

Supporting Information

A Restricted Open-Shell Hartree-Fock Method for a General Configuration State Function Featuring Arbitrarily Complex Spin-Couplings

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A. Geometry.....	S31

1. Ni chain

A. Geometries

i. 1 Ni:

Ni	0.00000000000000	0.00000000000000	0.00000000000000
O	2.08738999752000	0.00000000000000	0.00000000000000
O	-2.08738999752000	0.00000004408251	0.00000000000000
O	-0.0000000145727	2.08738999752000	0.00000000000000
O	0.0000000072864	-2.08738999752000	-0.00000000000000
O	-0.0000000072864	0.0000000072864	-2.08738999752000
O	0.0000000072864	0.0000000072864	2.08738999752000
H	2.65763473155719	0.78999235683467	-0.00000131854335
H	2.65763485984455	-0.78999226522986	-0.00000000000000
H	0.0000000076434	2.65763446560963	-0.78999254420468
H	0.00000081701211	2.65763458772359	0.78999243939734
H	-0.78999215339847	0.00000066219845	2.65763502439174
H	0.78999239892974	0.0000000092769	2.65763469199836
H	-2.65763480169159	0.78999234525531	0.00000098542597
H	-2.65763477981872	-0.78999227327541	-0.00000000000000
H	-0.00000015005059	-2.65763446565846	0.78999254456285
H	-0.00000085447791	-2.65763459603914	-0.78999243697144
H	-0.78999241156412	-0.00000009255474	-2.65763467469341
H	0.78999214302993	0.0000000092769	-2.65763503766959

ii. 2 Ni:

Ni	0.00023500000000	-0.03373900000000	0.01222700000000
O	2.08762500000000	-0.03373900000000	0.01238000000000
O	-2.08715500000000	-0.03373900000000	0.01207400000000
O	0.00023400000000	2.05353900000000	0.03382800000000
O	0.00023700000000	-2.12101700000000	-0.00937400000000
O	0.00038800000000	-0.01213900000000	-2.07505100000000
O	0.00008300000000	-0.05534000000000	2.09950500000000
H	2.61058100000000	0.71468400000000	-0.32528900000000
H	2.56534500000000	-0.85014500000000	-0.21914900000000
H	-0.00163000000000	2.88884100000000	-0.46497400000000
H	-0.00089600000000	2.23334200000000	0.99682200000000
H	-2.61018800000000	0.71460900000000	-0.32563500000000
H	-2.56494200000000	-0.85019200000000	-0.21913500000000
H	-0.00038700000000	-2.40844200000000	0.92301900000000
H	-0.00104300000000	-2.88919300000000	-0.60427300000000
H	-0.77788000000000	0.16732800000000	-2.63125000000000
H	0.77877800000000	0.16729300000000	-2.63110300000000
Ni	-0.00007000000000	-0.07694100000000	4.18678400000000
O	-0.00007100000000	2.01033700000000	4.20838500000000
O	-0.00006900000000	-2.16421900000000	4.16518300000000
O	-0.00022200000000	-0.09854200000000	6.27406200000000
O	2.08732000000000	-0.07694100000000	4.18693600000000
O	-2.08746000000000	-0.07694100000000	4.18663100000000
H	0.77786000000000	2.56448000000000	4.39857400000000
H	-0.77701800000000	2.56455500000000	4.40237500000000
H	-0.78503000000000	-2.62371100000000	4.51544300000000
H	0.78502100000000	-2.62366600000000	4.51521700000000
H	0.00089400000000	0.65369200000000	6.89081700000000
H	-0.00039400000000	-0.90243900000000	6.82099200000000
H	2.69821900000000	0.57470400000000	4.57292600000000
H	2.09496900000000	0.02452600000000	3.20133300000000
H	-2.69838200000000	0.57470800000000	4.57257500000000
H	-2.09494600000000	0.02444600000000	3.20101500000000

iii. 3 Ni:

Ni	-0.02982700000000	-0.01276000000000	-0.00029800000000
O	2.05735600000000	-0.01482900000000	-0.02964200000000
O	-2.11701000000000	-0.01069000000000	0.02904700000000
O	-0.02764500000000	2.07461400000000	0.00772500000000
O	-0.03200900000000	-2.10013300000000	-0.00832000000000
O	-0.05916300000000	-0.00470700000000	-2.08746600000000
O	-0.00049100000000	-0.02081200000000	2.08687100000000
H	2.58156100000000	0.76700300000000	-0.28339700000000
H	1.95713400000000	0.01326100000000	0.96063300000000
H	0.42762100000000	2.65403800000000	-0.63063500000000
H	0.32787200000000	2.24275300000000	0.90379900000000
H	-2.45395000000000	0.89258600000000	-0.12579300000000
H	-2.05016500000000	-0.10005400000000	1.01314300000000
H	-0.02157400000000	-2.12294300000000	0.97976200000000
H	0.81299100000000	-2.50513000000000	-0.28193300000000
H	-0.85823200000000	-0.42713300000000	-2.45500200000000
H	0.69116200000000	-0.40004200000000	-2.56706100000000
Ni	0.02884500000000	-0.02886500000000	4.17403900000000
O	0.03102800000000	2.05850900000000	4.18206200000000
O	0.02666300000000	-2.11623800000000	4.16601600000000
O	0.05818200000000	-0.03691800000000	6.26120700000000
O	2.11602800000000	-0.03093400000000	4.14469500000000
O	-2.05833700000000	-0.02679500000000	4.20338300000000
H	-0.68230600000000	2.53857200000000	4.63874800000000
H	-0.19549700000000	2.02716300000000	3.21930200000000
H	-0.89097700000000	-2.39596700000000	3.98828400000000
H	0.11777600000000	-2.09627500000000	5.14794900000000
H	2.40054300000000	0.88319500000000	4.33265500000000
H	2.07654200000000	-0.10517600000000	3.16187700000000
H	-2.00636500000000	0.17844500000000	5.17019600000000
H	-2.54573200000000	0.69777300000000	3.77292500000000
Ni	0.08751800000000	-0.04497000000000	8.34837600000000
O	0.08970000000000	2.04240300000000	8.35639800000000
O	0.08533500000000	-2.13234400000000	8.34035300000000
O	-1.99966500000000	-0.04290100000000	8.37772000000000
O	2.17470000000000	-0.04704000000000	8.31903200000000
O	0.11685300000000	-0.05302300000000	10.43554400000000
H	0.55164200000000	0.73567800000000	10.81096300000000
H	0.51387900000000	-0.81514800000000	10.89472800000000
H	-0.80858600000000	2.38131100000000	8.53407700000000
H	0.16097700000000	1.99316500000000	7.36982800000000
H	-0.69708400000000	-2.65468000000000	8.59617100000000
H	0.04249700000000	-2.01304500000000	7.35259000000000
H	-2.19089500000000	-0.38382700000000	7.48086900000000
H	-2.57156900000000	-0.49953600000000	9.02187800000000
H	2.58306100000000	-0.89721200000000	8.57071000000000
H	2.17961100000000	-0.04034000000000	7.33064900000000

iv. 4 Ni:

Ni	0.03694200000000	0.09357200000000	0.00222500000000
O	2.12135500000000	-0.01784400000000	0.00491200000000
O	-2.04747100000000	0.20498800000000	-0.00046200000000
O	0.14831400000000	2.17781900000000	0.02883600000000
O	-0.07443100000000	-1.99067500000000	-0.02438600000000
O	0.04104500000000	0.12000200000000	-2.08499300000000
O	0.03283800000000	0.06714200000000	2.08944400000000
H	2.06613900000000	0.02448100000000	0.99628500000000
H	2.59947300000000	-0.83679000000000	-0.21611600000000
H	-0.71274800000000	2.60022400000000	-0.15529600000000
H	0.18084200000000	2.07133100000000	1.01667500000000

H	-1.93148200000000	0.20515300000000	0.99253600000000
H	-2.45300400000000	-0.65762100000000	-0.21171400000000
H	0.13403100000000	-2.01507800000000	0.94107000000000
H	0.56291700000000	-2.55589600000000	-0.49637600000000
H	-0.79411700000000	0.33133800000000	-2.53968200000000
H	0.70572600000000	0.73335500000000	-2.44979100000000
Ni	0.02873500000000	0.04071200000000	4.17666200000000
O	0.14010700000000	2.12495900000000	4.20327400000000
O	-0.08263700000000	-2.04353500000000	4.15005100000000
O	0.02463200000000	0.01428200000000	6.26388100000000
O	2.11314800000000	-0.07070300000000	4.17934900000000
O	-2.05567800000000	0.15212800000000	4.17397500000000
H	1.08187800000000	2.34074500000000	4.34112800000000
H	0.05055700000000	2.03724900000000	3.21956000000000
H	-0.84478000000000	-2.42371700000000	3.67878900000000
H	-0.30075900000000	-2.03755900000000	5.11440900000000
H	2.00987000000000	-0.26205800000000	5.14841500000000
H	2.30538800000000	-0.93026400000000	3.76085000000000
H	-2.02164000000000	0.14815200000000	5.16421000000000
H	-2.57718300000000	-0.62814100000000	3.91746800000000
Ni	0.02052800000000	-0.01214800000000	8.35110000000000
O	0.13190100000000	2.07209900000000	8.37771100000000
O	-0.09084400000000	-2.09639500000000	8.32448800000000
O	-2.06388400000000	0.09926800000000	8.34841300000000
O	2.10494100000000	-0.12356300000000	8.35378700000000
O	0.01642500000000	-0.03857800000000	10.43831800000000
H	-0.54404800000000	2.59824300000000	8.83883900000000
H	-0.02409600000000	2.16166300000000	7.40756400000000
H	0.79793500000000	-2.38740200000000	8.60424700000000
H	-0.02755200000000	-1.96685100000000	7.34068400000000
H	-2.41721400000000	0.95350100000000	8.04262800000000
H	-1.97217200000000	0.16346900000000	9.33395400000000
H	2.38466700000000	0.71248000000000	8.77157900000000
H	2.04281500000000	0.06940700000000	7.38311000000000
Ni	0.01232200000000	-0.06500800000000	12.52553700000000
O	0.12369500000000	2.01923900000000	12.55214800000000
O	-0.09905000000000	-2.14925500000000	12.49892600000000
O	-2.07209100000000	0.04640700000000	12.52285000000000
O	2.09673500000000	-0.17642400000000	12.52822400000000
O	0.00821900000000	-0.09143800000000	14.61275600000000
H	0.18414300000000	0.74582900000000	15.07853100000000
H	0.63714700000000	-0.73845000000000	14.98280400000000
H	0.12170700000000	1.87545100000000	11.55963200000000
H	-0.74610800000000	2.41427500000000	12.75483800000000
H	-0.89278600000000	-2.64417300000000	12.77005100000000
H	-0.11720000000000	-2.10178600000000	11.50772600000000
H	-2.63365300000000	-0.60027200000000	12.98762300000000
H	-2.05402400000000	-0.18737500000000	11.56160400000000
H	2.51568100000000	0.68694800000000	12.70603100000000
H	2.06785300000000	-0.25691100000000	11.54147900000000

v. 5 Ni:

Ni	0.12893400000000	0.03779500000000	0.00112800000000
O	2.21517600000000	-0.02364300000000	0.03304300000000
O	-1.95730700000000	0.09923200000000	-0.03078800000000
O	0.19021900000000	2.12425900000000	0.01153000000000
O	0.06764900000000	-2.04867000000000	-0.00927500000000
O	0.16114200000000	0.04725500000000	-2.08599300000000
O	0.09672700000000	0.02833500000000	2.08824800000000
H	2.08131100000000	-0.01020000000000	1.02236000000000
H	2.52119700000000	-0.93036300000000	-0.16287700000000
H	-0.68844700000000	2.51529500000000	-0.15503000000000

H	0.24299300000000	2.02334900000000	1.00223900000000
H	-1.82524200000000	0.08916400000000	0.96422000000000
H	-2.48394900000000	-0.69128300000000	-0.24736600000000
H	-0.09252700000000	-2.02488800000000	0.96929100000000
H	-0.61807700000000	-2.59883300000000	-0.42703400000000
H	-0.56607700000000	0.51881600000000	-2.53059200000000
H	0.97973400000000	0.46068400000000	-2.41845300000000
Ni	0.06451900000000	0.01887600000000	4.17536800000000
O	0.12580400000000	2.10534000000000	4.18577000000000
O	0.00323400000000	-2.06758800000000	4.16496600000000
O	0.03231100000000	0.00941700000000	6.26248800000000
O	2.15076000000000	-0.04256100000000	4.20728300000000
O	-2.02172300000000	0.08031300000000	4.14345200000000
H	-0.70220500000000	2.33566200000000	3.72381100000000
H	-0.10615000000000	2.03716200000000	5.14677800000000
H	0.19136400000000	-2.05736600000000	5.13593900000000
H	0.84852100000000	-2.28546400000000	3.72904300000000
H	2.08295600000000	0.18037800000000	5.16956300000000
H	2.39784300000000	0.78585400000000	3.75432800000000
H	-2.00806700000000	-0.10485800000000	5.11589800000000
H	-2.24128500000000	-0.76728300000000	3.71423600000000
Ni	0.00010400000000	-0.00004300000000	8.34960800000000
O	0.06138900000000	2.08642100000000	8.36001000000000
O	-0.06118100000000	-2.08650700000000	8.33920600000000
O	-2.08613800000000	0.06139500000000	8.31769200000000
O	2.08634500000000	-0.06148000000000	8.38152300000000
O	-0.03210400000000	-0.00950200000000	10.43672800000000
H	0.87059100000000	2.26962600000000	8.87358200000000
H	0.34380700000000	2.03106200000000	7.41367500000000
H	-0.34335900000000	-2.02929800000000	9.28560600000000
H	-0.87078900000000	-2.26910000000000	7.82604600000000
H	-2.31156900000000	0.88347100000000	7.84423000000000
H	-2.01500500000000	0.31207900000000	9.27358900000000
H	2.31002400000000	-0.88498100000000	8.85333600000000
H	2.01318500000000	-0.31083500000000	7.42530300000000
Ni	-0.06431100000000	-0.01896200000000	12.52384800000000
O	-0.00302700000000	2.06750300000000	12.53425000000000
O	-0.12559600000000	-2.10542600000000	12.51344600000000
O	-2.15055300000000	0.04247600000000	12.49193200000000
O	2.02193000000000	-0.08039900000000	12.55576400000000
O	-0.09651900000000	-0.02842100000000	14.61096800000000
H	-0.18926400000000	2.05556500000000	11.56284400000000
H	-0.84912300000000	2.28637800000000	12.96806500000000
H	0.70138800000000	-2.34020800000000	12.97489600000000
H	0.10583300000000	-2.03894500000000	11.55227100000000
H	-2.39571000000000	-0.78663200000000	12.94469800000000
H	-2.08109600000000	-0.18030100000000	11.52962500000000
H	2.24348600000000	0.76660900000000	12.98504200000000
H	2.00978800000000	0.10449100000000	11.58334900000000
Ni	-0.12872600000000	-0.03788000000000	16.69808800000000
O	-0.06744200000000	2.04858400000000	16.70849000000000
O	-0.19001100000000	-2.12434400000000	16.68768600000000
O	-2.21496800000000	0.02355700000000	16.66617300000000
O	1.95751500000000	-0.09931700000000	16.73000400000000
O	-0.16093400000000	-0.04733900000000	18.78520800000000
H	-0.98005400000000	-0.45975500000000	19.11763600000000
H	0.56598000000000	-0.51904400000000	19.23016800000000
H	0.61526100000000	2.60188500000000	17.12707200000000
H	0.09279200000000	2.02666700000000	15.72999600000000
H	0.68864000000000	-2.51535500000000	16.85440400000000
H	-0.24186700000000	-2.02249800000000	15.69692900000000
H	-2.52146100000000	0.93005900000000	16.86239400000000
H	-2.08197600000000	0.01010500000000	15.67678400000000
H	1.82176200000000	-0.08850900000000	15.73511600000000
H	2.48162500000000	0.69296400000000	16.94614599999999

vi. 6 Ni:

Ni	-0.08614600000000	0.07092100000000	0.00057800000000
O	2.00118500000000	0.07094800000000	-0.01512100000000
O	-2.17347700000000	0.07089500000000	0.01627700000000
O	-0.08605400000000	2.15825200000000	0.01628700000000
O	-0.08623700000000	-2.01641000000000	-0.01513000000000
O	-0.10184500000000	0.08663000000000	-2.08669400000000
O	-0.07044700000000	0.05521200000000	2.08785000000000
H	1.84846900000000	0.06862600000000	0.97873400000000
H	2.50589500000000	-0.73767500000000	-0.21614800000000
H	0.80877900000000	2.51907600000000	-0.13096800000000
H	-0.15376100000000	2.04347800000000	1.00626800000000
H	-2.03871200000000	0.08143100000000	1.00674400000000
H	-2.50052700000000	-0.82883200000000	-0.17745600000000
H	0.04963000000000	-1.97439900000000	0.96892500000000
H	0.60813800000000	-2.57890400000000	-0.40080600000000
H	-0.90675200000000	0.52878500000000	-2.41543000000000
H	0.64053000000000	0.55086500000000	-2.51348000000000
Ni	-0.05474700000000	0.03950400000000	4.17512200000000
O	-0.05465600000000	2.12683500000000	4.19083000000000
O	-0.05483900000000	-2.04782700000000	4.15941300000000
O	-0.03904800000000	0.02379500000000	6.26239400000000
O	2.03258400000000	0.03953000000000	4.15942200000000
O	-2.14207800000000	0.03947700000000	4.19082100000000
H	0.11106700000000	2.04166070000000	5.16730700000000
H	0.80846600000000	2.33903500000000	3.78970700000000
H	-0.92479600000000	-2.24413100000000	3.76418100000000
H	-0.21059900000000	-1.97384500000000	5.13901200000000
H	1.98068800000000	-0.12466100000000	5.13667400000000
H	2.22492500000000	-0.82697100000000	3.75580600000000
H	-2.03965200000000	0.22586200000000	5.16124200000000
H	-2.35358500000000	0.89507800000000	3.77190100000000
Ni	-0.02334900000000	0.00808700000000	8.34966500000000
O	-0.02325700000000	2.09541800000000	8.36537400000000
O	-0.02344100000000	-2.07924400000000	8.33395700000000
O	-2.11068000000000	0.00806000000000	8.36536500000000
O	2.06398200000000	0.00811300000000	8.33396600000000
O	-0.00765000000000	-0.00762200000000	10.43693700000000
H	-0.28693500000000	1.99832300000000	9.31637900000000
H	-0.83453000000000	2.34108600000000	7.88342400000000
H	0.23682800000000	-2.07214100000000	9.28713300000000
H	0.78963300000000	-2.26415600000000	7.82779500000000
H	-2.00560800000000	-0.23180400000000	7.40688600000000
H	-2.35734000000000	-0.81860300000000	8.81924300000000
H	1.99438200000000	0.23268700000000	9.29713300000000
H	2.24727200000000	0.84880000000000	7.87370500000000
Ni	0.00804900000000	-0.02333100000000	12.52420900000000
O	0.00814100000000	2.06400000000000	12.53991700000000
O	0.00795800000000	-2.11066100000000	12.50850100000000
O	-2.07928200000000	-0.02335700000000	12.53990900000000
O	2.09538000000000	-0.02330400000000	12.50851000000000
O	0.02374800000000	-0.03903900000000	14.61148100000000
H	0.84847800000000	2.24771800000000	13.00063600000000
H	0.23304800000000	1.99529100000000	11.57682200000000
H	-0.81850500000000	-2.35788200000000	12.05457100000000
H	-0.23210600000000	-2.00571400000000	13.46694100000000
H	-2.26364100000000	0.78972300000000	13.04626900000000
H	-2.07188800000000	0.23722100000000	11.58681400000000
H	2.34071200000000	-0.83568000000000	12.98877800000000
H	1.99772600000000	-0.28533100000000	11.55704900000000

