

Supporting Information

Revisiting magnetic exchange coupling in heterodinuclear complexes through the decomposition method in KS-DFT

April 28, 2023

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1 Structures

1.1 (1)

1.1.1 X-ray

Cu	2.76366750537716	5.25094054303288	10.42490024225420
Cr	1.30145180878724	4.72113061351623	13.95360066789094
N	-0.69720037702259	5.39392637967764	13.60559788460752
N	1.05931883231097	5.85676847484017	15.78220816965559
N	0.19832905108307	3.24293329712899	15.08768259352760
N	1.94883849639250	3.76888060459839	11.23546582648046
N	2.64707198907015	6.42125963199789	11.90910733385213
N	3.84587888585807	6.74690396330043	9.71907104366455
N	3.38032601246552	3.86264218881608	9.14866672538418
O	1.12614943909939	3.57977970313662	12.36010186323300
O	2.03089385540158	6.31754020325966	13.17794015435533
O	0.85771227729197	5.83456639260601	9.30850946694740
O	2.98085362618782	4.06463951662015	14.53694680339246
C	-1.05609520410961	6.43209035535718	14.66541918745401
C	0.10616393668157	6.92778371485414	15.35911579883155
C	0.48604210472663	4.90857628505094	16.81938456967863
C	0.64519981471499	3.53931575193399	16.46616813833278
C	-1.25852818497418	3.38057612942392	14.75413030954471
C	-1.56905296398500	4.25231449180181	13.62844900733944
C	-0.89322134086327	6.05287645953495	12.27767344441868
C	2.35035500120657	6.39796021690262	16.13301273672628
C	0.68248834581414	1.94538600536217	14.74544299054135
C	2.04593324781059	2.60020736617066	10.67381512959485
C	1.42271495406842	1.31108627509918	11.01114770145178
C	2.94614971612780	2.71622382225513	9.40565786237045
C	3.09490504092278	1.39173799328627	8.53311837486910
C	3.94708377071226	7.76961382118967	10.39558315064406
C	4.63782652268099	9.07698210072738	10.21841267558317
C	3.21082306827422	7.57015352953734	11.78442453036194
C	3.40433217554997	8.71883203882379	12.81176548362805
C	4.31718317397939	4.11694589325188	8.01990633991132
C	4.37410943029925	6.63146855951521	8.24021375322270
C	4.62545956425279	5.25369010121465	7.95181613878451
C	4.02684480724833	3.97699790548835	13.69012310436156
H	-1.76620618404348	5.96081257005541	15.36303577711124
H	-1.61442728237600	7.26146387269723	14.20541628354504
H	0.69047814572957	7.59365949529995	14.70894233844088
H	-0.19877262142740	7.53742229009443	16.23230318779745
H	-0.57317796041004	5.17581790900796	16.96056200927686
H	0.96017899725398	5.11558014284555	17.79349273892532
H	1.70705054996860	3.25345524374033	16.48694244235387
H	0.12181557094643	2.88662015845369	17.19210613200804
H	-1.76305883845646	3.74400764795674	15.66595402470852
H	-1.68630924527368	2.37850298298415	14.59604038707793
H	-2.63797972102862	4.53890430963312	13.64702101619741
H	-1.40439581110441	3.71776625864413	12.68035175837189
H	-0.31223075313540	6.98245715039313	12.24257805084375
H	-1.96089550085209	6.28071181829787	12.11861449569433
H	-0.53268759182560	5.39026665868124	11.48219429507015
H	3.03846291719066	5.58254943334721	16.38474045905425
H	2.27356010875403	7.09370267195000	16.99074639073132

H	2.77693104689385	6.92709651850829	15.27517321182610
H	0.38507301282159	1.67938652010872	13.72507417744869
H	0.28451248197622	1.17206307888436	15.43078366330262
H	1.77965217322354	1.92973365525274	14.79353372093968
H	1.59717164998711	0.55053741115156	10.24737082768986
H	0.33852304221284	1.44068388769219	11.16169588428116
H	3.49401134344998	0.57501867420257	9.15178943921249
H	3.75389411359647	1.53670388189204	7.66975473731312
H	2.09447520248489	1.10512011389377	8.17500493791947
H	3.91579900017592	9.90376798040788	10.29255605474690
H	5.15313967983203	9.16332386077853	9.25221726754439
H	5.37822064499299	9.21770478394680	11.01959380598474
H	3.15778314751472	9.68656150238994	12.35613086445905
H	4.46062264339264	8.73981376188945	13.12478162341874
H	3.72491781382726	3.74051005913095	7.14410238423323
H	5.13537499163571	3.38026278414297	8.08371618341334
H	5.28106011351334	7.23029089342870	8.11303256236835
H	3.56758116797839	7.10878905894518	7.64652690906787
H	5.61475520043820	5.27563068994796	8.50691090151323
H	5.09656972456080	5.38043353227916	6.94215083520089
H	4.94538587670370	3.66562975339731	14.23106541465432
H	4.29468071106231	4.93841255805490	13.19438970473552
H	3.89636974112714	3.22477947523851	12.87859855947079
H	1.81456340916106	0.93864424772625	11.97348451823466
H	2.78143290873053	8.56758097610736	13.69775249239794
H	0.28145212076384	5.24558127689697	8.79916093457314
H	0.46905387459111	6.71614812030952	9.20813739394273

1.1.2 Optimised geometry

Cu	2.86301792772240	5.17586917166928	10.44841240218980
Cr	1.19386139673246	4.78888541943906	13.81097073887710
N	-0.94942337191361	5.36877014501213	13.80579333909710
N	1.14472377784439	5.87549093554504	15.69896088897256
N	0.41884497992443	3.17670170138268	15.05791876485822
N	1.70959881602649	3.67258342833243	11.14784565371403
N	2.50663700682730	6.57876637083047	11.86149072865731
N	4.10334897884036	6.61359187110589	9.79463700460079
N	3.40484744906235	3.73076608020112	9.16069354201374
O	0.86389827182326	3.75960709162994	12.13997841432298
O	1.69712712082600	6.46694742253055	12.88229196401885
O	0.99314551891916	5.95430656493404	9.08713136553834
O	2.90209092411970	4.12360156051234	14.11079204366778
C	-1.20931593252006	6.27184922155439	14.97206247419237
C	0.07833548923401	6.89606513413528	15.50239797068503
C	0.81500015381069	4.91315407273679	16.80291038811832
C	1.04123120101208	3.46586404526469	16.38079289093248
C	-1.07698867124085	3.24075736750288	15.09994790662233
C	-1.64059449246644	4.05693096830486	13.94066273710556
C	-1.35036793628549	6.02622095120154	12.54067770638593
C	2.44146801185390	6.53980179462037	15.97530316241004
C	0.87062720034563	1.84607921482500	14.58220831998566
C	1.69774795500720	2.61858990079409	10.37845981499141
C	0.76162231597650	1.46843685040427	10.59017426059845
C	2.71704134386066	2.64162843432833	9.29245902648181
C	2.85881154155639	1.41768329749498	8.43547773676779
C	4.00468613057997	7.72220850261623	10.45530463511454

