

The optimised coordinates of the ferromagnetic state ($\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow$) for the calculation of coupling constants are given below:

Mn	-0.51434000	-0.71891200	-1.13915800
Mn	-2.45719700	-0.61492700	1.66364300
Mn	-3.78636200	-1.87353300	-0.87808000
Mn	-5.34608400	0.64769300	0.47854100
Mn	0.51414300	0.71919300	1.13933200
Mn	2.45696500	0.61503500	-1.66364200
Mn	3.78639300	1.87334600	0.87806900
Mn	5.34579600	-0.64793400	-0.47886400
K	2.46232900	-2.34369200	0.51406100
K	-2.46261600	2.34396600	-0.51400300
O	3.78534300	0.34952400	-0.32070400
O	5.20413800	-1.20520000	1.40053400
O	4.74752100	-2.99402600	-0.79507800
O	6.72067700	-2.01872400	-0.68408500
O	0.28630900	2.76217200	0.14987300
O	2.35415000	2.64484900	-0.70389100
O	6.72038400	0.94197400	-0.22453300
O	5.33685800	2.69783300	0.02581000
O	5.46111900	-0.40375500	-2.42262700
O	3.85551000	1.08526500	-2.96649500
O	-1.14128900	0.08331200	0.48650500
O	0.83351500	-1.16193200	2.33615400
O	-2.44796700	1.39192000	2.57104400
O	-0.21423900	1.57619700	2.73789100
O	-1.27588700	-1.26844900	3.09215100
O	2.26313200	1.17169900	1.77450700
O	5.08462100	0.84511100	2.30933200
O	-3.72130700	-3.47366300	-1.95049500
O	-2.64249200	-2.73412000	-3.78355800
O	-3.78552000	-0.34961700	0.32061200
O	-5.20432500	1.20478100	-1.40090600
O	-4.74820900	2.99385400	0.79456800
O	-6.72121600	2.01827900	0.68344700
O	-0.28631600	-2.76190400	-0.14975400
O	-2.35413400	-2.64474300	0.70406500
O	-6.72045000	-0.94242400	0.22438700
O	-5.33676300	-2.69816500	-0.02588800
O	-5.46145800	0.40383300	2.42236800
O	-3.85578000	-1.08502100	2.96647900
O	1.14107800	-0.08302200	-0.48639000
O	-0.83381700	1.16215400	-2.33603300
O	2.44758400	-1.39159900	-2.57127900
O	0.21385800	-1.57598800	-2.73775500
O	1.27558900	1.26880700	-3.09199800
O	-2.26322400	-1.17167800	-1.77447100
O	-5.08462700	-0.84560800	-2.30950000
O	3.72181200	3.47328800	1.95073900
O	2.64384700	2.73317200	3.78406500

N	2.54171600	-4.77454700	2.13767000
N	-2.54147000	4.77503000	-2.13728700
C	5.24109700	-0.38495500	2.39070800
C	5.53148600	-1.01122200	3.73052000
C	5.99249600	-3.06947200	-0.82971600
C	6.71076600	-4.36956300	-1.05522300
C	1.29323800	3.28419900	-0.38052600
C	1.30885500	4.76751200	-0.64820800
C	6.47416300	2.16900100	-0.19684200
C	7.60296000	3.14110200	-0.42696400
C	4.91545200	0.43902800	-3.18954900
C	-1.40875000	1.88237700	3.06694200
C	-1.53082200	2.94724700	4.12661800
C	-0.02800600	-1.51277700	3.16885500
C	0.42065500	-2.26446100	4.39878100
C	5.58278800	0.66739000	-4.51913300
C	2.66254400	-5.78081200	2.69834500
C	2.81379200	-7.04316600	3.40096000
C	-3.29305600	-3.58685700	-3.17068200
C	-3.66826000	-4.89358400	-3.82686500
C	-5.24114600	0.38444700	-2.39100800
C	-5.53144100	1.01056900	-3.73090700
C	-5.99320000	3.06915100	0.82900100
C	-6.71167900	4.36921200	1.05400700
C	-1.29317900	-3.28401900	0.38067700
C	-1.30867200	-4.76732800	0.64836000
C	-6.47411500	-2.16942800	0.19675700
C	-7.60283500	-3.14162300	0.42685100
C	-4.91574000	-0.43877000	3.18944300
C	1.40827500	-1.88188500	-3.06723200
C	1.53076300	-2.94648900	-4.12715300
C	0.02770700	1.51313200	-3.16867700
C	-0.42094700	2.26496500	-4.39851300
C	-5.58294000	-0.66688700	4.51913500
C	-2.66139900	5.78167100	-2.69748000
C	-2.81153400	7.04450300	-3.39947300
C	3.29422700	3.58605200	3.17121000
C	3.67004500	4.89242600	3.82774500
H	3.57783000	-6.94985500	4.17678300
H	3.11404000	-7.82622600	2.70021800
H	1.86704200	-7.32782000	3.86684600
H	-3.57306500	6.95121500	-4.17776000
H	-3.11463900	7.82669800	-2.69899500
H	-1.86357700	7.33036400	-3.86215400
H	2.24468600	1.64690800	2.66108000
H	-2.24439400	-1.64721900	-2.66087000
H	-4.75336500	-4.92222100	-3.96433200
H	-3.40257200	-5.73063100	-3.17601300
H	-3.17233100	-4.98924400	-4.79284400
H	-7.86303000	-3.60167200	-0.53172700
H	-7.27531400	-3.94221300	1.09369400

H	-8.47602800	-2.63047800	0.83188300
H	-5.29081900	-1.63212600	4.93300200
H	-6.66624000	-0.58908700	4.41785100
H	-5.24705700	0.12037100	5.20224200
H	-7.25956800	4.31630500	1.99929200
H	-7.44712500	4.52492900	0.26053000
H	-6.00384800	5.19759200	1.08519000
H	-2.49180400	2.87300000	4.63650400
H	-1.47074200	3.92484000	3.63598500
H	-0.69829400	2.87993000	4.82892100
H	3.17464600	4.98777600	4.79402700
H	3.40419000	5.72980500	3.17738800
H	4.75522900	4.92077900	3.96465000
H	2.03741500	5.22146100	0.03163700
H	1.65793900	4.95512700	-1.66659900
H	0.32640600	5.21270400	-0.48626200
H	7.27549400	3.94172100	-1.09379900
H	7.86321200	3.60112600	0.53160900
H	8.47610300	2.62988400	-0.83201700
H	5.28969300	1.63210600	-4.93351600
H	5.24817300	-0.12061800	-5.20199400
H	6.66615000	0.59091100	-4.41742300
H	6.61079300	-1.17956900	3.80703400
H	5.03883600	-1.98242500	3.81282000
H	5.21530100	-0.34626200	4.53422000
H	7.25720200	-4.31695400	-2.00137300
H	6.00295600	-5.19801000	-1.08511800
H	7.44742100	-4.52493500	-0.26281200
H	2.48403600	-2.85958700	-4.64949800
H	1.49254700	-3.92398500	-3.63407100
H	0.68831200	-2.89226500	-4.81854200
H	-0.91047800	1.55352600	-5.07165700
H	0.42335200	2.72381900	-4.91325700
H	-1.16144800	3.01797400	-4.11813600
H	-5.21503800	0.34559800	-4.53451200
H	-5.03893900	1.98184700	-3.81321500
H	-6.61076500	1.17872800	-3.80759000
H	-0.42366300	-2.72304900	4.91372800
H	1.16095700	-3.01767800	4.11843300
H	0.91045000	-1.55300200	5.07171100
H	-0.32620800	-5.21245400	0.48632600
H	-1.65765200	-4.95497100	1.66678200
H	-2.03726000	-5.22131900	-0.03142400

The optimised coordinates of the non-ferromagnetic state ($\uparrow\uparrow\downarrow\uparrow\uparrow\uparrow\uparrow$) for the calculation of coupling constants are given below:

Mn	0.51271300	0.72482800	-1.13686300
Mn	2.45865600	0.61732300	1.66159400
Mn	3.78639100	1.87386000	-0.87589300
Mn	5.34230100	-0.64918000	0.47603900
Mn	-0.51273500	-0.71841500	1.13942800
Mn	-2.45410200	-0.61692900	-1.66307000
Mn	-3.78609500	-1.87313500	0.87821000
Mn	-5.34458200	0.64620500	-0.48332300
K	-2.46442500	2.34253200	0.51950500
K	2.45617500	-2.34991700	-0.50644600
O	-3.78433100	-0.35079300	-0.32205000
O	-5.20583500	1.20516000	1.39617200
O	-4.74535200	2.99150700	-0.79938000
O	-6.71899800	2.01690300	-0.69191800
O	-0.28561300	-2.76252600	0.14920900
O	-2.35377400	-2.64588200	-0.70326900
O	-6.71942200	-0.94313600	-0.22716000
O	-5.33611500	-2.69871400	0.02602600
O	-5.45820700	0.39808200	-2.42676200
O	-3.85050200	-1.09011600	-2.96696800
O	1.14207600	-0.08175000	0.48467800
O	-0.83130200	1.16053700	2.33896200
O	2.44878200	-1.39548400	2.56580200
O	0.21527000	-1.57647100	2.73708500
O	1.28017800	1.26710600	3.08975800
O	-2.26229000	-1.17087600	1.77372800
O	-5.08524700	-0.84394100	2.30761300
O	3.73683100	3.47608700	-1.94696000
O	2.65259100	2.74311800	-3.78009500
O	3.78989200	0.35908500	0.32755300
O	5.19668900	-1.20470600	-1.39865400
O	4.74296100	-2.99835600	0.79413800
O	6.71584600	-2.02260200	0.67844100
O	0.27939200	2.76213300	-0.14262700
O	2.34937500	2.65647900	0.70788000
O	6.72049300	0.94046000	0.21642200
O	5.33572800	2.69633900	-0.02965400
O	5.46594600	-0.40559500	2.41806000
O	3.85660900	1.07740800	2.97046100
O	-1.14089800	0.08518600	-0.48490000
O	0.84107000	-1.15530500	-2.33572000
O	-2.45017500	1.38861300	-2.57215400
O	-0.21677200	1.57724200	-2.73622500
O	-1.26918600	-1.27018700	-3.08872800
O	2.25700400	1.19863700	-1.76562800
O	5.07513900	0.84228300	-2.31488700
O	-3.72208600	-3.47161300	1.95280100
O	-2.64714600	-2.72778000	3.78637700

N	-2.55102200	4.76925800	2.14837400
N	2.54336600	-4.77330000	-2.14049300
C	-5.24385500	0.38598700	2.38715100
C	-5.53839200	1.01312900	3.72566000
C	-5.99023200	3.06742600	-0.83643200
C	-6.70761900	4.36772100	-1.06346600
C	-1.29330100	-3.28534900	-0.37902600
C	-1.31043900	-4.76934800	-0.64258000
C	-6.47328900	-2.17014800	-0.19788000
C	-7.60201800	-3.14246300	-0.42738200
C	-4.91086100	-0.44515800	-3.19195400
C	1.41028000	-1.88390500	3.06444400
C	1.53105000	-2.94641000	4.12662900
C	0.03240300	1.51291500	3.16832100
C	-0.41193900	2.26807600	4.39761100
C	-5.57620300	-0.67593200	-4.52212400
C	-2.67276400	5.77434200	2.71096000
C	-2.82516400	7.03522800	3.41596300
C	3.30916000	3.59125600	-3.16712500
C	3.69432000	4.89485100	-3.82394500
C	5.22351400	-0.38849000	-2.39309600
C	5.49117800	-1.02299700	-3.73386000
C	5.98799300	-3.07301400	0.82670800
C	6.70705900	-4.37262500	1.05337800
C	1.28972300	3.29158800	0.37510300
C	1.30914300	4.78024700	0.61283700
C	6.47228100	2.16653700	0.19908800
C	7.59564500	3.14002100	0.44940900
C	4.91792800	0.43220800	3.18916500
C	-1.41169700	1.88223800	-3.06579000
C	-1.53275000	2.94768200	-4.12485800
C	-0.02034700	-1.50941100	-3.16716300
C	0.42939100	-2.25945300	-4.39777200
C	5.58541600	0.65477700	4.51971500
C	2.67208000	-5.77793000	-2.70235000
C	2.83331500	-7.03825000	-3.40638400
C	-3.29667500	-3.58181700	3.17433900
C	-3.67408700	-4.88663800	3.83303900
H	-3.60497200	6.94631600	4.17645800
H	-3.10402700	7.82411800	2.71292600
H	-1.88485100	7.30855100	3.90126400
H	3.61473000	-6.94536800	-4.16475400
H	3.11459900	-7.82528200	-2.70223000
H	1.89586900	-7.31694400	-3.89417100
H	-2.24482600	-1.64400000	2.66132800
H	2.24400800	1.66477500	-2.65712600
H	4.77902800	4.91233300	-3.96642100
H	3.44025700	5.73413700	-3.17140000
H	3.19519500	4.99594100	-4.78772200
H	7.86222600	3.61208500	-0.50152200
H	7.25994200	3.93173400	1.12277300

