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Supporting Information

Exchange Couplings and Magneto-Structural Correlations of Trinuclear $M^{II}-U^{IV}-M^{II}$ ($M^{II} = Co, Ni, Cu$) Complexes

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Exchange Couplings and Magneto-Structural Correlations of Trinuclear $M^{II}-U^{IV}-M^{II}$ ($M^{II} = Co, Ni, Cu$) Complexes. Theory Meets Experiment.

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Supplementary Information

Optimized coordinates

Co2UL				Ni2UL			
U	4.34666900	2.38065700	2.23798400	U	9.21954300	22.72684200	25.20238100
Co	3.41612400	1.31506100	5.64923100	Ni	8.41292900	23.38148100	28.68416700
Co	5.17622100	2.94482900	-1.28768000	Ni	10.32715500	21.71527500	21.87216800
O	4.54439800	4.65271900	2.69117600	O	11.50032700	22.92582500	25.40062800
O	3.85793300	2.95591000	4.56968400	O	9.96353600	23.32961700	27.41616800
O	3.63002700	0.62331800	3.79478200	O	7.56023000	23.16626300	26.91961200
O	4.27255800	0.28534100	1.32740400	O	7.05438100	22.44735000	24.49594600
O	6.54613000	2.20238900	3.00029700	O	9.20848600	20.61179800	26.10906000
O	6.02990900	2.82293600	0.50354600	O	9.92008700	20.98685400	23.65222300
O	3.62178900	2.98361300	-0.03357000	O	9.76258200	23.31600400	22.90601800
O	2.07037800	2.76060400	2.02817300	O	9.10149000	24.95431100	24.79456200
N	2.51246200	2.49327000	7.06223800	N	9.62084100	24.23697100	30.10854500
N	2.38615200	-0.40030800	6.17683600	N	6.61275600	23.93074300	29.49529900
N	7.03214700	3.49888900	-2.09251500	N	11.29548300	19.98978100	21.33210300
N	4.00621000	3.79115600	-2.72194800	N	11.16851400	22.90947700	20.42560300
N	5.29127200	0.90034800	6.59925500	N	8.48457455	21.54568290	29.30731405
N	5.16770900	0.97514600	-1.82395700	N	8.50982400	21.37878800	20.93446900
C	3.69318200	4.24410000	4.85222900	C	11.23733600	23.62189400	27.62704000
C	4.14624900	5.17353500	3.82135800	C	12.09159500	23.38970400	26.49940100
C	3.98424300	6.53652300	4.07592800	C	13.45495800	23.66915700	26.63102100
H	4.25608300	7.14875900	3.43110900	H	14.11278500	23.48811900	25.77960300
C	3.40212100	7.03794700	5.33199700	C	13.96700600	24.18867200	27.84075700
H	3.30876100	7.95353100	5.46487700	H	15.03354000	24.40554500	27.91769900
C	3.00397100	6.18885000	6.28314000	C	13.13724300	24.43581300	28.92111900
H	2.66073800	6.51851600	7.08182100	H	13.53942600	24.84980900	29.84791300
C	3.11105900	4.68319200	6.07053200	C	11.74080000	24.15473700	28.83983000
C	2.53717500	3.74544600	7.07762400	C	10.90473100	24.45200300	29.96839900
H	2.14177100	4.14575400	7.81895700	H	11.43427900	24.91750200	30.81785800
C	1.87542200	1.89350000	8.27914200	C	9.04482500	24.58599300	31.40853100
H	1.35920100	2.58053400	8.72953600	H	9.75575900	25.22074900	31.96935500
H	2.57287100	1.60538900	8.88619500	H	8.91395100	23.65561600	31.99133200
C	0.94732200	0.69257500	7.98680500	C	7.67651800	25.30754600	31.35513700
C	1.77108000	-0.51804600	7.48885400	C	6.55636200	24.34142000	30.90046700
H	2.47127400	-0.69119000	8.13507200	H	6.61926500	23.43375400	31.52807000
H	1.18895700	-1.29373000	7.48046200	H	5.57762300	24.81158300	31.10897900
C	2.20218000	-1.41423800	5.34038900	C	5.47019200	23.86606200	28.86199600
H	1.67497500	-2.10958300	5.66349800	H	4.56461100	24.16581700	29.41723800
C	2.69368900	-1.58461200	4.02977000	C	5.22791600	23.43389900	27.51303700
C	2.48774900	-2.86726100	3.37655800	C	3.88353800	23.34479100	27.04695500
H	2.07312400	-3.55568000	3.84233900	H	3.06951100	23.59876000	27.72867500
C	2.87766100	-3.06810700	2.14986300	C	3.61732300	22.93642900	25.75043700
H	2.74036800	-3.90335300	1.76521000	H	2.58374100	22.86379200	25.40868300
C	3.52019300	-2.01677800	1.35677800	C	4.66258100	22.61660900	24.85718000
H	3.77555800	-2.17330000	0.47697000	H	4.44608000	22.30039900	23.83568200
C	3.73711500	-0.78122500	1.95404000	C	5.99848000	22.70525800	25.26269600
C	3.36642400	-0.56652600	3.30522300	C	6.27219600	23.10525900	26.61295100
C	-0.09610500	1.05132900	7.00349100	C	7.34172700	25.71983900	32.80253600
H	0.31577400	1.27433800	6.16424700	H	6.37302800	26.23747200	32.84733700
H	-0.59310600	1.80762100	7.32520100	H	8.10576800	26.40303900	33.19995000
H	-0.69195700	0.30750300	6.88040200	H	7.29036900	24.84566900	33.46952300
C	0.31577400	0.29919200	9.29183000	C	7.73872200	26.55283200	30.45853400
H	-0.32401100	0.96683500	9.55059700	H	6.77653600	27.08540600	30.46788600
H	0.99400100	0.22716500	9.96742100	H	7.97198800	26.29259100	29.41815900
H	-0.12631000	-0.54574900	9.19112100	H	8.51312900	27.24748300	30.81576900
C	7.33144600	2.83124700	0.83924400	C	10.16542100	19.77273900	24.13082100
C	7.59779500	2.42262700	2.24218000	C	9.74526600	19.56669000	25.48717100

