

Selective Coordination of Cyanate and Thiocyanate in the End-On Mode:

Synthesis, Structures and Properties of $[\text{Ni}^{\text{II}}_2(\text{L})(\mu_{1,1}\text{-NCO})]^+$ and

$[\text{Ni}^{\text{II}}_2(\text{L})(\mu_{1,1}\text{-NCS})]^+$ (L^{2-} = Macrocyclic N_6S_2 Ligand)

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† Electronic supplementary information (ESI) available: MS and IR spectra for new compounds. Calculated coordinates for complexes **3** and **4**. Crystallographic data in CIF format for **3**. CCDC 1815491 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif. For ESI and or other electronic format see DOI: 10.1039/_____

SUPPORTING INFORMATION

1) Spectrophotometric titration of $[\text{Ni}_2\text{L}][\text{ClO}_4]_2$ (**1**) with $\text{N}(\text{n-Bu})_4\text{NO}_2$.

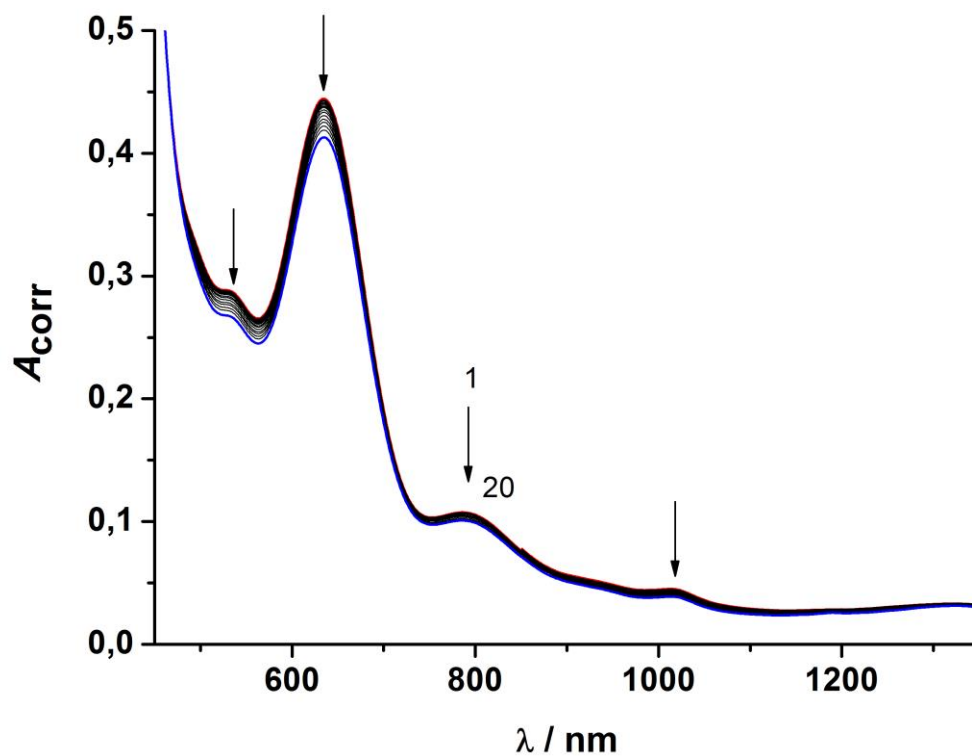


Fig S1. Spectrophotometric titration of $[\text{Ni}_2\text{L}][\text{ClO}_4]_2$ (**1**) as a function of increasing amounts of $\text{N}(\text{n-Bu})_4\text{NO}_2$ added in $25 \mu\text{L}$ increments. Solvent: MeCN/MeOH (1/1 v/v), $T = 298(1) \text{ K}$. Left: $[\mathbf{1}]_0 = 1.00 \cdot 10^{-3} \text{ M}$, $[\text{N}(\text{n-Bu})_4\text{NO}_2] = 6.94 \cdot 10^{-3} \text{ M}$ (spectra 1–11: 0–1.0 equiv.), $\text{N}(\text{n-Bu})_4\text{NO}_2 = 6.94 \cdot 10^{-2} \text{ M}$ (spectra 12–20: 2–9.8 equiv.), $I = 0.1 \text{ M N}(\text{n-Bu})_4\text{ClO}_4$.

2) ESI-MS spectra for Complex 3.