H	8.46717100	2.62712100	0.85582700
H	5.29167000	1.61737500	4.93857000
H	6.66881900	0.57949300	4.41761600
H	5.25128100	-0.13653500	5.19898800
H	7.25122800	-4.31963400	2.00083100
H	7.44571900	-4.52722900	0.26271300
H	5.99999800	-5.20176600	1.08181200
H	2.51071000	-2.90435900	4.60323000
H	1.41381500	-3.92422700	3.64713400
H	0.72642000	-2.84281300	4.85683400
H	-3.18020400	-4.98017200	4.80027400
H	-3.40766700	-5.72552600	3.18485900
H	-4.75949200	-4.91417900	3.96836100
H	-2.03904800	-5.22068500	0.03895100
H	-1.66026000	-4.95946500	-1.66024400
H	-0.32835300	-5.21511100	-0.47997500
H	-7.27420800	-3.94402100	-1.09291700
H	-7.86292200	-3.60115800	0.53165100
H	-8.47485900	-2.63171900	-0.83368100
H	-5.28637900	-1.64368500	-4.93176400
H	-5.23592800	0.10743400	-5.20754000
H	-6.65942800	-0.59415400	-4.42347400
H	-6.61871400	1.17535200	3.80121800
H	-5.05131800	1.98723200	3.80662100
H	-5.21918700	0.35125100	4.53072900
H	-7.25371500	4.31463500	-2.00977900
H	-5.99930400	5.19572300	-1.09366100
H	-7.44452300	4.52418500	-0.27148800
H	-2.51616300	2.91408200	-4.59422700
H	-1.40285800	3.92360000	-3.64487000
H	-0.73459600	2.83870900	-4.86146900
H	0.92082800	-1.54746700	-5.06892100
H	-0.41446200	-2.71690800	-4.91446900
H	1.16871000	-3.01367500	-4.11741200
H	5.15332200	-0.36607400	-4.53540700
H	5.00547600	-1.99886800	-3.79941800
H	6.57024000	-1.18179500	-3.83161800
H	0.43392500	2.73024000	4.90678200
H	-1.15524400	3.01859700	4.11809500
H	-0.89673200	1.55791800	5.07553200
H	0.32713100	5.22422400	0.44478800
H	1.66170500	4.98802400	1.62609300
H	2.03648700	5.21878300	-0.07832200

The optimised coordinates of the non-ferromagnetic state ($\uparrow\downarrow\uparrow\uparrow\uparrow\uparrow\uparrow$) for the calculation of coupling constants are given below:

Mn	-0.51478600	-0.72103600	-1.13677100
Mn	-2.46063700	-0.60873500	1.65310800
Mn	-3.78069700	-1.87910600	-0.87302900
Mn	-5.35223000	0.64135900	0.47032800
Mn	0.51367300	0.71911100	1.13696900
Mn	2.45486400	0.62184400	-1.66567100
Mn	3.78724700	1.86851600	0.88049300
Mn	5.34422000	-0.64717500	-0.49068200
K	2.46417000	-2.33830100	0.51623100
K	-2.46227400	2.34358800	-0.50116200
O	3.78451600	0.35032300	-0.32593400
O	5.20801300	-1.20939600	1.38810100
O	4.74169900	-2.99050400	-0.80918100
O	6.71692800	-2.01895800	-0.70319800
O	0.28534700	2.76312600	0.15597000
O	2.35325900	2.64736500	-0.69746100
O	6.71834300	0.94270400	-0.23340500
O	5.33581700	2.69762900	0.02915100
O	5.45638600	-0.39634000	-2.43379300
O	3.85103600	1.09595600	-2.96937000
O	-1.13692400	0.06832800	0.49329000
O	0.82316400	-1.16830700	2.33563500
O	-2.44188200	1.41545300	2.55015500
O	-0.20692200	1.57088300	2.73690400
O	-1.28967100	-1.24761900	3.08868200
O	2.26680400	1.15967200	1.77528700
O	5.09043800	0.83735700	2.30505800
O	-3.70868700	-3.48008900	-1.94162100
O	-2.63725100	-2.73794700	-3.77800400
O	-3.79178300	-0.35453700	0.32763300
O	-5.21105900	1.18999600	-1.40694800
O	-4.76118200	2.99773700	0.77894500
O	-6.72767200	2.00795100	0.67085800
O	-0.28114700	-2.76191300	-0.15988300
O	-2.34458100	-2.65701100	0.70749900
O	-6.72110500	-0.95733000	0.21715300
O	-5.32876100	-2.70791400	-0.02435700
O	-5.47268600	0.40473200	2.41231900
O	-3.85388300	-1.06597200	2.96872400
O	1.13946100	-0.07914300	-0.48799000
O	-0.83781500	1.16579400	-2.33049000
O	2.44534200	-1.38279900	-2.57655100
O	0.21161400	-1.56996600	-2.73920100
O	1.27060800	1.27890000	-3.08878800
O	-2.26414700	-1.17015100	-1.77285300
O	-5.08348700	-0.86195500	-2.31067400
O	3.72190700	3.46334600	1.96028000
O	2.65133400	2.71164100	3.79324200

N	2.55668000	-4.75880500	2.15395700
N	-2.53968300	4.77858000	-2.11964800
C	5.24945200	-0.39270500	2.38101500
C	5.54811000	-1.02360900	3.71683800
C	5.98641400	-3.06823100	-0.84831300
C	6.70144700	-4.36909800	-1.07931200
C	1.29253300	3.28626700	-0.37323000
C	1.30803400	4.77004400	-0.63782400
C	6.47234600	2.16965200	-0.19931300
C	7.60065000	3.14262100	-0.42818700
C	4.91003200	0.44954800	-3.19672300
C	-1.40161800	1.88721200	3.05995300
C	-1.51747500	2.94069800	4.13179400
C	-0.04311600	-1.50303600	3.16882000
C	0.39376800	-2.24629900	4.40808200
C	5.57475600	0.68200600	-4.52689100
C	2.68000200	-5.75717400	2.72804300
C	2.83434900	-7.00970100	3.44738400
C	-3.28160900	-3.59328900	-3.16233600
C	-3.64999500	-4.90379500	-3.81465800
C	-5.24303200	0.36706200	-2.39558400
C	-5.53077100	0.99075400	-3.73709300
C	-6.00612500	3.06428500	0.81323100
C	-6.73458600	4.35962300	1.03362100
C	-1.27962000	-3.28775400	0.38427200
C	-1.27541200	-4.76826200	0.66915400
C	-6.46884400	-2.18289900	0.19561500
C	-7.59229200	-3.16014100	0.43040600
C	-4.91839600	-0.42623700	3.18656100
C	1.40597100	-1.87385600	-3.07123900
C	1.52714600	-2.93635100	-4.13332100
C	0.02175000	1.52060400	-3.16313800
C	-0.42951500	2.27471300	-4.39070000
C	-5.58293600	-0.64601200	4.51899500
C	-2.66540200	5.78686400	-2.67559800
C	-2.82289500	7.05177800	-3.37221700
C	3.29760100	3.56913500	3.18260500
C	3.67196900	4.87344700	3.84410400
H	3.58710500	-6.89978000	4.23201100
H	3.15149700	-7.79784000	2.75990800
H	1.88436400	-7.29832700	3.90415400
H	-3.60029300	6.96389900	-4.13529700
H	-3.10788100	7.83421400	-2.66443800
H	-1.88289200	7.33362000	-3.85323100
H	2.24979000	1.62949300	2.66441800
H	-2.24402300	-1.64816700	-2.65816100
H	-4.73519900	-4.93969500	-3.94954600
H	-3.37738200	-5.73759500	-3.16251700
H	-3.15558700	-4.99838100	-4.78151800
H	-7.84791000	-3.62875100	-0.52523600
H	-7.26134800	-3.95390300	1.10371500

H	-8.46913300	-2.65116500	0.83024400
H	-5.27294300	-1.59875000	4.94845900
H	-6.66747600	-0.59114000	4.41517800
H	-5.26456400	0.15875300	5.18995600
H	-7.28854000	4.30332400	1.97512700
H	-7.46569900	4.51045100	0.23515800
H	-6.03232300	5.19254300	1.06894900
H	-2.48031300	2.86783500	4.63841700
H	-1.44916700	3.92340000	3.65255100
H	-0.68726600	2.85913300	4.83527800
H	3.18016300	4.96245700	4.81282400
H	3.40074400	5.71316900	3.19899200
H	4.75760300	4.90467500	3.97670900
H	2.03528900	5.22285400	0.04418100
H	1.65873500	4.95983900	-1.65523800
H	0.32515300	5.21451900	-0.47659700
H	7.27147300	3.94621600	-1.09058700
H	7.86355900	3.59838700	0.53169300
H	8.47262900	2.63311500	-0.83787400
H	5.28512300	1.65044700	-4.93502000
H	5.23398300	-0.10031600	-5.21324700
H	6.65799900	0.59966900	-4.42883700
H	6.62746100	-1.19522800	3.78484500
H	5.05348300	-1.99379900	3.79962400
H	5.23940100	-0.36043400	4.52489100
H	7.24018500	-4.31706700	-2.02992300
H	5.99244500	-5.19670700	-1.10375700
H	7.44431900	-4.52535300	-0.29293600
H	2.48598500	-2.85831000	-4.64666500
H	1.47205000	-3.91489100	-3.64400000
H	0.69171600	-2.87040100	-4.83228000
H	-0.92024600	1.56451200	-5.06426800
H	0.41352600	2.73496500	-4.90625900
H	-1.16963000	3.02695500	-4.10722600
H	-5.21918900	0.32132200	-4.53882200
H	-5.03154200	1.95833400	-3.82271200
H	-6.60890600	1.16644600	-3.81319600
H	-0.45484900	-2.70610400	4.91486600
H	1.14179800	-2.99671500	4.14148300
H	0.87028400	-1.52825100	5.08362700
H	-0.28756300	-5.20285300	0.51104000
H	-1.62086000	-4.94871400	1.69006100
H	-1.99857800	-5.23976600	-0.00445500

The optimised coordinates of the non-ferromagnetic state ($\downarrow\downarrow\uparrow\uparrow\downarrow\uparrow\uparrow$) for the calculation of coupling constants are given below:

Mn	0.50976800	0.72608800	-1.13533800
Mn	2.46102900	0.61144800	1.65394400
Mn	3.78309300	1.87808800	-0.87342300
Mn	5.34570100	-0.64888900	0.46845100
Mn	-0.51526100	-0.71604200	1.12586800
Mn	-2.46102200	-0.61510500	-1.65747300
Mn	-3.78419300	-1.87361200	0.87695400
Mn	-5.35153900	0.64181600	-0.47916500
K	-2.46754600	2.34444100	0.51093100
K	2.45132600	-2.35292000	-0.49079600
O	-3.79322400	-0.35385500	-0.33048500
O	-5.21465500	1.19534100	1.39773800
O	-4.75598900	2.99497700	-0.79150700
O	-6.72482900	2.00962900	-0.68827000
O	-0.28379800	-2.75749000	0.15846500
O	-2.34786700	-2.65580900	-0.70566100
O	-6.72351700	-0.95285100	-0.21996700
O	-5.33339700	-2.70394400	0.03037400
O	-5.47026400	0.39383300	-2.42132500
O	-3.85184500	-1.08147900	-2.96683300
O	1.13302000	-0.06793300	0.48459100
O	-0.82405700	1.17353100	2.32719100
O	2.43423500	-1.41622000	2.53640500
O	0.20025600	-1.55802900	2.73631700
O	1.28667400	1.24392000	3.08709400
O	-2.26852600	-1.16205600	1.77327000
O	-5.08883100	-0.85296500	2.31047900
O	3.73229500	3.47821900	-1.94308000
O	2.65820900	2.74366700	-3.78160300
O	3.78847700	0.35453500	0.32787300
O	5.19618500	-1.20038200	-1.40656400
O	4.75665900	-3.00609000	0.78222300
O	6.72168400	-2.01458300	0.66464700
O	0.27690500	2.76382800	-0.14992200
O	2.34301300	2.65693300	0.71103100
O	6.71866400	0.94597500	0.21546000
O	5.33014300	2.70084100	-0.01677400
O	5.46944600	-0.41423300	2.41038900
O	3.85397000	1.05708700	2.97438500
O	-1.14102600	0.07667200	-0.48888200
O	0.82873100	-1.16051500	-2.32811400
O	-2.44989100	1.39999300	-2.56040000
O	-0.21649300	1.57543600	-2.73940500
O	-1.28178600	-1.26177400	-3.08541700
O	2.25711700	1.19434900	-1.76601600
O	5.07903900	0.85163100	-2.31112100
O	-3.70785300	-3.47829000	1.94023100
O	-2.60929400	-2.75775000	3.76922400