C	4.76575749861257	8.98259186280183	10.16215303894306
C	3.05353984834960	7.73548621304563	11.60294317972226
C	2.78602615159196	8.95883461150143	12.42501311805981
C	4.44907311970713	3.91883081984866	8.15426585916965
C	5.00070044676340	6.40290370156145	8.66108175049114
C	5.49376765174850	4.95723579191917	8.56592576782714
C	4.16079889668596	4.41323510905606	13.59596580105205
H	-1.71437688074827	5.70299910762346	15.76355130185082
H	-1.91018557560651	7.07260094635669	14.68837957353335
H	0.46743983952412	7.62494476433690	14.77842031178384
H	-0.12501677510738	7.44036001560119	16.44320976786666
H	-0.22428832455113	5.07213644425709	17.11975990314919
H	1.43222547274435	5.13014461826028	17.68815791963685
H	2.11556060820510	3.27516913960978	16.26383545980943
H	0.65046600539980	2.78151264980231	17.15594746570716
H	-1.39397990179557	3.66519916357988	16.06123434172023
H	-1.50332674907823	2.22609740722742	15.06954066798442
H	-2.73012143349248	4.19309833528617	14.07053377576454
H	-1.48460967713237	3.52017062306214	12.99460017714629
H	-0.83281145000406	6.98882270695242	12.44697355795028
H	-2.44077082946124	6.19668111348701	12.51518626686775
H	-1.05994428633121	5.39407088022649	11.69188369593415
H	3.21758200818149	5.77800171461018	16.11427726020550
H	2.37092051418827	7.16485616931139	16.88211711708016
H	2.71537971343836	7.17026622977616	15.12093191429605
H	0.39555669134399	1.62244494710449	13.62014049344844
H	0.59974201042998	1.06371133329700	15.31170068261572
H	1.95843602969305	1.87051900770231	14.44426330926149
H	0.51033959482730	0.96353162691341	9.64812146575219
H	-0.16622288936414	1.82058225957983	11.05872137366159
H	2.88391201084224	0.50848176211019	9.05456634899434
H	3.75194421018455	1.43567742992934	7.80187804778708
H	1.98113315145087	1.32445649583873	7.77215401474684
H	4.08173846816910	9.74165997290059	9.74347748448480
H	5.58044851151892	8.83939453689332	9.44446341798062
H	5.18376162254343	9.40886179999444	11.08672780095542
H	2.88458510976651	9.87916677054670	11.83529061972485
H	3.49140353324793	9.03281874215727	13.27153468289668
H	3.97093318714158	4.22984676175821	7.20629847495822
H	4.96587074956425	2.96848017444605	7.95011022817802
H	5.87549121531276	7.06720762934664	8.72452620435034
H	4.46283617738665	6.67552718405771	7.73330355464972
H	5.96507312941803	4.65928994563081	9.51828142777134
H	6.29297668866117	4.93170810774153	7.80781999358256
H	4.92687366389410	3.79691936665521	14.10048924556984
H	4.45370542249181	5.47458316499507	13.73223480031746
H	4.24743900211042	4.18700994434470	12.50865796923881
H	1.20862999886950	0.71224928984198	11.25992089500452
H	1.77271713643123	8.91532254661505	12.84406172016326
H	0.51268950675702	5.40134277826467	8.45397323134802
H	0.89157706799604	6.85843876332290	8.75574763808067

1.2 (2)

1.2.1 X-ray

Cu	-0.35449955198693	7.79414544205942	19.50400503948715
Mn	2.63481813763938	6.15974312216652	18.54396231498957
N	4.76178569993520	6.80404261725285	18.98691497479860
N	3.50444991180430	4.27015549373308	18.99463395758036
N	3.46844019139722	5.77698785217562	16.65113688488782
N	0.97848069023099	8.44102259069217	18.16446428437634
N	0.88911894464339	6.76298671928094	20.66873403862947
N	-1.47707323211501	7.65069576806137	21.10221073456224
N	-1.37675089457399	9.27182124195811	18.65695051048612
O	2.25410071752577	7.96297643569064	18.01899805095681
O	2.15163951876369	6.33955071355770	20.37523731914849
O	-1.17711506242647	6.24049506447927	18.23880644495996
O	0.82181674542948	5.31305150859629	17.92665570855229
C	5.54991504378234	5.65114733314887	19.44353523568948
C	4.62301921207105	4.57502839766088	19.91338394052993
C	3.98585354650430	3.63645384182554	17.72448874447560
C	3.40102857670358	4.27540422722569	16.52771794481712
C	4.86194913241996	6.31496083950497	16.57117660198273
C	5.20652835474526	7.27058094844007	17.62790842148492
C	4.80423604900398	7.94073956599577	19.97850877874557
C	2.52382929481915	3.34858953085571	19.66311022377892
C	2.63805355389245	6.36522734991758	15.55037748175909
C	0.62594849412816	9.45052987600467	17.44127120256207
C	1.50134340838899	10.09590897901050	16.44461946045893
C	-0.77137003137981	9.85547196040324	17.67887609045475
C	-1.36267779493977	10.87682048941672	16.76326306737840
C	-0.92380761796747	7.07231656445838	22.09743097140958
C	-1.54354767288274	6.89882928477559	23.46550041384287
C	0.47132594053977	6.55679272295427	21.87299240320346
C	1.29617766188045	5.85152500408105	22.87026956924366
C	-2.80732204350009	9.59240410540547	19.01468377035980
C	-2.82274898447274	8.23947313991105	21.17880362512635
C	-3.05157310086533	9.53337669662538	20.33107632496830
C	-0.39292675621822	5.44637411513724	17.65893102210707
C	-0.94263046171759	4.56567530309855	16.55063646323873
H	6.20618946367204	5.29348893136203	18.63581557427284
H	6.22901879484841	5.92399766491999	20.26783234283466
H	4.15788398963125	4.88672816077425	20.86095463485109
H	5.18573987634821	3.64900572227088	20.13634377560132
H	3.75303254052940	2.55989336022832	17.72897640331076
H	5.08389824393506	3.69364682785085	17.70132983976025
H	3.91179193783096	3.94448579244489	15.60615860595766
H	2.33560493563407	4.02892119760635	16.43213952236694
H	5.01653790423861	6.78458252902496	15.58665402232053
H	5.55447300579340	5.45949713938421	16.57775537776390
H	6.29387711033362	7.47336757501342	17.61251347317134
H	4.70721478189837	8.23578789445478	17.45773106207977
H	4.12001511817221	8.73034300959396	19.64436905663533
H	5.82743133944094	8.34383528958924	20.06939269632258
H	4.46645606527987	7.57435099035691	20.95585914723647
H	1.68852152719138	3.16075885851602	18.97950934595759
H	2.14232987006462	3.83016851731737	20.56974902796428
H	3.02059198685046	2.40133384105114	19.92816923730777
H	2.68228219591392	7.45773228280614	15.60691388324820
H	1.60010192718197	6.03703217311561	15.66646949280295
H	3.02392918042587	6.02913723740841	14.57373636026268
H	1.36875778358203	11.18799678881396	16.43500061622408

H	1.27065998233486	9.73873113636608	15.42513941102107
H	2.55365383852414	9.87049782216070	16.65340413129493
H	-0.94757345803161	10.78858762177097	15.75022350573368
H	-1.12162950179883	11.89593629922335	17.11746820991055
H	-2.45335853442792	10.79748989515684	16.68493022380607
H	-1.26684291993857	5.92542902708884	23.89509296809610
H	-2.63690886038494	6.96051986770275	23.44803114528886
H	-1.16085504395822	7.67646340445971	24.15086036709904
H	0.97474357852042	6.05313425997331	23.90015806074475
H	2.34995134959785	6.14345618344034	22.76613663052403
H	1.24271275953316	4.75801613519525	22.71843281289239
H	-2.03721967947463	4.50027392291680	16.60160377822330
H	-0.50228658310420	3.55908820120623	16.59101558183340
H	-0.67632776279527	5.00618680377944	15.57397165748274
H	-3.08717337951800	8.48535417220275	22.21507708945521
H	-3.52667437241582	7.45894635328362	20.83295766537957
H	-4.11104237269437	9.78335768932551	20.51748442438000
H	-2.50192114329257	10.33677208585503	20.86221602788370
H	-3.41107706980587	8.86773305164283	18.42932643473193
H	-3.06125602686911	10.58462943778403	18.61285435493101