C	8.89933200	2.35891000	2.60725100	C	9.93260500	18.30377000	26.05945600
H	9.11625500	2.08880600	3.47027400	H	9.59545900	18.14254000	27.08414100
C	9.94275900	2.69411700	1.70086800	C	10.56162000	17.26929400	25.33506400
H	10.82143400	2.67056900	2.00019800	H	10.70447900	16.29550500	25.80614200
C	9.69837800	3.04178900	0.42381800	C	11.01471400	17.48165300	24.04487900
H	10.40406400	3.24125100	-0.14966500	H	11.52422800	16.68782200	23.49513900
C	8.34741400	3.10412100	-0.04476000	C	10.82966700	18.74632100	23.41173600
C	8.15245800	3.47811200	-1.42811400	C	11.36769000	18.93036700	22.09480200
H	8.91306200	3.73159400	-1.89809000	H	11.91125700	18.05562000	21.69749100
C	7.04313100	3.91997400	-3.48845800	C	11.89316500	19.86855000	20.00008600
H	7.01018100	3.12212800	-4.03816200	H	11.08059400	19.69754100	19.27021600
H	7.89709300	4.34798600	-3.66050300	H	12.54800500	18.97817300	19.96909300
C	5.97499100	4.83971400	-3.95983300	C	12.70396400	21.09589200	19.52317200
C	4.64050300	4.14298400	-4.03676400	C	11.76702900	22.29396000	19.23991200
H	4.02817700	4.71089500	-4.52772100	H	12.33132400	23.05639800	18.67171000
H	4.75308400	3.32574500	-4.54730400	H	10.95165600	21.93906100	18.58340900
C	2.74036800	4.07511100	-2.52892200	C	11.16494300	24.21567900	20.45935100
H	2.30926800	4.42278400	-3.27445000	H	11.64788300	24.74519800	19.61952300
C	1.91935600	3.94490700	-1.39034800	C	10.62410500	25.07905200	21.47044500
C	0.53544300	4.42416900	-1.40573400	C	10.78017800	26.48792000	21.30974300
H	0.18946400	4.79261900	-2.18762900	H	11.25833300	26.86330700	20.40295000
C	-0.24438200	4.34521600	-0.32310900	C	10.34803600	27.36076400	22.29255500
H	-1.10658200	4.69150300	-0.35667900	H	10.47417300	28.43589700	22.15748100
C	0.19770200	3.76899300	0.83085200	C	9.76438900	26.87664400	23.48258500
H	-0.37892900	3.71358700	1.55819600	H	9.44813900	27.56203300	24.27037600
C	1.52395200	3.24679200	0.95533900	C	9.59930100	25.50416200	23.68632900
C	2.35045600	3.37561100	-0.21960200	C	9.99770600	24.59938500	22.64814600
C	5.99970400	6.08357900	-3.04505700	C	13.34542100	20.70591100	18.17670100
H	5.57135000	6.81770800	-3.49125500	H	14.01492700	19.84233100	18.29807600
H	6.90858400	6.31628400	-2.84503700	H	13.94115000	21.53732100	17.77418200
H	5.53290800	5.88827300	-2.22959200	H	12.58356000	20.44144500	17.42712900
C	6.26605300	5.35360500	-5.42151600	C	13.79841300	21.46918500	20.53387600
H	6.35666600	4.60285300	-6.01178500	H	14.48378000	20.62337500	20.69159200
H	7.07882700	5.86472500	-5.42431400	H	13.37427200	21.74847100	21.50678900
H	5.53840000	5.90628000	-5.71665000	H	14.39114900	22.31932100	20.16602000
C	6.29900300	1.79376900	6.35587500	C	9.65911855	21.00089190	29.69011105
H	6.13974300	2.50712200	5.78099200	H	10.52114955	21.66845490	29.68972705
C	7.58681100	1.65802500	6.96292800	C	9.77786955	19.66358390	30.05659805
H	8.25405500	2.29657900	6.85242700	H	10.75050255	19.27321390	30.35557005
C	7.79000500	0.46264000	7.76300700	C	8.64509055	18.84691090	30.01991205
H	8.60827100	0.31581400	8.17703400	H	8.70781455	17.79442790	30.29871705
C	6.73559500	-0.48757300	7.91686800	C	7.43375355	19.40482590	29.60412705
H	6.83444600	-1.27295300	8.40502900	H	6.52485655	18.80703190	29.54125205
C	5.56860400	-0.14959600	7.28463800	C	7.39466455	20.75133890	29.25414205
H	4.87664700	-0.76737300	7.36436600	H	6.47300855	21.22262790	28.91124105
C	6.23310200	0.16483300	-1.73443800	C	8.00337100	20.13457300	20.79145000
H	7.00194300	0.64963500	-1.54840500	H	8.63916200	19.31739700	21.13254300
C	6.52416300	-1.23001300	-1.84214100	C	6.74305900	19.89671100	20.25252400
H	7.27103700	-1.70096400	-1.55120300	H	6.38211200	18.87241100	20.16085000
C	5.47249900	-1.65941000	-2.45199100	C	5.96224000	20.98268700	19.84885400
H	5.54389100	-2.47110800	-2.90238500	H	4.96907300	20.82824600	19.42704400
C	4.23137000	-1.01393000	-2.49815000	C	6.47874100	22.27094600	20.01032500
H	3.51744700	-1.54167200	-2.77649900	H	5.90517800	23.15260500	19.72631400
C	3.89637500	0.35598400	-2.17364200	C	7.74823500	22.42885100	20.55731700
H	3.05614200	0.75352200	-2.18483200	H	8.18116600	23.41657700	20.71561200