N	-2.55470700	4.76553100	2.14829100
N	2.53929100	-4.77147700	-2.13325800
C	-5.25113600	0.37605500	2.38932800
C	-5.54696300	1.00541900	3.72649200
C	-6.00074400	3.06420800	-0.83043500
C	-6.72542700	4.36058300	-1.05683800
C	-1.28521800	-3.28711100	-0.37686500
C	-1.28725500	-4.77091800	-0.64239600
C	-6.47269500	-2.17869700	-0.19234300
C	-7.59750400	-3.15551900	-0.42243800
C	-4.91599900	-0.44165700	-3.18979300
C	1.39316100	-1.86057700	3.07212200
C	1.52181300	-2.81102300	4.23499600
C	0.04037900	1.50633700	3.16202200
C	-0.39608000	2.25502400	4.39815900
C	-5.57691900	-0.66951400	-4.52256000
C	-2.67763800	5.76809100	2.71509900
C	-2.83162000	7.02591100	3.42523300
C	3.30887800	3.59330300	-3.16529000
C	3.69194800	4.89954500	-3.81811100
C	5.23025900	-0.37832600	-2.39604300
C	5.50870300	-1.00523600	-3.73794600
C	6.00163700	-3.07157300	0.81087500
C	6.73248800	-4.36590500	1.02932600
C	1.28399600	3.29177900	0.37577700
C	1.29974900	4.77947400	0.62011100
C	6.46911300	2.17222400	0.20028700
C	7.59473400	3.14578400	0.43984800
C	4.91800000	0.41511100	3.18820900
C	-1.41186000	1.88378700	-3.06463300
C	-1.53293100	2.94020700	-4.13289100
C	-0.03327200	-1.50798800	-3.16104000
C	0.41269500	-2.25828300	-4.39282900
C	5.58848000	0.63026000	4.51845700
C	2.67533100	-5.77231000	-2.70013400
C	2.84567600	-7.02802100	-3.41025800
C	-3.26331800	-3.60533100	3.15323900
C	-3.62369900	-4.92308700	3.79579900
H	-3.59747200	6.92718800	4.19859200
H	-3.13079000	7.81308400	2.72864900
H	-1.88624200	7.30844700	3.89517400
H	3.70103000	-6.96146000	-4.08722900
H	3.01957900	-7.83845300	-2.69797800
H	1.94847200	-7.25359100	-3.99211500
H	-2.23715700	-1.64741400	2.65324300
H	2.24413000	1.65957300	-2.65676400
H	4.77744300	4.92279900	-3.95355000
H	3.42935900	5.73676700	-3.16625600
H	3.19839100	4.99929300	-4.78488500
H	7.85211600	3.61760500	-0.51374100
H	7.26527800	3.93763600	1.11611800

H	8.47012300	2.63305000	0.83807500
H	5.24223100	1.55592200	4.97791800
H	6.67297900	0.62893000	4.39800500
H	5.32132700	-0.20838100	5.16982000
H	7.28567400	-4.31005000	1.97134600
H	7.46445700	-4.51409600	0.23119300
H	6.03179400	-5.20022500	1.06303600
H	1.77221100	-2.22712900	5.12715300
H	2.34417000	-3.50665300	4.05478000
H	0.58457800	-3.33943300	4.41058600
H	-3.11672700	-5.02857400	4.75502100
H	-3.36011100	-5.74977400	3.13099100
H	-4.70702900	-4.96027200	3.94461100
H	-2.01651700	-5.22944900	0.03354500
H	-1.62855800	-4.96272600	-1.66265100
H	-0.30251100	-5.20842300	-0.47371000
H	-7.26717500	-3.95394800	-1.09049500
H	-7.85488900	-3.61780300	0.53581400
H	-8.47314200	-2.64758400	-0.82623100
H	-5.28356000	-1.63539800	-4.93417800
H	-5.23604900	0.11635100	-5.20482800
H	-6.66064000	-0.59066400	-4.42726400
H	-6.62275900	1.19987500	3.78790800
H	-5.03281800	1.96481200	3.81728500
H	-5.25641900	0.33259000	4.53318900
H	-7.27179200	4.30478100	-2.00282600
H	-6.02160200	5.19238900	-1.08706000
H	-7.46273800	4.51285700	-0.26440500
H	-2.52506800	2.91991100	-4.58422300
H	-1.37437500	3.91863100	-3.66695300
H	-0.75082300	2.80779600	-4.88288800
H	0.89931600	-1.54549800	-5.06668400
H	-0.43244600	-2.71764200	-4.90573000
H	1.15491000	-3.01048800	-4.11494700
H	5.20518100	-0.33154800	-4.53916900
H	4.99608000	-1.96586900	-3.82317700
H	6.58421200	-1.19585500	-3.81500400
H	0.45340000	2.71117400	4.90680300
H	-1.13848700	3.00937800	4.12698800
H	-0.87953700	1.54152700	5.07360900
H	0.31684100	5.22191800	0.45323900
H	1.65131100	4.98392500	1.63437300
H	2.02631300	5.22272100	-0.06889000

The optimised coordinates of the non-ferromagnetic state ($\downarrow\downarrow\downarrow\uparrow\uparrow\downarrow\uparrow\uparrow$) for the calculation of coupling constants are given below:

Mn	-0.51575600	-0.71786800	-1.13581000
Mn	-2.46841400	-0.60449500	1.65646100
Mn	-3.77623800	-1.88504100	-0.87603600
Mn	-5.35266700	0.63781300	0.45161000
Mn	0.50961800	0.71985000	1.12692400
Mn	2.46054100	0.61157500	-1.65485800
Mn	3.77970400	1.87232200	0.88084600
Mn	5.34814600	-0.64594100	-0.46820600
K	2.45577700	-2.34947900	0.49662300
K	-2.45438600	2.35793300	-0.49083800
O	3.78980600	0.35121500	-0.32547600
O	5.20398500	-1.19866800	1.40771600
O	4.75738200	-2.99952600	-0.78529400
O	6.72434800	-2.01179800	-0.67039700
O	0.28356400	2.76212600	0.16016500
O	2.34702800	2.65438100	-0.70535500
O	6.72054900	0.94845400	-0.20918700
O	5.33078500	2.70056600	0.03565400
O	5.47112400	-0.40205500	-2.41040000
O	3.85297400	1.07004000	-2.96532400
O	-1.13884100	0.07250400	0.48479100
O	0.81425200	-1.17515400	2.32302300
O	-2.44014000	1.42748500	2.53105900
O	-0.20619600	1.56129200	2.73737600
O	-1.29281700	-1.23153100	3.09370700
O	2.26260600	1.16337700	1.77636100
O	5.08010500	0.85096700	2.31750400
O	-3.68993700	-3.50175000	-1.92479100
O	-2.59516600	-2.78757800	-3.75828100
O	-3.79248600	-0.36220300	0.32722300
O	-5.20632800	1.17192700	-1.42398400
O	-4.77190600	2.99953900	0.75355600
O	-6.73398300	2.00217600	0.63581700
O	-0.28587000	-2.76089600	-0.16151600
O	-2.34560000	-2.64260500	0.71241400
O	-6.72126700	-0.96472200	0.20355400
O	-5.32350100	-2.71191200	-0.02968600
O	-5.48483800	0.41820400	2.39360400
O	-3.86518100	-1.04159300	2.97634700
O	1.13550400	-0.07087500	-0.48790900
O	-0.82644100	1.17219500	-2.32527100
O	2.43895600	-1.40698800	-2.55148300
O	0.20564800	-1.55903400	-2.74719000
O	1.28342300	1.25840600	-3.08647900
O	-2.26614400	-1.17593700	-1.77853900
O	-5.07564500	-0.88145100	-2.32436500
O	3.70330900	3.47847500	1.94194100
O	2.60240900	2.76118800	3.77078700

N	2.54717100	-4.76460800	2.14374500
N	-2.53210000	4.78350300	-2.12390700
C	5.23754800	-0.37857300	2.39869000
C	5.52304300	-1.00787000	3.73809400
C	6.00240100	-3.06718600	-0.81707600
C	6.72990500	-4.36242300	-1.04114000
C	1.28554300	3.28825100	-0.37742600
C	1.29006800	4.77140000	-0.64695900
C	6.47032800	2.17444200	-0.18374700
C	7.59616500	3.15037400	-0.41261100
C	4.91871700	0.43099600	-3.18275300
C	-1.39899500	1.86711800	3.07066700
C	-1.52711700	2.81478300	4.23582800
C	-0.04743100	-1.49906500	3.16457700
C	0.39239200	-2.24203200	4.40295300
C	5.58751500	0.65672600	-4.51200800
C	2.68492600	-5.76300000	2.71449600
C	2.85758100	-7.01571900	3.42934900
C	-3.24348500	-3.63542000	-3.13592500
C	-3.59264700	-4.96072600	-3.76895800
C	-5.23010700	0.34764700	-2.41226600
C	-5.50037000	0.97281900	-3.75667700
C	-6.01730500	3.06146900	0.77826600
C	-6.75211200	4.35531200	0.98697900
C	-1.28367900	-3.28014800	0.38839200
C	-1.28623600	-4.75876800	0.68083800
C	-6.46445600	-2.18903500	0.19348600
C	-7.58130300	-3.16922400	0.44698700
C	-4.93252700	-0.40221300	3.18054900
C	1.39878600	-1.85781100	-3.08418200
C	1.53013000	-2.81174200	-4.24385800
C	0.03665800	1.51534600	-3.15874400
C	-0.40600200	2.27305500	-4.38718600
C	-5.60808100	-0.60835500	4.50966100
C	-2.65562700	5.79394400	-2.67642400
C	-2.81035200	7.06169600	-3.36849100
C	3.25761300	3.60749900	3.15430800
C	3.61832000	4.92582600	3.79550200
H	3.66262000	-6.91994600	4.16221700
H	3.11079000	-7.81382300	2.72699900
H	1.93336700	-7.28051600	3.94908100
H	-3.58004600	6.97515900	-4.13948900
H	-3.10459200	7.83978300	-2.65970000
H	-1.86661300	7.34880400	-3.83896100
H	2.23069400	1.64996900	2.65565400
H	-2.23387100	-1.66931500	-2.65536800
H	-4.67556400	-5.00796000	-3.91790500
H	-3.32249000	-5.78024400	-3.09793400
H	-3.08435400	-5.06918600	-4.72714400
H	-7.83818300	-3.65341700	-0.50048800
H	-7.24302500	-3.95116200	1.13047200

H	-8.45941700	-2.65961300	0.84322200
H	-5.24995800	-1.52109100	4.98548000
H	-6.69162600	-0.62712200	4.38163500
H	-5.36046500	0.24490100	5.14960000
H	-7.31312300	4.30145600	1.92443800
H	-7.47763300	4.49968700	0.18225300
H	-6.05323500	5.19102500	1.02357900
H	-1.76981400	2.22747100	5.12791000
H	-2.35349400	3.50697600	4.06127500
H	-0.59135800	3.34684300	4.40846800
H	3.11034400	5.03299200	4.75400500
H	3.35616300	5.75184400	3.12929700
H	4.70150900	4.96233300	3.94551300
H	2.01973700	5.23052000	0.02814900
H	1.63218700	4.95995700	-1.66755000
H	0.30593500	5.21086900	-0.47979800
H	7.26784000	3.94801800	-1.08259800
H	7.85151200	3.61391500	0.54557800
H	8.47252200	2.64141800	-0.81355200
H	5.25049400	1.59273300	-4.95726500
H	5.30682100	-0.16888500	-5.17428800
H	6.67225700	0.64060200	-4.39573900
H	6.59644000	-1.21389700	3.80324800
H	4.99824400	-1.96149200	3.82913300
H	5.23678800	-0.33044300	4.54244500
H	7.27092400	-4.30890600	-1.99039400
H	6.02841200	-5.19643400	-1.06475900
H	7.47190300	-4.50927600	-0.25215400
H	1.76297800	-2.22842100	-5.14115200
H	2.36369500	-3.49511200	-4.06862700
H	0.59847500	-3.35352900	-4.40830900
H	-0.89980700	1.56630900	-5.06219400
H	0.44154400	2.72759500	-4.90043600
H	-1.14166900	3.03018700	-4.10528900
H	-5.20248300	0.29359000	-4.55525600
H	-4.97688900	1.92743900	-3.84414000
H	-6.57344700	1.17560700	-3.83583600
H	-0.45590600	-2.69409500	4.91723500
H	1.13280200	-2.99885400	4.13324400
H	0.87918800	-1.52560900	5.07291600
H	-0.30341400	-5.20077300	0.51284500
H	-1.62012800	-4.93140100	1.70698800
H	-2.02140800	-5.22808900	0.01886100

The optimised coordinates of the non-ferromagnetic state ($\downarrow\downarrow\uparrow\uparrow\uparrow\uparrow\downarrow$) for the calculation of coupling constants are given below:

Mn	0.50808400	0.72728500	-1.12909600
Mn	2.46289900	0.61220000	1.65289000
Mn	3.78565900	1.87094000	-0.87895100
Mn	5.34483900	-0.65507000	0.46979200
Mn	-0.51670300	-0.71568600	1.12813300
Mn	-2.46745600	-0.60987300	-1.65925100
Mn	-3.78201800	-1.87669900	0.87728300
Mn	-5.35157200	0.64201500	-0.46839100
K	-2.46189000	2.34928400	0.51146500
K	2.44943200	-2.35170600	-0.49607800
O	-3.79429800	-0.36010200	-0.33375200
O	-5.21273900	1.18259000	1.40697200
O	-4.75650500	2.99974100	-0.77102000
O	-6.72468200	2.01293800	-0.66579000
O	-0.28849000	-2.75978200	0.15746500
O	-2.35149000	-2.64399500	-0.70802400
O	-6.72371000	-0.95607600	-0.21235000
O	-5.33035100	-2.70512100	0.03358900
O	-5.48057000	0.41002400	-2.40932000
O	-3.86225500	-1.05703100	-2.97754400
O	1.13361800	-0.06673600	0.48457500
O	-0.82441200	1.17295400	2.32892500
O	2.43418100	-1.41322300	2.53866400
O	0.20031600	-1.55648800	2.73810400
O	1.28794800	1.24852800	3.08439300
O	-2.27149500	-1.16463700	1.77540800
O	-5.08415300	-0.86604400	2.31879500
O	3.73461600	3.46906300	-1.95163400
O	2.65683000	2.73319800	-3.78756400
O	3.78965000	0.35078500	0.32739600
O	5.19497500	-1.20962200	-1.40456400
O	4.74933200	-3.00971000	0.78619200
O	6.71724800	-2.02392700	0.66905800
O	0.28068200	2.76607600	-0.14758300
O	2.34897800	2.65640000	0.70732900
O	6.72015600	0.93685900	0.21192300
O	5.33500500	2.69369900	-0.02578800
O	5.46972400	-0.41569700	2.41121300
O	3.85584200	1.05843000	2.97257100
O	-1.14182800	0.07624900	-0.48637500
O	0.82134800	-1.16303200	-2.32740800
O	-2.44810600	1.41500200	-2.54486400
O	-0.21391100	1.57572900	-2.73198100
O	-1.28832700	-1.24312500	-3.08924600
O	2.25861600	1.18625100	-1.76709200
O	5.08043000	0.84015100	-2.31461300
O	-3.69810400	-3.48828500	1.93396700
O	-2.60500000	-2.76607600	3.76540700