1.2.2 Optimised geometry

Cu	-0.42514727334690	7.79744781692613	19.40856719482002
Mn	2.58702586607219	6.14768819791618	18.43795974598449
N	4.79636338654549	6.84359123408208	18.94363305128277
N	3.50192495272334	4.24180063122407	18.94634018549775
N	3.55868436887054	5.75854313037908	16.53210816193726
N	0.97813850447715	8.48037749970935	18.10350095184245
N	0.86312188760544	6.79927959173238	20.62413526199526
N	-1.54505566148667	7.67761986085634	21.08325808647526
N	-1.43970213106754	9.32511612723738	18.57181750831532
O	2.17786191453727	7.96114589832659	17.92030842903116
O	2.05766395542868	6.35241422183226	20.28390891628889
O	-1.12223198608353	6.15132227519324	18.30103097951474
O	0.84779927928841	5.25219330257064	17.73376668487211
C	5.52344125487438	5.65612458093446	19.45547132231804
C	4.56401882488597	4.56936696465488	19.94431340451660
C	4.06414169233570	3.61981572561753	17.69828054768224
C	3.49599781800597	4.26965763399303	16.44439423230343
C	4.97394624898550	6.26368262955936	16.52496781701833
C	5.25229093598406	7.29774965956902	17.61471248098845
C	4.80855694784306	7.94985872538543	19.91857353985845
C	2.49931893209153	3.33198086253039	19.55826351486939
C	2.79151767497723	6.35958152759109	15.41307418857162
C	0.64228025958889	9.55772061982879	17.45976533754133
C	1.55528074776173	10.28082099777222	16.51851556749525
C	-0.76790003837381	9.99828828615101	17.69913362970023
C	-1.27598228486558	11.15621656522834	16.88804280837614
C	-0.95403839123190	7.10986421985543	22.08055910874499
C	-1.54925238560047	6.84354000924465	23.43332295139751
C	0.44841816288564	6.64256494804366	21.84539875032831
C	1.26880973172978	5.99746237731010	22.91941859774437
C	-2.83854417406296	9.55786122281648	18.91253260412114
C	-2.92798949797531	8.14214420763612	21.08367809896070
C	-3.09160097775808	9.51409563737360	20.42277876578476
C	-0.43540963983053	5.28009851116028	17.72370711916624

C	-1.13927094375055	4.19540942490490	16.93652362374539
H	6.19150164772161	5.26276080998012	18.67654690128870
H	6.18704132435536	5.93413138488895	20.29081257125396
H	4.04536133644353	4.91094566220947	20.85040806946577
H	5.12764438969642	3.65752127440025	20.21030279851102
H	3.83989754320950	2.54216408343594	17.68303240300980
H	5.15846700637420	3.69933480826530	17.72164069419414
H	4.03765690453682	3.91174219109885	15.55065275867774
H	2.43828696336280	4.00265282417939	16.32879421171248
H	5.20109181071327	6.70628861515658	15.54269494860195
H	5.65448868879644	5.40952220912991	16.62837424672575
H	6.33256300152806	7.53951088101114	17.60841690048649
H	4.71336531586755	8.22924786045295	17.39041625066351
H	4.16289074532109	8.76274541697972	19.56088586294324
H	5.83000224712861	8.34226287439859	20.07307575793980
H	4.41311906998447	7.60054391075243	20.88079705328661
H	1.71078933178149	3.11816829674120	18.82876308605948
H	2.05081942527098	3.81820881827208	20.43223815598842
H	2.97993033002829	2.39102856431046	19.87331798973091
H	2.84931308445924	7.45199075696103	15.47738048701914
H	1.74138021172439	6.05355507355502	15.48600697068482
H	3.20424763166250	6.02787156723317	14.44547773017442
H	1.48108795361034	11.37058571189342	16.64855165132774
H	1.29567757263046	10.06192824647597	15.46761132477404
H	2.59539032675985	9.97548278095124	16.68319366357485
H	-1.03058011731022	11.01549524780785	15.82394359335876
H	-0.77850001571573	12.08769266235701	17.20766189501403
H	-2.35775499849347	11.30195759823176	16.97051709481780
H	-1.43028686334252	5.78090247773266	23.69658971234456
H	-2.61293623128433	7.09267757249222	23.49854220885657
H	-1.01236469181802	7.42239723637211	24.20272397018968
H	1.12422257787285	6.49422238904898	23.88874098928718
H	2.33413209723267	6.03430060826367	22.66090629745217
H	0.98591279133900	4.93819306060966	23.05166008141169
H	-2.21076802764922	4.17010790523536	17.17026837577056
H	-0.68523750864189	3.21268744414135	17.13301129715333
H	-1.01968059239170	4.39915470174885	15.85860037692822
H	-3.33649441867859	8.19175640420271	22.10285420101073
H	-3.52411157044256	7.39368839204653	20.53026092616694
H	-4.13406093557423	9.83081722046651	20.58621139779630
H	-2.45789758996805	10.25839605062041	20.93414269883307
H	-3.43251807022716	8.76859243976782	18.41681195086474
H	-3.19249765993856	10.52232084097324	18.52242727555402

1.3 (3)

Cu	-0.41252984646625	7.87716001787187	19.46135503548289
Mn	2.56277110050203	6.15316943557589	18.42005709961383
N	4.83396910103445	6.77675220812177	18.87873468798177
N	3.62817242937164	4.08765938029672	18.92499521344200
N	3.70854659890538	5.62848383921711	16.40943933368895
N	0.98328482477079	8.66417895968094	18.15437373008498
N	0.85554292713254	6.89155752063135	20.75856906836533
N	-1.60090670234409	7.73202451087564	21.13128908578680
N	-1.49393618702271	9.39613822351277	18.60744075890219
O	2.17131641544684	8.20181006451019	17.94084931129445
O	2.03100929519378	6.43388681697193	20.47832018138993