Cu2UL

Th	1.481610	9.768624	3.205659
Cu	2.586031	8.685641	-0.132030
Cu	0.234528	10.965100	6.472171
O	-0.834479	9.874639	2.605277
O	0.967584	8.958814	0.923664
O	3.287281	9.058531	1.668029
O	3.660679	9.760489	4.113023
O	1.160622	7.476175	3.740841
O	0.661423	9.330130	5.539270
O	0.766264	11.596075	4.729705
O	1.850979	11.925404	2.415111
N	1.575368	7.759582	-1.540346
N	4.400199	8.317212	-0.874765
N	-0.159404	9.976980	8.133680
N	-0.263639	12.776938	7.093199
N	2.618710	10.930855	-0.679165
C	-0.312548	8.801366	0.578649
C	-1.287637	9.288144	1.477863
C	-2.612221	9.137255	1.130131
H	-3.274236	9.481018	1.684329
C	-2.979395	8.458915	-0.073350
H	-3.879753	8.377567	-0.296116
C	-2.049238	7.938023	-0.885631
H	-2.310079	7.449933	-1.632713
C	-0.674227	8.124337	-0.613965
C	0.301479	7.616566	-1.543063

NiUZnL

U	9.21954300	22.72684199	25.20238099
Ni	8.41292900	23.38148099	28.68416699
Zn	10.30933887	21.83740210	21.67290855
O	11.47638751	23.00514849	25.41318720
O	9.93225477	23.41318447	27.42671070
O	7.54586164	23.09843803	26.92076947
O	7.08160176	22.38214004	24.49468283
O	9.38007052	20.62666648	26.02710041
O	10.00510792	21.04982171	23.55753080
O	9.77719506	23.42737244	22.88155779
O	9.06625407	24.94297363	24.85196365
N	9.56828987	24.26653148	30.09628417
N	6.59862774	23.84795262	29.47511049
N	11.47235751	20.17611732	21.21001540
N	11.31460083	23.16473878	20.43004040
N	8.54259642	21.45284849	29.31436361
N	8.45892792	21.47228763	20.75777523
C	11.20268688	23.72040325	27.63095394
C	12.05967967	23.49290531	26.50753622
C	13.41741572	23.79930458	26.63670330
H	14.07907256	23.62461633	25.78705321
C	13.91878823	24.33587708	27.84340768
H	14.98109002	24.57258891	27.91935863
C	13.08488825	24.57248829	28.92370084
H	13.47986547	24.99565252	29.84936469
C	11.69543850	24.26405042	28.84155260

