3.92057700	0.43647100	9.81468600
S	4.03932100	2.78216300	8.74143100
C	4.00819700	1.33282500	10.88932200
H	3.85615600	-0.64049800	9.92830800
C	4.08165100	2.66713800	10.49521000
H	4.02022900	1.02175900	11.92786200
C	4.18596900	3.85863600	11.27658800
H	4.24515800	4.79098800	10.72346400
C	4.21971100	3.89270700	12.64711600

H	4.15783900	2.95583100	13.19088200
C	4.32730500	5.05787700	13.45813400
C	4.35747100	6.40800400	13.15619800
C	4.41886500	4.94365400	14.98319400
C	4.28012400	6.96283600	11.85347000
N	4.20922700	7.34142300	10.75432700
C	4.44950200	7.16155700	14.38736600
C	4.52804200	8.51214800	14.63198900
C	4.55443200	9.48239100	13.58805300
C	4.58867600	8.98699400	15.97715300
N	4.57966100	10.30880600	12.76832200
N	4.63354300	9.38734400	17.06924900
O	4.41905600	6.31138500	15.44021400
C	5.81315600	4.40380600	15.40828500
F	6.04014000	3.17084000	14.89318400
F	5.91934700	4.32362600	16.73843800
F	6.78097900	5.21184500	14.95077000
C	3.23848500	4.20151100	15.60912100
C	3.30397100	2.85825900	16.00281400
C	2.02725400	4.89440400	15.74505100
C	2.17410400	2.22485300	16.52481400
H	4.22760100	2.29895500	15.92089700
C	0.90354900	4.25786100	16.26755200
H	1.96516700	5.93837100	15.45763300
C	0.97249100	2.91906900	16.65827100
H	2.24264900	1.18587900	16.83450700
H	-0.02453600	4.81206300	16.37296100
H	0.09718500	2.42360300	17.06849100
S	3.58232300	-1.78649200	0.63701900
S	3.35520500	1.61467100	0.95579900
C	3.71640800	0.27331500	4.78489000
C	3.54207900	1.04833600	3.62135300
C	3.81289400	-1.12150800	4.62977400
C	3.45654800	0.47859600	2.34818200
H	3.47636500	2.12909000	3.70868300
C	3.72918100	-1.70079900	3.36950400
H	3.96424800	-1.76273600	5.49260000
C	3.55000100	-0.92472300	2.21305800
H	3.81383200	-2.77790100	3.26444100
S	-9.12543100	-1.69596100	-9.29852200
S	-9.36547400	1.69597200	-8.97588300
C	-7.53560800	-2.58635800	-9.53684900
H	-6.72306300	-1.88258100	-9.72999500
H	-7.29565800	-3.21303400	-8.67550700

H	-7.68194300	-3.22162800	-10.41468100
C	-7.92910000	2.84194200	-9.01033700
H	-8.17180800	3.59527300	-9.76476700
H	-7.78512500	3.33286300	-8.04573700
H	-7.01944500	2.31411900	-9.30491000

The one-electron-oxidized species of 2

C	-4.41741800	0.75772900	-0.67708300
C	-5.65216700	0.19434100	-0.67226800
C	-8.15309000	-0.35074700	-1.08125400
C	-7.75149700	-1.21775200	-0.11126200
C	-10.26202600	-1.72320500	-0.48092200
C	-11.53562000	-2.24922200	-0.43096300
C	-14.07934200	-2.79159900	-0.78128600
C	-13.66616700	-3.65964500	0.18896200
C	-3.57144900	3.41929000	-0.93580200
C	-2.25213600	3.98725100	-0.95610700
H	-1.41672800	3.62782800	-1.54036900
C	-2.23458600	5.07528100	-0.02992000
C	-3.54210200	5.18284500	0.55301300
H	-3.82964500	5.89373300	1.31628400
C	-4.37161500	4.17609100	-0.01496200
H	-5.40784800	3.98569700	0.22938100
C	-2.63473100	1.32761100	1.40907600
C	-1.31683300	1.89911700	1.40618400
H	-0.50085100	1.60539900	0.76093900
C	-1.29973000	2.95241000	2.37105600
C	-2.60100800	3.02447700	2.97268200
H	-2.90616900	3.74685700	3.71797400
C	-3.41967400	2.01371500	2.39534200
H	-4.45888800	1.82121400	2.62481800
Fe	-2.74313300	3.30344100	0.92198600
S	-4.06654700	2.01440400	-1.90470300
S	-3.14720300	0.00572000	0.33817600
S	-6.96388200	0.74685500	-1.76057200
S	-6.07204100	-1.18077900	0.39711900
S	-9.82634900	-0.41021200	-1.57643400
S	-8.94866900	-2.30665300	0.54365100
S	-12.85185500	-1.70314400	-1.43990200
S	-11.96892600	-3.55714500	0.66735700
C	4.23996700	2.93488500	0.01166200
H	4.40034200	2.27997000	0.86733100
C	5.19030500	2.97492300	-0.95487400
H	5.06017300	3.62499200	-1.81798800