Ni	0.03944800000000	-0.05474800000000	16.69875300000000
O	0.03953900000000	2.03258300000000	16.71446100000000
O	0.03935600000000	-2.14207900000000	16.68304500000000
O	-2.04788300000000	-0.05477400000000	16.71445200000000
O	2.12677900000000	-0.05472100000000	16.68305300000000
O	0.05514700000000	-0.07045600000000	18.78602500000000
H	-0.82722500000000	2.22389500000000	17.11805099999999
H	-0.12446700000000	1.98069100000000	15.73717000000000
H	0.89472400000000	-2.35342600000000	17.10254600000000
H	0.22640600000000	-2.04031200000000	15.71272600000000
H	-1.97338700000000	-0.21040900000000	15.73482600000000
H	-2.24227200000000	-0.92520300000000	17.10965000000000
H	2.33823800000000	0.80781100000000	17.08588700000000
H	2.04354800000000	0.11217700000000	15.70675600000000
Ni	0.07084600000000	-0.08616500000000	20.87329700000000
O	0.07093800000000	2.00116600000000	20.88900500000000
O	0.07075400000000	-2.17349600000000	20.85758800000000
O	-2.01648500000000	-0.08619200000000	20.88899599999999
O	2.15817700000000	-0.08613800000000	20.85759699999999
O	0.08654600000000	-0.10187400000000	22.96056800000000
H	0.55080900000000	0.64038200000000	23.38751300000000
H	0.52851100000000	-0.90686300000000	23.28933400000000
H	0.06861200000000	1.84824100000000	19.89516800000000
H	-0.73747900000000	2.50620600000000	21.08997000000000
H	-0.82895500000000	-2.50064000000000	21.05119600000000
H	0.08123600000000	-2.03792300000000	19.86717800000000
H	-2.57827200000000	0.60866900000000	21.27480300000000
H	-1.97441300000000	0.04982900000000	19.90498100000000
H	2.51878400000000	0.80880500000000	21.00467300000000
H	2.04291700000000	-0.15393100000000	19.86765300000000

vii. 7 Ni:

Ni	-0.06894700000000	0.12001500000000	-0.00106500000000
O	2.01841500000000	0.12609000000000	-0.00995100000000
O	-2.15630900000000	0.11394100000000	0.00782100000000
O	-0.07493500000000	2.20730000000000	0.01908600000000
O	-0.06295800000000	-1.96726900000000	-0.02121700000000
O	-0.07789100000000	0.14014100000000	-2.08833900000000
O	-0.06000200000000	0.09989000000000	2.08620900000000
H	1.83730500000000	0.13348500000000	0.97972900000000
H	2.35189400000000	-0.77186700000000	-0.19784300000000
H	0.81662900000000	2.58000800000000	-0.11821900000000
H	-0.14220400000000	2.06002800000000	1.00352400000000
H	-2.07704600000000	0.16478300000000	0.99924300000000
H	-2.67460500000000	-0.68782500000000	-0.18246300000000
H	-0.21827600000000	-1.91269100000000	0.95798300000000
H	-0.78082300000000	-2.49621700000000	-0.41176300000000
H	-0.71197500000000	0.80867200000000	-2.40812500000000
H	0.77415200000000	0.36650900000000	-2.50257800000000
Ni	-0.05105800000000	0.07976400000000	4.17348200000000
O	-0.05704600000000	2.16704800000000	4.19363400000000
O	-0.04507000000000	-2.00752000000000	4.15333100000000
O	-0.04211400000000	0.05963900000000	6.26075600000000
O	2.03630400000000	0.08583900000000	4.16459600000000
O	-2.13842000000000	0.07369000000000	4.18236900000000
H	0.85098700000000	2.42599700000000	4.43619200000000
H	-0.04339200000000	2.06623600000000	3.20661000000000
H	0.01165600000000	-1.90743600000000	5.14713200000000
H	0.76777100000000	-2.45710900000000	3.86448900000000
H	1.98182800000000	-0.06420500000000	5.14626200000000
H	2.49226100000000	-0.67948300000000	3.77466500000000
H	-2.00995400000000	0.17072600000000	5.16537600000000
H	-2.37392400000000	-0.86355400000000	4.05081400000000

Ni	-0.03316900000000	0.03951300000000	8.34803000000000
O	-0.03915800000000	2.12679800000000	8.36818100000000
O	-0.02718100000000	-2.04777100000000	8.32787900000000
O	-2.12053100000000	0.03343900000000	8.35691600000000
O	2.05419300000000	0.04558800000000	8.33914400000000
O	-0.02422500000000	0.01938800000000	10.43530400000000
H	-0.85108500000000	2.29706000000000	8.88118700000000
H	-0.30260300000000	2.13059900000000	7.41536100000000
H	0.14541600000000	-1.97237000000000	9.30501800000000
H	0.83997500000000	-2.22099500000000	7.91701500000000
H	-2.04273900000000	-0.25386000000000	7.41249200000000
H	-2.34236500000000	-0.76416700000000	8.87148700000000
H	1.93174600000000	0.17873100000000	9.32128000000000
H	2.27269100000000	0.92825300000000	7.98808600000000
Ni	-0.01528000000000	-0.00073700000000	12.52257800000000
O	-0.02126900000000	2.08654700000000	12.54272900000000
O	-0.00929200000000	-2.08802200000000	12.50242700000000
O	-2.10264300000000	-0.00681200000000	12.53146400000000
O	2.07208200000000	0.00533700000000	12.51369100000000
O	-0.00633600000000	-0.02086300000000	14.60985200000000
H	0.82502700000000	2.31468400000000	12.96863800000000
H	0.17786000000000	2.00826500000000	11.57177400000000
H	-0.86152400000000	-2.31757500000000	12.08933200000000
H	-0.19461800000000	-2.01402000000000	13.47660800000000
H	-2.27654200000000	0.81754000000000	13.02312300000000
H	-2.04245200000000	0.24242300000000	11.57307200000000
H	2.00441200000000	-0.24187400000000	13.47270100000000
H	2.24330600000000	-0.82140400000000	12.02505700000000
Ni	0.00260900000000	-0.04098800000000	16.69712500000000
O	-0.00338000000000	2.04629600000000	16.71727700000000
O	0.00859700000000	-2.12827200000000	16.67697400000000
O	-2.08475400000000	-0.04706300000000	16.70601200000000
O	2.08997100000000	-0.03491400000000	16.68823900000000
O	0.01155300000000	-0.06111400000000	18.78439900000000
H	-0.87245100000000	2.21783000000000	17.12514700000000
H	-0.17490000000000	1.96565500000000	15.73985000000000
H	0.17022600000000	-2.10247800000000	17.65397500000000
H	0.87091900000000	-2.30839900000000	16.25908400000000
H	-1.96799300000000	-0.19081200000000	15.72542800000000
H	-2.32401300000000	-0.92030000000000	17.06759700000000
H	2.01291200000000	0.27659100000000	17.62465400000000
H	2.30266100000000	0.74881600000000	16.14869800000000
Ni	0.02049800000000	-0.08123900000000	20.87167300000000
O	0.01450900000000	2.00604500000000	20.89182400000000
O	0.02648600000000	-2.16852300000000	20.85152200000000
O	-2.06686500000000	-0.08731300000000	20.88055900000000
O	2.10786000000000	-0.07516500000000	20.86278699999999
O	0.02944200000000	-0.10136400000000	22.95894700000000
H	-0.05358700000000	1.91363100000000	19.89895599999999
H	-0.80321900000000	2.43511100000000	21.19745099999999
H	-0.00080600000000	-2.06422100000000	21.83833300000000
H	0.94627900000000	-2.43027200000000	20.65925199999999
H	-2.52866700000000	0.74238300000000	21.09160600000000
H	-1.98193500000000	-0.11028100000000	19.88924900000000
H	2.32927900000000	0.81778600000000	21.18572400000000
H	1.95950800000000	0.02207500000000	19.87908400000000

Ni	0.03838600000000	-0.12149000000000	25.04622099999999
O	0.03239800000000	1.96579400000000	25.06637200000000
O	0.04437500000000	-2.20877400000000	25.02607000000000
O	-2.04897600000000	-0.12756400000000	25.05510700000000
O	2.12574900000000	-0.11541500000000	25.03733499999999
O	0.04733100000000	-0.14161500000000	27.13349400000000
H	0.74548700000000	2.50519000000000	25.45136800000000
H	0.17856100000000	1.91361300000000	24.08582199999999
H	-0.84524500000000	-2.58317600000000	25.17301300000000
H	0.09409800000000	-2.05420700000000	24.04120000000000
H	-2.39175800000000	0.76760500000000	25.23879799999999
H	-1.89889800000000	-0.14792800000000	24.06347400000000
H	2.01539100000000	-0.15083200000000	24.04612500000000
H	2.63001100000000	0.69552700000000	25.22712200000000
H	-0.80752800000000	-0.35811000000000	27.54730600000000
H	0.67392800000000	-0.81643400000000	27.45460100000000

viii. 8 Ni:

Ni	-0.08238700000000	0.06788100000000	0.00048100000000
O	2.00497000000000	0.06308200000000	-0.01028300000000
O	-2.16974400000000	0.07267900000000	0.01124400000000
O	-0.07753400000000	2.15523800000000	0.01118100000000
O	-0.08724000000000	-2.01947600000000	-0.01021900000000
O	-0.09312600000000	0.07860600000000	-2.08685400000000
O	-0.07164800000000	0.05715600000000	2.08781500000000
H	1.83476700000000	0.06593600000000	0.98239100000000
H	2.51256700000000	-0.74748100000000	-0.19538600000000
H	0.82240200000000	2.50964100000000	-0.11886100000000
H	-0.15367600000000	2.02437800000000	1.00013600000000
H	-2.02224400000000	0.09177900000000	1.00125800000000
H	-2.49304600000000	-0.83107000000000	-0.16855600000000
H	0.02927400000000	-1.94241200000000	0.97698200000000
H	0.63170200000000	-2.57510800000000	-0.35889900000000
H	-0.90018000000000	0.52773800000000	-2.40046400000000
H	0.64624600000000	0.56358400000000	-2.49527200000000
Ni	-0.06090900000000	0.04643100000000	4.17515000000000
O	-0.05605600000000	2.13378800000000	4.18585000000000
O	-0.06576300000000	-2.04092600000000	4.16445000000000
O	-0.05017100000000	0.03570600000000	6.26248500000000
O	2.02644700000000	0.04163300000000	4.16438700000000
O	-2.14826600000000	0.05122900000000	4.18591400000000
H	0.09311800000000	2.02597500000000	5.16538300000000
H	0.81859600000000	2.33093300000000	3.80243000000000
H	-0.94551500000000	-2.22270800000000	3.78437000000000
H	-0.20807600000000	-1.93539000000000	5.14610200000000
H	1.91552600000000	-0.09374500000000	5.14734000000000
H	2.21107600000000	-0.84236500000000	3.79684200000000
H	-2.04233000000000	0.20542700000000	5.16441900000000
H	-2.35134200000000	0.92202200000000	3.79604400000000
Ni	-0.03943200000000	0.02498200000000	8.34982000000000
O	-0.03457800000000	2.11233900000000	8.36052000000000
O	-0.04428500000000	-2.06237500000000	8.33912000000000
O	-2.12678800000000	0.02978000000000	8.36058400000000
O	2.04792500000000	0.02018300000000	8.33905600000000
O	-0.02869300000000	0.01425700000000	10.43715500000000
H	-0.29947800000000	2.02660600000000	9.31205100000000
H	-0.85574500000000	2.27259700000000	7.85786300000000
H	0.20881500000000	-2.04243200000000	9.29478600000000
H	0.77773300000000	-2.21426500000000	7.83585700000000
H	-2.28277600000000	-0.77326600000000	7.82789900000000
H	-2.05619300000000	-0.26435900000000	9.30328000000000
H	2.01335800000000	0.24441800000000	9.30277900000000
H	2.20627400000000	0.85869000000000	7.86619800000000