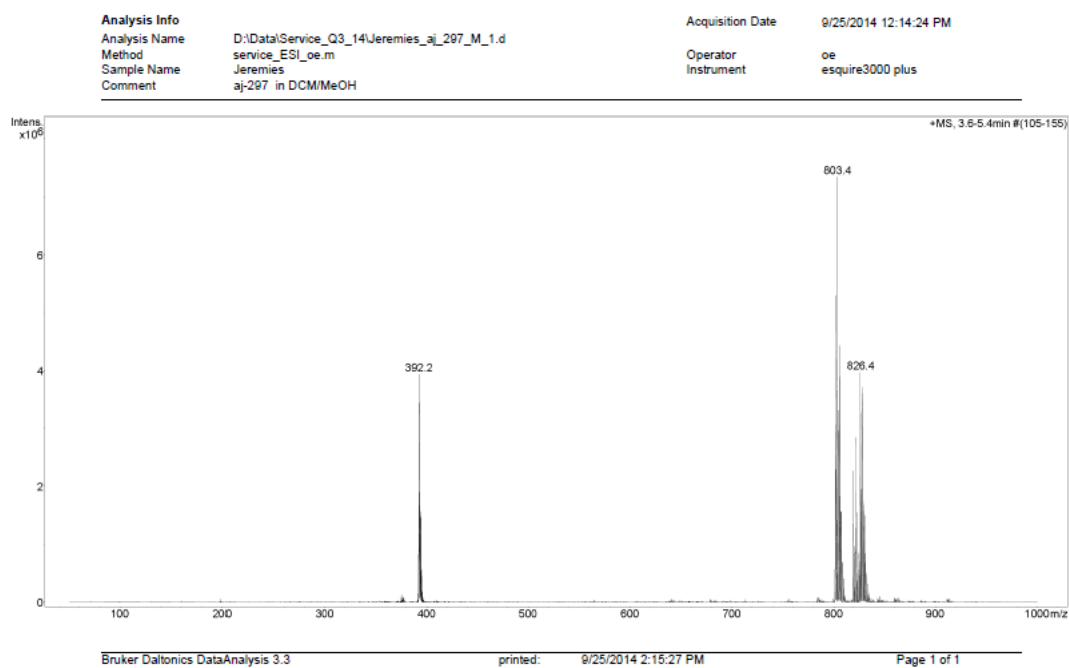


Fig. S2. m/z (ESI+, CH₂Cl₂/MeOH): C₆₃H₈₄BN₇Ni₂OS₂ (1147.72) [Ni₂L(OCN)-BPh₄]⁺ calcd.: 826.33; found 826.4.

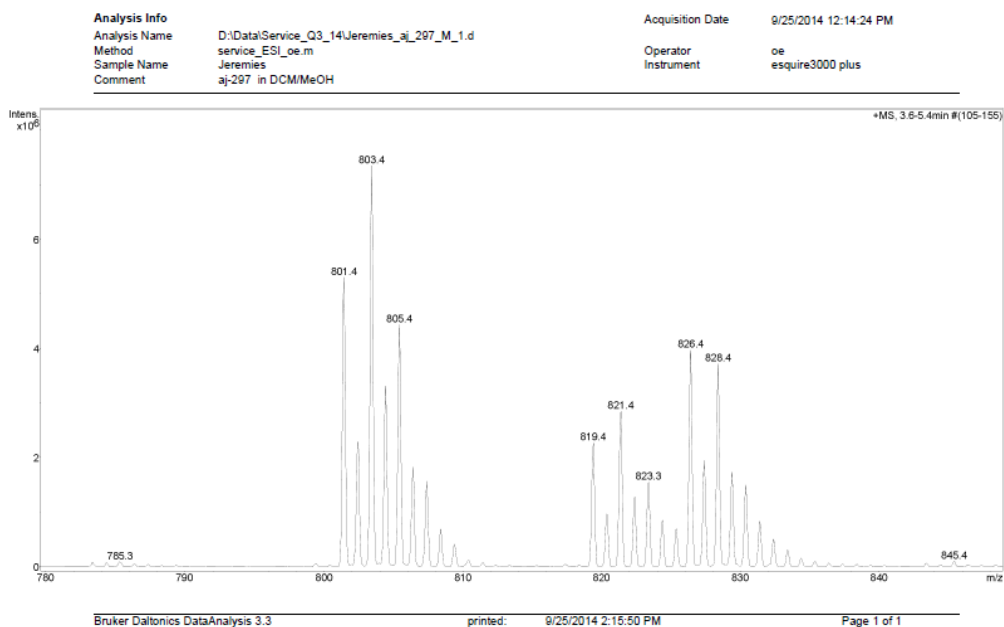


Fig. S3. m/z (ESI+, CH₂Cl₂/MeOH): C₆₃H₈₄BN₇Ni₂OS₂ (1147.72) [Ni₂L(OCN)-BPh₄]⁺ calcd.: 826.33; found 826.4.

3) Infrared spectroscopy.