N	-2.54142600	4.77100500	2.14868100
N	2.52904300	-4.76621400	-2.14464100
C	-5.24320900	0.36287700	2.39899500
C	-5.52748800	0.99385300	3.73786300
C	-6.00138100	3.06810900	-0.80580500
C	-6.72754600	4.36499600	-1.02529800
C	-1.29008600	-3.28155600	-0.38352400
C	-1.29738700	-4.76257800	-0.66315800
C	-6.46957600	-2.18095500	-0.19496500
C	-7.58818400	-3.15995600	-0.44533900
C	-4.92726500	-0.41623000	-3.18950300
C	1.39337100	-1.85922300	3.07339400
C	1.52236100	-2.81196200	4.23432400
C	0.04146200	1.50874800	3.16130000
C	-0.39404400	2.25929200	4.39667500
C	-5.59460500	-0.62774200	-4.52185800
C	-2.65639900	5.77621900	2.71245700
C	-2.80037500	7.03733200	3.41883600
C	3.30876300	3.58315900	-3.17313800
C	3.69074500	4.88899200	-3.82755700
C	5.23159400	-0.39001900	-2.39601700
C	5.51271600	-1.02061800	-3.73564500
C	5.99412300	-3.07875100	0.81586000
C	6.72105800	-4.37490900	1.03641400
C	1.29101200	3.29315700	0.37311700
C	1.31168200	4.78170000	0.61168400
C	6.47291900	2.16357700	0.19281400
C	7.60057300	3.13563100	0.42899800
C	4.91938200	0.41584200	3.18737700
C	-1.40883100	1.89029400	-3.05410000
C	-1.52754200	2.94543900	-4.12394100
C	-0.04058000	-1.49607500	-3.16549000
C	0.40225100	-2.23411000	-4.40575300
C	5.59030800	0.63327000	4.51702400
C	2.64763900	-5.76774500	-2.71419500
C	2.79607800	-7.02436000	-3.42763900
C	-3.25300900	-3.61640600	3.14628800
C	-3.60376900	-4.93863700	3.78501100
H	-3.55703900	6.94296800	4.20172600
H	-3.10690200	7.82182300	2.72242400
H	-1.84909800	7.32072200	3.87619300
H	3.57793200	-6.93365200	-4.18581600
H	3.06992900	-7.81930500	-2.72946500
H	1.85566000	-7.29022500	-3.91686800
H	-2.24022500	-1.65209200	2.65493200
H	2.24421700	1.64915600	-2.65850200
H	4.77606400	4.91246300	-3.96433500
H	3.42871800	5.72671400	-3.17610800
H	3.19596900	4.98783600	-4.79380500
H	7.85888900	3.60362700	-0.52622400
H	7.27279000	3.93049000	1.10254700

H	8.47493800	2.62248200	0.82894200
H	5.24690000	1.56157400	4.97329500
H	6.67481500	0.62801400	4.39689200
H	5.32012300	-0.20222200	5.17118600
H	7.27172200	-4.32032400	1.97999800
H	7.45484900	-4.52512900	0.24035500
H	6.01811600	-5.20740300	1.06839200
H	1.76704800	-2.22910200	5.12875600
H	2.34818900	-3.50370700	4.05521900
H	0.58664900	-3.34447600	4.40567000
H	-3.09731500	-5.04268600	4.74466600
H	-3.33254300	-5.76145000	3.11844900
H	-4.68697600	-4.98494400	3.93210300
H	-2.03094800	-5.22427600	0.00593400
H	-1.63601600	-4.94317500	-1.68637100
H	-0.31493100	-5.20547000	-0.49535900
H	-7.25029800	-3.94637700	-1.12385300
H	-7.84810800	-3.63838800	0.50423300
H	-8.46430200	-2.65054500	-0.84622000
H	-5.28426500	-1.57702400	-4.95864500
H	-5.27910100	0.18218300	-5.18794200
H	-6.67897300	-0.57517800	-4.41507600
H	-6.60219600	1.19166900	3.80691700
H	-5.00964000	1.95160800	3.82464700
H	-5.23314200	0.32032300	4.54257300
H	-7.27202900	4.31418800	-1.97267000
H	-6.02480400	5.19791400	-1.04947800
H	-7.46650600	4.51151200	-0.23336000
H	-2.50026100	2.88860300	-4.61323500
H	-1.43163700	3.92701600	-3.64725900
H	-0.71181100	2.84917900	-4.84252000
H	0.88552800	-1.51406000	-5.07431100
H	-0.44411400	-2.68906600	-4.92061400
H	1.14626500	-2.98809400	-4.13788600
H	5.21490700	-0.34744800	-4.53943000
H	4.99650100	-1.97936200	-3.82080500
H	6.58767800	-1.21599800	-3.80811800
H	0.45611900	2.71413800	4.90532500
H	-1.13459000	3.01510100	4.12437700
H	-0.87962200	1.54750300	5.07237900
H	0.32942600	5.22620200	0.44644100
H	1.66734200	4.98906000	1.62391700
H	2.03707500	5.22018400	-0.08158300

The optimised coordinates of the non-ferromagnetic state ($\downarrow\uparrow\downarrow\uparrow\uparrow\uparrow\uparrow$) for the calculation of coupling constants are given below:

Mn	-0.51221500	0.71787800	1.12589500
Mn	-2.46513100	0.61448200	-1.65803700
Mn	-3.77668500	1.87815800	0.88490100
Mn	-5.34784900	-0.64079700	-0.46205800
Mn	0.51047300	-0.71984400	-1.13569200
Mn	2.46287500	-0.61322200	1.65762900
Mn	3.77745500	-1.88554200	-0.88096100
Mn	5.34765600	0.64133700	0.46197000
K	2.45700000	2.34917500	-0.49673300
K	-2.45561300	-2.35484500	0.49019900
O	3.78248100	-0.35446900	0.31560400
O	5.19681800	1.18865000	-1.41825000
O	4.76797300	2.99423200	0.77098600
O	6.73266600	2.00332500	0.64871800
O	0.28662400	-2.76407600	-0.15617500
O	2.34951100	-2.64578800	0.71065800
O	6.71436800	-0.95614700	0.21771000
O	5.32632200	-2.70938100	-0.02596000
O	5.46654300	0.41577200	2.40656800
O	3.86058400	-1.06537700	2.97052500
O	-1.13972700	-0.07319100	-0.48633200
O	0.82276100	1.16823700	-2.32797000
O	-2.44663900	-1.40641000	-2.55183100
O	-0.21344100	-1.56441400	-2.74507900
O	-1.28651100	1.25768200	-3.08976600
O	2.25962900	-1.18095500	-1.77915600
O	5.07723800	-0.86626800	-2.31625900
O	-3.69243200	3.49159900	1.93802600
O	-2.58750000	2.77913600	3.76630500
O	-3.79010200	0.35993500	-0.32336200
O	-5.19805400	-1.18915800	1.41368300
O	-4.76551700	-2.99318800	-0.77754000
O	-6.73173800	-2.00534100	-0.65312700
O	-0.28384100	2.75959200	0.15629500
O	-2.34817700	2.65282200	-0.70762300
O	-6.71701100	0.95734400	-0.20855300
O	-5.32680700	2.70770100	0.04649000
O	-5.47330100	-0.40695600	-2.40556800
O	-3.86152900	1.07006800	-2.96734100
O	1.13476000	0.06973200	0.48462800
O	-0.82523700	-1.17460400	2.32313200
O	2.44160000	1.41057800	2.54028000
O	0.20748400	1.55837200	2.73572000
O	1.28274000	-1.24698200	3.09010400
O	-2.26316200	1.17150700	1.77963400
O	-5.07416600	0.86028900	2.32397300
O	3.70271300	-3.49598200	-1.93657300
O	2.59788800	-2.78665200	-3.76605000

N	2.54256400	4.77511800	-2.12915200
N	-2.55094700	-4.77253700	2.13370100
C	5.22936900	0.36384500	-2.40484500
C	5.50774900	0.98564500	-3.74918600
C	6.01351700	3.06046500	0.79429200
C	6.74393600	4.35638500	1.00442500
C	1.28794600	-3.28416500	0.38617900
C	1.29632000	-4.76476600	0.66835500
C	6.46486900	-2.18262100	0.19496300
C	7.59093400	-3.15675500	0.42969200
C	4.92172600	-0.41827900	3.18385400
C	-1.40694000	-1.85943400	-3.08378400
C	-1.53978200	-2.81167900	-4.24470400
C	-0.03923800	1.51232100	-3.16211700
C	0.40532000	2.26801400	-4.39107100
C	5.59662800	-0.63338500	4.51190800
C	2.67649300	5.78297800	-2.68395300
C	2.84438200	7.04747400	-3.37891100
C	-3.24172100	3.62500200	3.14779700
C	-3.59451300	4.94798900	3.78383900
C	-5.22124500	-0.37047900	2.40611500
C	-5.48164700	-1.00324200	3.74909000
C	-6.01111800	-3.06062900	-0.80213000
C	-6.73931900	-4.35680600	-1.01914500
C	-1.28484900	3.28580200	-0.38241500
C	-1.28717900	4.76789700	-0.65734300
C	-6.46487800	2.18255200	-0.18476900
C	-7.58546600	3.16059500	-0.42988000
C	-4.92546700	0.42670900	-3.18071100
C	1.40023500	1.85831500	3.07326800
C	1.52930000	2.81002400	4.23501500
C	0.03603500	-1.50761700	3.16160000
C	-0.40641600	-2.25493700	4.39652800
C	-5.59900200	0.64757500	-4.50850200
C	-2.69344900	-5.77359800	2.69858300
C	-2.87218800	-7.02960200	3.40613100
C	3.25518200	-3.63001500	-3.14767300
C	3.61620000	-4.95012100	-3.78497500
H	3.64222300	6.96305600	-4.12098700
H	3.10559100	7.83306400	-2.66546900
H	1.91566700	7.32248100	-3.88514700
H	-3.70033700	-6.94505900	4.11421000
H	-3.09391600	-7.82956100	2.69529800
H	-1.96102700	-7.28384200	3.95344900
H	2.22699100	-1.67101400	-2.65675400
H	-2.22659500	1.66276800	2.65668900
H	-4.67697400	4.98976800	3.93762700
H	-3.33133700	5.76960600	3.11261800
H	-3.08256900	5.05773900	4.73994000
H	-8.45902100	2.65224100	-0.83767500
H	-7.84969700	3.62935400	0.52333200

H	-7.24792600	3.95417000	-1.10014000
H	-5.25922100	1.57871200	-4.96168000
H	-6.68324000	0.63813200	-4.38643900
H	-5.32675100	-0.18451400	-5.16613100
H	-7.29433300	-4.30223900	-1.96017100
H	-7.46952300	-4.50656100	-0.21969900
H	-6.03695100	-5.18967800	-1.05424000
H	-1.76567600	-2.22594100	-5.14225300
H	-2.37811700	-3.49014600	-4.07338600
H	-0.61077100	-3.35871800	-4.40668500
H	3.10678700	-5.06113600	-4.74227100
H	3.35595000	-5.77408000	-3.11548400
H	4.69918400	-4.98603000	-3.93661300
H	2.03180000	-5.22718800	0.00186900
H	1.63268500	-4.94328600	1.69269100
H	0.31467000	-5.20890300	0.49915600
H	7.84927500	-3.62273200	-0.52650600
H	8.46582000	-2.64597100	0.83152800
H	7.26144200	-3.95278300	1.10102200
H	5.25155600	-1.55845600	4.97332800
H	5.33300300	0.20630200	5.16331600
H	6.68063900	-0.63287400	4.38689200
H	6.58235300	1.18176800	-3.82486400
H	4.99034500	1.94326900	-3.83976000
H	5.20919000	0.30712900	-4.54818100
H	7.30935700	4.30159800	1.93916600
H	6.04191700	5.18919800	1.04679100
H	7.46528200	4.50631500	0.19693600
H	1.77214500	2.22608300	5.12924800
H	2.35634300	3.50073600	4.05749300
H	0.59407700	3.34363500	4.40559900
H	-0.89637600	-1.54152000	5.06734500
H	0.44083800	-2.70797400	4.91164700
H	-1.14502400	-3.01188000	4.12206200
H	-5.17602000	-0.32933500	4.54930600
H	-4.95978800	-1.95957700	3.82669500
H	-6.55460100	-1.20362800	3.83601100
H	-0.44104600	2.72450100	-4.90454800
H	1.14314700	3.02328900	-4.10985600
H	0.89708300	1.55946200	-5.06568400
H	-0.30281900	5.20672100	-0.48988700
H	-1.62687100	4.95302900	-1.67939000
H	-2.01780500	5.23027800	0.01446700