C	6.41643100	2.22159700	-0.96870700
C	7.39540700	2.27326100	-1.96026700
S	6.88246200	1.09950800	0.28336000
C	8.49247600	1.43353200	-1.72031600
H	7.30228200	2.91247700	-2.83185300
C	8.38692400	0.70971200	-0.53398500
H	9.34167000	1.35196600	-2.38908200
C	9.27715800	-0.23805000	0.06149500
H	8.95346600	-0.66905800	1.00353800
C	10.48235300	-0.61976000	-0.46606600
H	10.80608000	-0.17857100	-1.40319500
C	11.38579900	-1.56355200	0.10684100
C	11.28724800	-2.39029600	1.21011300
C	12.75489200	-1.82747700	-0.52690900
C	10.16535200	-2.48425800	2.07312300
N	9.20456900	-2.50390000	2.73085700
C	12.50093100	-3.17200600	1.31809200
C	12.90114100	-4.11188800	2.23763600
C	12.09725200	-4.48003600	3.35567800
C	14.16572000	-4.75726100	2.08815400
N	11.47040300	-4.80782600	4.28032500
N	15.19202600	-5.29388200	1.97279600
O	13.31478400	-2.88651700	0.27685100
C	13.70881200	-0.62343700	-0.28413600
F	13.21170800	0.51156500	-0.83413400
F	14.91628600	-0.84662100	-0.80808500
F	13.84532000	-0.40322200	1.03173800
C	12.67287500	-2.28476400	-1.98273700
C	12.88758000	-1.42010000	-3.06449700
C	12.32226800	-3.61909800	-2.23276400
C	12.75546400	-1.88940000	-4.37313300
H	13.17239000	-0.38804200	-2.90257300
C	12.19320000	-4.08188600	-3.54050600
H	12.16864100	-4.30411100	-1.40600100
C	12.40804100	-3.21765300	-4.61603700
H	12.93681300	-1.21125400	-5.20205300
H	11.93121700	-5.12098000	-3.71692300
H	12.31237000	-3.57999100	-5.63551500
S	-0.90211500	6.17824000	0.36749900
S	0.04040000	4.01846700	2.83539700
C	2.99430300	3.69208200	0.04923500
C	2.14422300	3.53048700	1.16251400
C	2.58345200	4.58518700	-0.95795900
C	0.93906400	4.22437100	1.28934900

H	2.43980700	2.85598100	1.96099700
C	1.38467500	5.27936200	-0.84513400
H	3.20082700	4.74652400	-1.83592500
C	0.54447700	5.11861400	0.26832000
H	1.08848700	5.97277400	-1.62606200
S	-15.69885400	-2.74258800	-1.48066900
S	-14.74534400	-4.83906300	0.92514900
C	-16.50436400	-1.44507500	-0.45074700
H	-16.52974900	-1.74475300	0.59835600
H	-16.00128000	-0.48324700	-0.56906100
H	-17.52638600	-1.36662800	-0.83081200
C	-13.69565100	-5.61708500	2.20668200
H	-14.34962700	-6.34616500	2.69170200
H	-12.84747200	-6.14864400	1.76764300
H	-13.36226000	-4.89278400	2.95402300