H	-0.041317	7.114044	-2.246678	C	10.84499846	24.52999323	29.96615440
C	2.285362	7.060249	-2.648744	H	11.35227901	25.00690838	30.82241890
H	1.654664	6.892304	-3.365942	C	8.98292347	24.58065581	31.40277873
H	2.597212	6.200843	-2.325461	H	9.67137982	25.23608434	31.96727711
C	3.467037	7.827810	-3.208376	H	8.89050302	23.63950731	31.97526769
C	4.639792	7.806816	-2.268411	C	7.58923642	25.24738171	31.35947656
H	4.957213	6.892304	-2.203211	C	6.51618674	24.24054278	30.88600306
H	5.352084	8.332957	-2.662327	H	6.61356376	23.32867873	31.50322301
C	5.492406	8.487781	-0.176583	H	5.51702591	24.66558501	31.09277436
H	6.284572	8.302779	-0.627548	C	5.45287277	23.74602099	28.84795329
C	5.650699	8.919452	1.184464	H	4.54295725	24.01159871	29.41274726
C	6.945663	9.016545	1.738662	C	5.21204319	23.31115007	27.50045991
H	7.684310	8.834167	1.206197	C	3.87174133	23.19072382	27.02920108
C	7.133230	9.370804	3.042659	H	3.04831851	23.42205260	27.70759357
H	7.996922	9.449528	3.379525	C	3.62191630	22.78128810	25.72963936
C	6.051989	9.616161	3.868524	C	2.59206454	22.68540057	25.38265478
H	6.211949	9.848397	4.756872	C	4.67841596	22.49032778	24.83803279
C	4.744999	9.533501	3.439292	H	4.47341274	22.17531878	23.81387503
C	4.537449	9.177930	2.067378	C	6.00798606	22.60897010	25.25257591
C	3.053680	9.239597	-3.667491	C	6.206349911	23.00869576	26.60354116
H	2.765476	9.749992	-2.906826	C	7.23403779	25.62090109	32.81234428
H	2.334965	9.172681	-4.300473	H	6.24510864	26.09846202	32.86220905
H	3.803537	9.675204	-4.080423	H	7.96835845	26.32766287	33.22438826
C	3.928543	7.034007	-4.439023	H	7.21540407	24.73415779	33.46419062
H	4.200611	6.153608	-4.170073	C	7.60053437	26.50889336	30.48355706
H	4.670195	7.484047	-4.851955	H	6.61585475	26.99880550	30.49700933
H	3.205737	6.968404	-5.066571	H	7.84905624	26.27638649	29.44007375
C	0.439321	8.082351	5.897869	H	8.34179376	27.23127191	30.85620396
C	0.713334	7.081242	4.909005	C	10.38543857	19.87628778	24.03711343
C	0.534957	5.748179	5.251304	C	10.01691941	19.63101623	25.40085878
H	0.720211	5.088207	4.623755	C	10.33930816	18.40340537	25.97998781
C	0.062030	5.361118	6.571601	H	10.03991951	18.21872895	27.01269633
H	-0.061927	4.464974	6.788933	C	11.05746579	17.42992849	25.24921724
C	-0.195042	6.353043	7.492548	H	11.30769847	16.47967270	25.72333478
H	-0.493990	6.116870	8.340146	C	11.46170158	17.67928150	23.95139463
C	-0.017281	7.726780	7.180133	H	12.04182588	16.93753436	23.39826476
C	-0.224912	8.685903	8.193447	C	11.13820646	18.91483774	23.31133465
H	-0.442521	8.339517	9.027461	C	11.65159400	19.14163760	21.99233598
C	-0.443091	10.726172	9.380627	H	12.29166417	18.32786937	21.60771847
H	0.394001	11.051566	9.747376	C	12.13953632	20.14497303	19.90651476
H	-0.832062	10.117372	10.029909	H	11.37401181	20.00081448	19.12228541
C	-1.382344	11.900475	9.193178	H	12.81982911	19.27464594	19.85978507
C	-0.700123	13.052472	8.503146	C	12.94744014	21.42070738	19.54748441
H	-1.305965	13.810849	8.497713	C	12.00753239	22.62085635	19.25971164
H	0.079197	13.305702	9.024745	H	12.59822004	23.41979785	18.77510610
C	-0.166142	13.835778	6.362418	H	11.24934993	22.28861118	18.52686765
H	-0.444930	14.633517	6.750900	C	11.35536580	24.46270650	20.58922069
C	0.323813	13.918439	5.012238	H	11.92056188	25.04177620	19.83752594
C	0.409370	15.225260	4.444456	C	10.77758078	25.25814622	21.63290983
H	0.076753	15.953459	4.917155	C	10.99349539	26.66951131	21.59349768
C	0.980921	15.423383	3.194792	H	11.53928889	27.09317060	20.74739061
H	1.004678	16.270980	2.814460	C	10.53567966	27.48306197	22.61291048
C	1.520941	14.323868	2.515627	H	10.70790293	28.55933609	22.56894395
H	1.960156	14.465572	1.708779	C	9.86690390	26.93249771	23.72874091
C	1.420858	13.024919	3.010059	H	9.53075369	27.56808008	24.54931927
C	0.821303	12.867470	4.273306	C	9.64555210	25.55767709	23.81376653
C	-1.752472	12.404310	10.616708	C	10.06804511	24.71300532	22.73572240
H	-0.954818	12.669348	11.081256	C	13.68840597	21.11619121	18.22968390
H	-2.185573	11.698416	11.102990	H	14.37312736	20.26546094	18.35491732
H	-2.347520	13.154814	10.546074	H	14.28548312	21.98181365	17.90952845
C	-2.688654	11.464868	8.459679	H	12.98663552	20.87021317	17.41768537
H	-2.470466	11.147347	7.579482	C	13.96202419	21.76260850	20.64892437
H	-3.283012	12.215372	8.391763	H	14.65217197	20.92208160	20.81373740
H	-3.114893	10.762910	8.956828	H	13.46846528	21.98773203	21.60273975
C	3.746100	11.556713	-1.054064	H	14.56174965	22.63918803	20.36245435
H	4.537277	11.069935	-1.035047	C	9.72604813	20.93888552	29.71867471
C	3.808765	12.879279	-1.464280	H	10.56639855	21.63305863	29.74630607
H	4.621319	13.280773	-1.668029	C	9.88015076	19.60220707	30.07093742
C	2.618089	13.578612	-1.559363	H	10.85872483	19.24096616	30.38713911
H	2.608457	14.448515	-1.888079	C	8.77640147	18.74755076	29.99818214
C	1.465442	12.978996	-1.165447	H	8.86740727	17.69411463	30.26443116
H	0.660652	13.444781	-1.157297	C	7.55663172	19.27325046	29.56251487
C	1.527176	11.653806	-0.776965	H	6.66901687	18.64752812	29.47097040
H	0.724208	11.236567	-0.567782	C	7.48022287	20.62107770	29.22874010
				H	6.55063803	21.06496639	28.87146794
				C	8.01839219	20.21374045	20.51684555
				H	8.70803444	19.40883169	20.77537020
				C	6.76370392	19.94760959	19.98330747
				H	6.45872128	18.91467683	19.81569609
				C	5.91162779	21.01691159	19.68058143
				H	4.92013696	20.83987753	19.26375999
				C	6.36047781	22.31842610	19.93691973
				H	5.73186617	23.18543834	19.73356288
				C	7.62707671	22.50446975	20.47665872
				H	8.00387955	23.49972831	20.71383620