The optimised coordinates of the non-ferromagnetic state ($\downarrow\uparrow\uparrow\downarrow\uparrow\uparrow\uparrow$) for the calculation of coupling constants are given below:

Mn	-0.51132500	0.71975500	1.12565100
Mn	-2.46177200	0.61278100	-1.65564000
Mn	-3.78249700	1.87433400	0.87986300
Mn	-5.34515400	-0.64617400	-0.46248400
Mn	0.51323700	-0.71921400	-1.13596300
Mn	2.46368900	-0.60942100	1.65790300
Mn	3.78180500	-1.88243700	-0.87818500
Mn	5.34733800	0.64801300	0.46327900
K	2.45491900	2.35295600	-0.49988000
K	-2.44809800	-2.35898900	0.48944800
O	3.78385000	-0.35033000	0.31673000
O	5.19657900	1.19358400	-1.41748100
O	4.76407400	3.00039900	0.76971400
O	6.73023300	2.01213900	0.64996800
O	0.29121300	-2.76329900	-0.15258400
O	2.35407300	-2.64269000	0.71378500
O	6.71685100	-0.94741400	0.22042100
O	5.33165200	-2.70307200	-0.02195100
O	5.46572900	0.42295800	2.40799000
O	3.86115100	-1.05979100	2.97189200
O	-1.13839800	-0.07458600	-0.48594500
O	0.82567100	1.16510100	-2.33088700
O	-2.44222000	-1.40874900	-2.55116500
O	-0.20907000	-1.56742900	-2.74368900
O	-1.28425300	1.25311800	-3.09083500
O	2.26277700	-1.18143500	-1.77707600
O	5.08026200	-0.86229800	-2.31374600
O	-3.72037700	3.48338700	1.94056800
O	-2.60969700	2.77400300	3.76714400
O	-3.78930200	0.35750700	-0.32520200
O	-5.20182600	-1.19497000	1.40942200
O	-4.75161700	-3.00300100	-0.78038200
O	-6.71899300	-2.01593600	-0.66374000
O	-0.28663400	2.75698800	0.14604400
O	-2.35460400	2.64808100	-0.70960200
O	-6.72383400	0.94534600	-0.20019100
O	-5.33226000	2.69726100	0.03352100
O	-5.47537800	-0.40460500	-2.40278200
O	-3.85814900	1.06598600	-2.96540600
O	1.13587800	0.07325300	0.48379800
O	-0.82620600	-1.17040600	2.32522200
O	2.44241400	1.41459000	2.53959300
O	0.20821300	1.56229100	2.73373200
O	1.28263800	-1.24303400	3.08991800
O	-2.25752100	1.18894600	1.76837300
O	-5.07284000	0.85177300	2.32556700
O	3.70979900	-3.49406800	-1.93229500
O	2.60420900	-2.78799100	-3.76256000

N	2.53266900	4.77932100	-2.13108500
N	-2.54012900	-4.77248400	2.13898500
C	5.23064500	0.36796700	-2.40334700
C	5.50874800	0.98882900	-3.74817000
C	6.00950800	3.06841700	0.79395300
C	6.73789700	4.36554600	1.00364100
C	1.29364300	-3.28252800	0.38845600
C	1.30516700	-4.76366000	0.66771500
C	6.46933100	-2.17429100	0.19872900
C	7.59691200	-3.14641000	0.43450400
C	4.92154800	-0.41150900	3.18530800
C	-1.40269800	-1.86157800	-3.08321000
C	-1.53523200	-2.81270300	-4.24510700
C	-0.03753300	1.50902900	-3.16410700
C	0.40569600	2.26600800	-4.39277500
C	5.59641500	-0.62559700	4.51355900
C	2.66418900	5.78407500	-2.69205600
C	2.82888100	7.04469600	-3.39478200
C	-3.27221300	3.61544600	3.15148700
C	-3.64034700	4.93143000	3.79363700
C	-5.22687100	-0.37790800	2.40377800
C	-5.49731500	-1.01386800	3.74321300
C	-5.99659800	-3.07061000	-0.81140000
C	-6.72411400	-4.36605500	-1.03526800
C	-1.29432800	3.28427800	-0.37834100
C	-1.31085500	4.77071900	-0.62747800
C	-6.47182000	2.17064900	-0.18782300
C	-7.59313200	3.14715500	-0.43577200
C	-4.92382800	0.42610800	-3.17884500
C	1.40086900	1.86282700	3.07150100
C	1.52920200	2.81572500	4.23233100
C	0.03583400	-1.50258600	3.16334100
C	-0.40579900	-2.24739700	4.40005600
C	-5.59570400	0.64666900	-4.50743100
C	-2.67481800	-5.77498300	2.70323400
C	-2.84369700	-7.03281600	3.40995400
C	3.26293200	-3.62971100	-3.14345800
C	3.62647400	-4.94958300	-3.77981100
H	3.65772100	6.97206700	-4.10337300
H	3.04187400	7.84432900	-2.68091700
H	1.91479900	7.29090800	-3.94090100
H	-3.64226200	-6.94120500	4.15039800
H	-3.10440100	-7.82505500	2.70371600
H	-1.91556200	-7.30323900	3.91970600
H	2.23100100	-1.67217400	-2.65434200
H	-2.23064700	1.66641300	2.65259400
H	-4.72275000	4.95777600	3.95140600
H	-3.39086400	5.75911500	3.12468400
H	-3.12687200	5.04442700	4.74854100
H	-7.85130100	3.62561000	0.51427500
H	-7.25892100	3.93384700	-1.11576800

H	-8.46940000	2.63556000	-0.83355900
H	-5.25493400	1.57771600	-4.96012200
H	-6.68015000	0.63758900	-4.38735000
H	-5.32242300	-0.18526400	-5.16485500
H	-7.27096000	-4.31036400	-1.98101500
H	-7.46123500	-4.51585500	-0.24223800
H	-6.02205800	-5.19938500	-1.06514200
H	-1.76109600	-2.22604900	-5.14206100
H	-2.37353700	-3.49140400	-4.07455100
H	-0.60620300	-3.35957400	-4.40754700
H	3.11709200	-5.06233400	-4.73691900
H	3.36806700	-5.77358200	-3.10965700
H	4.70949700	-4.98338800	-3.93167300
H	2.04153300	-5.22312100	0.00015700
H	1.64208500	-4.94352300	1.69163300
H	0.32444100	-5.20953800	0.49771200
H	7.26850300	-3.94251900	1.10626700
H	7.85629800	-3.61263800	-0.52129500
H	8.47083400	-2.63390800	0.83623900
H	5.25157800	-1.55046300	4.97556100
H	5.33263700	0.21447600	5.16440200
H	6.68043400	-0.62490800	4.38856900
H	6.58367600	1.18278300	-3.82497200
H	4.99306600	1.94735900	-3.83873300
H	5.20832500	0.31044300	-4.54658900
H	7.30043200	4.31319700	1.94027500
H	6.03484400	5.19766700	1.04231000
H	7.46160000	4.51468900	0.19813500
H	1.76605400	2.23198000	5.12831400
H	2.35956600	3.50297900	4.05711200
H	0.59542900	3.35314200	4.39888300
H	-0.89701900	-1.53306100	5.06896300
H	0.44194800	-2.69806500	4.91642300
H	-1.14327400	-3.00606100	4.12725100
H	-5.20512500	-0.33876000	4.54736700
H	-4.96871200	-1.96620100	3.82523200
H	-6.56939600	-1.22335600	3.81808700
H	-0.44166100	2.72019400	-4.90664700
H	1.14109900	3.02344000	-4.11095400
H	0.90006400	1.55904800	-5.06714100
H	-0.32994300	5.21527500	-0.45500300
H	-1.65511900	4.97063600	-1.64520100
H	-2.04375800	5.21465100	0.05426000

The optimised coordinates of the non-ferromagnetic state ($\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow\downarrow\uparrow$) for the calculation of coupling constants are given below:

Mn	-0.51181300	-0.71733100	-1.12935000
Mn	-2.46633900	-0.60864200	1.65596600
Mn	-3.77634300	-1.88072000	-0.88075200
Mn	-5.35022900	0.63846200	0.45854700
Mn	0.51023400	0.72490400	1.12764400
Mn	2.46629300	0.61586300	-1.65632700
Mn	3.78186600	1.87800100	0.88229200
Mn	5.34392800	-0.64919900	-0.46339400
K	2.44979700	-2.35573800	0.49181800
K	-2.45467400	2.35584800	-0.49565200
O	3.78897400	0.35991500	-0.32414500
O	5.18885100	-1.19809100	1.41132600
O	4.75617200	-3.00209800	-0.77817100
O	6.72380100	-2.01727600	-0.65119400
O	0.28454500	2.76417700	0.14821700
O	2.35118400	2.65568300	-0.71095100
O	6.71720300	0.94475300	-0.20932400
O	5.33176800	2.70019300	0.03656400
O	5.47130200	-0.41895400	-2.40575300
O	3.86309200	1.05909300	-2.97450800
O	-1.13883700	0.07304500	0.48446900
O	0.82356500	-1.16655300	2.32505400
O	-2.44290100	1.41965800	2.53622400
O	-0.20924100	1.56382900	2.73700700
O	-1.28598100	-1.23859000	3.08867100
O	2.25833000	1.19637300	1.77119800
O	5.07195400	0.85122800	2.32267400
O	-3.69009400	-3.49420800	-1.93443700
O	-2.59383300	-2.77575100	-3.76547500
O	-3.79170100	-0.36268200	0.32912900
O	-5.20558400	1.17877100	-1.41575400
O	-4.76446800	2.99827700	0.76569000
O	-6.72866100	2.00477500	0.64989100
O	-0.28568900	-2.76248000	-0.15831900
O	-2.34805400	-2.64477900	0.70870900
O	-6.72076600	-0.96117000	0.20273600
O	-5.32531400	-2.70919200	-0.03827800
O	-5.48206000	0.40932900	2.39956000
O	-3.86076500	-1.05121700	2.97623200
O	1.13725300	-0.06834300	-0.48376000
O	-0.82259100	1.17409000	-2.32529600
O	2.44098200	-1.41029900	-2.54123100
O	0.20719200	-1.55616400	-2.73956200
O	1.28798000	1.25180100	-3.08542600
O	-2.26522900	-1.16977600	-1.77804600
O	-5.07563100	-0.87081400	-2.32508100
O	3.72071200	3.48901200	1.93893900
O	2.60850500	2.78501000	3.76675300

N	2.53844400	-4.76810300	2.14346300
N	-2.54348000	4.77440100	-2.13801200
C	5.21493600	-0.37990900	2.40431700
C	5.47216400	-1.01492600	3.74679900
C	6.00155200	-3.07156300	-0.80065400
C	6.72828800	-4.36889700	-1.01561300
C	1.29196300	3.29140900	-0.37727000
C	1.30849300	4.77852800	-0.62382300
C	6.46834400	2.17077200	-0.19235700
C	7.59129300	3.14452000	-0.44350100
C	4.92505400	0.41260300	-3.18504400
C	-1.40268800	1.86542600	3.07218900
C	-1.53250700	2.81581400	4.23490900
C	-0.03917800	-1.49800600	3.16284700
C	0.40159300	-2.24183200	4.40044100
C	5.60057300	0.62489800	-4.51329400
C	2.67235000	-5.76919600	2.71039500
C	2.84019300	-7.02525100	3.42051400
C	-3.24259100	-3.62492900	-3.14561300
C	-3.59148300	-4.94885900	-3.78186200
C	-5.23161800	0.35840000	-2.40731900
C	-5.50559500	0.98954100	-3.74823300
C	-6.00968700	3.06237700	0.79361300
C	-6.74160100	4.35685700	1.00849700
C	-1.28704900	-3.28308500	0.38417900
C	-1.29475700	-4.76376900	0.66569600
C	-6.46551900	-2.18579600	0.18721300
C	-7.58377900	-3.16556100	0.43622400
C	-4.92874000	-0.41368500	3.18306400
C	1.40035000	-1.85681500	-3.07606500
C	1.52975000	-2.80748600	-4.23863000
C	0.04110200	1.51175600	-3.15918600
C	-0.39767200	2.26456200	-4.39200400
C	-5.60377500	-0.62578800	4.51152000
C	-2.67553100	5.77878900	-2.69951300
C	-2.84097700	7.03901200	-3.40278400
C	3.27165000	3.62449800	3.14931600
C	3.63984100	4.94226000	3.78768600
H	3.64980600	-6.93727000	4.14930800
H	3.08409800	-7.82292400	2.71439000
H	1.91696900	-7.28525800	3.94440900
H	-3.64467900	6.95380800	-4.13841800
H	-3.09231800	7.83149700	-2.69343500
H	-1.91435100	7.30464100	-3.91777400
H	2.23008200	1.67584400	2.65428800
H	-2.23213000	-1.65890600	-2.65650400
H	-4.67438400	-4.99605800	-3.93091300
H	-3.32111600	-5.76995800	-3.11284200
H	-3.08315600	-5.05492500	-4.74030500
H	-8.46117000	-2.65656000	0.83484800
H	-7.84138700	-3.64500400	-0.51346800