Ni	-0.01795400000000	0.00353200000000	12.52449000000000
O	-0.01310100000000	2.09088900000000	12.53519000000000
O	-0.02280800000000	-2.08382500000000	12.51379000000000
O	-2.10531100000000	0.00833000000000	12.53525300000000
O	2.06940300000000	-0.00126600000000	12.51372600000000
O	-0.00721500000000	-0.00719300000000	14.61182400000000
H	0.75643500000000	2.29613700000000	13.09794100000000
H	0.32458400000000	2.02875300000000	11.60721500000000
H	-0.87828800000000	-2.29455800000000	12.09658700000000
H	-0.21624500000000	-1.97809500000000	13.48459200000000
H	-2.23075900000000	0.74245200000000	13.16737800000000
H	-2.08489900000000	0.40671100000000	11.63336000000000
H	1.98322900000000	-0.21241200000000	13.48145600000000
H	2.24910900000000	-0.84855900000000	12.06506700000000
Ni	0.00352400000000	-0.01791800000000	16.69915900000000
O	0.00837700000000	2.06943900000000	16.70985900000000
O	-0.00133000000000	-2.10527400000000	16.68845900000000
O	-2.08383300000000	-0.01311900000000	16.70992300000000
O	2.09088000000000	-0.02271600000000	16.68839600000000
O	0.01426200000000	-0.02864200000000	18.78649400000000
H	-0.83807400000000	2.25355500000000	17.15831700000000
H	-0.20282500000000	1.98489700000000	15.74202800000000
H	0.40015000000000	-2.08796000000000	17.58895700000000
H	0.73005800000000	-2.23228800000000	16.05341500000000
H	-1.97921000000000	-0.20641400000000	15.73899100000000
H	-2.29609600000000	-0.86835100000000	17.12689800000000
H	2.02996300000000	0.31603400000000	17.61603599999999
H	2.29914500000000	0.74546100000000	16.12491700000000
Ni	0.02500100000000	-0.03936700000000	20.87382900000000
O	0.02985500000000	2.04799000000000	20.88452899999999
O	0.02014800000000	-2.12672400000000	20.86312900000000
O	-2.06235500000000	-0.03456900000000	20.88459200000000
O	2.11235800000000	-0.04416500000000	20.86306499999999
O	0.03574000000000	-0.05009200000000	22.96116400000000
H	0.86945700000000	2.20340900000000	21.35639099999999
H	0.25325300000000	2.01032700000000	19.92058900000000
H	-0.27391700000000	-2.05325400000000	19.92054600000000
H	-0.78383200000000	-2.27835200000000	21.39567900000000
H	-2.21217100000000	0.78763300000000	21.38815000000000
H	-2.04146100000000	0.21880500000000	19.92903200000000
H	2.26985500000000	-0.86581500000000	21.36580500000000
H	2.02644800000000	-0.30911000000000	19.91160200000000
Ni	0.04647900000000	-0.06081700000000	25.04849900000000
O	0.05133200000000	2.02654000000000	25.05919800000000
O	0.04162500000000	-2.14817400000000	25.03779900000000
O	-2.04087800000000	-0.05601800000000	25.05926200000000
O	2.13383600000000	-0.06561500000000	25.03773500000000
O	0.05721700000000	-0.07154100000000	27.13583300000000
H	-0.83170700000000	2.21572000000000	25.42672300000000
H	-0.08452900000000	1.91677800000000	24.07623399999999
H	0.91166900000000	-2.35490400000000	25.42744899999999
H	0.19589300000000	-2.04328500000000	24.05918899999999
H	-1.93478200000000	-0.19860100000000	24.07762599999999
H	-2.22657500000000	-0.93517900000000	25.43885600000000
H	2.33643600000000	0.80886200000000	25.41863299999999
H	2.02506200000000	0.08189000000000	24.05787300000000

Ni	0.06795600000000	-0.08226600000000	29.22316800000000
O	0.07280900000000	2.00509100000000	29.23386800000000
O	0.06310200000000	-2.16962300000000	29.21246799999999
O	-2.01940100000000	-0.07746800000000	29.23393099999999
O	2.15531300000000	-0.08706400000000	29.21240500000000
O	0.07869400000000	-0.09299100000000	31.31050299999999
H	0.07467600000000	1.83484600000000	28.24122400000000
H	-0.73539200000000	2.51627300000000	29.41946000000000
H	-0.84260900000000	-2.48784200000000	29.39153499999999
H	0.08404700000000	-2.02266900000000	28.22244900000000
H	-2.57220900000000	0.64463300000000	29.58055200000000
H	-1.94004500000000	0.03701100000000	28.24648000000000
H	2.51430500000000	0.81082300000000	29.34400800000000
H	2.02376900000000	-0.16092000000000	28.22328699999999
H	0.56416600000000	0.64568600000000	31.71961700000000
H	0.52661800000000	-0.90081600000000	31.62390600000000

ix. 9 Ni:

Ni	-0.08688900000000	0.10264100000000	-0.00183700000000
O	2.00046900000000	0.10729600000000	-0.01237200000000
O	-2.17424700000000	0.09798500000000	0.00869800000000
O	-0.09148900000000	2.18999700000000	0.00922000000000
O	-0.08228900000000	-1.98471500000000	-0.01289400000000
O	-0.09744900000000	0.11367400000000	-2.08917100000000
O	-0.07633000000000	0.09160700000000	2.08549700000000
H	1.80653100000000	0.11810800000000	0.97568700000000
H	2.33717200000000	-0.79097600000000	-0.19130600000000
H	0.80765800000000	2.54943500000000	-0.11232800000000
H	-0.16984900000000	2.03226100000000	0.99231900000000
H	-2.08002400000000	0.15263000000000	0.99924200000000
H	-2.70940500000000	-0.69571900000000	-0.16843000000000
H	-0.22277600000000	-1.89975100000000	0.96819800000000
H	-0.82501500000000	-2.49868100000000	-0.37572100000000
H	-0.72512400000000	0.79241700000000	-2.39961600000000
H	0.75895400000000	0.34618300000000	-2.49061700000000
Ni	-0.06577000000000	0.08057400000000	4.17283200000000
O	-0.07037000000000	2.16793000000000	4.18388800000000
O	-0.06117000000000	-2.00678200000000	4.16177500000000
O	-0.05521100000000	0.06954000000000	6.26016600000000
O	2.02158800000000	0.08522900000000	4.16229700000000
O	-2.15312800000000	0.07591800000000	4.18336700000000
H	0.82893700000000	2.41941400000000	4.46370200000000
H	-0.01906200000000	2.06167300000000	3.19868200000000
H	-0.00440800000000	-1.88800700000000	5.15553100000000
H	0.75366100000000	-2.45782200000000	3.88092000000000
H	1.95208800000000	-0.05993800000000	5.14530900000000
H	2.46433000000000	-0.69200100000000	3.78086600000000
H	-2.01497600000000	0.17577800000000	5.16592100000000
H	-2.38384300000000	-0.86316100000000	4.05677400000000
Ni	-0.04465100000000	0.05850700000000	8.34750000000000
O	-0.04925100000000	2.14586300000000	8.35855700000000
O	-0.04005100000000	-2.02884900000000	8.33644300000000
O	-2.13200900000000	0.05385100000000	8.35803500000000
O	2.04270700000000	0.06316200000000	8.33696500000000
O	-0.03409200000000	0.04747300000000	10.43483400000000
H	-0.84297800000000	2.29546000000000	8.90585900000000
H	-0.34876300000000	2.14156800000000	7.41688200000000
H	0.12670800000000	-1.92758700000000	9.31457300000000
H	0.83289800000000	-2.19175000000000	7.93361800000000
H	-2.06152700000000	-0.28759900000000	7.43237000000000
H	-2.32693600000000	-0.71296300000000	8.92806600000000
H	1.91101400000000	0.19947400000000	9.31854800000000
H	2.24595000000000	0.94818600000000	7.98253500000000