O	-1.10036994579782	6.21850112898329	18.34226309374194
O	0.81703922547511	5.25001894413918	17.68751591865157
C	5.56940379720874	5.60863905536017	19.41501510223071
C	4.64504195783662	4.49180121599878	19.91602623768615
C	4.19455866852344	3.51310959973425	17.68060751298913
C	3.62806858464984	4.15421013195238	16.40735592734091
C	5.09257855820927	6.15603935926724	16.45653602307950
C	5.29591755915041	7.21450458229070	17.54712069425300
C	4.82320994029895	7.89747463863493	19.83133532780593
C	2.61945339012003	3.20040024643486	19.52352442218056
C	2.94102740637798	6.20506387194789	15.29530483457421
C	0.57907706786249	9.73429919749555	17.51279349183923
C	1.48846781736007	10.45673292990947	16.56319693787301
C	-0.83133896040068	10.10264416363989	17.74769775905512
C	-1.38899891848350	11.24712058362225	16.94051647850832
C	-1.02059830427691	7.17667312173690	22.14789913768794
C	-1.66445458009804	6.91158959214445	23.48453704119295
C	0.37456156695273	6.72850546153700	21.96786106847749
C	1.19521715519596	6.05645232977202	23.02831419966338
C	-2.90239251999191	9.56344143304584	18.91894949313564
C	-2.99142549799437	8.15095220623033	21.09026546971162
C	-3.18438037005526	9.51693874323865	20.42430060659623
C	-0.45509233499054	5.33624125475043	17.73425227474467
C	-1.23295819981420	4.28466099755053	16.95884076242877
H	6.25019224777301	5.21767222361552	18.64503603197313
H	6.22452851368702	5.91268678076543	20.24998282190341
H	4.09770096409731	4.84438109229839	20.80401655685512
H	5.26682148315282	3.63042945423451	20.23674748429263
H	3.99918488131768	2.42737716609260	17.63342079102251
H	5.29009463121129	3.60818179961647	17.69889211937606
H	4.14808898252757	3.71973545915962	15.52831686645078
H	2.56159766430364	3.89942458351533	16.31850374097126
H	5.37080238540361	6.60156549366511	15.48518083234784
H	5.79621227450384	5.32453457825772	16.60216918305570
H	6.36575506128264	7.50973296382043	17.56277758835779
H	4.71756909295196	8.11591114246771	17.29124141805676
H	4.17227212573228	8.69522128850468	19.44830248169784
H	5.84004009160511	8.30373030181642	19.99972359313481
H	4.40773226076166	7.56169240566358	20.79079084399248
H	1.83791413650454	2.98207152795620	18.78374978307316
H	2.14509320078613	3.71009317978061	20.37393459694853
H	3.06264057316218	2.24841071861487	19.87590977702170
H	2.95498042668142	7.30171544604903	15.36741895460774
H	1.89582529369059	5.87382107545324	15.36419775786962
H	3.35116507103628	5.90355628810050	14.31107746086605
H	1.20600045403890	11.50930726058415	16.43294895003226
H	1.48942818880017	9.98127908627249	15.56566117449888
H	2.52025350956783	10.40728934720095	16.93893224049798
H	-1.16019930638883	11.10446234699162	15.87278691594361
H	-0.91012993940853	12.19270325386820	17.24489539309052
H	-2.47261329963548	11.36529074907934	17.04313146007147
H	-1.59436080166572	5.84016361506054	23.73040051007325
H	-2.71915001039543	7.20083076187591	23.52619312728865
H	-1.12709677614142	7.45608294861526	24.27731385625383
H	0.80198356006982	6.22545599921857	24.03794881905037
H	2.22951736176174	6.42860024118255	22.98308014468232
H	1.24759304292355	4.96572060866127	22.85990565124624

H	-2.29503064574554	4.29519511004589	17.23599883459550
H	-0.80518489123862	3.28474591311370	17.12697062072924
H	-1.14643579872371	4.49717490291014	15.87953420228039
H	-3.44003079981387	8.18938525327435	22.09456355205714
H	-3.55323397740987	7.38964632835020	20.51705367138468
H	-4.23800791027908	9.80697028689795	20.57089189165177
H	-2.57433232170949	10.27592502105513	20.94342836959979
H	-3.45611121062822	8.74423706024964	18.42332327185968
H	-3.30285280999388	10.50675316935960	18.51722333775228

1.4 (4)

Cu	2.77031206776782	5.26010275722342	10.34581248374374
Fe	1.22897242343180	4.86170412021233	13.70925777441106
N	-1.00519635979173	5.35316448609994	13.80508819876958
N	1.10261307404681	5.97519029836747	15.68715041336392
N	0.47558108810561	3.20851482361350	15.07086872623991
N	1.64253745913345	3.71154701750422	11.06070346882877
N	2.41539645542408	6.68492700322306	11.77081907742000
N	4.11992070468529	6.66855487648282	9.78422715053476
N	3.34996862692355	3.78039975462190	9.08010042905626
O	0.79980875053428	3.78966736796141	12.06068091763023
O	1.53157977597293	6.59060692664759	12.73417080017479
O	0.93609762071641	5.99563786487758	9.09557936245541
Cl	3.41516300341917	4.26064562915279	13.83804825891128
C	-1.27757135892374	6.24910674773616	14.96755234593149
C	-0.01090122193585	6.93593170709792	15.47071948137858
C	0.81776048341541	4.99977855305864	16.78551692208933
C	1.10086357509543	3.55651980157185	16.37530691053627
C	-1.01852316887241	3.22855666783631	15.11723462883073
C	-1.62469520235368	4.01227598084625	13.95509922507447
C	-1.43312340786238	5.98472967803606	12.53712489654186
C	2.36225351502235	6.70995250038885	15.95574882091676
C	0.96423813455877	1.88677412433035	14.60885178519578
C	1.70750019456388	2.62262795822975	10.34850653464081
C	0.85881753638328	1.41864318887829	10.61780943299405
C	2.72234058323995	2.66294112909118	9.25238302747974
C	2.91698196555670	1.41620736670357	8.43904867382125
C	4.07573358277026	7.75237086207728	10.48747245248369
C	4.92068749134276	8.97354553301282	10.26740617577675
C	3.08486217229355	7.79077116343172	11.60594356567413
C	2.90884135338169	8.99432235568804	12.47854680557186
C	4.37084306232491	4.00827530459719	8.06053248350634
C	5.02039636811615	6.45145865555666	8.65518059975419
C	5.45381080016527	4.98985910629930	8.51518423923516
H	-1.74216118915430	5.66544817704252	15.77301687226707
H	-2.01804919789952	7.01738621497524	14.69365204073917
H	0.33925251662363	7.66568909841923	14.72725333179847
H	-0.23446278243441	7.49383561520000	16.39988122193778
H	-0.22627471730218	5.11360091286079	17.10579909706460
H	1.42643862834105	5.24149881858840	17.67101104441321
H	2.18347200361913	3.40503467217653	16.26053694174058
H	0.75240801965762	2.87159326607668	17.17109712981068
H	-1.34566214108897	3.64932956888357	16.07709437091971
H	-1.41240051388826	2.20011790586112	15.09895822334163
H	-2.71864085358913	4.09656944549775	14.09690679024600
H	-1.45628798693665	3.47715378229926	13.00972591617880

H	-0.99513419670885	6.98805258123696	12.46340658726834
H	-2.53379874279490	6.06468683092751	12.48964020841464
H	-1.06706902420585	5.39097025196854	11.68936185354653
H	3.18440168649494	5.99854720730470	16.09975855510827
H	2.25786531529533	7.34115004764734	16.85593675336493
H	2.60560165757485	7.34515997061490	15.09509559589855
H	0.49481469329897	1.64246821885953	13.64836433104514
H	0.71428949495478	1.10183410025715	15.34417057154738
H	2.05227975010797	1.92415889024301	14.46770354809668
H	0.58862814983580	0.89264300563271	9.69208637464889
H	-0.06113025625900	1.71786733752144	11.13508579971824
H	2.99130506517293	0.53351146626668	9.09161142448899
H	3.80453828279012	1.45215553760653	7.79842879206172
H	2.04077555575308	1.25675838484559	7.78660243642257
H	4.29863907110389	9.78402931053894	9.84834993129240
H	5.75370112844787	8.80474574556352	9.57701565068447
H	5.32598967323841	9.34533067927508	11.22038901171555
H	2.94039071894188	9.92596214994622	11.89643040859939
H	3.71168601593288	9.05549037871222	13.23429872139133
H	3.87116811488702	4.39911118092954	7.15404899205639
H	4.85345650100511	3.06306008181951	7.77022561356480
H	5.92130860922500	7.07694034341316	8.74453098981449
H	4.50065920556751	6.77583081906342	7.73373956690923
H	5.90551744568845	4.63934006938992	9.45912041786351
H	6.25664695973865	4.96003635957821	7.76080111040962
H	1.39168931823437	0.69672332081545	11.26221770766465
H	1.94916749578147	8.93784290954296	13.00543283488282
H	0.42095318129089	5.49506153523693	8.44628541712066
H	0.59627619500623	6.90060249690360	9.04136174496574