ZnUCoL

U	9.21954300	22.72684200	25.20238100
Ni	8.41292900	23.38148100	28.68416700
Zn	10.32715500	21.71527500	21.87216800
O	11.50032700	22.92582500	25.40062800
O	9.96353600	23.32961700	27.41616800
O	7.56023000	23.16626300	26.91961200
O	7.05438100	22.44735000	24.49594600
O	9.20848600	20.61179800	26.10906000
O	9.92008700	20.98685400	23.65222300
O	9.76258200	23.31600400	22.90601800
O	9.10149000	24.95431100	24.79456200
N	9.62084100	24.23697100	30.10854500
N	6.61275600	23.93074300	29.49529900
N	11.29548300	19.98978100	21.33210300
N	11.16851400	22.90947700	20.42560300
N	8.48457455	21.54568290	29.30731405
N	8.54707863	21.38568586	20.95369149
C	11.23733600	23.62189400	27.62704000
C	12.09159500	23.38970400	26.49940100
C	13.45495800	23.66915700	26.63102100
H	14.11278500	23.48811900	25.77960300
C	13.96700600	24.18867200	27.84075700
H	15.03354000	24.40554500	27.91769900
C	13.13724300	24.43581300	28.92111900
C	13.53942600	24.84980900	29.84791300
C	11.74080000	24.15473700	28.83983000
C	10.90473100	24.45200300	29.96839900
H	11.43427900	24.91750200	30.81785800
C	9.04482500	24.58599300	31.40853100
H	9.75575900	25.22074900	31.96935500
H	8.91395100	23.65561600	31.99133200
C	7.67651800	25.30754600	31.35513700
C	6.55636200	24.34142000	30.90046700
H	6.61926500	23.43375400	31.52807000
H	5.57762300	24.81158300	31.10897900
C	5.47019200	23.86606200	28.86199600
H	4.56461100	24.16581700	29.41723800
C	5.22791600	23.43389900	27.51303700
C	3.88353800	23.34479100	27.04695500
H	3.06951100	23.59876000	27.72867500
C	3.61732300	22.93642900	25.75043700
H	2.58374100	22.86379200	25.40868300
C	4.66258100	22.61660900	24.85718000
H	4.44608000	22.30039900	23.83568200
C	5.99848000	22.70525800	25.26269600
C	6.27219600	23.10525900	26.61295100
C	7.34172700	25.71983900	32.80253600
H	6.37302800	26.23747200	32.84733700
H	8.10576800	26.40303900	33.19995000
H	7.29036900	24.84566900	33.46952300
C	7.73872200	26.55283200	30.45853400
H	6.77653600	27.08540600	30.46788600
H	7.97198800	26.29259100	29.41815900
H	8.51312900	27.24748300	30.81576900
C	10.16542100	19.77273900	24.13082100
C	9.74526600	19.56669000	25.48717100
C	9.93260500	18.30377000	26.05945600
H	9.59545900	18.14254000	27.08414100
C	10.56162000	17.26929400	25.33506400
H	10.70447900	16.29550500	25.80614200
C	11.01471400	17.48165300	24.04487900
H	11.52422800	16.68782200	23.49513900
C	10.82966700	18.74632100	23.41173600
C	11.36769000	18.93036700	22.09480200
H	11.91125700	18.05562000	21.69749100
C	11.89316500	19.86855000	20.00086600
H	11.08059400	19.69754100	19.27021600
H	12.54800500	18.97817300	19.96909300
C	12.70396400	21.09589200	19.52317200
C	11.76702900	22.29396000	19.23991200
H	12.33132400	23.05639800	18.67171000
H	10.95165600	21.93906100	18.58340900
C	11.16494300	24.21567900	20.45935100
H	11.64788300	24.74519800	19.61952300
C	10.62410500	25.07905200	21.47044500
C	10.78017800	26.48792000	21.30974300
H	11.25833300	26.86330700	20.40295000
C	10.34803600	27.36076400	22.29255500
H	10.47417300	28.43589700	22.15748100
C	9.76438900	26.87664400	23.48258500
H	9.44813900	27.56203300	24.27037600
C	9.59930100	25.50416200	23.68632900
C	9.99770600	24.59938500	22.64814600
C	13.34542100	20.70591100	18.17670100
H	14.01492700	19.84233100	18.29807600