Ni	-0.02353200000000	0.03644000000000	12.52216800000000
O	-0.02813200000000	2.12379600000000	12.53322500000000
O	-0.01893200000000	-2.05091600000000	12.51111100000000
O	-2.11089000000000	0.03178400000000	12.53270300000000
O	2.06382600000000	0.04109600000000	12.51163300000000
O	-0.01297300000000	0.02540600000000	14.60950200000000
H	0.81549900000000	2.34361000000000	12.96874300000000
H	0.18095200000000	2.02866600000000	11.56484000000000
H	-0.87483800000000	-2.26424200000000	12.09681600000000
H	-0.20656400000000	-1.95305000000000	13.48411600000000
H	-2.26223300000000	0.84896500000000	13.04414700000000
H	-2.04240600000000	0.29986500000000	11.57971500000000
H	1.99573900000000	-0.19441400000000	13.47411400000000
H	2.22181700000000	-0.79335800000000	12.03168200000000
Ni	-0.00241300000000	0.01437300000000	16.69683600000000
O	-0.00701300000000	2.10172900000000	16.70789300000000
O	0.00218700000000	-2.07298300000000	16.68577900000000
O	-2.08977100000000	0.00971700000000	16.70737100000000
O	2.08494500000000	0.01902900000000	16.68630100000000
O	0.00814600000000	0.00334000000000	18.78417000000000
H	-0.83193900000000	2.25468600000000	17.20604300000000
H	-0.25901700000000	2.04548500000000	15.75005300000000
H	0.25369500000000	-2.01659000000000	17.64378400000000
H	0.82763300000000	-2.22429100000000	16.18796600000000
H	-1.99167500000000	-0.18446100000000	15.73570400000000
H	-2.30628500000000	-0.84161500000000	17.12929199999999
H	1.98686400000000	0.21085800000000	17.65850900000000
H	2.30095200000000	0.87164600000000	16.26675100000000
Ni	0.01870600000000	-0.00769400000000	20.87150500000000
O	0.01410600000000	2.07966200000000	20.88256100000000
O	0.02330600000000	-2.09505000000000	20.86044799999999
O	-2.06865200000000	-0.01235000000000	20.88204000000000
O	2.10606400000000	-0.00303800000000	20.86097000000000
O	0.02926500000000	-0.01872700000000	22.95883900000000
H	0.86802300000000	2.29375200000000	21.30050600000000
H	0.20467900000000	1.98408200000000	19.91013300000000
H	-0.82312800000000	-2.31291200000000	20.42939600000000
H	-0.18170600000000	-1.99697600000000	21.82977300000000
H	-2.22758600000000	0.81877200000000	21.36751200000000
H	-2.00342800000000	0.22845400000000	19.92098099999999
H	2.03584800000000	-0.26201700000000	21.81673700000000
H	2.25890800000000	-0.82520800000000	20.35816000000000
Ni	0.03982500000000	-0.02976100000000	25.04617300000000
O	0.03522500000000	2.05759500000000	25.05723000000000
O	0.04442500000000	-2.11711700000000	25.03511600000000
O	-2.04753300000000	-0.03441600000000	25.05670800000000
O	2.12718300000000	-0.02510500000000	25.03563800000000
O	0.05038400000000	-0.04079400000000	27.13350699999999
H	-0.82387500000000	2.22275400000000	25.48872500000000
H	-0.15552300000000	1.96755900000000	24.08379699999999
H	0.33501600000000	-2.11044700000000	25.97994600000000
H	0.84328100000000	-2.26628700000000	24.49523900000000
H	-1.91914200000000	-0.17408900000000	24.07571000000000
H	-2.26125300000000	-0.91570000000000	25.41389100000000
H	2.02449400000000	0.27598900000000	25.97501900000000
H	2.31890700000000	0.77014900000000	24.50506300000000
Ni	0.06094400000000	-0.05182800000000	29.22084099999999
O	0.05634400000000	2.03552800000000	29.23189800000000
O	0.06554400000000	-2.13918300000000	29.20978400000000
O	-2.02641400000000	-0.05648300000000	29.23137599999999
O	2.14830200000000	-0.04717200000000	29.21030599999999
O	0.07150300000000	-0.06286100000000	31.30817499999999

H	0.85323900000000	2.46125100000000	29.59253799999999
H	0.18257500000000	1.94584100000000	28.24505900000000
H	-0.84984500000000	-2.37507700000000	28.97133699999999
H	0.05704400000000	-2.01659600000000	30.19569600000000
H	-2.22744100000000	0.81012500000000	29.63071800000000
H	-1.94614800000000	0.10580100000000	28.25277000000000
H	2.60191300000000	0.80682600000000	29.32087900000000
H	1.99808700000000	-0.15107400000000	28.22734600000000
Ni	0.08206300000000	-0.07389400000000	33.39550900000000
O	0.07746300000000	2.01346200000000	33.40656600000000
O	0.08666300000000	-2.16124900000000	33.38445300000000
O	-2.00529500000000	-0.07854900000000	33.40604500000000
O	2.16942100000000	-0.06923800000000	33.38497400000000
O	0.09262300000000	-0.08492600000000	35.48284400000000
H	-0.81139500000000	2.37779000000000	33.57780700000000
H	0.10149100000000	1.87842800000000	32.41814900000000
H	-0.63007800000000	-2.73779000000000	33.70323600000000
H	-0.01919700000000	-2.05188700000000	32.40151000000000
H	-2.52148300000000	-0.88084100000000	33.60362300000000
H	-1.82964700000000	-0.09965600000000	32.41612600000000
H	2.49755100000000	-0.97120300000000	33.56434700000000
H	2.03618600000000	-0.04975300000000	32.39548200000000
H	0.89676500000000	0.36773600000000	35.79837000000000
H	-0.64981800000000	0.39328800000000	35.89328200000000

x. 10 Ni:

Ni	-0.08067600000000	-0.03164800000000	-0.05728200000000
O	2.00656300000000	-0.05422400000000	-0.06839200000000
O	-2.16791400000000	-0.00907300000000	-0.04617200000000
O	-0.05811700000000	2.05561700000000	-0.06041500000000
O	-0.10323400000000	-2.11891400000000	-0.05415100000000
O	-0.09181900000000	-0.03466000000000	-2.14464000000000
O	-0.06953300000000	-0.02863700000000	2.03007600000000
H	2.52074600000000	0.75502800000000	-0.24047700000000
H	1.82096900000000	-0.05898700000000	0.92310400000000
H	0.67937700000000	2.60479800000000	-0.37936900000000
H	0.04218400000000	1.94960000000000	0.92777800000000
H	-2.47517300000000	0.90239200000000	-0.21395900000000
H	-2.00821200000000	-0.03791700000000	0.94253700000000
H	-0.17808000000000	-1.97441000000000	0.93414400000000
H	0.79437600000000	-2.48172500000000	-0.17609200000000
H	-0.90437900000000	-0.48294100000000	-2.44500400000000
H	0.64091600000000	-0.54056900000000	-2.53935600000000
Ni	-0.05839000000000	-0.02562500000000	4.11743400000000
O	-0.03583100000000	2.06164100000000	4.11430200000000
O	-0.08094800000000	-2.11289100000000	4.12056600000000
O	-0.04724600000000	-0.02261300000000	6.20479200000000
O	2.02884900000000	-0.04820000000000	4.10632400000000
O	-2.14562800000000	-0.00305000000000	4.12854400000000
H	-0.17506600000000	1.94872900000000	5.09648800000000
H	-0.91672700000000	2.24695900000000	3.73868900000000
H	0.79552900000000	-2.31282700000000	3.74305800000000
H	0.06290100000000	-2.00303400000000	5.10191900000000
H	1.90448500000000	0.07742000000000	5.09099100000000
H	2.21724900000000	0.83969500000000	3.75053700000000
H	-2.03251300000000	-0.14997100000000	5.10884200000000
H	-2.35274000000000	-0.87648000000000	3.74712400000000
Ni	-0.03610300000000	-0.01960200000000	8.29215000000000
O	-0.01354500000000	2.06766400000000	8.28901800000000
O	-0.05866200000000	-2.10686800000000	8.29528200000000
O	-2.12334200000000	0.00297300000000	8.30326000000000
O	2.05113500000000	-0.04217700000000	8.28104000000000
O	-0.02496000000000	-0.01659000000000	10.37950800000000

H	0.19221300000000	1.98019900000000	9.25792300000000
H	0.83939700000000	2.20950900000000	7.83731000000000
H	-0.25367400000000	-2.01745700000000	9.26611900000000
H	-0.91576800000000	-2.25697600000000	7.85427200000000
H	-2.02057300000000	0.20285700000000	9.27256800000000
H	-2.27322700000000	0.85835100000000	7.85885200000000
H	2.19292900000000	-0.90084700000000	7.84034100000000
H	1.95583400000000	-0.23648100000000	9.25265100000000
Ni	-0.01381700000000	-0.01357900000000	12.46686600000000
O	0.00874100000000	2.07368700000000	12.46373400000000
O	-0.03637600000000	-2.10084400000000	12.46999800000000
O	-2.10105600000000	0.00899600000000	12.47797600000000
O	2.07342100000000	-0.03615400000000	12.45575600000000
O	-0.00267400000000	-0.01056700000000	14.55422400000000
H	-0.20446700000000	2.00797800000000	13.43112100000000
H	-0.83640200000000	2.23577800000000	12.00402800000000
H	0.80170200000000	-2.26265900000000	11.99730900000000
H	0.18963000000000	-2.03785700000000	13.43414500000000
H	-2.00612200000000	-0.25664700000000	13.42965500000000
H	-2.25189000000000	-0.81135200000000	11.97094400000000
H	2.03307000000000	0.20290900000000	13.41620800000000
H	2.22615300000000	0.79372900000000	11.96595900000000
Ni	0.00846900000000	-0.00755500000000	16.64158200000000
O	0.03102800000000	2.07971000000000	16.63845000000000
O	-0.01409000000000	-2.09482100000000	16.64471400000000
O	-2.07877000000000	0.01502000000000	16.65269200000000
O	2.09570700000000	-0.03013000000000	16.63047200000000
O	0.01961200000000	-0.00454400000000	18.72894000000000
H	0.24618900000000	1.99654000000000	17.60551100000000
H	0.87753900000000	2.23823700000000	16.18025800000000
H	-0.20316400000000	-1.98539600000000	17.61641700000000
H	-0.87394900000000	-2.28246300000000	16.22544300000000
H	-2.24131200000000	0.73436000000000	17.29157100000000
H	-2.02179000000000	0.42803400000000	15.75703100000000
H	2.25299100000000	-0.89124500000000	16.20033700000000
H	2.01208600000000	-0.21473700000000	17.60427400000000
Ni	0.03075500000000	-0.00153200000000	20.81629800000000
O	0.05331400000000	2.08573400000000	20.81316700000000
O	0.00819600000000	-2.08879800000000	20.81943000000000
O	-2.05648300000000	0.02104300000000	20.82740799999999
O	2.11799300000000	-0.02410700000000	20.80518899999999
O	0.04189800000000	0.00148000000000	22.90365700000000
H	-0.13365900000000	1.97195000000000	21.78599100000000
H	-0.80056000000000	2.31563900000000	20.40355300000000
H	0.85286400000000	-2.26369000000000	20.36395100000000
H	0.22226100000000	-2.00639400000000	21.78700100000000
H	-2.27959700000000	-0.80626500000000	21.29138300000000
H	-1.94079800000000	-0.22395100000000	19.86854400000000
H	2.03665100000000	0.20156300000000	21.76970000000000
H	2.27999700000000	0.81572500000000	20.33572299999999
Ni	0.05304100000000	0.00449100000000	24.99101500000000
O	0.07560000000000	2.09175700000000	24.98788300000000
O	0.03048200000000	-2.08277400000000	24.99414600000000
O	-2.03419700000000	0.02706600000000	25.00212400000000
O	2.14027900000000	-0.01808400000000	24.97990500000000
O	0.06418400000000	0.00750300000000	27.07837299999999
H	0.33163700000000	2.00485700000000	25.94382400000000
H	0.90358100000000	2.23881800000000	24.49360600000000
H	-0.07789400000000	-1.95346600000000	25.97857899999999
H	-0.85649400000000	-2.29841500000000	24.65389900000000
H	-2.23130200000000	0.89705700000000	25.39449400000000
H	-1.90280800000000	0.20073400000000	24.02730700000000
H	2.21983900000000	-0.71421500000000	24.29704499999999
H	2.19233600000000	-0.46052300000000	25.85539600000000