1.5 (4a)

Cu	-0.40407961217047	7.87936779260820	19.45495163755998
Fe	2.55445730839809	6.12762971669394	18.41132924936701
N	4.66508255246021	6.83475554059126	18.91973355210751
N	3.55953513546685	4.16054349844517	18.92251644382352
N	3.63568925909654	5.69070380580438	16.46900525468975
N	0.97378109860960	8.53881665247875	18.07675253255166
N	0.85648678800972	6.80493628382038	20.67100210408868
N	-1.54091434425457	7.73210149940005	21.13477060716826
N	-1.41291702435371	9.42684354149217	18.62558906352866
O	2.15860390320388	8.00150830819855	17.87197379428629
O	2.03023442462846	6.31913613710886	20.32186356286698
O	-1.02124861533011	6.17553424080139	18.31530870782215
O	0.94053208080080	5.26413599536892	17.73583123495790
C	5.45503628589704	5.69406716916629	19.47259670137008
C	4.56533965305124	4.54605980745534	19.94571450769032
C	4.17712865978714	3.57952852238969	17.69121219814759
C	3.61919202346637	4.20572097605418	16.41559883303248
C	5.01839054585631	6.25561352808675	16.51342825228421
C	5.17786650058655	7.30798725010859	17.60795978814484
C	4.61268731443098	7.95618815103919	19.88569868151129
C	2.56254918459124	3.22818520297530	19.49714602760784
C	2.87231158249989	6.25339400288110	15.33170908405566
C	0.60917493609120	9.58528216575855	17.39170499439057
C	1.48537303757022	10.25035983856403	16.37663518258078
C	-0.77857656981601	10.05220017752448	17.68920976800351

C	-1.37435103080208	11.17949694234105	16.88885347876443
C	-0.97135067871907	7.11934262726170	22.11923099954483
C	-1.57893005988767	6.85295703983783	23.46680730889379
C	0.41097297677557	6.60160319788622	21.87733027998319
C	1.18531599320599	5.85909198569499	22.92149308383457
C	-2.78164462611753	9.74207127778346	19.01697102898637
C	-2.89980218106648	8.26171061342272	21.14790393568639
C	-2.99794396273414	9.66082115686075	20.53098437149844
C	-0.36012725652637	5.30282097724804	17.73908824855499
C	-1.04981450358271	4.19205942510486	16.98391640673859
H	6.16577891788510	5.34265309724528	18.71263355077398
H	6.07520369093391	6.03452514588109	20.31728159433326
H	4.00650261384730	4.84905191215817	20.84255554935054
H	5.19466965035651	3.68103549047761	20.22604902424449
H	4.00494330250053	2.49159147250920	17.65820876595015
H	5.26760767659059	3.70307940754293	17.74010854901168
H	4.18799825398490	3.83710654936807	15.54163172652636
H	2.57164139763108	3.90418128152905	16.27794124248391
H	5.27537749335223	6.70749779609880	15.54184052179241
H	5.73853256180698	5.43924276062713	16.65490509722532
H	6.24029960534097	7.60595766847071	17.68310750447579
H	4.60562507595883	8.21000166481202	17.34808612086504
H	3.94697418104159	8.73948176599828	19.50171906207831
H	5.61915477120071	8.38004957836934	20.04850607596870
H	4.21279607412764	7.59857319739562	20.84222934284011
H	1.81661872668789	2.97557673028608	18.73387958916858
H	2.05160255275116	3.71164533642924	20.33926869103409
H	3.04925249135562	2.30266103392027	19.85121340015111
H	2.87444127364459	7.34851112975305	15.39421330665864
H	1.83422348984017	5.90156476566261	15.37740590611631
H	3.31638595324915	5.94259693592315	14.36958951130276
H	1.49698345459719	11.34232570144733	16.51738848586794
H	1.12642290294585	10.05702119359516	15.35073985982750
H	2.51107219074074	9.87388198274511	16.45831543968804
H	-0.72117911211582	11.50811268369501	16.07363757723234
H	-1.57033085649031	12.05271609526087	17.53419522624895
H	-2.33775165683221	10.87634621135870	16.45036418503632
H	-1.49451561568833	5.78376926824943	23.71614134552692
H	-2.63438197943938	7.13444647316089	23.53332777691541
H	-1.02539039789008	7.40455283451516	24.24465616545075
H	1.04382666952805	6.29854856179266	23.91851722474786
H	2.25469245365720	5.87051476220927	22.67779258895379
H	0.86167442182932	4.80471510451845	22.98004392516587
H	-2.13809973568224	4.32877689504244	16.99820358765632
H	-0.79496912065026	3.22076997717211	17.43826973560157
H	-0.69095121254355	4.16260618958102	15.94313402704838
H	-3.30828220660389	8.29859420523175	22.16785022571456
H	-3.53184012665306	7.55989720825938	20.57301011880384
H	-4.01401580707573	10.03571353270501	20.73436708534549
H	-2.30600912469759	10.34824350886421	21.04689445744357
H	-3.45003593439624	9.02203611910002	18.50833858715338
H	-3.07151973975020	10.74525172278029	18.67164733609424

1.6 (5a)

Cu	-1.94887209298901	0.00340039883802	-0.00266436114211
Co	1.63498380932708	-0.00349692629127	-0.01111061776448