The two-electron-oxidized species of 2

C	4.96596700	-4.56301700	0.42524900
C	5.96579600	-5.48450300	0.35052600
C	7.84681400	-7.18070200	0.89480000
C	7.78184900	-7.13946300	-0.47007800
C	9.66627600	-8.82565800	0.07547700
C	10.67828700	-9.76880900	0.00328400
C	12.53629400	-11.54231200	0.52580200
C	12.45268700	-11.50944600	-0.84494000
C	4.49110200	-2.40142500	2.14931000
C	3.39082500	-1.48433900	2.22787300
H	2.34269200	-1.74860400	2.22664700
C	3.93700300	-0.16225500	2.27554400
C	5.36914700	-0.26734400	2.23413500
H	6.05878900	0.56638100	2.22863500
C	5.71253000	-1.64457800	2.17172300
H	6.71254300	-2.05245400	2.11602800
C	4.36013000	-2.29812600	-1.11749700
C	3.26366900	-1.37292000	-1.05549600
H	2.21715800	-1.63403900	-0.98337500
C	3.81504700	-0.05366100	-1.05603500
C	5.24473200	-0.16603500	-1.13463700
H	5.93978000	0.66310700	-1.12563000
C	5.58143900	-1.54586500	-1.18647800
H	6.57970400	-1.95958300	-1.22944400
Fe	4.52602500	-1.13919900	0.54944900
S	4.31010000	-4.16659000	2.04241500
S	4.17244100	-4.06506400	-1.10144900

S	6.72257300	-6.19495900	1.80560400
S	6.58260400	-6.10005900	-1.21020000
S	9.04519300	-8.22415500	1.60951400
S	8.90255600	-8.13796200	-1.35475600
S	11.45404300	-10.46597400	1.39688000
S	11.29238500	-10.37265900	-1.52955700
C	-2.13969500	1.22729400	-0.61417900
H	-2.02241100	1.20459100	-1.69690800
C	-3.40682600	1.30259900	-0.10462500
H	-3.55590700	1.35045400	0.97163600
C	-4.60914300	1.34808800	-0.86903500
C	-5.90604600	1.48635200	-0.33867600
S	-4.67216300	1.24910700	-2.61174400
C	-6.90737900	1.51901400	-1.30183900
H	-6.08655700	1.56416200	0.72794700
C	-6.42067600	1.39985200	-2.61664700
H	-7.96091700	1.62178600	-1.06954600
C	-7.11398500	1.37954800	-3.85508800
H	-6.50631900	1.24532800	-4.74390700
C	-8.47757600	1.52816700	-3.99117000
H	-9.08024300	1.69103000	-3.10309900
C	-9.19963200	1.50080600	-5.21431600
C	-8.80829200	1.18524300	-6.50769600
C	-10.69185900	1.84103900	-5.26491800
C	-7.50553500	0.78962800	-6.90376300
N	-6.40972800	0.47403400	-7.13934400
C	-9.96189300	1.28214600	-7.36880100
C	-10.08915500	1.08336000	-8.73011600
C	-8.98148400	0.73830600	-9.55347700
C	-11.36445600	1.22598800	-9.34764900
N	-8.09319600	0.45441600	-10.25129700
N	-12.40529300	1.33592600	-9.85808200
O	-11.05303100	1.59209400	-6.64494000
C	-10.88750200	3.37594700	-5.09173800
F	-10.39799700	3.78253500	-3.89582000
F	-12.17208300	3.71635100	-5.16442400
F	-10.20979500	4.03007600	-6.04727700
C	-11.54923100	0.97666300	-4.34593000
C	-12.07502600	1.44473000	-3.13353500
C	-11.78049400	-0.35367500	-4.72722500
C	-12.82473400	0.59014900	-2.32227300
H	-11.92721200	2.46969900	-2.81713000
C	-12.53145900	-1.19948100	-3.91454500
H	-11.39442900	-0.72632000	-5.67048400