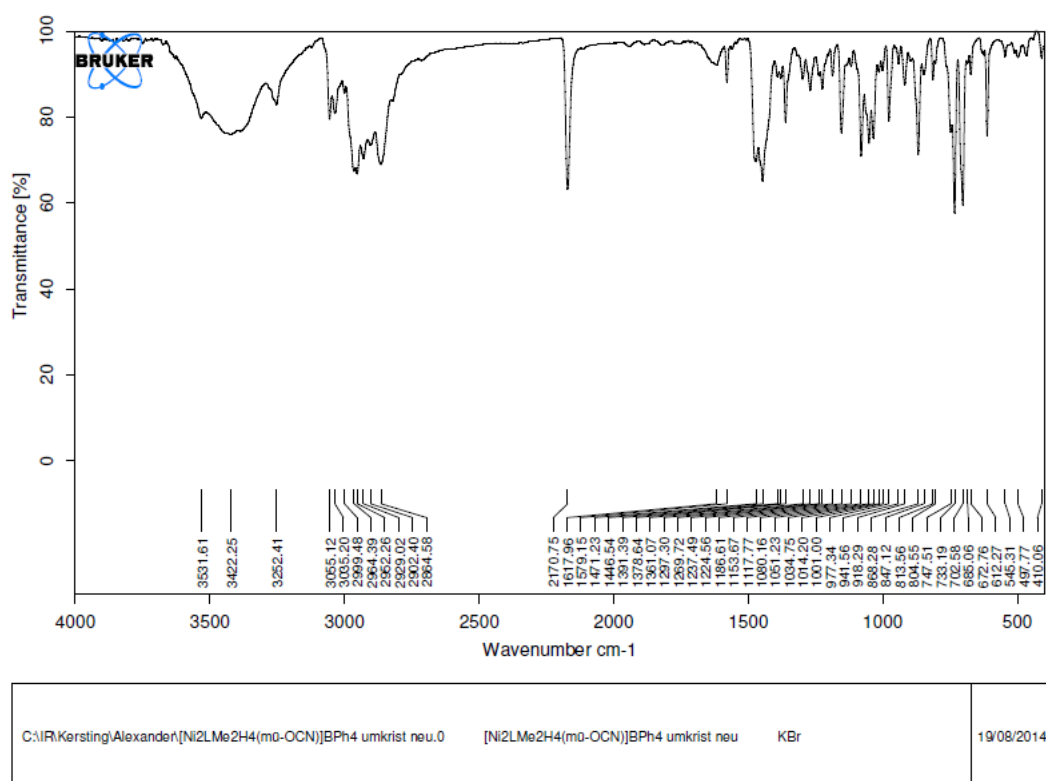


Fig. S4. Infrared spectrum of 3.

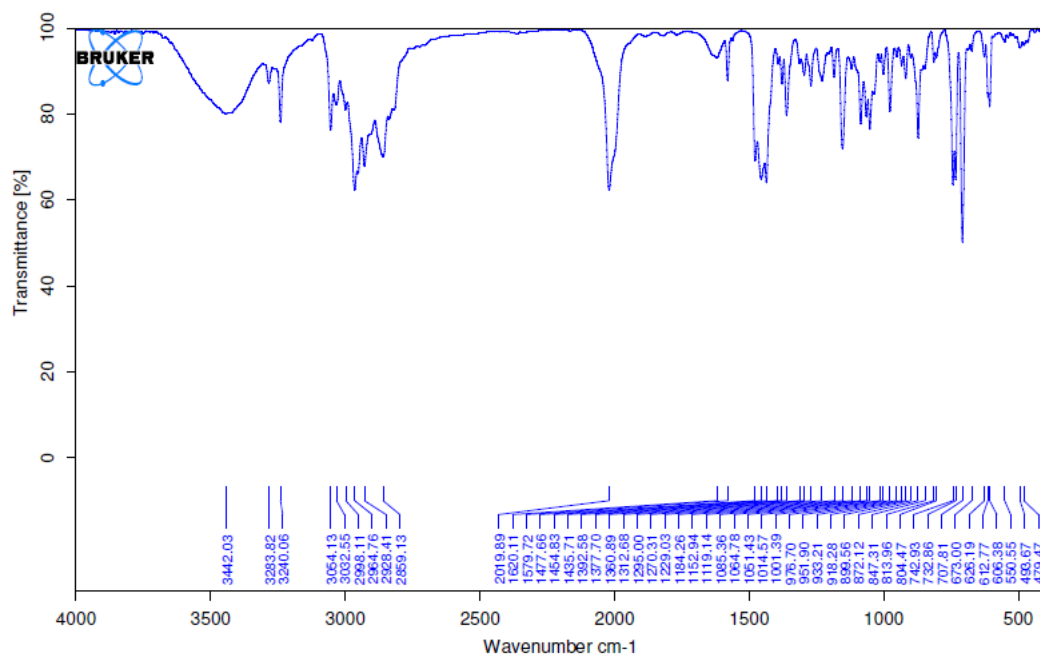


Fig. S5. Infrared spectrum of 4.

Table S1. Cartesian Coordinates of $[\text{Ni}_2\text{L}(\mu_{1,1}\text{-NCO})]^+$ (PBE0, RIJONX, TZV(P), TZV/J, ZORA).