NiThNiL

Th	9.50668400	22.68695700	25.27112800
Ni	8.35622900	23.38004500	28.81442100
Ni	10.49989700	21.75151600	21.73024900
O	11.79190800	22.93704700	25.80809000
O	10.00608300	23.40667000	27.05030500
O	7.64353800	23.08802300	26.94127000
O	7.29936900	22.35589300	24.45805000
O	9.58837600	20.45232400	26.05946600
O	10.24872100	20.95090400	23.58007300
O	10.19242500	23.34954900	22.91956100
O	9.40527100	24.99323300	24.78490000
N	9.41097900	24.25684700	30.32210900
N	6.48266500	23.86673900	29.44853100
N	11.33425500	19.99927700	21.09807900
N	11.27681600	22.96704000	20.29060200
N	8.44222400	21.39825400	29.41616400
N	8.56663400	21.51276800	21.04203900
C	11.26343200	23.64297900	27.99418300
C	12.24233500	23.38248100	26.97117400
C	13.58946200	23.62084100	27.27489300
H	14.33670500	23.41754700	26.50631900
C	13.97237100	24.12306300	28.53596100
H	15.02912300	24.30535000	28.73897000
C	13.02921200	24.39404100	29.51313600
H	13.33067400	24.79122600	30.48432300
C	11.64544400	24.15353500	29.26348600
C	10.70226200	24.46523200	30.30040900
H	11.15017800	24.93469400	31.19365300
C	8.71472100	24.62832700	31.55695700
H	9.35949900	25.29611800	32.15784200
H	8.55316400	23.71169100	32.15350200
C	7.34116500	25.31328600	31.36100900
C	6.29106100	24.30646400	30.83367000
H	6.32107900	23.41501400	31.48625200
H	5.28629400	24.75409400	30.94383600
C	5.40199100	23.76073800	28.71979100
H	4.44691400	24.04703800	29.19358100
C	5.27224600	23.30054300	27.36485500
C	3.96035700	23.17480700	26.81832700
H	3.10055700	23.41407900	27.44710500
C	3.78525500	22.75122300	25.51222900
H	2.77727300	22.64895600	25.10680000
C	4.89363100	22.45693400	24.69028200
H	4.74973500	22.13413300	23.65791800
C	6.20435500	22.58257000	25.16943700
C	6.38540200	22.99114300	26.53892500
C	6.86549700	25.75381100	32.75989100
H	5.88531700	26.24797700	32.70124700
H	7.57361700	26.46638200	33.20589900
H	6.77215800	24.89644300	33.44412900
H	7.45366600	26.53742200	30.44072100
C	6.47908100	27.03721600	30.34130100
H	7.79609300	26.26147600	29.43510300
H	8.16657700	27.26642900	30.85311800
C	10.43090500	19.70329600	23.98558600
C	10.06173400	19.43619000	25.35227500
C	10.23624300	18.13371300	25.83732000
H	9.95059700	17.92567600	26.86984000
C	10.78038000	17.11785200	25.02339700
H	10.91208500	16.11562800	25.43437300
C	11.15766500	17.37993200	23.71819000
H	11.59077800	16.59564300	23.09452300
C	10.98834800	18.68533400	23.16764600
C	11.42872100	18.91311700	21.82051000
H	11.90701700	18.03702800	21.34813800
C	11.83710800	19.09952800	19.72481700
H	10.97171500	19.81720300	19.04347500
H	12.43894900	18.98893100	19.61128800
C	12.68535400	21.11525300	19.25343200
C	11.80100100	22.37021900	19.05847600
H	12.38138500	23.12691100	18.49944700
H	10.94431500	22.08362600	18.42165800
C	11.30599800	24.27295100	20.36006100
H	11.75678200	24.81112700	19.50806800
C	10.81632100	25.12866100	21.40400000
C	10.89440900	26.53960200	21.21256300
H	11.30594700	26.92392900	20.27125900
C	10.45477300	27.40447200	22.20056600
H	10.51644600	28.48232400	22.04243800
C	9.93505000	26.91460500	23.41650500
H	9.60049600	27.60034200	24.19668600
C	9.85086200	25.53807400	23.66280800
C	10.28650500	24.63845500	22.62691600
C	13.24050200	20.74667700	17.86320200
H	13.87757800	19.85282000	17.92232000