C	-13.05511700	-0.72996000	-2.70772500
H	-13.23990600	0.96850100	-1.39289400
H	-12.71399000	-2.22245000	-4.22945600
H	-13.64651300	-1.38739600	-2.07746800
S	3.08943300	1.38187600	2.45931000
S	2.98292300	1.50944400	-1.00427700
C	-0.90226200	1.19961400	0.13471300
C	0.31718900	1.20445400	-0.58080300
C	-0.83467000	1.19000500	1.54478000
C	1.55901300	1.21452400	0.05433400
H	0.29205700	1.23771800	-1.66605700
C	0.39241000	1.18816700	2.18951400
H	-1.74021800	1.18237900	2.14241300
C	1.60520900	1.19798200	1.47315500
H	0.42932800	1.18450200	3.27408300
S	13.55533600	-12.62779300	1.47363500
S	13.42758700	-12.54946500	-1.86354000
C	15.16365600	-11.72591500	1.47453500
H	15.54095500	-11.59839800	0.45870100
H	15.06925200	-10.76511500	1.98367600
H	15.84657000	-12.36876000	2.03613400
C	12.93736300	-12.05597100	-3.55524700
H	13.53819500	-12.69000600	-4.21201500
H	11.88017800	-12.26152500	-3.74252400
H	13.18107300	-11.00987000	-3.75793800

Compound 3

C	-10.51387605	0.64423796	-0.88668717
C	-10.12091863	-0.65184795	-0.95091605
C	-8.10424433	0.61420787	0.15489835
C	-6.83514295	0.98459433	0.42548550
C	-4.62737779	2.38936129	0.54782664
C	-4.21287206	1.04554371	0.47902262
S	-12.04167831	1.28843744	-1.49459294
S	-11.05388239	-1.97554578	-1.65492853
S	-9.47015159	1.74918259	0.05608777
S	-8.61389020	-1.07287685	-0.08411785
S	-6.36212470	2.67785431	0.71836705
S	-5.49433895	-0.17877307	0.58264698
C	-2.86592267	0.72582203	0.37774158
C	-1.89124675	1.74553696	0.35151738
C	-2.32593086	3.08430742	0.42427667
C	-3.67498533	3.40946677	0.51744205
H	-2.57038091	-0.31690280	0.31993924

H	-1.58893541	3.88233192	0.40149502
H	-3.98394014	4.44939184	0.56394752
C	-0.46272946	1.48133416	0.24995183
H	0.16309416	2.37349720	0.25572739
C	0.14724546	0.27428630	0.15114732
H	-0.44861435	-0.63624541	0.13633536
C	1.56424224	0.04465346	0.05825253
C	2.18193169	-1.20076483	-0.05573689
S	2.76407881	1.31241136	0.07749353
C	3.57965575	-1.13953234	-0.12698138
H	1.61412376	-2.12475136	-0.08494177
C	4.08487222	0.15807518	-0.06865677
H	4.21267657	-2.01528999	-0.21675160
C	5.42981909	0.63061337	-0.10326054
H	5.56111211	1.70607311	-0.03290217
C	6.53985707	-0.16867093	-0.21840138
H	6.40014973	-1.24200550	-0.29665627
C	7.89172476	0.27102614	-0.23995266
C	8.47322166	1.51781619	-0.07813699
C	9.03685500	-0.72422142	-0.45622662
C	7.77490911	2.72827353	0.16161094
N	7.13185285	3.67958981	0.35724690
C	9.90946418	1.37942502	-0.15595331
C	10.92717049	2.30048756	-0.07493283
C	10.69010748	3.69557151	0.09493885
C	12.28468088	1.86760092	-0.16384551
N	10.54358456	4.84252245	0.23214545
N	13.39590922	1.52696758	-0.22974533
O	10.22997056	0.07238859	-0.30705502
C	9.08151570	-1.19464936	-1.93790944
F	7.93132439	-1.81761663	-2.29248573
F	10.09385818	-2.04248076	-2.14923939
F	9.23104026	-0.14035021	-2.75383691
C	9.05852483	-1.86139719	0.56479338
C	8.53617851	-3.13360516	0.29769079
C	9.58103773	-1.59173910	1.83719340
C	8.54002247	-4.11584654	1.28986325
H	8.13713206	-3.37530225	-0.67951661
C	9.58303318	-2.57574851	2.82312016
H	10.00243585	-0.61622449	2.05375368
C	9.06046604	-3.84179751	2.55354315
H	8.14022135	-5.10053632	1.06472937
H	9.99864808	-2.35182947	3.80128597
H	9.06485220	-4.60992427	3.32164775