Ni	0.07532700000000	0.01051500000000	29.16573100000000
O	0.09788600000000	2.09778000000000	29.16259900000000
O	0.05276800000000	-2.07675100000000	29.16886300000000
O	-2.01191100000000	0.03309000000000	29.17684100000000
O	2.16256600000000	-0.01206100000000	29.15462100000000
O	0.08647000000000	0.01352600000000	31.25308900000000
H	-0.07293000000000	2.05819600000000	30.13715000000000
H	-0.74399400000000	2.35381400000000	28.74525199999999
H	-0.80183200000000	-2.48598000000000	28.94747200000000
H	0.06413200000000	-1.93623400000000	30.15706000000000
H	-2.42682800000000	-0.76042400000000	29.55672300000000
H	-1.90522900000000	-0.12400800000000	28.19540399999999
H	2.41554200000000	0.89803800000000	29.39786599999999
H	1.98624600000000	0.02988300000000	28.17144599999999
Ni	0.09761300000000	0.01653800000000	33.34044700000000
O	0.12017200000000	2.10380300000000	33.33731500000000
O	0.07505400000000	-2.07072800000000	33.34357900000000
O	-1.98962500000000	0.03911300000000	33.35155700000000
O	2.18485200000000	-0.00603800000000	33.32933700000000
O	0.10875600000000	0.01955000000000	35.42780500000000
H	0.19155100000000	1.97000800000000	34.32004000000000
H	-0.80856900000000	2.36204400000000	33.19014400000000
H	-0.72673200000000	-2.53591000000000	33.63885400000000
H	-0.00348500000000	-1.93485800000000	32.35492300000000
H	-2.41188600000000	-0.78171500000000	33.65767100000000
H	-1.85160600000000	-0.04280100000000	32.36064700000000
H	2.42139600000000	-0.91894300000000	33.57767400000000
H	2.11417500000000	-0.01501600000000	32.33829400000000
Ni	0.11990000000000	0.02256300000000	37.51516300000000
O	0.14245800000000	2.10982900000000	37.51202900000000
O	0.09734100000000	-2.06470300000000	37.51829800000000
O	-1.96733900000000	0.04513800000000	37.52627700000000
O	2.20713800000000	-0.00001200000000	37.50405600000000
O	0.13104300000000	0.02557700000000	39.60252099999999
H	0.12540900000000	1.89931800000000	36.52886700000000
H	-0.62977000000000	2.67958800000000	37.68239200000000
H	-0.81795100000000	-2.36563700000000	37.67201299999999
H	0.16416100000000	-1.94158500000000	36.53238600000000
H	-2.47654000000000	0.80287400000000	37.86322900000000
H	-1.85644200000000	0.16481400000000	36.54112700000000
H	2.58636200000000	0.88609000000000	37.65710900000000
H	2.08783500000000	-0.04423100000000	36.51392000000000
H	0.61491500000000	0.77347200000000	39.99633099999998
H	0.59645200000000	-0.77319300000000	39.91338999999999

2. [Fe(SCH₃)₄]⁻

A. Geometry

Fe	0.000000000000000	0.000000000000000	0.000000000000000
S	-1.344228763000000	-1.344264597000000	1.229154000000000
S	1.344264597000000	-1.344228763000000	-1.229154000000000
S	1.344228763000000	1.344264597000000	1.229154000000000
S	-1.344264597000000	1.344228763000000	-1.229154000000000
C	-0.234560888000000	-2.195782737000000	2.286572000000000
C	2.195782737000000	-0.234560888000000	-2.286572000000000
C	0.234560888000000	2.195782737000000	2.286572000000000
C	-2.195782737000000	0.234560888000000	-2.286572000000000
H	0.551446256000000	-2.504371013000000	1.789726000000000
H	-0.699297872000000	-2.925393241000000	2.714291000000000
H	-0.081683162000000	-1.555481654000000	3.096647000000000
H	2.504371013000000	0.551446256000000	-1.789726000000000
H	2.925393241000000	-0.699297872000000	-2.714291000000000
H	1.555481654000000	-0.081683162000000	-3.096647000000000
H	-0.551446256000000	2.504371013000000	1.789726000000000
H	0.699297872000000	2.925393241000000	2.714291000000000
H	0.081683162000000	1.555481654000000	3.096647000000000
H	-2.504371013000000	-0.551446256000000	-1.789726000000000
H	-2.925393241000000	0.699297872000000	-2.714291000000000
H	-1.555481654000000	0.081683162000000	-3.096647000000000

B. Branching diagrams

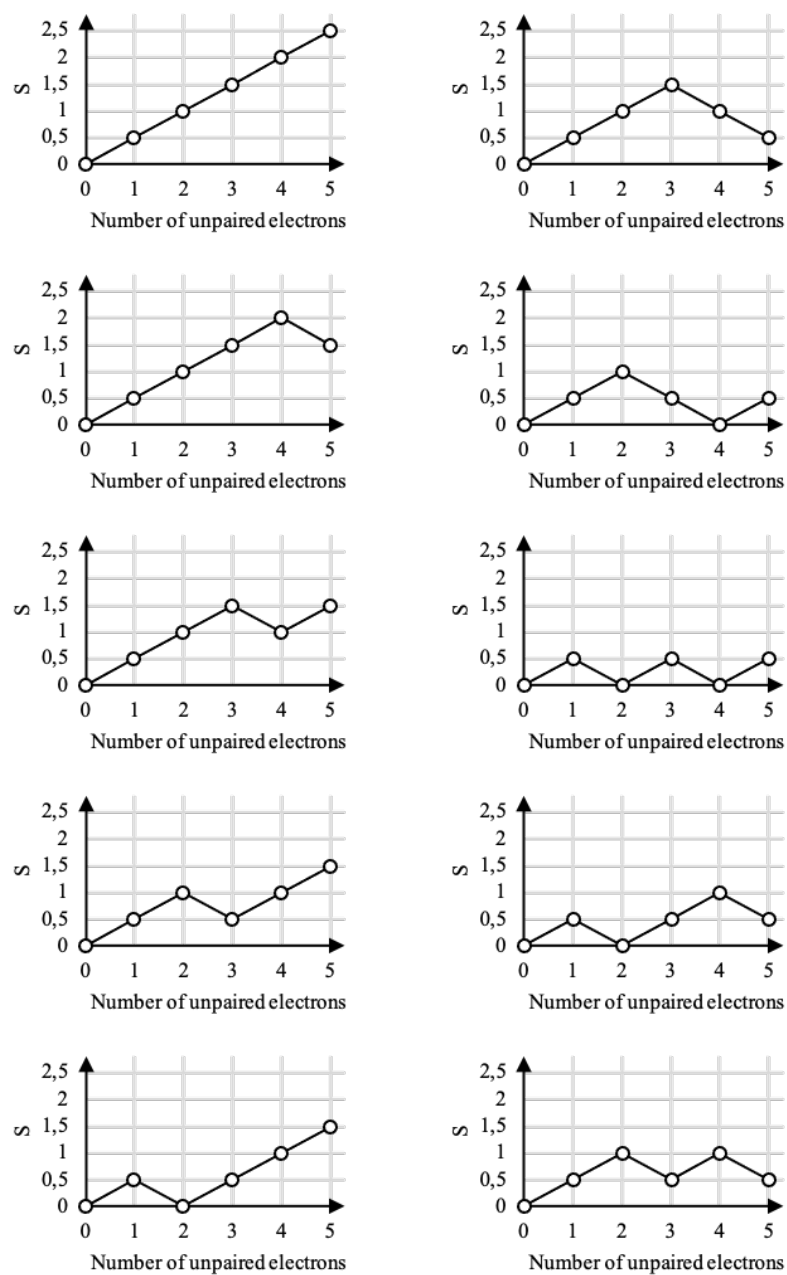


Figure S1. Branching diagrams for the sextet, quartet and doublet multiplicities of $[\text{Fe}(\text{SCH}_3)_4]^-$.

C. Sample Inputs

SAHF calculation for 5 electrons in 5 orbitals and $S = \frac{3}{2}$ of $[\text{Fe}(\text{SCH}_3)_4]^-$, using AVAS for the initial guess orbitals:

```

# [Fe(SCH3)4]- Quartet SAHF

! Def2-TZVP TightSCF

%pal
nproc 8
end

%scf
avas
system
norb 5
nel 5
center 0
type d
end
end
HFTyp ROHF
ROHF_CASE SAHF
ROHF_NumOp 2
ROHF_NEL[1] 5
ROHF_NORB[1] 5
end

*xyz -1 4
Fe 0.000000000000000 0.000000000000000 0.000000000000000
S -1.344228763000000 -1.344264597000000 1.229154000000000
S 1.344264597000000 -1.344228763000000 -1.229154000000000
S 1.344228763000000 1.344264597000000 1.229154000000000
S -1.344264597000000 1.344228763000000 -1.229154000000000
C -0.234560888000000 -2.195782737000000 2.286572000000000
C 2.195782737000000 -0.234560888000000 -2.286572000000000
C 0.234560888000000 2.195782737000000 2.286572000000000
C -2.195782737000000 0.234560888000000 -2.286572000000000
H 0.551446256000000 -2.504371013000000 1.789726000000000
H -0.699297872000000 -2.925393241000000 2.714291000000000
H -0.081683162000000 -1.555481654000000 3.096647000000000
H 2.504371013000000 0.551446256000000 -1.789726000000000
H 2.925393241000000 -0.699297872000000 -2.714291000000000
H 1.555481654000000 -0.081683162000000 -3.096647000000000
H -0.551446256000000 2.504371013000000 1.789726000000000
H 0.699297872000000 2.925393241000000 2.714291000000000
H 0.081683162000000 1.555481654000000 3.096647000000000
H -2.504371013000000 -0.551446256000000 -1.789726000000000
H -2.925393241000000 0.699297872000000 -2.714291000000000
H -1.555481654000000 0.081683162000000 -3.096647000000000
end