H	13.94115000	21.53732100	17.77418200	H	13.85025400	21.56606300	17.45696000
H	12.58356000	20.44144500	17.42712900	H	12.43134300	20.53912100	17.14631000
C	13.79841300	21.46918500	20.53387600	C	13.84641200	21.39230900	20.21992100
H	14.48378000	20.62337500	20.69159200	H	14.49281000	20.50710700	20.31110700
H	13.37427200	21.74847100	21.50678900	H	13.48751400	21.65332000	21.22366600
H	14.39114900	22.31932100	20.16602000	H	14.46447800	22.22498000	19.85394900
C	9.65911855	21.00089190	29.69011105	C	9.60320100	20.87058300	29.85404300
H	10.52114955	21.66845490	29.68972705	H	10.44312300	21.56132100	29.94164700
C	9.77786955	19.66358390	30.05659805	C	9.73839100	19.52058600	30.16836400
H	10.75050255	19.27321390	30.35557005	H	10.70023300	19.14299900	30.51488300
C	8.64509055	18.84691090	30.01991205	C	8.63653500	18.67761100	30.01763400
H	8.70781455	17.79442790	30.29871705	H	8.71250400	17.61511900	30.25235400
C	7.43375355	19.40482590	29.60412705	C	7.43937000	19.21850600	29.54682400
H	6.52485655	18.80703190	29.54125205	H	6.55581300	18.59813300	29.39529500
C	7.39466455	20.75133890	29.25414205	C	7.38326600	20.57883300	29.25480000
H	6.47300855	21.22262790	28.91124105	H	6.47267100	21.04059200	28.87080900
C	8.04062563	20.14147086	20.81067249	C	7.94209900	20.32195800	21.14164500
H	8.67641663	19.32429486	21.15176549	H	8.54779700	19.49135700	21.50555200
C	6.78031363	19.90360886	20.27174649	C	6.59928800	20.15382700	20.81508400
H	6.41936663	18.87930886	20.18007249	H	6.13931200	19.17127600	20.91872600
C	5.99949463	20.98958486	19.86807649	C	5.86805300	21.25786900	20.37508000
H	5.00632763	20.83514386	19.44626649	H	4.81321000	21.15845000	20.11659300
C	6.51599563	22.27784386	20.02954749	C	6.50906200	22.49430200	20.28624100
H	5.94243263	23.15950286	19.74553649	H	5.97703300	23.38924400	19.96530000
C	7.78548963	22.43574886	20.57653949	C	7.85538300	22.58183500	20.63067400
H	8.21842063	23.42347486	20.73483449	H	8.39249900	23.53043500	20.59283600