H	-7.24659400	-3.95113300	1.11607100
H	-5.24588300	-1.54096700	4.98281500
H	-6.68738700	-0.64336900	4.38397800
H	-5.35529200	0.22422200	5.15543400
H	-7.29470800	4.30315700	1.95068500
H	-7.47372700	4.50223600	0.21000000
H	-6.04165400	5.19189500	1.03990400
H	-1.76489800	2.22931000	5.13028300
H	-2.36585800	3.50016900	4.06278300
H	-0.60044400	3.35643900	4.40080300
H	3.12651300	5.05769600	4.74236600
H	3.38993200	5.76802500	3.11652700
H	4.72227400	4.96927400	3.94504800
H	2.04241100	5.22119800	0.05761900
H	1.65123200	4.98037300	-1.64168100
H	0.32796200	5.22304300	-0.44901600
H	7.85732600	3.61782100	0.50696300
H	8.46323800	2.63164900	-0.84905900
H	7.25532800	3.93528400	-1.11785500
H	5.25429400	1.54805800	-4.97763800
H	5.33884700	-0.21714600	-5.16241800
H	6.68450700	0.62655000	-4.38757400
H	6.54209600	-1.23260400	3.82881500
H	4.93560200	-1.96291200	3.82759300
H	5.18031700	-0.33585800	4.54774500
H	7.28442200	-4.31595400	-1.95607300
H	6.02479700	-5.20081300	-1.05074900
H	7.45738300	-4.51893300	-0.21521500
H	1.76944900	-2.22229500	-5.13291300
H	2.35870000	-3.49636600	-4.06303800
H	0.59548000	-3.34311100	-4.40818400
H	-0.88638600	1.55438800	-5.06714300
H	0.45122000	2.71933600	-4.90284100
H	-1.13644400	3.02078800	-4.11600900
H	-5.22340800	0.30841400	-4.55083400
H	-4.96954000	1.93704700	-3.83803600
H	-6.57623600	1.20798000	-3.81747700
H	-0.44652100	-2.69220500	4.91645700
H	1.13941600	-3.00057100	4.12879700
H	0.89212400	-1.52687500	5.06919400
H	-0.31259600	-5.20733500	0.49792400
H	-1.63288300	-4.94306200	1.68930500
H	-2.02886200	-5.22597300	-0.00245100

The optimised coordinates of the non-ferromagnetic state ($\downarrow\downarrow\uparrow\downarrow\uparrow\uparrow\uparrow$) for the calculation of coupling constants are given below:

Mn	0.51003400	0.72523700	-1.12565900
Mn	2.46936300	0.60578400	1.65586400
Mn	3.78244700	1.87641500	-0.87984700
Mn	5.34420500	-0.65716600	0.45399600
Mn	-0.51137100	-0.72087700	1.12876300
Mn	-2.46712900	-0.60646800	-1.65627400
Mn	-3.78388600	-1.87618000	0.88330000
Mn	-5.34812000	0.65445700	-0.46065000
K	-2.45501000	2.35247100	0.51019900
K	2.44516300	-2.36123200	-0.49731400
O	-3.78612200	-0.34582500	-0.31449600
O	-5.19647000	1.20056500	1.42013800
O	-4.75989100	3.00491300	-0.76673000
O	-6.72836700	2.02125900	-0.64764200
O	-0.29434000	-2.76420200	0.14650500
O	-2.35998000	-2.64007800	-0.71241900
O	-6.71907800	-0.93917100	-0.21398800
O	-5.33602400	-2.69633700	0.03008400
O	-5.46882000	0.42705000	-2.40501400
O	-3.86497900	-1.05627700	-2.96959800
O	1.13822100	-0.07316600	0.48302600
O	-0.81748000	1.16570000	2.33173700
O	2.44301900	-1.42390300	2.53347800
O	0.20932000	-1.56913000	2.73410500
O	1.29401600	1.23696000	3.08974400
O	-2.26323100	-1.17523100	1.77783600
O	-5.08067000	-0.85420200	2.31910300
O	3.72139600	3.49174100	-1.93015400
O	2.60579900	2.79621900	-3.75918100
O	3.78987200	0.35372700	0.32085700
O	5.18644500	-1.19913100	-1.42228600
O	4.75578300	-3.01120000	0.76150900
O	6.72360300	-2.02668400	0.63511000
O	0.28650400	2.76188200	-0.13952900
O	2.35369700	2.64919900	0.71810800
O	6.71850800	0.93674100	0.20431400
O	5.33402000	2.69414200	-0.03280500
O	5.47461600	-0.43424200	2.39706500
O	3.86848500	1.04302500	2.97365900
O	-1.13825600	0.07453600	-0.48269100
O	0.82490500	-1.16231600	-2.32830100
O	-2.44575800	1.41675300	-2.53816900
O	-0.21188700	1.56859500	-2.73230200
O	-1.28574600	-1.24109500	-3.08800400
O	2.25719100	1.19998500	-1.76925600
O	5.06952300	0.85379900	-2.32544200
O	-3.71097000	-3.48718100	1.93828900
O	-2.60178800	-2.78149700	3.76662600

N	-2.51704700	4.77599300	2.14667100
N	2.51840200	-4.77732800	-2.14438800
C	-5.23199500	0.37606800	2.40689600
C	-5.51301100	0.99841600	3.75043200
C	-6.00518600	3.07600300	-0.79074300
C	-6.73052500	4.37516900	-0.99821400
C	-1.30014500	-3.28196300	-0.39004300
C	-1.31612200	-4.76355800	-0.66655100
C	-6.47312400	-2.16636400	-0.19046300
C	-7.60233200	-3.13728300	-0.42356000
C	-4.92557600	-0.40800300	-3.18228000
C	1.40270800	-1.87108100	3.06848100
C	1.53313700	-2.82448900	4.22872000
C	0.04768300	1.49865200	3.16602400
C	-0.38862700	2.24713100	4.40232800
C	-5.60178800	-0.62296900	-4.50971000
C	-2.60820700	5.78981400	2.69927600
C	-2.72218100	7.06181100	3.39148300
C	3.27086200	3.63243700	-3.13938100
C	3.64003100	4.95211000	-3.77326800
C	5.21094400	-0.37721900	-2.41216900
C	5.46527800	-1.00663300	-3.75781900
C	6.00117400	-3.08121700	0.78169300
C	6.72780600	-4.37974900	0.98972400
C	1.29482600	3.28665300	0.38652500
C	1.31331600	4.77331600	0.63618000
C	6.47054300	2.16298300	0.19237300
C	7.59461800	3.13492700	0.44552400
C	4.93025800	0.39493500	3.18019100
C	-1.40512800	1.86855700	-3.06869000
C	-1.53542000	2.82545800	-4.22600800
C	-0.03846700	-1.49701200	-3.16420100
C	0.40252200	-2.24137200	-4.40148700
C	5.60799800	0.60188000	4.50816400
C	2.63610300	-5.78479800	-2.70356300
C	2.78356800	-7.04883200	-3.40397600
C	-3.26181900	-3.62292100	3.14866300
C	-3.62479000	-4.94279200	3.78550500
H	-3.40649300	6.96669900	4.23826000
H	-3.10630400	7.82432700	2.70928800
H	-1.74247500	7.37630900	3.75984200
H	3.54763000	-6.95915200	-4.18020000
H	3.08180600	-7.83142400	-2.70184900
H	1.83587600	-7.33172700	-3.86901900
H	-2.22987100	-1.66445600	2.65532800
H	2.22807800	1.68273100	-2.65046500
H	4.72218500	4.97780400	-3.93278800
H	3.39300700	5.77566700	-3.09834300
H	3.12498000	5.07222200	-4.72644300
H	7.85978800	3.61138600	-0.50360400
H	7.26020500	3.92355500	1.12314400

H	8.46668400	2.61990000	0.84808000
H	5.26340500	1.52379000	4.97623500
H	6.69174400	0.60279400	4.38083900
H	5.34630200	-0.24211800	5.15475800
H	7.29175200	-4.32868200	1.92558800
H	7.45012600	-4.52976800	0.18315600
H	6.02353300	-5.21080100	1.02919300
H	1.76997900	-2.24083400	5.12478200
H	2.36404800	-3.51083000	4.05257900
H	0.60000800	-3.36283500	4.39597100
H	-3.11410400	-5.05573400	4.74190300
H	-3.36753700	-5.76685300	3.11497300
H	-4.70760400	-4.97636700	3.93889000
H	-2.05042200	-5.22009900	0.00528100
H	-1.65818300	-4.94453000	-1.68856100
H	-0.33558500	-5.21120800	-0.50015400
H	-7.27557600	-3.93524200	-1.09393100
H	-7.86179100	-3.60117300	0.53335800
H	-8.47576800	-2.62429100	-0.82573100
H	-5.25827600	-1.54873000	-4.97091400
H	-5.33764500	0.21603300	-5.16178800
H	-6.68569500	-0.62101800	-4.38381800
H	-6.58829600	1.19124500	3.82506600
H	-4.99872500	1.95773100	3.84060900
H	-5.21329800	0.32142800	4.55030900
H	-7.30016800	4.32301900	-1.93051500
H	-6.02493300	5.20481400	-1.04309900
H	-7.44774500	4.52830400	-0.18762500
H	-1.76714100	2.24410700	-5.12489800
H	-2.36944100	3.50803500	-4.05004400
H	-0.60379200	3.36788800	-4.38835200
H	0.89668700	-1.52771200	-5.06890600
H	-0.44579500	-2.68934500	-4.91924100
H	1.13757200	-3.00243600	-4.12867800
H	5.15656800	-0.33038600	-4.55488700
H	4.94306300	-1.96270800	-3.83587200
H	6.53787500	-1.20671700	-3.84985800
H	0.46149600	2.69851900	4.91412500
H	-1.12659400	3.00555500	4.13024700
H	-0.87776700	1.53500200	5.07508900
H	0.33280700	5.21897500	0.46416900
H	1.65849700	4.97271100	1.65370300
H	2.04621500	5.21655700	-0.04599800

The optimised coordinates of the non-ferromagnetic state ($\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow\downarrow$) for the calculation of coupling constants are given below:

Mn	-0.51259500	0.71864300	1.12981900
Mn	-2.46677500	0.60955700	-1.65682300
Mn	-3.77689400	1.87937400	0.88080400
Mn	-5.35019800	-0.63962600	-0.45895100
Mn	0.51268200	-0.71877700	-1.13023400
Mn	2.46686000	-0.60964500	1.65653900
Mn	3.77690000	-1.87945900	-0.88103600
Mn	5.35023400	0.63964800	0.45876500
K	2.45351400	2.35446600	-0.49217000
K	-2.45336800	-2.35466600	0.49178300
O	3.79170700	-0.36180700	0.32944400
O	5.20531800	1.18016100	-1.41534200
O	4.76360700	2.99861600	0.76741100
O	6.72831300	2.00635100	0.65004600
O	0.28654100	-2.76384200	-0.16244900
O	2.34808000	-2.64531400	0.70675900
O	6.72063700	-0.96015500	0.20405600
O	5.32536100	-2.70817900	-0.03796200
O	5.48180100	0.41175700	2.39996900
O	3.86207100	-1.05054700	2.97637800
O	-1.13756500	-0.06956300	-0.48597600
O	0.81971200	1.17639400	-2.32262400
O	-2.43834900	-1.41868000	-2.53768600
O	-0.20453700	-1.55559500	-2.74202100
O	-1.28860900	1.24261800	-3.08976400
O	2.26658800	-1.16766500	-1.77912700
O	5.07676500	-0.86935400	-2.32491200
O	-3.69134200	3.49214700	1.93563200
O	-2.59626600	2.77211800	3.76673600
O	-3.79159800	0.36169600	-0.32963200
O	-5.20511300	-1.18012200	1.41521600
O	-4.76394000	-2.99875200	-0.76704400
O	-6.72848900	-2.00616300	-0.64990500
O	-0.28650900	2.76380700	0.16190100
O	-2.34818200	2.64521200	-0.70696500
O	-6.72066500	0.96007500	-0.20414200
O	-5.32544400	2.70813100	0.03792200
O	-5.48167500	-0.41181400	-2.40013600
O	-3.86197400	1.05047100	-2.97665300
O	1.13763200	0.06939400	0.48562400
O	-0.81953000	-1.17659900	2.32229300
O	2.43839400	1.41852200	2.53751000
O	0.20456300	1.55571500	2.74147800
O	1.28871700	-1.24239800	3.08966200
O	-2.26651500	1.16749900	1.77877600
O	-5.07674400	0.86941600	2.32475300
O	3.69177100	-3.49222400	-1.93586900
O	2.59655100	-2.77235100	-3.76695600