```

CSF-ROHF calculation for the CSF $[+ + - + +]$ with $S = \frac{3}{2}$ of $[\text{Fe}(\text{SCH}_3)_4]^-$, using the converged SAHF orbitals as initial guess:

```

# [Fe(SCH3)4]- Quartet ROHF [++-++] CSF

! Def2-TZVP TightSCF MOREAD

%moinp "fesch3_quart_sahf.gbw"

%pal
nproc 8
end

%scf
HFTyp ROHF
ROHF_CASE USER_CSF
ROHF_REF {1 1 -1 1 1} end
MaxIter 1000
end

*xyz -1 4
Fe 0.000000000000000 0.000000000000000 0.000000000000000
S -1.34422876300000 -1.34426459700000 1.229154000000000
S 1.34426459700000 -1.34422876300000 -1.229154000000000
S 1.34422876300000 1.34426459700000 1.229154000000000
S -1.34426459700000 1.34422876300000 -1.229154000000000
C -0.23456088800000 -2.19578273700000 2.286572000000000
C 2.19578273700000 -0.23456088800000 -2.286572000000000
C 0.23456088800000 2.19578273700000 2.286572000000000
C -2.19578273700000 0.23456088800000 -2.286572000000000
H 0.55144625600000 -2.50437101300000 1.789726000000000
H -0.69929787200000 -2.92539324100000 2.714291000000000
H -0.08168316200000 -1.55548165400000 3.096647000000000
H 2.50437101300000 0.55144625600000 -1.789726000000000
H 2.92539324100000 -0.69929787200000 -2.714291000000000
H 1.55548165400000 -0.08168316200000 -3.096647000000000
H -0.55144625600000 2.50437101300000 1.789726000000000
H 0.69929787200000 2.92539324100000 2.714291000000000
H 0.08168316200000 1.55548165400000 3.096647000000000
H -2.50437101300000 -0.55144625600000 -1.789726000000000
H -2.92539324100000 0.69929787200000 -2.714291000000000
H -1.55548165400000 0.08168316200000 -3.096647000000000
end

```

3. $[\text{Fe}_2\text{S}_2(\text{SCH}_3)_4]^{2-}$

A. Geometry

Fe	0.0000000000000000	0.0000000000000000	-1.34356781200000
Fe	0.0000000000000000	0.0000000000000000	1.34356781200000
S	1.07173350100000	1.37336608200000	0.00000000000000
S	1.34671428400000	-1.34590148600000	-2.65162144900000
S	-1.34671428400000	1.34590148600000	-2.65162144900000
S	-1.07173350100000	-1.37336608200000	0.00000000000000
S	-1.34671428400000	1.34590148600000	2.65162144900000
S	1.34671428400000	-1.34590148600000	2.65162144900000
C	-2.48566330400000	0.36254339300000	-3.60079527600000
H	-3.31993751600000	0.59673175500000	-3.50588279500000
H	-2.34744650700000	0.38829290300000	-4.46338059000000
H	-2.47240470900000	-0.48571120300000	-3.40416734300000
C	2.48566330400000	-0.36254339300000	-3.60079527600000
H	3.31993751600000	-0.59673175500000	-3.50588279500000
H	2.34744650700000	-0.38829290300000	-4.46338059000000
H	2.47240470900000	0.48571120300000	-3.40416734300000
C	2.48566330400000	-0.36254339300000	3.60079527600000
H	2.34744650700000	-0.38829290300000	4.46338059000000
H	3.31993751600000	-0.59673175500000	3.50588279500000
H	2.47240470900000	0.48571120300000	3.40416734300000
C	-2.48566330400000	0.36254339300000	3.60079527600000
H	-3.31993751600000	0.59673175500000	3.50588279500000
H	-2.47240470900000	-0.48571120300000	3.40416734300000
H	-2.34744650700000	0.38829290300000	4.46338059000000

B. Sample Inputs

SAHF calculation for 10 electrons in 10 orbitals and $S = 0$ of $[\text{Fe}_2\text{S}_2(\text{SCH}_3)_4]^{2-}$, using AVAS for the initial guess orbitals:

```

# [Fe2S2(SCH3)4]2- SAHF with AVAS Guess Orbitals

! Def2-TZVP TightSCF

%pal
nproc 8
end

%scf
avas
system
nel 10
norb 10
center 0,1
type d,d
end
end
HFTyp ROHF
ROHF_Case SAHF
ROHF_NumOp 2
ROHF_NEL[1] 10
ROHF_NORB[1] 10
end

*xyz -2 1
Fe 0.000000000 0.000000000 -1.343567812
Fe 0.000000000 0.000000000 1.343567812
S 1.071733501 1.373366082 0.000000000
S 1.346714284 -1.345901486 -2.651621449
S -1.346714284 1.345901486 -2.651621449
S -1.071733501 -1.373366082 0.000000000
S -1.346714284 1.345901486 2.651621449
S 1.346714284 -1.345901486 2.651621449
C -2.485663304 0.362543393 -3.600795276
H -3.319937516 0.596731755 -3.505882795
H -2.347446507 0.388292903 -4.463380590
H -2.472404709 -0.485711203 -3.404167343
C 2.485663304 -0.362543393 -3.600795276
H 3.319937516 -0.596731755 -3.505882795
H 2.347446507 -0.388292903 -4.463380590
H 2.472404709 0.485711203 -3.404167343
C 2.485663304 -0.362543393 3.600795276
H 2.347446507 -0.388292903 4.463380590
H 3.319937516 -0.596731755 3.505882795
H 2.472404709 0.485711203 3.404167343
C -2.485663304 0.362543393 3.600795276
H -3.319937516 0.596731755 3.505882795
H -2.472404709 -0.485711203 3.404167343
H -2.347446507 0.388292903 4.463380590
end

```

CSF-ROHF calculation for the CSF [++++--] with $S = 0$ of $[\text{Fe}_2\text{S}_2(\text{SCH}_3)_4]^{2-}$, using the converged SAHF orbitals as initial guess:

```

# [Fe2S2(SCH3)4]2- AF-ROHF with localized SAHF orbitals

! Def2-TZVP TightSCF MOREAD

%moinp "fe2sch_sahf.loc"

%pal
nproc 8
end

%scf
Rotate {88,94,90} {92,96,90} end
HFTyp ROHF
ROHF_Case AF_CSF
ROHF_AFORBS 5,5
MaxIter 500
end

*xyz -2 1
Fe 0.000000000 0.000000000 -1.343567812
Fe 0.000000000 0.000000000 1.343567812
S 1.071733501 1.373366082 0.000000000
S 1.346714284 -1.345901486 -2.651621449
S -1.346714284 1.345901486 -2.651621449
S -1.071733501 -1.373366082 0.000000000
S -1.346714284 1.345901486 2.651621449
S 1.346714284 -1.345901486 2.651621449
C -2.485663304 0.362543393 -3.600795276
H -3.319937516 0.596731755 -3.505882795
H -2.347446507 0.388292903 -4.463380590
H -2.472404709 -0.485711203 -3.404167343
C 2.485663304 -0.362543393 -3.600795276
H 3.319937516 -0.596731755 -3.505882795
H 2.347446507 -0.388292903 -4.463380590
H 2.472404709 0.485711203 -3.404167343
C 2.485663304 -0.362543393 3.600795276
H 2.347446507 -0.388292903 4.463380590
H 3.319937516 -0.596731755 3.505882795
H 2.472404709 0.485711203 3.404167343
C -2.485663304 0.362543393 3.600795276
H -3.319937516 0.596731755 3.505882795
H -2.472404709 -0.485711203 3.404167343
H -2.347446507 0.388292903 4.463380590
end

```

4. $[\text{Gd}_2\text{Cl}_{11}]^{5-}$

A. Geometry

Cl	2.82651000000000	0.00000000000000	0.00000000000000
Cl	0.00000000000000	2.82651000000000	0.00000000000000
Cl	0.00000000000000	-2.82651000000000	-0.00000000000000
Cl	0.00000000000000	0.00000000000000	-2.82651000000000
Cl	0.00000000000000	-0.00000000000000	2.82651000000000
Cl	-2.82651000000000	0.00000000000000	0.00000000000000
Cl	-5.65302000000000	2.82651000000000	0.00000000000000
Cl	-5.65302000000000	-2.82651000000000	-0.00000000000000
Cl	-5.65302000000000	0.00000000000000	-2.82651000000000
Cl	-5.65302000000000	0.00000000000000	2.82651000000000
Cl	-8.47953000000000	0.00000000000000	0.00000000000000
Gd	0.00000000000000	0.00000000000000	0.00000000000000
Gd	-5.65302000000000	0.00000000000000	0.00000000000000

B. Molecular Orbitals

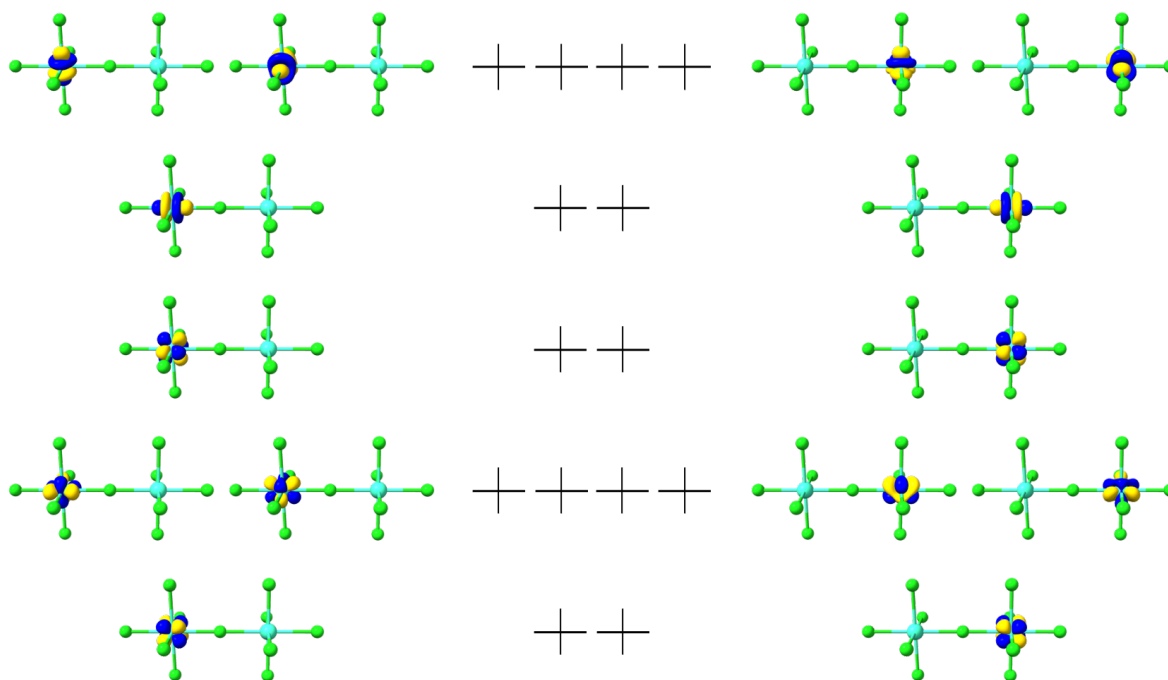


Figure S2. CSF-ROHF molecular orbitals for the CSF $[+++++-----]$ of $[\text{Gd}_2\text{Cl}_{11}]^{5-}$.