Ni	0.02615878920445	0.04461848470771	0.12866853685897
Ni	-0.04392443522105	3.19845215481705	0.13904978799377
S	0.06600643816248	1.63042535447890	-1.74638106323756
S	1.70421806684405	1.64939110508339	1.00245746463946
N	1.45080164099838	4.49660758295575	-0.46690849440496
N	-0.44971152363412	4.62748069748973	1.87605428495873
N	-1.56986758043167	4.19574193216995	-0.81914207894918
N	-0.32196731706976	-1.40167264584645	1.85775898858333
N	-1.46341466522153	-1.00344206252314	-0.83363518728572
N	1.56869964237265	-1.18773546744209	-0.49466348296774
C	2.84352634228018	1.68202371634106	-0.36330762244990
C	3.27492515605195	2.90131979808531	-0.89392449291996
C	4.13634689758404	2.91818382473896	-1.98435339033940
H	4.45963649938357	3.87152972435689	-2.38891809945498
C	4.59117758591957	1.73697544857118	-2.54883513749689
C	4.18422778957388	0.52854738879775	-2.00568587299575
H	4.54590080019413	-0.40348607597173	-2.42703526941810
C	3.32329762868400	0.49051098162899	-0.91516933482031
C	2.84974252242948	4.19427487296087	-0.27625051256713
H	3.03382170741802	4.14916232802734	0.80740890068082
H	3.46866949678210	5.00910751454041	-0.66185026520747
C	1.19936673388706	5.90803832718709	-0.43283312500694
H	0.23242376494463	6.11456360523497	-0.89619993227267
H	1.97416652833546	6.44563099075357	-0.98793698589976
C	1.17150044517929	6.40256525962499	1.01868326720136
H	2.04462327215861	6.04061155944959	1.56651737230196
H	1.25024741695916	7.49221660562734	1.00265026426727
C	-0.12924103873139	6.06203426971498	1.70208876061545
H	-0.91934183032740	6.51389224688610	1.10667899447280
H	-0.16616048160949	6.54179310484450	2.68903438099148
C	0.31051855520153	4.10187967874781	3.01555655721449
H	0.09394845267889	4.67263630392066	3.92751426201544
H	1.37898259768361	4.14954508797592	2.81300842582654
H	0.04473947618767	3.05869275341772	3.18047787489916
C	-1.88851676648518	4.54785347113405	2.22023146327665
H	-2.06238400548318	5.15919003170904	3.11713414257135
H	-2.09865539600316	3.52255205891997	2.51334009995847
C	-2.86498857362783	5.01835371512572	1.15377489692142
H	-2.76936682767586	6.09403626973475	0.99771459369962
H	-3.86567020162130	4.88246559251336	1.57417579439709
C	-2.86217260791583	4.33105052213759	-0.20473717350230
H	-3.29054186447817	3.32278774761959	-0.12056345849689
H	-3.54514240441847	4.86885885564339	-0.87210513817378
C	-1.62672368908676	4.10436052436807	-2.26516520352699
H	-2.21954592091875	4.93656021182377	-2.65676234048222
H	-0.60757521469705	4.18231961471748	-2.64965753617145
C	-2.24702187081663	2.79638338213873	-2.69704941968752
C	-1.57651718429130	1.59943327051946	-2.40811412232434
C	-2.19886547423367	0.37827276811981	-2.70327316522502
C	-3.44380218342531	0.36611640721180	-3.32137413129381
H	-3.91825853973537	-0.58338515984987	-3.54516493962263
C	-4.08461277024666	1.55260908884473	-3.64721940427535
C	-3.49155260658147	2.76208033840922	-3.31510076887958
H	-4.00371404840492	3.69305062893235	-3.53366267825230

C	-1.52623655554379	-0.90607418567597	-2.27914285164862
H	-0.50540118447407	-0.94137148223484	-2.66542549041479
H	-2.08634932477012	-1.75884123868263	-2.67451959471154
C	-2.74786295571209	-1.19488025509409	-0.21771067170106
H	-3.40826292007563	-1.75870511172375	-0.88650017950805
H	-3.21965001920035	-0.20659899824547	-0.12907245034476
C	-2.72035977205468	-1.88747168465181	1.13794387702398
H	-2.57995816368585	-2.95756907043996	0.97702938795493
H	-3.72516813106928	-1.79532124157436	1.56016788452132
C	-1.76228423206632	-1.38188670050295	2.20483044674899
H	-2.01290430651232	-0.36720463237918	2.50268930057890
H	-1.90864922433144	-2.00411422319514	3.09901314146944
C	0.41797875846581	-0.85320004078021	3.00012803090473
H	0.22308429015232	-1.43686291497968	3.90876596030971
H	0.11248256960820	0.17810005935577	3.17040032905856
H	1.48722165328280	-0.85904304031297	2.79688788943592
C	0.05537519170070	-2.82141715351301	1.67582022584867
H	-0.71589220987600	-3.30086375701490	1.07725157990523
H	0.03736586856562	-3.30746184810683	2.66013191700901
C	1.36874431894956	-3.10514944981090	0.99070196744288
H	2.22646752253452	-2.70799252216841	1.53809788306177
H	1.49310770876489	-4.19050897981715	0.97237857304723
C	1.37468363502104	-2.60820667990419	-0.46027985224990
H	2.16900011862566	-3.11438640144920	-1.01728366125197
H	0.41563863880273	-2.85280363206456	-0.92160518650463
C	2.95633891462886	-0.83045053896099	-0.31954958131915
H	3.60081479190212	-1.61193624082410	-0.73137078656685
H	3.15771972364580	-0.80166519860223	0.76184052523928
H	5.26375427164790	1.75812792552894	-3.39843630685758
H	-5.05167258796237	1.53458356678772	-4.13525409488228
N	-1.27760613828362	1.59664765104835	0.93448044497599
C	-2.41024044515925	1.57262829250318	1.30847993633339
O	-3.53658703022693	1.54738393635941	1.68791212035423

Table S2. Cartesian Coordinates of $[\text{Ni}_2\text{L}(\mu_{1,1}\text{-OCN})]^+$ (PBE0, RIJONX, TZV(P), TZV/J, ZORA).

