

SUPPORTING INFORMATION

A Selenium-Containing Diarylamido Pincer Ligand: Synthesis and Coordination Chemistry with Group 10 Metals

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Table S1. Conditions Used in the Attempted Preparation of [(N(C₇H₆SeMe)₂)NiL_n].

Nickel(II) Source	Base/Reactant	Solvent	Temperature (°C)	Time (h)
NiCl ₂ (DME)	Et ₃ N	THF	70	14
	ⁿ BuLi	THF	23	18
	Ag(OTf)	CH ₂ Cl ₂	23	24
NiCl ₂	Et ₃ N	THF	80	1
	DMAP	toluene	100	24
NiBr ₂	Et ₃ N	THF	70	2
	ⁿ BuLi/TMEDA	THF	23	2
Ni(OTf) ₂	Et ₃ N	THF	70	2
NiCl ₂ •6H ₂ O	Et ₃ N	MeOH/ CH ₂ Cl ₂	23	48
	Et ₃ N	toluene	100	1

Table S2. Crystal Data for Compounds **1**, **1-Pd**, **3-Pd**, and **3-Pt**.

Compound	1	1-Pd	3-Pd	3-Pt
Empirical formula	C ₁₇ H ₂₁ NSe ₂	C ₁₇ H ₂₁ Cl ₂ NPdSe ₂	C ₁₆ H ₁₈ CINPdSe ₂	C ₁₆ H ₁₈ CINPtSe ₂
Formula weight	397.27	574.57	524.08	612.77
Temperature/K	295	295	295	150
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic
Space group	<i>P2₁/c</i>	<i>C2/c</i>	<i>C2/c</i>	<i>C2/c</i>
a/Å	14.5262(10)	31.4104(17)	15.1538(5)	14.9179(6)
b/Å	8.1591(6)	8.4136(5)	9.5448(3)	9.5125(4)
c/Å	14.4769(10)	17.2474(10)	12.7299(4)	12.6401(5)
α/°	90	90	90	90
β/°	100.438(4)	121.645(3)	111.1590(10)	110.272(2)
γ/°	90	90	90	90
Volume/Å ³	1687.4(2)	3880.3(4)	1717.12(10)	1682.61(12)
Z	4	8	4	4
ρ _{calc} /g/cm ³	1.564	1.967	2.027	2.419
μ/mm ⁻¹	4.373	4.982	5.468	12.817
F(000)	792	2224	1008	1136
Crystal size/mm ³	0.2 × 0.2 × 0.15	0.3 × 0.2 × 0.1	0.18 × 0.08 × 0.05	0.16 × 0.049 × 0.041
2θ range for data collection/°	5.704 to 52.732	5.388 to 50.05	6.742 to 50.048	5.63 to 61.016
Reflections collected	25900	27222	14295	31503
Independent reflections [R _{int}]	3455 [0.0515]	3426 [0.1133]	1512 [0.0288]	2580 [0.0454]
Data/restraints/parameters	3455/0/186	3426/0/213	1512/0/99	2580/0/99
Goodness-of-fit on F ²	1.057	0.967	1.2	1.091
R ₁ [I >= 2σ(I)], wR ₂ [all data]	0.0335, 0.0822	0.0261, 0.0480	0.0232, 0.0605	0.0256, 0.0372
Largest diff. peak/hole / e Å ⁻³	0.53/-0.56	0.38/-0.41	0.46/-0.63	0.75/-1.21

Table S3. Atomic coordinates (Å) and energies for **3-Pd** (C_2 -symmetric isomer).