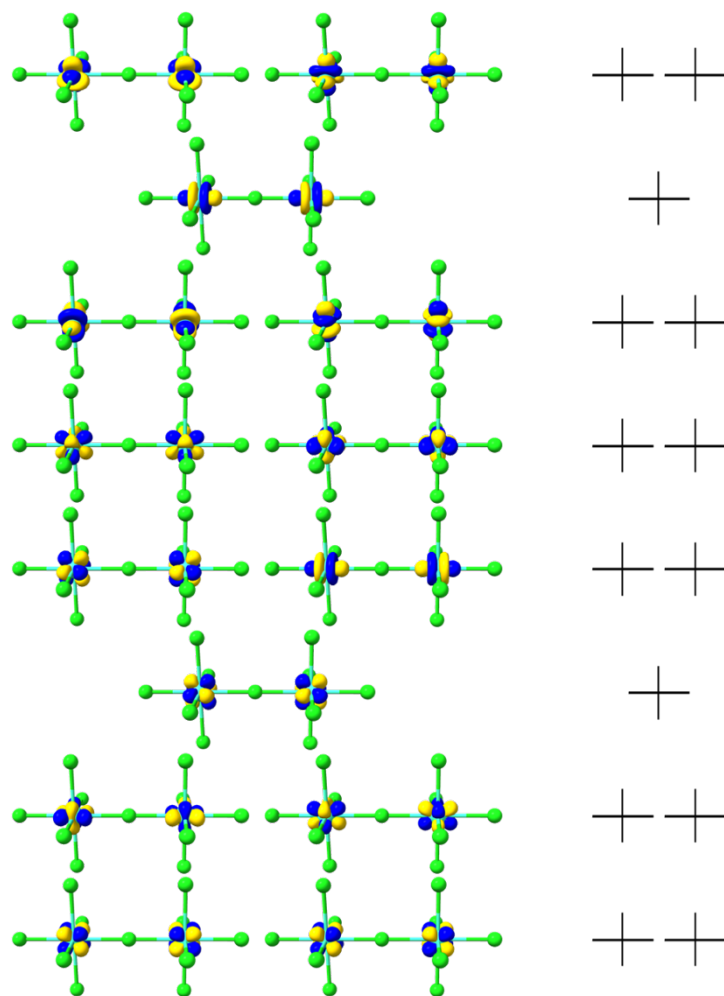


Figure S3. HS-ROHF molecular orbitals for $[\text{Gd}_2\text{Cl}_{11}]^{5-}$.

5. $[\text{Fe}_4\text{S}_4(\text{SCH}_3)_4]^{2-}$

A. Geometry

S	0.04000000000000	-1.78000000000000	-1.29000000000000
S	-0.04000000000000	1.78000000000000	-1.29000000000000
S	1.78000000000000	-0.04000000000000	1.29000000000000
S	-1.78000000000000	0.04000000000000	1.29000000000000
Fe	0.05000000000000	-1.37000000000000	1.01000000000000
Fe	-1.38000000000000	0.05000000000000	-1.00000000000000
Fe	-0.05000000000000	1.38000000000000	1.00000000000000
Fe	1.37000000000000	-0.05000000000000	-1.01000000000000
S	0.24000000000000	3.30000000000000	2.14000000000000
S	-0.24000000000000	-3.29000000000000	2.14000000000000
S	-3.29000000000000	-0.24000000000000	-2.14000000000000
S	3.29000000000000	0.24000000000000	-2.14000000000000
C	-3.80000000000000	-1.84000000000000	-1.38000000000000
H	-3.91000000000000	-1.71000000000000	-0.29000000000000
H	-4.76000000000000	-2.17000000000000	-1.81000000000000
H	-3.03000000000000	-2.60000000000000	-1.56000000000000
C	3.80000000000000	1.83000000000000	-1.38000000000000
H	3.91000000000000	1.71000000000000	-0.29000000000000
H	4.76000000000000	2.16000000000000	-1.81000000000000
H	3.03000000000000	2.59000000000000	-1.55000000000000
C	-1.83000000000000	-3.80000000000000	1.38000000000000
H	-2.16000000000000	-4.76000000000000	1.81000000000000
H	-2.59000000000000	-3.03000000000000	1.55000000000000
H	-1.70000000000000	-3.91000000000000	0.29000000000000
C	1.84000000000000	3.80000000000000	1.38000000000000
H	2.17000000000000	4.76000000000000	1.81000000000000
H	2.60000000000000	3.03000000000000	1.56000000000000
H	1.71000000000000	3.91000000000000	0.29000000000000

6. $[\text{Cu}_3(\text{OH})_3(\text{en})_3]^{3+}$

A. Geometry

Cu	0.07390700000000	1.73092000000000	0.01728100000000
Cu	1.81809500000000	-1.29635400000000	-0.06114800000000
Cu	-1.76965100000000	-1.21814100000000	0.07267000000000
O	-1.11343200000000	0.44627400000000	0.92915300000000
O	1.23194000000000	0.41405300000000	-0.88164600000000
O	0.00802500000000	-2.01785300000000	-0.04229800000000
H	-0.67662500000000	0.15321200000000	1.75194100000000
H	0.84086100000000	0.17106800000000	-1.74256200000000
H	-0.01157100000000	-2.97021000000000	0.15205400000000
N	-0.62089900000000	3.27656000000000	1.18293300000000
N	0.82029800000000	3.26233500000000	-1.13975700000000
C	-0.52146500000000	4.56387700000000	0.42541700000000
H	-1.58160500000000	3.09354300000000	1.48805800000000
C	0.77778000000000	4.54127000000000	-0.36247200000000
H	-0.56199500000000	5.43010500000000	1.10083200000000
H	-1.38740900000000	4.62578800000000	-0.24858200000000
H	1.77207700000000	3.04496800000000	-1.45056000000000
H	1.64541000000000	4.55438200000000	0.31203600000000
H	0.85628700000000	5.41479800000000	-1.02501300000000
H	0.25669200000000	3.35170300000000	-1.99421900000000
H	-0.05715100000000	3.32866500000000	2.04053600000000
N	3.76166100000000	-0.70464200000000	-0.29823400000000
N	2.69106900000000	-2.94869100000000	0.83010000000000
C	4.12438700000000	-2.63407000000000	1.13987200000000
H	2.20605000000000	-3.26122700000000	1.67785100000000
C	4.68937700000000	-1.84646900000000	-0.02897100000000
H	4.70222700000000	-3.55162700000000	1.32005400000000
H	4.14384100000000	-2.03907700000000	2.06385900000000
H	4.73442000000000	-2.46528500000000	-0.93626000000000
H	5.70837200000000	-1.49381700000000	0.18460900000000
H	3.89700700000000	-0.32506600000000	-1.24067700000000
H	3.94736000000000	0.07036700000000	0.34860100000000
H	2.64871500000000	-3.73410900000000	0.16832600000000
N	-2.72036100000000	-2.88368800000000	-0.70205800000000
N	-3.66319300000000	-0.44825300000000	0.09463100000000
C	-4.66373900000000	-1.54643800000000	-0.08398300000000
H	-3.81394600000000	0.06029000000000	0.97155200000000
C	-4.10940100000000	-2.50669200000000	-1.12204100000000
H	-5.64255200000000	-1.15021300000000	-0.38851000000000
H	-4.79163500000000	-2.04603500000000	0.88649400000000
H	-4.04250600000000	-2.02529900000000	-2.10774600000000
H	-4.74848100000000	-3.39476100000000	-1.22706700000000
H	-2.20327300000000	-3.28730700000000	-1.49016700000000
H	-2.76412000000000	-3.61553600000000	0.01812800000000
H	-3.75470400000000	0.24348600000000	-0.65837700000000

7. [Co(¹L_N)₂]

A. Geometry

Co	0.19114500000000	-0.17442700000000	-0.06452000000000
N	1.55368800000000	1.05392800000000	-0.06859800000000
N	1.55831300000000	-1.39562900000000	-0.13419400000000
N	-1.17597600000000	1.04675200000000	0.00680900000000
N	-1.17128200000000	-1.40292200000000	-0.05634000000000
C	2.82159500000000	-0.88598400000000	-0.15190100000000
H	1.49470000000000	-2.41478500000000	-0.15872200000000
C	2.81865900000000	0.55037000000000	-0.11335200000000
C	4.03879100000000	1.25450100000000	-0.12470900000000
C	4.04451700000000	-1.58355000000000	-0.20029800000000
C	5.23765700000000	-0.86651400000000	-0.21031000000000
C	5.23482300000000	0.54392300000000	-0.17277100000000
C	-2.43909900000000	0.53691400000000	0.03167800000000
H	-1.11233700000000	2.06589900000000	0.03213300000000
C	-2.43609700000000	-0.89954800000000	-0.00493100000000
C	-3.65606000000000	-1.60389300000000	0.01389000000000
C	-4.85196200000000	-0.89344700000000	0.06773700000000
C	-4.85485600000000	0.51707400000000	0.10352800000000
C	-3.66189700000000	1.23433000000000	0.08609200000000
H	-5.80501200000000	1.05123300000000	0.14563700000000
H	-3.66543000000000	2.32626900000000	0.11374600000000
H	-3.65494800000000	-2.69584600000000	-0.01371600000000
H	-5.79991900000000	-1.43294400000000	0.08247400000000
H	6.18291400000000	1.08325500000000	-0.18162400000000
H	4.03773600000000	2.34638000000000	-0.09539200000000
H	4.04801700000000	-2.67541700000000	-0.22961200000000
H	6.18790900000000	-1.40080600000000	-0.24754300000000
H	-1.10390200000000	-2.42178200000000	-0.08253700000000
H	1.48644500000000	2.07268600000000	-0.03874500000000