CoThCoL

Th	9.50668400	22.68695700	25.27112800
Co	8.35622900	23.38004500	28.81442100
Co	10.49989700	21.75151600	21.73024900
O	11.79190800	22.93704700	25.80809000
O	10.00608300	23.40667000	27.65030500
O	7.64353800	23.08802300	26.94127000
O	7.29936900	22.35589300	24.45805000
O	9.58837600	20.45232400	26.05946600
O	10.24872100	20.95090400	23.58007300
O	10.19242500	23.34954900	22.91956100
O	9.40527100	24.99323300	24.78490000
N	9.41097900	24.25684700	30.32210900
N	6.48266500	23.86673900	29.44853100
N	11.33425500	19.99927700	21.09807900
N	11.27681600	22.96704000	20.29060200
N	8.44222400	21.39825400	29.41616400
N	8.67513490	21.52616730	21.08066355
C	11.26343200	23.64297900	27.99418300
C	12.24233500	23.38248100	26.97117400
C	13.58946200	23.62084100	27.27489300
H	14.33670500	23.41754700	26.50631900
C	13.97237100	24.12306300	28.53596100
H	15.02912300	24.30535000	28.73897000
C	13.02921200	24.39404100	29.51313600
H	13.33067400	24.79122600	30.48432300
C	11.64544400	24.15353500	29.26348600
C	10.70226200	24.46523200	30.30040900
H	11.15017800	24.93469400	31.19365300
C	8.71472100	24.62832700	31.55695700
H	9.35949900	25.29611800	32.15784200
H	8.55316400	23.71169100	32.15350200
C	7.34116500	25.31328600	31.36100900
C	6.29106100	24.30646400	30.83367000
H	6.32107900	23.41501400	31.48625200
H	5.28629400	24.75409400	30.94383600
C	5.40199100	23.76073800	28.71979100
H	4.44691400	24.04703800	29.19358100
C	5.27224600	23.30054300	27.36485500
C	3.96035700	23.17480700	26.81832700
H	3.10055700	23.41407900	27.44710500
C	3.78525500	22.75122300	25.51222900
H	2.77727300	22.64895600	25.10680000
C	4.89363100	22.45693400	24.69028200
H	4.74973500	22.13413300	23.65791800
C	6.20435500	22.58257000	25.16943700
C	6.38540200	22.99114300	26.53892500
C	6.86549700	25.75381100	32.75989100
H	5.88531700	26.24797700	32.70124700
H	7.57361700	26.46638200	33.20589900
H	6.77215800	24.89644300	33.44412900
C	7.45366600	26.53742200	30.44072100
H	6.47908100	27.03721600	30.34130100
H	7.79609300	26.26147600	29.43510300
H	8.16657700	27.26642900	30.85311800
C	10.43090500	19.70329600	23.98558600
C	10.06173400	19.43619000	25.35227500
C	10.23624300	18.13371300	25.83732000
H	9.95059700	17.92567600	26.86984000
C	10.78038000	17.11785200	25.02339700

H	10.91208500	16.11562800	25.43437300
C	11.15766500	17.37993200	23.71819000
H	11.59077800	16.59564300	23.09452300
C	10.98834800	18.68533400	23.16764600
C	11.42872100	18.91311700	21.82051000
H	11.90701700	18.03702800	21.34813800
C	11.83710800	19.90952800	19.72481700
H	10.97171500	19.81720300	19.04347500
H	12.43894900	18.98893100	19.61128800
C	12.68535400	21.11525300	19.25343200
C	11.80100100	22.37021900	19.05847600
H	12.38138500	23.12691100	18.49944700
H	10.94431500	22.08362600	18.42165800
C	11.30599800	24.27295100	20.36006100
H	11.75678200	24.81112700	19.50806800
C	10.81632100	25.12866100	21.40400000
C	10.89440900	26.53960200	21.21256300
H	11.30594700	26.92392900	20.27725900
C	10.45477300	27.40447200	22.20056600
H	10.51644600	28.48232400	22.04243800
C	9.93505000	26.91460500	23.41650500
H	9.60049600	27.60034200	24.19668600
C	9.85086200	25.53807400	23.66280800
C	10.28650500	24.63845500	22.62691600
C	13.24050200	20.74667700	17.86320200
H	13.87757800	19.85282000	17.92232000
H	13.85025400	21.56606300	17.45696000
H	12.43134300	20.53912100	17.14631000
C	13.84641200	21.39230900	20.21992100
H	14.49281000	20.50710700	20.31110700
H	13.48751400	21.65332000	21.22366600
H	14.46447800	22.22498000	19.85394900
C	9.60320100	20.87058300	29.85404300
H	10.44312300	21.56132100	29.94164700
C	9.73839100	19.52058600	30.16836400
H	10.70023300	19.14299900	30.51488300
C	8.63653500	18.67761100	30.01763400
H	8.71250400	17.61511900	30.25235400
C	7.43937000	19.21850600	29.54682400
H	6.55581300	18.59813300	29.39529500
C	7.38326600	20.57883300	29.25480000
H	6.47267100	21.04059200	28.87080900
C	8.05059990	20.33535730	21.18026955
H	8.65629790	19.50475630	21.54417655
C	6.70778890	20.16722630	20.85370855
H	6.24781290	19.18467530	20.95735055
C	5.97655390	21.27126830	20.41370455
H	4.92171090	21.17184930	20.15521755
C	6.61756290	22.50770130	20.32486555
H	6.08553390	23.40264330	20.00392455
C	7.96388390	22.59523430	20.66929855
H	8.50099990	23.54383430	20.63146055