Ni	0.02409404729081	-0.03791260828705	0.14119311259415
Ni	-0.03795217158663	3.29352702181177	0.14672829927000
S	-0.05070091410070	1.63342764058988	-1.61251407122760
S	1.59961137625041	1.65608910515205	1.05372381825769
N	1.47639247149162	4.50954505020480	-0.47468141826955
N	-0.40441838922916	4.72552173521843	1.79868959548566
N	-1.60082881283689	4.21224415330140	-0.79295417278066
N	-0.28379204601716	-1.50327224181316	1.78281240010693
N	-1.49845393577925	-1.01379357946366	-0.80987871956626
N	1.58443532834593	-1.18924938318057	-0.49576697621048
C	2.82532939653195	1.68535373655891	-0.24042180628646
C	3.30544546724915	2.90153658596443	-0.73814948514958
C	4.24525225289516	2.91383771959727	-1.76183562244012
H	4.60171027250071	3.86597324842229	-2.14003840567500
C	4.73687979666033	1.73151870287097	-2.29059403419112
C	4.28955917697788	0.52634919184579	-1.77410140488892
H	4.68150133297016	-0.40782858349426	-2.16189985548164
C	3.35006905445366	0.49291875907611	-0.75046317797337
C	2.85017075814335	4.20263580607812	-0.15700197197646

H	2.93753760540358	4.15146736631553	0.93827877492120
H	3.51043339195659	5.00877404538229	-0.48701018365971
C	1.23712534419743	5.91630409711131	-0.59898185394362
H	0.31180415280866	6.08142681309662	-1.15330828143127
H	2.06042761402413	6.39914199209361	-1.13364851409206
C	1.09826395198863	6.53466092439606	0.79752013713238
H	1.97059871599090	6.29934754415911	1.41125810008475
H	1.08995923737513	7.62049395710053	0.67716910950474
C	-0.20439849902959	6.15163763555862	1.45620867097141
H	-0.99815604467965	6.44044792363229	0.77133026715922
H	-0.34370221465172	6.74188121592571	2.37111161877767
C	0.44554570422240	4.36616539875825	2.93957774173721
H	0.25483900900491	5.02923182042067	3.79179862942682
H	1.49764464585416	4.43251712370558	2.67114362680968
H	0.23962513667726	3.33967758386679	3.23780162054442
C	-1.81577796746067	4.57968843086699	2.23402515526539
H	-1.96610355929731	5.20838387744985	3.12174675321466
H	-1.95265005735206	3.55222240532159	2.56146663558995
C	-2.87814999996984	4.96403763759042	1.21656398278733
H	-2.88110275676331	6.04325242409320	1.05633810199855
H	-3.84017692249086	4.74098268365253	1.68584321031850
C	-2.87685237777714	4.26416110154780	-0.13526715439064
H	-3.22464549456305	3.22754999911309	-0.01294126593930
H	-3.62172085091180	4.73752620168391	-0.78449999071325
C	-1.69748294929830	4.10941356189975	-2.23554903419021
H	-2.30562849528094	4.93888661663786	-2.60960782879814
H	-0.69198338700183	4.19893992737128	-2.65258977883398
C	-2.31984043090208	2.80071170157606	-2.66048629844970
C	-1.66671462650788	1.60274853332243	-2.34367137793002
C	-2.27008515136379	0.38081449745589	-2.66779552633710
C	-3.49209047309584	0.36950741640314	-3.32951719677233
H	-3.95559216593090	-0.57988644132252	-3.57503235418881
C	-4.12329967318554	1.55631875572856	-3.67193805074741
C	-3.54116080346009	2.76604655495863	-3.32244920372642
H	-4.04321692938613	3.69717908237387	-3.56208026149656
C	-1.59475557242221	-0.90453291672711	-2.25208117340775
H	-0.58517773163607	-0.94841177357812	-2.66643631505103
H	-2.16715495411014	-1.75498729945461	-2.63491038508313
C	-2.77166800120009	-1.13472618796815	-0.15627625155355
H	-3.49350440674956	-1.63224540312263	-0.81339676684621
H	-3.16628149227875	-0.11725578701597	-0.01778751722429
C	-2.74115367656370	-1.85312262968910	1.18543110374671
H	-2.68998009840177	-2.92863028351649	1.00963488532650
H	-3.71452035252093	-1.68553018287836	1.65453894147342
C	-1.70259756256899	-1.43016523608901	2.21214998586578
H	-1.89089056323726	-0.41492263136449	2.55146559717338
H	-1.82599801498634	-2.07608954466207	3.09178718323829
C	0.54297678932504	-1.10501933249452	2.92818297322812
H	0.37877873573264	-1.77622438759167	3.77971778745449
H	0.28886254601791	-0.08919642185431	3.22550350361202
H	1.59832465256716	-1.12268251972067	2.66455095392266
C	-0.01170393856907	-2.91782964930352	1.44131549791178
H	-0.79337786554295	-3.25104727555632	0.76265240130068
H	-0.11463047823398	-3.51201698525496	2.35834123231110
C	1.30451871482655	-3.23281814018127	0.77458736703213
H	2.16699410594100	-2.95529615828796	1.38478755035864
H	1.35130360243140	-4.31739437382266	0.65166100443330