ATOM	CHARGE	X	Y	Z
PD	46.0	6.4278827311	1.4423649015	2.9679585382
SE	34.0	6.0429809906	1.6027434711	5.3466495242
SE	34.0	6.8128945993	1.6024900478	0.5892316016
CL	17.0	6.4272566725	-0.8865003348	2.9677514907
N	7.0	6.4285114283	3.4588639964	2.9679130699
C	6.0	6.7238033625	4.1130834735	4.1530012606
C	6.0	6.5653860086	3.4482509173	5.3892876699
C	6.0	7.2597146420	5.4207261351	4.2327330013
C	6.0	6.8176621259	4.0698970553	6.6130423178
C	6.0	7.5311944205	6.0220550599	5.4524870898
C	6.0	7.2990256708	5.3760407524	6.6763358259
C	6.0	7.7074856502	0.8007844014	5.9683853259
C	6.0	7.5797475276	6.0619230767	7.9882594438
C	6.0	6.1332747174	4.1131500287	1.7828648658
C	6.0	6.2906758122	3.4480662291	0.5465790196
C	6.0	5.5983816435	5.4212031428	1.7032346397
C	6.0	6.0380513452	4.0697097098	-0.6771195108
C	6.0	5.3264713138	6.0225797304	0.4835783359
C	6.0	5.5573156361	5.3760884448	-0.7403240191
C	6.0	5.1487689232	0.8001095365	-0.0329505715
C	6.0	5.2754965154	6.0617615768	-2.0521890115
H	1.0	7.4944050767	5.9585483363	3.3137959673
H	1.0	6.6501200920	3.5124792119	7.5404530780
H	1.0	7.9526012783	7.0320849542	5.4539949540
H	1.0	8.5514978954	1.3013785249	5.4794643949
H	1.0	7.6659632120	-0.2539051442	5.6647164425
H	1.0	7.7717384781	0.8959827257	7.0598240601
H	1.0	7.4062639141	5.3882281846	8.8398627331
H	1.0	6.9339828032	6.9445632137	8.1244764386
H	1.0	8.6237000629	6.4104055847	8.0430528563
H	1.0	5.3647923610	5.9592836363	2.6223525001
H	1.0	6.2046183843	3.5120012949	-1.6045379677
H	1.0	4.9058881066	7.0329830216	0.4821627420
H	1.0	4.3042924683	1.3000752802	0.4558161514
H	1.0	5.1908891492	-0.2545887822	0.2704844967
H	1.0	5.0848734520	0.8953760036	-1.1243856742
H	1.0	5.4513695855	5.3887798276	-2.9038090699
H	1.0	5.9187589725	6.9463859793	-2.1878641388
H	1.0	4.2306629710	6.4072467945	-2.1075698723

Electronic Energy (Hartrees): -6065.3606105070
Total Gibbs Energy Correction (kJ mol⁻¹): +647.714

Table S4. Atomic coordinates (Å) and energies for **3-Pd** (asymmetric isomer).

ATOM	CHARGE	X	Y	Z
PD	46.0	6.4068408382	1.4280164782	3.0166123513
SE	34.0	5.9882553562	1.6076045739	5.3867840691
SE	34.0	6.8037409870	1.5845962520	0.6347886436
CL	17.0	6.5362857740	-0.8913733053	3.0680518136
N	7.0	6.4269011704	3.4497406432	3.0038723031
C	6.0	6.7169490227	4.1040068317	4.1906950387
C	6.0	6.5386094318	3.4454019008	5.4277229942
C	6.0	7.2697785681	5.4046807674	4.2714947100
C	6.0	6.7897410539	4.0675989215	6.6514858938
C	6.0	7.5403193012	6.0060563746	5.4914854751
C	6.0	7.2896401158	5.3667919596	6.7151188707
C	6.0	7.6236219069	0.7797800971	6.0498775436
C	6.0	7.5682170036	6.0525832415	8.0275268743
C	6.0	6.1506311317	4.1072849067	1.8163006075
C	6.0	6.3165195527	3.4360152999	0.5840777678
C	6.0	5.6303039400	5.4196690606	1.7275983857
C	6.0	6.0487396936	4.0424498720	-0.6439171642
C	6.0	5.3703076257	6.0155467387	0.5019858849
C	6.0	5.5895806255	5.3565328927	-0.7169482439
C	6.0	8.7454883140	1.7625926633	0.6239773731
C	6.0	5.3047504596	6.0319613143	-2.0334246287
H	1.0	7.5174659788	5.9373869402	3.3528781057
H	1.0	6.6062988390	3.5158271267	7.5792158483
H	1.0	7.9754585887	7.0102496990	5.4934456126
H	1.0	8.4878197161	1.3021094676	5.6225450434
H	1.0	7.5955850245	-0.2593554942	5.6944651895
H	1.0	7.6380728025	0.8260931695	7.1461672467
H	1.0	7.3922403720	5.3790500962	8.8787653080
H	1.0	6.9228350060	6.9356792521	8.1623563686
H	1.0	8.6120694235	6.4003724683	8.0847311236
H	1.0	5.3959487853	5.9658432587	2.6416511196
H	1.0	6.1854223135	3.4653958306	-1.5641181012
H	1.0	4.9593212708	7.0299029044	0.4925459900
H	1.0	9.0705871720	2.0706582377	-0.3779637319
H	1.0	9.1560758090	0.7752575483	0.8740137039
H	1.0	9.0438484898	2.5006759567	1.3777802015
H	1.0	5.4633068759	5.3471900505	-2.8790412215
H	1.0	5.9583242114	6.9064574934	-2.1845029516
H	1.0	4.2643074485	6.3908885097	-2.0830014185

Electronic Energy (Hartrees): -6065.3597385468

Total Gibbs Energy Correction (kJ mol⁻¹): +644.916

Table S5. Atomic coordinates (Å) and energies for **3-Pt**.