C	-9.87481662	-2.64935876	-2.89344484
H	-8.94954208	-2.98736691	-2.42270607
H	-10.38168916	-3.50554686	-3.34672434
H	-9.65662707	-1.90765420	-3.66473805
C	-11.46314248	2.59525282	-2.65024237
H	-12.36963365	3.06600967	-3.04017121
H	-10.86092393	3.34646854	-2.13546047
H	-10.89757977	2.15863588	-3.47613232

Compound 4

C	-6.40192900	1.55413100	-1.05748700
C	-5.86418100	0.25876400	-1.25466200
C	-8.90544000	1.36521200	0.18164800
C	-8.41976800	1.40971300	1.52828600
H	-7.44075000	1.75292200	1.83377600
C	-9.43573600	0.88062300	2.37842700
H	-9.35787100	0.74810200	3.44963900
C	-10.55341600	0.52011600	1.56698200
H	-11.47278900	0.06712900	1.91394200
C	-10.22717400	0.80931100	0.20791600
H	-10.84702400	0.62195600	-0.65844000
C	-7.64193000	-1.65859900	-0.26055400
C	-7.11848200	-1.66058600	1.07245400
H	-6.15646900	-1.26768400	1.37188300
C	-8.10872800	-2.22375900	1.93163200
H	-8.02760500	-2.32941400	3.00555900
C	-9.23803800	-2.58227400	1.13568000
H	-10.16395100	-3.00839200	1.49892300
C	-8.95795600	-2.22678700	-0.21815800
H	-9.62342500	-2.33445100	-1.06408700
Fe	-8.86665600	-0.54176800	0.96702800
S	-8.13132500	1.96810200	-1.30040400
S	-6.84732500	-1.15715200	-1.76887100
C	-4.48750300	0.06179600	-1.14672900
C	-3.60149200	1.11773200	-0.84895500
C	-4.15372700	2.39494100	-0.65205200
C	-5.52580600	2.60521200	-0.75596800
H	-4.10709600	-0.94120200	-1.30766200
H	-3.49955000	3.23149300	-0.41940400
H	-5.93395800	3.60039700	-0.61049700
C	-2.15676100	0.94596400	-0.73941900
H	-1.61227900	1.84834400	-0.46166000
C	-1.45035100	-0.19051600	-0.95316300
H	-1.96698600	-1.10296100	-1.24395300

C	-0.02203300	-0.33808200	-0.84332600
C	0.69630100	-1.50621700	-1.09535200
S	1.06021300	0.94565100	-0.37066600
C	2.08050700	-1.37285000	-0.91736200
H	0.21105600	-2.42637000	-1.40311300
C	2.46965300	-0.09527300	-0.51965700
H	2.78407200	-2.18319600	-1.07173000
C	3.76592400	0.43303600	-0.23871800
H	3.80216000	1.47364400	0.06867400
C	4.93801800	-0.27342500	-0.33636200
H	4.89400600	-1.31019900	-0.65329000
C	6.24269000	0.22261700	-0.05916900
C	6.69585500	1.43138500	0.44129400
C	7.48077400	-0.64834100	-0.29737800
C	5.87748600	2.52675100	0.81712800
N	5.14014900	3.38109800	1.10523300
C	8.13660600	1.38284600	0.55047500
C	9.05692300	2.31345600	0.97208200
C	8.68778900	3.62459700	1.39198300
C	10.44422800	1.97718100	0.99926200
N	8.43266100	4.70518000	1.74252300
N	11.57761500	1.71367200	1.03162400
O	8.57645200	0.15752000	0.17941600
C	7.75877100	-0.79940700	-1.81987700
F	6.71545100	-1.38621300	-2.45559600
F	8.84970400	-1.53868600	-2.04372000
F	7.93795300	0.40684700	-2.37824200
C	7.45295700	-1.97073300	0.46914900
C	7.04292900	-3.17676300	-0.11526400
C	7.80501700	-1.95520200	1.82597100
C	6.98806600	-4.34400900	0.64902700
H	6.77832000	-3.22288400	-1.16421300
C	7.74934000	-3.12335100	2.58365700
H	8.14069100	-1.03368100	2.28856600
C	7.33836800	-4.32246100	1.99835800
H	6.67727100	-5.27296100	0.17938200
H	8.03323900	-3.09464400	3.63162200
H	7.29791900	-5.23342200	2.58866800