C	1.40262218343728	-2.60470828943714	-0.62101746032605
H	2.23984775963713	-3.05068341340963	-1.16605367224006
H	0.47927950069648	-2.80696112937460	-1.16645721311255
C	2.94637834665909	-0.83045810968777	-0.18177004022757
H	3.63624053473669	-1.60689747301314	-0.52218605260575
H	3.03660507053577	-0.78805034414187	0.91357838387596
H	5.47128058025337	1.74919840577600	-3.08730166045188
H	-5.07442188492936	1.53826070649865	-4.19022873462038
O	-1.34766929541761	1.58493292502230	1.14383801032456
C	-2.51203808860208	1.56029433483162	1.54475974632205
N	-3.62095628618148	1.53768503736870	1.92756504963812

Table S3. Cartesian Coordinates of $[\text{Ni}_2\text{L}(\mu_{1,1}\text{-NCS})]^+$ (PBE0, RIJONX, TZV(P), TZV/J, ZORA).

Ni	0.02778612928015	0.02220142616632	0.14148903957112
Ni	-0.00958318893918	3.23415948352166	-0.18245432140700
S	-0.25115221795760	1.44758360756474	-1.82434054056157
S	1.78097362532918	1.71792229444160	0.61221441123522
N	1.39156182232513	4.37378071061936	-1.17356335823456
N	-0.08448274953147	4.90620029136278	1.34966540859315
N	-1.67625815145581	4.12967596285282	-0.96924437205705
N	-0.02745268664418	-1.31397459780431	1.96613091303310
N	-1.61351272043038	-1.04838294558743	-0.46582051485600
N	1.46945727433853	-1.25093872919377	-0.60362832215123
C	2.77695707392546	1.58249091726558	-0.85680582595712
C	3.16682978706183	2.72779587098275	-1.55789369491816
C	3.92959572368879	2.61059493293370	-2.71381907880181
H	4.22031999479291	3.50811603468823	-3.24926716903275
C	4.32867355402056	1.36753652218398	-3.17878509132440
C	3.96389430089328	0.23376407729382	-2.47045130536823
H	4.28235349403188	-0.74483240431774	-2.81393663674032
C	3.20116705422713	0.33095259689719	-1.31261180489313
C	2.80245646569809	4.08844121172536	-1.05716177182019
H	3.06938077128175	4.15769982890469	0.00754706226461
H	3.39228514993337	4.84756893952176	-1.57731404968469
C	1.13932316220884	5.76813646373304	-1.38777315273852
H	0.12094867045305	5.90501352188479	-1.75524638841668
H	1.83686555760306	6.17059339117865	-2.12900264183533
C	1.29909867723744	6.52810145396096	-0.06636760039990
H	2.26495212120265	6.30519220709270	0.39243727445904
H	1.30919748430715	7.59633021194387	-0.29541131897911
C	0.13500029114519	6.28664502369680	0.86234398079393
H	-0.75830208759289	6.59635316464678	0.32542040880395
H	0.22034512913084	6.94451391771364	1.73763150199568
C	0.89971616383722	4.59771766122962	2.39264280711424
H	0.83949920594031	5.32398802138804	3.21280682242244
H	1.90830740247086	4.61224810372145	1.98445708785070
H	0.71310320289137	3.60125520316687	2.78977185970240
C	-1.42433402552635	4.88742992290485	1.98413111862380
H	-1.42757226610245	5.62114049690563	2.80259486634192
H	-1.55144756919042	3.91403490638950	2.44961830903592
C	-2.60552297330542	5.20882010769054	1.08137329472725
H	-2.58545377391164	6.25777569933323	0.78258865834627
H	-3.49850538636430	5.10746388290391	1.70407904728029
C	-2.83782169602836	4.35348181262370	-0.15650873020822