N	3.01112957151721	-0.10129548474461	-1.80573642566037
N	3.19310865926899	1.50708114784170	0.60755508945224
N	3.20651165313066	-1.42049932036887	0.77874139902515
N	-0.78106451762450	-1.57421740644829	-0.62897085585685
N	-0.77314854496466	1.56080144796145	-0.64533553030865
N	-3.31958650763010	1.52114217115378	-0.04214257642362
N	-3.34548716212043	-1.48328070865625	-0.10493069151045
O	0.49121764423011	-1.51810455612547	-0.84145456351352
O	0.50026170436042	1.51324634014329	-0.85778459939131
O	-1.47805115269186	0.00622417015059	2.04474364048266
O	0.76252440793280	0.00333526494297	1.87235335204200
C	4.04165267845917	0.95819087367887	-1.68044425970095
C	3.63288885955842	2.05387427821666	-0.69228901790472
C	4.26704369039439	0.78428408274649	1.33876735474289
C	3.82631628204415	-0.59527009509813	1.83929364383188
C	4.13962873304330	-1.77049209407570	-0.32070098392279
C	3.55376363511858	-1.47117965702239	-1.70328608804112
C	2.22017057160386	0.06086425234911	-3.03735041971375
C	2.58239736831409	2.55208512406209	1.44423529989500
C	2.56368788512998	-2.61493304718201	1.35017091376715
C	-1.44103658409071	-2.69042752214381	-0.83568912472789
C	-0.77002282699885	-3.92899481849171	-1.35467384426002
C	-2.87144758140487	-2.62979022147741	-0.47740947367236
C	-3.70240192896005	-3.89006180929220	-0.51901427201159
C	-2.85016781451124	2.64896667868838	-0.47067389440429
C	-3.62511082697962	3.93761249078095	-0.57217590511363
C	-1.42353893108991	2.68011458064510	-0.85589430873741
C	-0.71527274141047	3.89791944869240	-1.37290924319111
C	-4.71355119131261	-1.29239464995866	0.34566066841328
C	-4.66141998675504	1.29916281411497	0.46545689345031
C	-5.31295670403864	0.03903527250500	-0.11779653783149
C	-0.32421857552317	0.00705479698845	2.53273897849677
C	-0.19187560327935	-0.00574503101839	4.04939277388901
H	4.99510719022758	0.50647921510206	-1.37418759280603
H	4.24204354715819	1.42355822275310	-2.66085670982560
H	2.78091657817916	2.61604159694331	-1.10229482537827
H	4.47445902654019	2.76651734293180	-0.57116357695723
H	4.60772898747517	1.37688243960259	2.20479181958482
H	5.14837586521637	0.68735896612858	0.68861180774731
H	4.69787381027431	-1.10979912036206	2.29260904172453
H	3.06376853253262	-0.47055677652049	2.62034676809712
H	4.40863194427189	-2.83971373999526	-0.27582919374553
H	5.08533366866084	-1.22691800732568	-0.18420162081991
H	4.32684422257948	-1.66122310722672	-2.47591146524043
H	2.71744614805903	-2.15726886263415	-1.90146380656727
H	1.38924792553068	-0.65748611247683	-3.03453271508991
H	2.84064615081655	-0.09674942359286	-3.94115296516392
H	1.78891619095655	1.06988631520532	-3.06594670858053
H	2.20623683412875	2.10237265723248	2.37202269949006
H	1.72712228662131	2.98824595542028	0.91133586993585
H	3.30720950022187	3.35135466094845	1.69130103808031
H	2.06259693479945	-3.17858209334036	0.55162918178294
H	1.79899123187877	-2.29935679695073	2.07128362573990
H	3.29813854411861	-3.27212783981047	1.85565852774114
H	-1.36034504895785	-4.40522462037544	-2.15232694231878
H	-0.61985283931612	-4.67957368372404	-0.55884758011152
H	0.21484504356124	-3.66377229285511	-1.75673697485767

H	-3.11247601180033	-4.76718766837149	-0.80496811735270
H	-4.53071173064904	-3.79061423550089	-1.23996417169600
H	-4.15026134569939	-4.09126274132343	0.46715220615148
H	-3.11037201278964	4.73319138175667	-0.01111391216900
H	-4.64837357961217	3.86070727989986	-0.1916222235457
H	-3.67171430474318	4.26794807231243	-1.62248069092854
H	-1.40350851505857	4.62932135515371	-1.81497791924141
H	0.02159203427352	3.59961192171881	-2.13278147068801
H	-0.15294567407732	4.40688459823718	-0.56915948023643
H	-1.17001526860600	0.10202816629378	4.53461150490324
H	0.48138584957379	0.80026846198292	4.38081002121345
H	0.26491126833439	-0.95699271336689	4.36932681298723
H	-5.32320423024160	2.15707508335050	0.27002172562077
H	-4.58684170807991	1.19317123974156	1.56387513114658
H	-6.37339105702804	0.04468184745781	0.18507024440558
H	-5.29897707647353	0.09136496714262	-1.22034896388965
H	-4.71458767186400	-1.32319900250926	1.45252216996024
H	-5.36964712005178	-2.10915519515875	0.00421701702252

1.7 (7a)

Cu	-0.33495980191822	7.85764502051730	19.45088327441128
Ni	2.66312718313450	6.12405892386586	18.43811018546302
N	4.70055683427874	6.81025382631941	18.91678714047116
N	3.52168014084707	4.16374651633446	18.94934080303183
N	3.59176080684046	5.68665185914051	16.48846249339511
N	1.03112886453893	8.55177780982790	18.10176941518130
N	0.91662458580124	6.84050515847432	20.69115892746005
N	-1.50789460175729	7.71395506778286	21.10463109269666
N	-1.38297218932087	9.38780137046489	18.63485939770512
O	2.20330351849846	8.04866490357106	17.89841942126291
O	2.08313179343058	6.37397476070005	20.38736347375261
O	-1.01903771901168	6.21754687322709	18.32074633956727
O	0.93211848783163	5.24538059170818	17.75519572242531
C	5.46209352335668	5.65521504496958	19.45806331813132
C	4.54482027733127	4.53299043200929	19.95048837852175
C	4.09728329893053	3.56967349291779	17.71407328018902
C	3.53531913931972	4.21044499395400	16.44356739918220
C	4.97928401234038	6.21713103405905	16.50490033235294
C	5.18846338482190	7.26664557099620	17.59785400858658
C	4.67352372569069	7.92771969834088	19.87631606205312
C	2.50406355310432	3.27671415258391	19.53738150644322
C	2.80830685579611	6.27356272578485	15.38891910422353
C	0.64590460143005	9.61602271156879	17.43607892946060
C	1.54293811824997	10.30961421740094	16.45263403816018
C	-0.74360427024560	10.02716414984419	17.70600955778925
C	-1.37212000144006	11.12119718667132	16.87727057134537
C	-0.92739172440450	7.14131604551774	22.11199613143826
C	-1.56229575700010	6.87326970487790	23.45182614594367
C	0.45861392979649	6.67489034068257	21.90881869774050
C	1.28651144405472	5.98731866612367	22.95381991718006
C	-2.77560076655850	9.64565286724017	18.96083728292957
C	-2.89247931448381	8.15459183773798	21.07535731088524
C	-3.05885027890489	9.54850525629273	20.46204082571557
C	-0.33445114299229	5.33546895514227	17.74602506829622
C	-1.08304217687787	4.29095335861435	16.92827848081065
H	6.14934198681643	5.27711671033609	18.68816337406261

H	6.10706048478462	5.97556226178349	20.29363688468928
H	4.00191827108294	4.87212994633978	20.84337056700189
H	5.16024397966808	3.65922212170734	20.24331604636130
H	3.89665917373046	2.48534884827158	17.67991187608671
H	5.19233910120806	3.66414235663408	17.73928000457228
H	4.07658704111694	3.81251520370018	15.56207040002224
H	2.47652306820082	3.94109799849164	16.33997558957018
H	5.23345393449840	6.66601816021264	15.52940202725551
H	5.68618527224556	5.38638831763687	16.63549362355495
H	6.25964498643497	7.54748281873448	17.63806311524651
H	4.61860336074357	8.17174083493258	17.34720709130034
H	4.00901167315949	8.71401837347990	19.49676035652904
H	5.68602448527393	8.34436061712674	20.03569913604229
H	4.27027272153302	7.57864357148264	20.83435670273221
H	1.72996191983786	3.06933231654838	18.78977771347744
H	2.02826443515523	3.78434185349871	20.38563650976691
H	2.95041007652264	2.32546485746351	19.88345104096409
H	2.82760209519701	7.36722242685228	15.47018020324371
H	1.76582080152289	5.94391816889717	15.47457962059724
H	3.20921083377475	5.97133878147218	14.40255548868866
H	1.46810593608665	11.40457740492931	16.53435116006257
H	1.29973165692906	10.03828994479446	15.40974741827968
H	2.58330795914866	10.01469462075049	16.63905479212998
H	-0.70096889691964	11.48680730223873	16.09267182176055
H	-1.65239558305950	11.98098941717013	17.50812807691694
H	-2.29243128483186	10.75846901494171	16.39339023892425
H	-1.51514882452495	5.79725162391914	23.68254742590155
H	-2.60912430370993	7.18686358988463	23.50974117794629
H	-1.00353375591900	7.39417549314348	24.24535903339192
H	0.88841592161613	6.12447895116700	23.96612722310985
H	2.31622159115259	6.37461381423885	22.92631884485114
H	1.35461439891823	4.90226014192376	22.75849801116801
H	-2.12601036622426	4.20581331814854	17.25999014818222
H	-0.58471587111874	3.31217088428145	16.97968924517232
H	-1.08625669663471	4.60613778703995	15.87076616332347
H	-3.34501036815746	8.15960359223266	22.07829086029811
H	-3.46268022653333	7.42522851831026	20.46995320218863
H	-4.10505441677572	9.85780319417703	20.62079739594676
H	-2.43066032063382	10.27309275177464	21.00810382701200
H	-3.39703760306210	8.90107138268760	18.42702820199213
H	-3.09529698276287	10.63817558137922	18.60730432547175