ATOM	CHARGE	X	Y	Z
PT	78.0	4.1740644939	8.1066836757	8.8929114108
SE	34.0	3.8448423588	7.9497300584	11.2714301176
SE	34.0	4.5033907745	7.9498808766	6.5142343206
CL	17.0	4.1734904858	10.4594415709	8.8928912899
N	7.0	4.1744916443	6.0851507709	8.8928572593
C	6.0	4.4762203977	5.4281601725	10.0765590897
C	6.0	5.0023484019	4.1169707654	10.1533305127
C	6.0	5.2813370557	3.5155304275	11.3710658614
C	6.0	5.0672532405	4.1654246726	12.5963467418
C	6.0	4.5982073611	5.4756702544	12.5355482268
C	6.0	4.3391486515	6.0970192493	11.3132417136
C	6.0	5.3561229306	3.4790158151	13.9061311655
C	6.0	5.5187145910	8.7276062250	11.8999084329
C	6.0	3.8729523656	5.4280727193	7.7091514050
C	6.0	3.3473644862	4.1166540837	7.6323709925
C	6.0	3.0684148448	3.5151672568	6.4146483601
C	6.0	3.2820234120	4.1652429246	5.1893850881
C	6.0	3.7507409254	5.4755987321	5.2501783830
C	6.0	4.0096855154	6.0970115239	6.4724745052
C	6.0	2.9921041079	3.4793608431	3.8795791197
C	6.0	2.8291826736	8.7272503077	5.8859052006
H	1.0	5.2263014605	3.5765481588	9.2335667570
H	1.0	5.6951464810	2.5024182407	11.3695906887
H	1.0	4.4472512476	6.0368235501	13.4635767905
H	1.0	4.7046794240	2.6018481005	14.0505236963
H	1.0	5.19744446817	4.1553857187	14.7584868974
H	1.0	6.3973429738	3.1218259827	13.9501267728
H	1.0	6.3559211398	8.2212095924	11.4057652671
H	1.0	5.5788532264	8.6253373035	12.9909254750
H	1.0	5.4863520068	9.7846442284	11.6025734566
H	1.0	3.1237810392	3.5760461031	8.5521130188
H	1.0	2.6550722089	2.5018648628	6.4161410766
H	1.0	3.9014250470	6.0368159915	4.3221496557
H	1.0	3.6371823357	2.5972187351	3.7383095121
H	1.0	3.1584100971	4.1534081191	3.0269082977
H	1.0	1.9481851269	3.1300020176	3.8327743004
H	1.0	1.9921334614	8.2201317327	6.3795601678
H	1.0	2.7692990372	8.6256817505	4.7947880355
H	1.0	2.8610182856	9.7841468863	6.1838709391

Electronic Energy (Hartrees): -6056.8549564644

Total Gibbs Energy Correction (kJ mol⁻¹): +646.957

Table S6. Atomic coordinates (Å) and energies for **E-Pd**.

ATOM	CHARGE	X	Y	Z
PD	46.0	8.6599316425	2.9414182656	3.6443486661
CL	17.0	8.6571887731	5.2711851298	3.6472738570
P	15.0	9.0749884784	2.7027871839	1.4065443559
P	15.0	8.2460981524	2.6936156804	5.8814703814
N	7.0	8.6633138179	0.8950991879	3.6403008295
C	6.0	8.4658472604	0.2440561075	2.4303874972
C	6.0	7.9741996716	-1.0776427802	2.2992268814
C	6.0	7.8112451231	-1.6673785695	1.0548336833
C	6.0	8.1064172677	-0.9965536297	-0.1425685445
C	6.0	8.5270860680	0.3257547346	-0.0267066032
C	6.0	8.6881429249	0.9450039765	1.2170236705
C	6.0	7.9433045733	-1.6741652521	-1.4785705196
C	6.0	10.7708290485	2.9856196854	0.7912029489
C	6.0	8.0062292073	3.6384713278	0.2632380551
C	6.0	8.8628210886	0.2404616035	4.8480235420
C	6.0	9.3597703078	-1.0796651958	4.9747854211
C	6.0	9.5255368050	-1.6727903946	6.2172229958
C	6.0	9.2279156941	-1.0071382212	7.4169564332
C	6.0	8.8015146249	0.3136054534	7.3054663093
C	6.0	8.6377159749	0.9362533552	6.0638196662
C	6.0	9.3945595849	-1.6881429598	8.7508574761
C	6.0	6.5508526360	2.9704943406	6.5011105254
C	6.0	9.3144278728	3.6263855272	7.0275204634
H	1.0	7.6845251598	-1.6377923816	3.1880128283
H	1.0	7.4217207700	-2.6895566899	1.0093169474
H	1.0	8.7195370459	0.9026597594	-0.9383114090
H	1.0	8.1122550621	-0.9721860752	-2.3082987903
H	1.0	8.6578932087	-2.5054350808	-1.5958016165
H	1.0	6.9321689890	-2.0959559862	-1.5961582632
H	1.0	9.6514901361	-1.6357964418	4.0841203305
H	1.0	9.9195183403	-2.6933616964	6.2591931613
H	1.0	8.6068103505	0.8868434573	8.2189093884
H	1.0	9.2233814531	-0.9893080803	9.5827578822
H	1.0	8.6833081584	-2.5225370729	8.8661963525
H	1.0	10.4074472381	-2.1061704268	8.8666304603
H	1.0	10.3631108106	3.3902030849	6.8007189530
H	1.0	9.1005754808	3.3873686980	8.0800150497
H	1.0	9.1512083607	4.6986960500	6.8442082034
H	1.0	10.8661172089	2.6947429488	-0.2660591089
H	1.0	11.4685906808	2.3918090726	1.3977650542
H	1.0	11.0179452213	4.0511694019	0.9076391099
H	1.0	5.8532430788	2.3751172908	5.8960631288
H	1.0	6.3000812342	4.0354422063	6.3867290894
H	1.0	6.4598964271	2.6782390259	7.5582177499
H	1.0	8.2210499796	3.4038762623	-0.7900220967
H	1.0	8.1683206012	4.7101820842	0.4510144636
H	1.0	6.9575784053	3.4000560330	0.4885751404