H	-3.21852846543528	3.36626773729160	0.14282488209620
H	-3.64087169292639	4.80090029739164	-0.75313518692914
C	-1.97802826483931	3.89418658683938	-2.36718393987343
H	-2.62534369898450	4.69538277512803	-2.73643423945520
H	-1.03971690244213	3.91230882493210	-2.92477957544742
C	-2.66757269969691	2.56299540471850	-2.55615959754129
C	-1.97319320522211	1.38685067205878	-2.24342556559660
C	-2.63732555440514	0.15591647969699	-2.32386887165818
C	-3.95789495408312	0.10792184215127	-2.75460707568991
H	-4.46444937324304	-0.84947076214517	-2.81215134666668
C	-4.63088708336925	1.26990329024749	-3.10313216287716
C	-3.98781449742967	2.49347878083212	-2.98475459008479
H	-4.51898540361879	3.40849825362283	-3.22371066322294
C	-1.91548020611444	-1.09533261453299	-1.88265036616264
H	-0.97526853526115	-1.19609944077844	-2.42870303462349
H	-2.54158371402351	-1.96870606007841	-2.08902655336321
C	-2.77567587306117	-1.13148785204725	0.37365223085406
H	-3.56892321847632	-1.69993408916596	-0.12397399573529
H	-3.17357417625088	-0.11162172645254	0.47545642677962
C	-2.53693630210522	-1.72641899430203	1.75515035937201
H	-2.48998708265871	-2.81254061471618	1.66462182747999
H	-3.43815110739997	-1.52814658379030	2.34199800212788
C	-1.37180112711712	-1.20743111272588	2.58265648306500
H	-1.52744920546065	-0.16605277003963	2.84961259926267
H	-1.36055525571056	-1.76914108124840	3.52695169572777
C	0.94275802628851	-0.78171410154292	2.92881212265524
H	0.90596723615524	-1.34150773896288	3.87130956859933
H	0.71952396822903	0.26468152334773	3.13115531979476
H	1.95146810790391	-0.83662946134643	2.52481048402938
C	0.22694074592844	-2.75755170947876	1.75555023107989
H	-0.64943540993712	-3.18085437416275	1.27161592264996
H	0.30584047862413	-3.23447641206493	2.74132439191664
C	1.41328694277344	-3.14281893505915	0.90687143075348
H	2.36221003628153	-2.79736854437790	1.32257971428532
H	1.46007475607576	-4.23431502360494	0.89724523711922
C	1.25558092795553	-2.66621576122420	-0.54145085509827
H	1.97485888246535	-3.18871576800818	-1.17956017174122
H	0.24720134075685	-2.90008291421949	-0.88694453488439
C	2.87233663301125	-0.91077297524058	-0.54818231492198
H	3.48328654598011	-1.74159075488675	-0.90983327721445
H	3.13939674205882	-0.75996371635148	0.50839101512229
H	4.92585401382884	1.28379242010001	-4.07906777783726
H	-5.65823846436138	1.22429174032123	-3.44376342673201
N	-1.17618888101555	1.71538241176921	1.06356890554335
C	-2.17969273543438	1.77193852702714	1.68640104531886
S	-3.56077009050852	1.84676311894682	2.52837304591497

Table S4. Cartesian Coordinates of $[\text{Ni}_2\text{L}(\mu_{1,1}\text{-SCN})]^+$ (PBE0, RIJONX, TZV(P), TZV/J, ZORA).

Ni	0.01517911265383	-0.09740324834604	0.23415423770658
Ni	-0.02401480564323	3.36751261072049	-0.11160372373685
S	-0.31228345862685	1.47181596407415	-1.61134027969435
S	1.77749724151794	1.71644655896207	0.70965080761267

N	1.41546597521877	4.39718821702601	-1.12758580669578
N	-0.10074947163288	5.11898722379561	1.29800169211403
N	-1.69209679626582	4.19636629609446	-0.93374937552509
N	-0.03446251073439	-1.52897159585922	1.95840631555063
N	-1.63115556995843	-1.10375160909001	-0.42484843737303
N	1.46661124896637	-1.27567199121724	-0.58171483830169
C	2.76522304457234	1.58378495948867	-0.76419331927316
C	3.16999480730337	2.73285879662404	-1.45233302038468
C	3.93440364893490	2.62137057717973	-2.60756138669365
H	4.23530722833042	3.52206102911959	-3.13186147189001
C	4.32480556177798	1.38011129076266	-3.08403911898266
C	3.95288262912297	0.24300377551574	-2.38521797429696
H	4.26921444043139	-0.73421330863808	-2.73438881344433
C	3.18861347946116	0.33381798702024	-1.22781467319238
C	2.81488811546987	4.09321467376997	-0.93913193929740
H	3.02770670552457	4.13007323292189	0.13849588511125
H	3.44437826956250	4.84826362104604	-1.41598583866855
C	1.18948901500781	5.76479175470410	-1.48705048329627
H	0.19647334179009	5.87307052657547	-1.92562160508156
H	1.93389184629674	6.09666909990909	-2.21691570314878
C	1.27975363745532	6.63665694175638	-0.22914070330241
H	2.23072067001968	6.47599409704070	0.28340122727669
H	1.27727353679375	7.68083750648529	-0.55068949192028
C	0.08605175937329	6.44797945676652	0.67463183233214
H	-0.79594473343822	6.65872934659648	0.07443977461691
H	0.11205610162658	7.19779520236031	1.47687189154925
C	0.90596290866335	4.91786662878544	2.34602294289693
H	0.86059465301369	5.72215780563416	3.09102317281059
H	1.90604377662708	4.89588586994264	1.91807406316902
H	0.73006337806942	3.96557525330669	2.84386307932500
C	-1.43183871205896	5.13898936753344	1.95661777182948
H	-1.42633716007233	5.93577423075366	2.71310827196529
H	-1.53938858121921	4.20035312827001	2.49523070469845
C	-2.62897603564660	5.37441031469042	1.04876121845267
H	-2.62815745078754	6.39663078347805	0.66802173424739
H	-3.51424748441741	5.30907618922848	1.68718595873763
C	-2.85133749499782	4.41718964335859	-0.11408106660077
H	-3.16599916230088	3.43672829949942	0.26891218545677
H	-3.69008198292217	4.77661554129871	-0.72033146615131
C	-1.99727771748715	3.90874537777052	-2.31904478746325
H	-2.64181977746728	4.70054170906051	-2.71301568507938
H	-1.06166647960029	3.90652293873225	-2.88161006954717
C	-2.69133005199219	2.57640230382957	-2.47390418407485
C	-2.00926018964726	1.40380902133082	-2.12112412582716
C	-2.65978825244462	0.16851236514902	-2.24542689200071
C	-3.96485094308877	0.11748326206660	-2.72033570558840
H	-4.46097780346324	-0.84288345199307	-2.80927579835401
C	-4.63368339074184	1.27799846444639	-3.08022565209440
C	-3.99600188770566	2.50244531711950	-2.94628563882312
H	-4.51740689618879	3.41539693894093	-3.21284501626710
C	-1.93245629968396	-1.09121123404436	-1.84062034889333
H	-0.99202960863706	-1.16861724205327	-2.39062292971663
H	-2.55286534628925	-1.96029960547537	-2.08052448710179
C	-2.79093741169433	-1.20047368101195	0.41728101554507
H	-3.61144016871204	-1.69655136835073	-0.11172367072875
H	-3.14318777728629	-0.17616722992287	0.60285520643027
C	-2.55207152326325	-1.90859035479520	1.74350961380574