1.8 (8a)

Cu	3.00270572608953	5.19295462599367	10.47037806962533
Cu	0.96994043249810	4.92773945007845	13.66308256313078
N	-1.24294522273699	5.39762182710881	13.92177322898894
N	1.14418844266519	5.95668441189120	15.52662989329731
N	0.51696102113622	3.24731021266564	14.90715289499437
N	1.77609354687390	3.71817775334588	11.10872724379973
N	2.53757636986657	6.62127800679663	11.82198440224683
N	4.32879683876420	6.59106125072162	9.90984858777305
N	3.62144419488841	3.72882197398494	9.25016536200084
O	0.86952540602987	3.80643972678558	12.04935786943738
O	1.61165519043080	6.55203087080983	12.74120429090111
O	1.27152012325955	5.83589052208657	8.93667066822193
C	-1.33019240296573	6.25737663563070	15.12397461641707

C	0.01060675645387	6.92061444775479	15.46413222424973
C	1.00429764043062	4.96782911966534	16.63637552306378
C	1.27553239339428	3.55164789061024	16.14794820894072
C	-0.96492843384517	3.22425016212676	15.13700829059226
C	-1.76099273900542	4.02973468544759	14.10659503472983
C	-1.82165103005017	6.04277095539339	12.73436638526074
C	2.43191889710579	6.67671178474092	15.64716094953796
C	0.97589867375334	1.95844086145055	14.34571052973930
C	1.77542356964943	2.68200442901295	10.31220893394187
C	0.76947325009011	1.57674888582578	10.41719505928199
C	2.86185795257950	2.68229851185381	9.29411527062963
C	2.98221318603609	1.49237462352582	8.38795765337760
C	4.16577962196927	7.71919627398965	10.52429867966414
C	4.94814500128443	8.97276578599114	10.25633525745026
C	3.10757071234531	7.77077178721143	11.56943582788664
C	2.73724827380390	9.03459689332944	12.28607968696260
C	4.73414526849115	3.89170228100155	8.31753873365729
C	5.33468273372451	6.35251256869660	8.87626643144020
C	5.78066397913280	4.88975802291779	8.81518011314997
H	-1.69870768829101	5.66951557506042	15.97678269958024
H	-2.07738663043658	7.05608585341491	14.98262979139506
H	0.26873933432245	7.64975952496325	14.68409028202426
H	-0.07907677063234	7.47209306208898	16.41887227013578
H	-0.00097180521494	5.04463750107023	17.06921859701979
H	1.69917173002123	5.21005003105295	17.45572289804528
H	2.34489952301778	3.43536243876144	15.91188923567697
H	1.04032819656269	2.82297309502098	16.94591641742634
H	-1.17335941061577	3.59375912417987	16.14906964707408
H	-1.32470702404957	2.18329991084882	15.12426865568255
H	-2.82700938115053	4.02362995704723	14.40910220824434
H	-1.70205894166438	3.53183511629442	13.12731690159450
H	-1.35247580215905	7.02417121174053	12.57654819230748
H	-2.91476570703872	6.18457081775466	12.82837916737665
H	-1.62326646870528	5.42268889386685	11.84819083720313
H	3.26216878837236	5.95596704959373	15.66360409340045
H	2.46302663921029	7.27107975555271	16.57741202864261
H	2.56020781560954	7.34077849045059	14.78680633827580
H	0.41975702994686	1.73514470971601	13.42938585671145
H	0.82603858825819	1.14204909592964	15.07430487216873
H	2.04397315896139	2.01850824303737	14.09531811413022
H	0.51384681264787	1.16577188416109	9.43108834879281
H	-0.14765207930080	1.94969345172378	10.89013157458028
H	2.85484106351217	0.55304507060329	8.94526923755766
H	3.93764995660738	1.45672021522231	7.85336251116034
H	2.17844990833625	1.52660531289745	7.63076735941028
H	4.30581422147269	9.70347098670578	9.73416638766262
H	5.83176587710053	8.80353767993943	9.63178795494504
H	5.26751184001763	9.44544381472635	11.19731532742476
H	2.82801618375789	9.91328057817867	11.63355668825058
H	3.38988089566786	9.21081600007567	13.15892717381051
H	4.33346560748949	4.22539611218003	7.34194345478396
H	5.23110452936777	2.92527867132241	8.13853906463509
H	6.22137232703750	6.98252429997760	9.04466262372818
H	4.91348661633972	6.65362287127736	7.89826679338969
H	6.16094864380096	4.57349806594663	9.80154940122944
H	6.63746004519018	4.83846638054212	8.12469751440352
H	1.14980932699764	0.74016839798275	11.02979951855092

H	1.70324685142197	8.96833088941030	12.64834415060806
H	0.36394135110650	5.86572670712057	9.27289028982917
H	1.32737947296039	6.55951591411402	8.29536703673630

2 Details of calculations

2.1 Details of Table 3

Table S11: Energy (E_h) and $\langle \hat{S}^2 \rangle$ of all determinants, the decomposition, J_Σ and $J_{\text{Yamaguchi}}$ in cm -1 for the eight compounds.

	(1)		(2)		(3)		(4)	
	E	$\langle \hat{S}^2 \rangle$	E	$\langle \hat{S}^2 \rangle$	E	$\langle \hat{S}^2 \rangle$	E	$\langle \hat{S}^2 \rangle$
HS.RO	-4192.372885	6.000	-4335.744341	8.750	-4336.056267	12.000	-4756.591095	12.000
HS.UFM	-4192.379754	6.027	-4335.754216	8.810	-4336.060005	12.008	-4756.597439	12.012
HS.U	-4192.379802	6.032	-4335.754837	8.847	-4336.060017	12.009	-4756.597516	12.014
BS.RO	-4192.372531	3.000	-4335.743198	4.750	-4336.055909	7.000	-4756.590207	7.000
BS.UFC	-4192.372538	3.000	-4335.743227	4.750	-4336.056941	6.991	-4756.591469	6.990
BS.UFM	-4192.379369	3.029	-4335.751979	4.813	-4336.059685	7.010	-4756.596709	7.016
BS.U	-4192.379489	3.032	-4335.753122	4.834	-4336.060855	6.999	-4756.598169	7.004
J_0	26		63		16		39	
ΔJ_{KE}	-1		-2		-45		-55	
ΔJ_{SP}	2		60		-2		-7	
J_Σ	28		121		-31		-23	
$J_{\text{Yamaguchi}}$	23		94		-37		-29	