N	2.54196100	4.77245800	-2.13558900
N	-2.54063100	-4.77306900	2.13475100
C	5.23195600	0.35995900	-2.40704300
C	5.50528500	0.99165500	-3.74781600
C	6.00881000	3.06342000	0.79502300
C	6.73994900	4.35799700	1.01185200
C	1.28693200	-3.28363700	0.38265100
C	1.29301100	-4.76355600	0.66822300
C	6.46542000	-2.18479200	0.18828100
C	7.58354200	-3.16455400	0.43786300
C	4.92914500	-0.41159700	3.18354800
C	-1.39743100	-1.86048400	-3.07586700
C	-1.52592600	-2.80974200	-4.23964500
C	-0.04261300	1.50642500	-3.16136700
C	0.39783200	2.25367700	-4.39696700
C	5.60362200	-0.62230900	4.51249300
C	2.67523200	5.77582300	-2.69863500
C	2.84232500	7.03472700	-3.40387400
C	-3.24466900	3.62184300	3.14719300
C	-3.59399900	4.94517300	3.78441100
C	-5.23180200	-0.35991900	2.40689800
C	-5.50502200	-0.99160700	3.74770300
C	-6.00915400	-3.06342500	-0.79431100
C	-6.74057800	-4.35817000	-1.00917400
C	-1.28716700	3.28365800	-0.38265200
C	-1.29378600	4.76375400	-0.66727900
C	-6.46549900	2.18472400	-0.18827300
C	-7.58372600	3.16444000	-0.43756200
C	-4.92906200	0.41152100	-3.18376500
C	1.39744500	1.86035800	3.07559200
C	1.52587700	2.80941600	4.23954300
C	0.04273400	-1.50626700	3.16124800
C	-0.39779500	-2.25319700	4.39701400
C	-5.60372100	0.62225200	-4.51261200
C	-2.67540100	-5.77516800	2.69969200
C	-2.84423400	-7.03257700	3.40717800
C	3.24513600	-3.62196000	-3.14744300
C	3.59475600	-4.94518600	-3.78471300
H	3.67351900	6.96032300	-4.10951800
H	3.05301600	7.83607300	-2.69124900
H	1.93010100	7.27969000	-3.95365200
H	-3.62311700	-6.93218300	4.16719100
H	-3.13297900	-7.81917000	2.70555400
H	-1.90771400	-7.31709100	3.89338400
H	2.23418900	-1.65660600	-2.65784900
H	-2.23403500	1.65640800	2.65750500
H	-4.67697900	4.99211300	3.93296500
H	-3.32339100	5.76687100	3.11622800
H	-3.08616800	5.05046200	4.74320200
H	-8.46037400	2.65567700	-0.83812200
H	-7.84292000	3.64234400	0.51248100

H	-7.24586700	3.95114300	-1.11575000
H	-5.24667000	1.53763200	-4.98415100
H	-6.68741200	0.63861400	-4.38558900
H	-5.35392300	-0.22775900	-5.15601700
H	-7.29406000	-4.30451400	-1.95114500
H	-7.47234000	-4.50404300	-0.21043600
H	-6.04026900	-5.19288500	-1.04105400
H	-1.76582500	-2.22336900	-5.13311300
H	-2.35425800	-3.49963700	-4.06526200
H	-0.59108900	-3.34417900	-4.40987400
H	3.08693200	-5.05055500	-4.74349900
H	3.32435200	-5.76696900	-3.11655300
H	4.67774500	-4.99186700	-3.93329300
H	2.02673600	-5.22846300	0.00153100
H	1.63072300	-4.94038400	1.69239700
H	0.31040000	-5.20649200	0.50143500
H	7.84207500	-3.64348600	-0.51183800
H	8.46052100	-2.65565800	0.83752100
H	7.24581400	-3.95050500	1.11699900
H	5.24791000	-1.53871800	4.98306000
H	5.35189000	0.22662500	5.15657500
H	6.68739400	-0.63664500	4.38601000
H	6.57478200	1.21614700	-3.81511700
H	4.96412600	1.93614600	-3.83908400
H	5.22813600	0.30867600	-4.55058100
H	7.28591100	4.30604800	1.95833700
H	6.04022500	5.19344900	1.03673000
H	7.47805100	4.50125800	0.21855100
H	1.76641800	2.22297900	5.13279300
H	2.35382300	3.49974100	4.06499700
H	0.59085900	3.34339900	4.41019600
H	-0.88873300	-1.53993000	5.06728500
H	0.45056500	-2.70404000	4.91222400
H	-1.13511900	-3.01177800	4.12365100
H	-5.22781600	-0.30862000	4.55044100
H	-4.96385400	-1.93609500	3.83893500
H	-6.57451400	-1.21609900	3.81508900
H	-0.45041700	2.70590000	-4.91115900
H	1.13639700	3.01109800	-4.12376600
H	0.88720100	1.54021200	-5.06818200
H	-0.31142800	5.20701100	-0.49986200
H	-1.63117700	4.94109500	-1.69147200
H	-2.02797900	5.22790600	-0.00057900

The optimised coordinates for Mn₈K₂(OH)(pivalate) (Fig. S14(a)) are:

Mn	-0.52182700	1.18558600	0.64704400
Mn	-2.52062800	-0.38696200	-1.61614500
Mn	-3.88347900	1.91224000	0.01076500
Mn	-5.30445700	-1.01067700	0.15840700
Mn	0.52182700	-1.18558600	-0.64704400
Mn	2.52062800	0.38696100	1.61614500
Mn	3.88347900	-1.91224000	-0.01076500
Mn	5.30445600	1.01067700	-0.15840600
K	2.29468200	1.94557600	-1.83623100
K	-2.29468200	-1.94557600	1.83623000
O	3.80358300	-0.00568300	0.25006100
O	5.15729000	0.54700600	-2.05306400
O	4.64414500	3.16806600	-1.00056000
O	6.65219100	2.33139000	-0.69363500
O	0.47759200	-2.42347600	1.24837000
O	2.56624300	-1.86989100	1.83300000
O	6.79676800	-0.44219400	0.31377200
O	5.50493500	-2.11387600	1.07211400
O	5.49858700	1.71111200	1.66573400
O	3.98041700	0.62395000	2.92490300
O	-1.14695500	-0.36579300	-0.31637600
O	0.73040600	-0.18551400	-2.61912600
O	-2.43688500	-2.56386700	-1.49525200
O	-0.20186500	-2.77657400	-1.54558300
O	-1.41091800	-0.41061100	-3.23927300
O	2.27986300	-1.86326200	-1.03463700
O	5.05310100	-1.68564900	-1.85044800
O	-3.93736000	3.84361600	0.10820500
O	-2.69612800	4.24961300	1.93578400
O	-3.80358300	0.00568300	-0.25006100
O	-5.15729000	-0.54700500	2.05306500
O	-4.64414600	-3.16806500	1.00056100
O	-6.65219200	-2.33138900	0.69363500
O	-0.47759200	2.42347500	-1.24837000
O	-2.56624300	1.86989100	-1.83300100
O	-6.79676800	0.44219400	-0.31377200
O	-5.50493400	2.11387600	-1.07211400
O	-5.49858700	-1.71111200	-1.66573400
O	-3.98041600	-0.62395000	-2.92490300
O	1.14695500	0.36579300	0.31637600
O	-0.73040600	0.18551400	2.61912600
O	2.43688500	2.56386600	1.49525300
O	0.20186500	2.77657400	1.54558300
O	1.41091800	0.41061000	3.23927300
O	-2.27986300	1.86326200	1.03463700
O	-5.05310000	1.68565000	1.85044800
O	3.93736000	-3.84361600	-0.10820500
O	2.69612800	-4.24961300	-1.93578400
C	5.18460600	-0.64768500	-2.52826400

C	5.40852000	-0.73790700	-4.01296400
C	5.88474500	3.29518200	-1.08014400
C	6.53793500	4.52963500	-1.62112500
C	1.50035900	-2.57599200	1.95456800
C	1.51620000	-3.63662900	3.02229300
C	6.62380400	-1.50978300	0.94633400
C	7.79770800	-2.17027900	1.61585400
C	5.03524600	1.30154000	2.77203900
C	-1.39082900	-3.22854600	-1.67370300
C	-1.49326700	-4.67612000	-2.07372800
C	-0.17556200	-0.19095900	-3.48024300
C	0.19327300	0.05767100	-4.91895700
C	5.82625600	1.64455200	4.00092800
C	-3.43154500	4.62527800	1.01159000
C	-3.81187700	6.07448500	0.85786100
C	-5.18460600	0.64768600	2.52826400
C	-5.40852000	0.73790800	4.01296400
C	-5.88474600	-3.29518100	1.08014500
C	-6.53793600	-4.52963400	1.62112700
C	-1.50035900	2.57599100	-1.95456900
C	-1.51619900	3.63662700	-3.02229400
C	-6.62380300	1.50978400	-0.94633400
C	-7.79770800	2.17027900	-1.61585400
C	-5.03524600	-1.30154100	-2.77203900
C	1.39082900	3.22854500	1.67370400
C	1.49326800	4.67611900	2.07372900
C	0.17556200	0.19095800	3.48024300
C	-0.19327300	-0.05767200	4.91895600
C	-5.82625700	-1.64455300	-4.00092800
C	3.43154600	-4.62527700	-1.01159100
C	3.81187700	-6.07448500	-0.85786100
H	2.26005600	-2.74115600	-1.51779500
H	-2.26005600	2.74115600	1.51779500
H	-4.89798900	6.17659500	0.93617200
H	-3.52293600	6.42792300	-0.13586100
H	-3.32766900	6.68110900	1.62282200
H	-8.01536300	3.11137800	-1.10144900
H	-7.54397800	2.41628200	-2.64985300
H	-8.67639500	1.52689200	-1.58575100
H	-5.24040800	-1.47783900	-4.90394400
H	-6.71799800	-1.00985900	-4.02549200
H	-6.16201100	-2.68188500	-3.94496800
H	-7.27035700	-4.90749700	0.90312800
H	-7.07919100	-4.27676800	2.53768100
H	-5.79359500	-5.29606900	1.83554800
H	-2.53429600	-4.97593400	-2.19030000
H	-1.00958400	-5.29700000	-1.31415800
H	-0.95382200	-4.83327300	-3.01195800
H	3.32767000	-6.68110900	-1.62282300
H	3.52293600	-6.42792300	0.13586100
H	4.89798900	-6.17659500	-0.93617200

H	2.33215300	-4.33660400	2.81846300
H	1.72391400	-3.17343700	3.99122800
H	0.57002900	-4.17647700	3.06279800
H	7.54397900	-2.41627800	2.64985400
H	8.01536100	-3.11137900	1.10145200
H	8.67639700	-1.52689200	1.58574800
H	5.24040800	1.47783700	4.90394500
H	6.16200900	2.68188500	3.94496900
H	6.71799900	1.00986000	4.02549100
H	6.41195200	-0.37001700	-4.24734700
H	4.69603700	-0.09246900	-4.53352600
H	5.30502600	-1.76608000	-4.35821200
H	7.27034900	4.90750200	-0.90312100
H	5.79359300	5.29606800	-1.83555200
H	7.07919700	4.27677000	-2.53767500
H	2.53429600	4.97593300	2.19030100
H	1.00958500	5.29700000	1.31415800
H	0.95382100	4.83327300	3.01195800
H	-0.73172300	0.81789200	5.29621100
H	0.68832600	-0.22907900	5.53629300
H	-0.87287100	-0.91256500	4.97300500
H	-5.30502700	1.76608100	4.35821100
H	-4.69603600	0.09247100	4.53352600
H	-6.41195100	0.37001800	4.24734700
H	-0.68832600	0.22907700	-5.53629400
H	0.87286900	0.91256500	-4.97300500
H	0.73172500	-0.81789300	-5.29621000
H	-0.57002700	4.17647400	-3.06280000
H	-1.72391400	3.17343600	-3.99122900
H	-2.33215100	4.33660400	-2.81846400
O	2.47476100	2.84248500	-4.40714000
H	1.94426100	3.53399800	-4.81564400
O	-2.47476300	-2.84248400	4.40713900
H	-1.94426100	-3.53399500	4.81564500
H	2.99082600	2.47263300	-5.13065200
H	-2.99082900	-2.47263200	5.13065100

The optimised coordinates for Mn₈K₂(O)(pivalic acid) (Fig. S14(a)) are:

Mn	0.62092400	1.17788300	-0.68194400
Mn	2.54850500	-0.55497600	1.60330400
Mn	3.71200400	1.87810100	-0.05340300
Mn	5.34289700	-1.00129900	-0.17334600
Mn	-0.50970600	-1.20414100	0.63035300
Mn	-2.46895600	0.40294300	-1.60810100
Mn	-3.88010700	-1.90202200	-0.00980200
Mn	-5.28850400	1.01189800	0.14207900
K	-2.26581200	1.89163200	1.79271300
K	2.32367600	-1.98746700	-1.77983400
O	-3.78784900	0.00000000	-0.24752200
O	-5.17665800	0.53559900	2.04101800
O	-4.61828000	3.15689400	1.01291200
O	-6.63251100	2.34800400	0.66942300
O	-0.48073200	-2.46439800	-1.25733300
O	-2.55853400	-1.87101100	-1.84519400
O	-6.79495200	-0.42494200	-0.34752900
O	-5.49935500	-2.09227600	-1.10876900
O	-5.46482200	1.71416000	-1.68286300
O	-3.93019100	0.63604600	-2.93121500
O	1.16992000	-0.44171500	0.33371500
O	-0.69568800	-0.23355500	2.62864400
O	2.40995600	-2.72624700	1.47966000
O	0.16764500	-2.83234800	1.53482300
O	1.44516800	-0.49802800	3.24099900
O	-2.28924900	-1.85648000	1.02717300
O	-5.08185500	-1.69554100	1.81871500
O	3.52489900	4.08065000	0.15982300
O	3.42966900	4.86085400	-1.89557300
O	3.77966700	-0.16181800	0.23125100
O	5.22605900	-0.39746000	-2.06592500
O	4.79219800	-3.09575300	-1.11012200
O	6.78078500	-2.22394700	-0.78152600
O	0.50780100	2.36770300	1.22380000
O	2.60837100	1.80737500	1.76222600
O	6.72325900	0.52701700	0.38193000
O	5.37496200	2.21709600	0.99020200
O	5.56230800	-1.81151300	1.61386300
O	4.01923200	-0.80562100	2.90826400
O	-1.10543900	0.35141000	-0.34048900
O	0.78050200	0.15149000	-2.61701000
O	-2.42629500	2.55680600	-1.48527500
O	-0.19737000	2.82556200	-1.57967300
O	-1.35728700	0.39144700	-3.24742000
O	2.26096300	1.84721300	-1.05553300
O	4.91804900	1.80931000	-1.77269400
O	-3.94063500	-3.83738800	0.07621900
O	-2.74528800	-4.25348800	1.93229900
C	-5.20558600	-0.66205500	2.50560300

C	-5.37767800	-0.77212200	3.99665600
C	-5.85859300	3.29763900	1.07519500
C	-6.50359600	4.53580900	1.61924500
C	-1.50293200	-2.59028100	-1.96954000
C	-1.52832600	-3.63616500	-3.05322700
C	-6.61839600	-1.48987700	-0.98402700
C	-7.79051700	-2.14746200	-1.66091500
C	-4.98718500	1.30873000	-2.78585100
C	1.33114700	-3.34315200	1.64835400
C	1.36917700	-4.80569400	2.00645400
C	0.21331000	-0.26386300	3.48596500
C	-0.15025800	-0.03171700	4.92995800
C	-5.76968500	1.65574000	-4.02023500
C	3.29529700	5.02133000	-0.58839800
C	2.86828300	6.36543400	-0.08907100
C	5.17686500	0.80824700	-2.48238300
C	5.42624900	1.01642900	-3.95171800
C	6.03864000	-3.18464000	-1.21087000
C	6.70729100	-4.36843000	-1.83933200
C	1.50585600	2.44089200	1.97055300
C	1.46055800	3.30116600	3.20334100
C	6.50509400	1.63481900	0.93218900
C	7.65117400	2.35488300	1.59394400
C	5.08709300	-1.45781500	2.73349300
C	-1.39004300	3.24869000	-1.66821500
C	-1.55418800	4.70127100	-2.04354700
C	-0.12660400	0.15208200	-3.47894900
C	0.24811000	-0.13011500	-4.91130100
C	5.87903200	-1.83450900	3.95289900
C	-3.45843900	-4.62280100	0.98866200
C	-3.83768800	-6.07154300	0.81927200
H	-2.27520100	-2.73052000	1.51045700
H	3.21866400	5.67552200	-2.37236700
H	3.57095100	7.13397500	-0.42473200
H	2.82407000	6.35858800	0.99834600
H	1.88233900	6.61408800	-0.49466100
H	7.74754300	3.35746400	1.16846200
H	7.43377700	2.47457200	2.65937200
H	8.58421500	1.80599400	1.47018500
H	5.26831500	-1.76885200	4.85271700
H	6.72275200	-1.14214500	4.04192800
H	6.28757000	-2.83972000	3.83535500
H	7.55509200	-4.69130500	-1.23091000
H	7.09811500	-4.07384900	-2.81855600
H	5.99922800	-5.18697400	-1.96832000
H	2.38593500	-5.12745500	2.23065800
H	0.97993000	-5.38715700	1.16472000
H	0.71537100	-4.99559100	2.86125500
H	-3.37688600	-6.68223400	1.59546300
H	-3.52105900	-6.42266700	-0.16688100
H	-4.92579600	-6.17199400	0.86599300

H	-2.36369300	-4.31936700	-2.87280500
H	-1.70933700	-3.15417300	-4.01848400
H	-0.59459100	-4.19787000	-3.08826100
H	-7.53513400	-2.38304900	-2.69700200
H	-8.00644200	-3.09404800	-1.15594800
H	-8.67121600	-1.50696500	-1.62638600
H	-5.18199100	1.47881300	-4.92019200
H	-6.09244100	2.69769800	-3.97066000
H	-6.66981800	1.03319600	-4.04669000
H	-6.08032200	-0.02164700	4.36292400
H	-4.40824500	-0.58356100	4.47089500
H	-5.70786900	-1.77449500	4.26979900
H	-7.22885000	4.92454200	0.89982200
H	-5.75373300	5.29437500	1.84248500
H	-7.05180900	4.28300000	2.53174500
H	-2.59687700	5.01170100	-1.97586100
H	-0.93159300	5.32543000	-1.39728300
H	-1.20231400	4.84407700	-3.07025300
H	0.79616900	0.73250900	-5.30438400
H	-0.63199200	-0.30639000	-5.52964600
H	0.92026400	-0.99178800	-4.94535600
H	5.84144300	2.00935600	-4.12943100
H	4.46430700	0.95434200	-4.47292300
H	6.08441000	0.24517700	-4.35321700
H	0.72911300	0.18948400	5.53512300
H	-0.87950300	0.77956200	4.99586800
H	-0.62611200	-0.93954400	5.31604000
H	0.47534600	3.74593500	3.34370900
H	1.73246900	2.70355900	4.07784300
H	2.21070200	4.09206300	3.10688400
O	-2.56862400	2.64910600	4.40530900
H	-2.07816300	3.29596600	4.92242800
O	2.50376700	-2.93245100	-4.34113800
H	1.93823100	-3.58452500	-4.76712000
H	-3.11826200	2.19097500	5.04930200
H	3.03777500	-2.57047900	-5.05558700

The optimised coordinates for Mn₈K₂(OH)₂ (Fig. S14(b)) are:

Mn	-0.52182700	1.18558600	0.64704400
Mn	-2.52062800	-0.38696200	-1.61614500
Mn	-3.88347900	1.91224000	0.01076500
Mn	-5.30445700	-1.01067700	0.15840700
Mn	0.52182700	-1.18558600	-0.64704400
Mn	2.52062800	0.38696100	1.61614500
Mn	3.88347900	-1.91224000	-0.01076500
Mn	5.30445600	1.01067700	-0.15840600
K	2.29468200	1.94557600	-1.83623100
K	-2.29468200	-1.94557600	1.83623000
O	3.80358300	-0.00568300	0.25006100
O	5.15729000	0.54700600	-2.05306400
O	4.64414500	3.16806600	-1.00056000
O	6.65219100	2.33139000	-0.69363500
O	0.47759200	-2.42347600	1.24837000
O	2.56624300	-1.86989100	1.83300000
O	6.79676800	-0.44219400	0.31377200
O	5.50493500	-2.11387600	1.07211400
O	5.49858700	1.71111200	1.66573400
O	3.98041700	0.62395000	2.92490300
O	-1.14695500	-0.36579300	-0.31637600
O	0.73040600	-0.18551400	-2.61912600
O	-2.43688500	-2.56386700	-1.49525200
O	-0.20186500	-2.77657400	-1.54558300
O	-1.41091800	-0.41061100	-3.23927300
O	2.27986300	-1.86326200	-1.03463700
O	5.05310100	-1.68564900	-1.85044800
O	-3.93736000	3.84361600	0.10820500
O	-2.69612800	4.24961300	1.93578400
O	-3.80358300	0.00568300	-0.25006100
O	-5.15729000	-0.54700500	2.05306500
O	-4.64414600	-3.16806500	1.00056100
O	-6.65219200	-2.33138900	0.69363500
O	-0.47759200	2.42347500	-1.24837000
O	-2.56624300	1.86989100	-1.83300100
O	-6.79676800	0.44219400	-0.31377200
O	-5.50493400	2.11387600	-1.07211400
O	-5.49858700	-1.71111200	-1.66573400
O	-3.98041600	-0.62395000	-2.92490300
O	1.14695500	0.36579300	0.31637600
O	-0.73040600	0.18551400	2.61912600
O	2.43688500	2.56386600	1.49525300
O	0.20186500	2.77657400	1.54558300
O	1.41091800	0.41061000	3.23927300
O	-2.27986300	1.86326200	1.03463700
O	-5.05310000	1.68565000	1.85044800
O	3.93736000	-3.84361600	-0.10820500
O	2.69612800	-4.24961300	-1.93578400
C	5.18460600	-0.64768500	-2.52826400

C	5.40852000	-0.73790700	-4.01296400
C	5.88474500	3.29518200	-1.08014400
C	6.53793500	4.52963500	-1.62112500
C	1.50035900	-2.57599200	1.95456800
C	1.51620000	-3.63662900	3.02229300
C	6.62380400	-1.50978300	0.94633400
C	7.79770800	-2.17027900	1.61585400
C	5.03524600	1.30154000	2.77203900
C	-1.39082900	-3.22854600	-1.67370300
C	-1.49326700	-4.67612000	-2.07372800
C	-0.17556200	-0.19095900	-3.48024300
C	0.19327300	0.05767100	-4.91895700
C	5.82625600	1.64455200	4.00092800
C	-3.43154500	4.62527800	1.01159000
C	-3.81187700	6.07448500	0.85786100
C	-5.18460600	0.64768600	2.52826400
C	-5.40852000	0.73790800	4.01296400
C	-5.88474600	-3.29518100	1.08014500
C	-6.53793600	-4.52963400	1.62112700
C	-1.50035900	2.57599100	-1.95456900
C	-1.51619900	3.63662700	-3.02229400
C	-6.62380300	1.50978400	-0.94633400
C	-7.79770800	2.17027900	-1.61585400
C	-5.03524600	-1.30154100	-2.77203900
C	1.39082900	3.22854500	1.67370400
C	1.49326800	4.67611900	2.07372900
C	0.17556200	0.19095800	3.48024300
C	-0.19327300	-0.05767200	4.91895600
C	-5.82625700	-1.64455300	-4.00092800
C	3.43154600	-4.62527700	-1.01159100
C	3.81187700	-6.07448500	-0.85786100
H	2.26005600	-2.74115600	-1.51779500
H	-2.26005600	2.74115600	1.51779500
H	-4.89798900	6.17659500	0.93617200
H	-3.52293600	6.42792300	-0.13586100
H	-3.32766900	6.68110900	1.62282200
H	-8.01536300	3.11137800	-1.10144900
H	-7.54397800	2.41628200	-2.64985300
H	-8.67639500	1.52689200	-1.58575100
H	-5.24040800	-1.47783900	-4.90394400
H	-6.71799800	-1.00985900	-4.02549200
H	-6.16201100	-2.68188500	-3.94496800
H	-7.27035700	-4.90749700	0.90312800
H	-7.07919100	-4.27676800	2.53768100
H	-5.79359500	-5.29606900	1.83554800
H	-2.53429600	-4.97593400	-2.19030000
H	-1.00958400	-5.29700000	-1.31415800
H	-0.95382200	-4.83327300	-3.01195800
H	3.32767000	-6.68110900	-1.62282300
H	3.52293600	-6.42792300	0.13586100
H	4.89798900	-6.17659500	-0.93617200

H	2.33215300	-4.33660400	2.81846300
H	1.72391400	-3.17343700	3.99122800
H	0.57002900	-4.17647700	3.06279800
H	7.54397900	-2.41627800	2.64985400
H	8.01536100	-3.11137900	1.10145200
H	8.67639700	-1.52689200	1.58574800
H	5.24040800	1.47783700	4.90394500
H	6.16200900	2.68188500	3.94496900
H	6.71799900	1.00986000	4.02549100
H	6.41195200	-0.37001700	-4.24734700
H	4.69603700	-0.09246900	-4.53352600
H	5.30502600	-1.76608000	-4.35821200
H	7.27034900	4.90750200	-0.90312100
H	5.79359300	5.29606800	-1.83555200
H	7.07919700	4.27677000	-2.53767500
H	2.53429600	4.97593300	2.19030100
H	1.00958500	5.29700000	1.31415800
H	0.95382100	4.83327300	3.01195800
H	-0.73172300	0.81789200	5.29621100
H	0.68832600	-0.22907900	5.53629300
H	-0.87287100	-0.91256500	4.97300500
H	-5.30502700	1.76608100	4.35821100
H	-4.69603600	0.09247100	4.53352600
H	-6.41195100	0.37001800	4.24734700
H	-0.68832600	0.22907700	-5.53629400
H	0.87286900	0.91256500	-4.97300500
H	0.73172500	-0.81789300	-5.29621000
H	-0.57002700	4.17647400	-3.06280000
H	-1.72391400	3.17343600	-3.99122900
H	-2.33215100	4.33660400	-2.81846400
O	2.47476100	2.84248500	-4.40714000
H	1.94426100	3.53399800	-4.81564400
O	-2.47476300	-2.84248400	4.40713900
H	-1.94426100	-3.53399500	4.81564500
H	2.99082600	2.47263300	-5.13065200
H	-2.99082900	-2.47263200	5.13065100