H	-2.51515606233561	-2.98451987299509	1.56649230280084
H	-3.44696550553576	-1.75100630073742	2.35202873878512
C	-1.37532167957339	-1.45831046721225	2.59430344906411
H	-1.52023295161155	-0.43339534831345	2.92679923801368
H	-1.35695517161846	-2.08152837337381	3.49824381252437
C	0.94844943913557	-1.07726807124614	2.95086364832032
H	0.91699313603290	-1.70852074925254	3.84691616162801
H	0.73323973225258	-0.04886031719932	3.23530559754954
H	1.95355158083047	-1.10977631252054	2.53513654639296
C	0.20911390411929	-2.95303692336131	1.63421186170981
H	-0.66632373888805	-3.32893694729571	1.11034143682478
H	0.27701636751334	-3.50853137830684	2.57841429838014
C	1.40360884562921	-3.27784922054460	0.77061606477872
H	2.34995452457467	-2.96910416890161	1.22018686790310
H	1.44638128240555	-4.36543484946087	0.67738439939084
C	1.26617744740378	-2.69266043197296	-0.63961349726299
H	2.00381551910700	-3.15574065412461	-1.30217379948679
H	0.26705074086253	-2.90919383838114	-1.02079797471088
C	2.86094531132181	-0.91566146353865	-0.47313524979489
H	3.50037890851229	-1.73332225451739	-0.81395398015109
H	3.08455661886428	-0.75683799331475	0.59180837675764
H	4.92406468168277	1.30030611050455	-3.98318567256221
H	-5.64939206088458	1.22940484893612	-3.45340601850348
S	-1.04125289874237	1.78516375101623	1.67078233635928
C	-2.68288278270696	1.79224204014215	1.99677512930066
N	-3.81892838582050	1.79916360622776	2.24966085125994

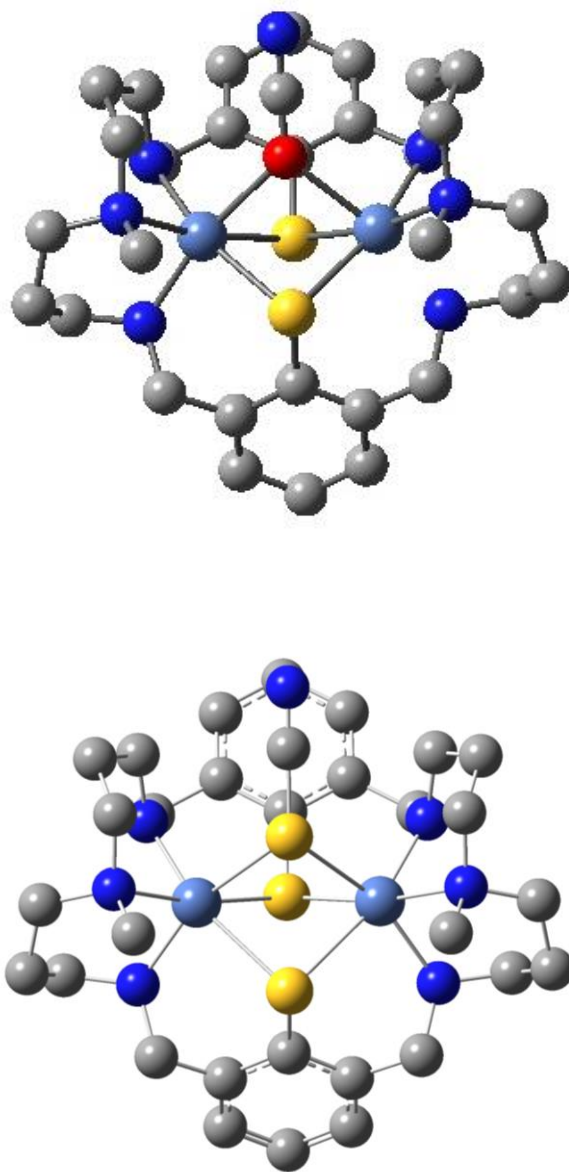


Fig. S6. Calculated structures of $[\text{Ni}_2\text{L}(\mu_{1,1}\text{-NCO})]^+$ (top) and $[\text{Ni}_2\text{L}(\mu_{1,1}\text{-SCN})]^+$ (bottom).

Hydrogen atoms are omitted for clarity.