	(4a)		(5a)		(7a)		(8)	
	E	$\langle \hat{S}^2 \rangle$	E	$\langle \hat{S}^2 \rangle$	E	$\langle \hat{S}^2 \rangle$	E	$\langle \hat{S}^2 \rangle$
HS.RO	-4448.442569	12.000	-4567.788209	6.000	-4693.334590	3.750	-4673.384863	2.000
HS.UFM	-4448.448626	12.012	-4567.794073	6.010	-4693.339814	3.759	-4673.388621	2.008
HS.U	-4448.448687	12.013	-4567.794088	6.010	-4693.339823	3.759	-4673.388629	2.008
BS.RO	-4448.441778	7.000	-4567.787839	3.000	-4693.334180	1.750	-4673.384266	1.000
BS.UFC	-4448.443525	6.987	-4567.788915	2.994	-4693.335377	1.741	-4673.386057	0.984
BS.UFM	-4448.447804	7.012	-4567.793711	3.010	-4693.339376	1.759	-4673.387944	1.007
BS.U	-4448.449786	6.996	-4567.794916	3.001	-4693.340674	1.748	-4673.389910	0.987
J_0	-48		-60		-93		-275	
ΔJ_{KE}	35		27		45		131	
ΔJ_{SP}	-77		-79		-131		-388	
J_Σ	1		-1		3		18	
$J_{\text{Yamaguchi}}$	-40		-52		-83		-240	

2.2 Details of Table 4

Table S12: Energy (E_h) and $\langle \hat{S}^2 \rangle$ of the determinants used to compute the direct exchange contribution of (5a).

	E	$\langle \hat{S}^2 \rangle$
HS.RO	-4567.78820865	6.000
$d_{x^2-y^2}^{\text{Cu}} t_{2g}^{\text{Co}} d_{z^2}^{\text{Co}} \bar{d}_{x^2-y^2}^{\text{Co}} \cdot \text{NO}$	-4567.73802402	3.000
$d_{x^2-y^2}^{\text{Cu}} t_{2g}^{\text{Co}} \bar{d}_{z^2}^{\text{Co}} d_{x^2-y^2}^{\text{Co}} \cdot \text{NO}$	-4567.73741458	3.000
$d_{x^2-y^2}^{\text{Cu}} \bar{t}_{2g}^{\text{Co}} d_{z^2}^{\text{Co}} d_{x^2-y^2}^{\text{Co}} \cdot \text{NO}$	-4567.74128104	3.000
$\bar{d}_{x^2-y^2}^{\text{Cu}} t_{2g}^{\text{Co}} d_{z^2}^{\text{Co}} d_{x^2-y^2}^{\text{Co}} \cdot \text{NO}$	-4567.78783907	3.000
$\bar{d}_{x^2-y^2}^{\text{Cu}} \bar{t}_{2g}^{\text{Co}} d_{z^2}^{\text{Co}} d_{x^2-y^2}^{\text{Co}} \cdot \text{NO}$	-4567.73821790	2.000

Table S13: Energy (E_h) and $\langle \hat{S}^2 \rangle$ of the determinants used to compute the direct exchange contribution of (7a).

	E	$\langle \hat{S}^2 \rangle$
HS.RO	-4693.33459046	3.750
$d_{x^2-y^2}^{\text{Cu}} d_{z^2}^{\text{Ni}} \bar{d}_{x^2-y^2}^{\text{Ni}} .\text{NO}$	-4693.30574320	1.750
$d_{x^2-y^2}^{\text{Cu}} \bar{d}_{z^2}^{\text{Ni}} d_{x^2-y^2}^{\text{Ni}} .\text{NO}$	-4693.30574320	1.750
$\bar{d}_{x^2-y^2}^{\text{Cu}} d_{z^2}^{\text{Ni}} \bar{d}_{x^2-y^2}^{\text{Ni}} .\text{NO}$	-4693.33418002	1.750

Table S14: Energy and $\langle \hat{S}^2 \rangle$ of the determinant corresponding to both relaxations of the $d_{x^2-y^2}$ orbitals ($\text{Cu} \rightarrow \text{M}$ and $\text{Cu} \leftarrow \text{M}$) and their associated t and U for (5a) and (7a). All energies are in E_h .

	(5a)				(7a)			
	E	$\langle \hat{S}^2 \rangle$	t	U	E	$\langle \hat{S}^2 \rangle$	t	U
$\text{Cu} \rightarrow \text{M}$	-4567.78840953	2.998	-0.013	0.328	-4693.33479631	1.748	-0.013	0.294
$\text{Cu} \leftarrow \text{M}$	-4567.78835601	2.997	-0.011	0.227	-4693.33476076	1.478	-0.012	0.244

2.3 Effect of the localisation scheme and the amount of Hartree-Fock exchange on the magnetic coupling of (2).

Table S15: Direct exchange and spin polarisation contributions obtained with the Pipek-Mezey (used throughout this work), Foster-Boys and IAO-BO localisation schemes for (2) in cm^{-1} .

localisation	Pipek-Mezey	Foster-Boys	IAO-BO
J_0	62.68	62.86	62.69
ΔJ_{SP}	59.97	61.13	59.96

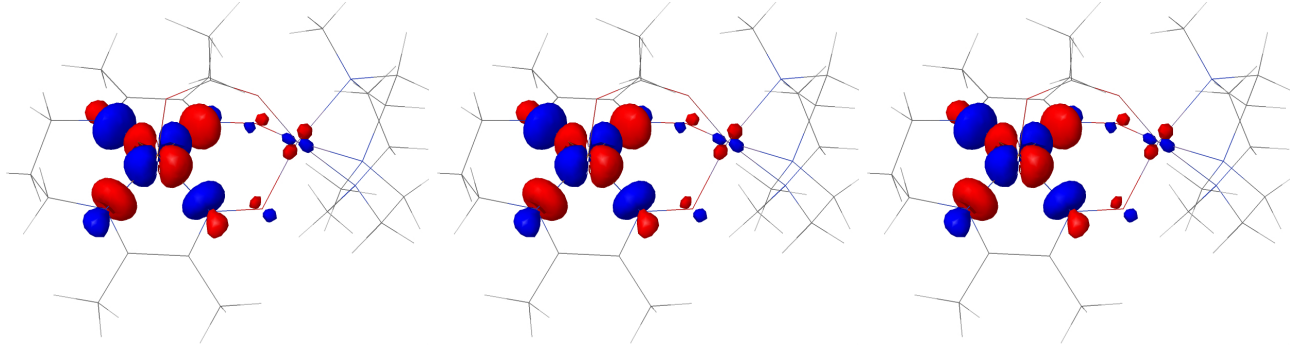


Figure S1: $d_{x^2-y^2}$ -like localized magnetic orbital of the Cu centre obtained from the $\Phi_{\text{HS,RO}}$ determinant for complexes (2) using the Pipek-Mezey (left), Foster-Boys (centre) and IAO-BO (right) localisation schemes. Isovalue = 0.05 a.u..

Table S16: $J_{\text{Yamaguchi}}$, J_{Σ} and decomposition computed with PBE0 at 30 and 50 % of Hartree-Fock exchange (HFX) for (2) in cm^{-1} .

	30 % HFX	50 % HFX
$J_{\text{Yamaguchi}}$	94	50
J_{Σ}	121	18
J_0	63	23
ΔJ_{KE}	-2	-1
ΔJ_{SP}	60	-4