Electronic Energy (Hartrees): -2025.0251629185

Total Gibbs Energy Correction (kJ mol⁻¹): +847.259

Table S7. Atomic coordinates (Å) and energies for **E-Pt**.

ATOM	CHARGE	X	Y	Z
PT	78.0	8.6603701276	2.9375495355	3.6443098343
CL	17.0	8.6555246417	5.2887722043	3.6479636047
P	15.0	9.0467611119	2.7035057710	1.4023057545
P	15.0	8.2755615032	2.6944492342	5.8851588936
N	7.0	8.6647211439	0.8943334614	3.6402909267
C	6.0	8.4758499074	0.2393355863	2.4288369514
C	6.0	7.9929396634	-1.0848613522	2.2987666205
C	6.0	7.8411902047	-1.6787213235	1.0551473925
C	6.0	8.1385806360	-1.0087191724	-0.1423666579
C	6.0	8.5461869891	0.3172384515	-0.0274319387
C	6.0	8.6961310416	0.9406636827	1.2155973520
C	6.0	7.9886592458	-1.6911566729	-1.4774183273
C	6.0	10.7292933500	3.0330236161	0.7780503299
C	6.0	7.9477756103	3.6209742718	0.2746513798
C	6.0	8.8550521349	0.2357672555	4.8496559558
C	6.0	9.3427991694	-1.0870703981	4.9756790203
C	6.0	9.4957598733	-1.6844867192	6.2174365788
C	6.0	9.1949909277	-1.0197309041	7.4170219062
C	6.0	8.7826231699	0.3050688554	7.3061385536
C	6.0	8.6314944984	0.9320694956	6.0651349256
C	6.0	9.3464502095	-1.7058809495	8.7499092394
C	6.0	6.5933391102	3.0163635514	6.5141892684
C	6.0	9.3734672196	3.6101699153	7.0152611392
H	1.0	7.7003650322	-1.6441152466	3.1868574832
H	1.0	7.4583473493	-2.7034080689	1.0102569705
H	1.0	8.7366290683	0.8945972839	-0.9391401310
H	1.0	8.1576645680	-0.9901138236	-2.3079722982
H	1.0	8.7100122789	-2.5174662031	-1.5876823116
H	1.0	6.9813098319	-2.1204218500	-1.5998997821
H	1.0	9.6382214611	-1.6423321121	4.0860279028
H	1.0	9.8822423588	-2.7079248454	6.2592546115
H	1.0	8.5892717281	0.8789749214	8.2194150445
H	1.0	9.1778898437	-1.0074340582	9.5826603551
H	1.0	8.6255983898	-2.5327975951	8.8583234785
H	1.0	10.3539577714	-2.1350119580	8.8702695871
H	1.0	10.4151045405	3.3559263385	6.7760613335
H	1.0	9.1661860667	3.3782932057	8.0704435969
H	1.0	9.2243444213	4.6842106697	6.8287229021
H	1.0	10.8248520356	2.7565942130	-0.2827862514
H	1.0	11.4462730781	2.4534517112	1.3754859820
H	1.0	10.9460593583	4.1040428414	0.9051295000
H	1.0	5.8767164886	2.4341790820	5.9189426837
H	1.0	6.3713452766	4.0866045228	6.3892215293
H	1.0	6.5028688145	2.7382749261	7.5750633398
H	1.0	8.1560471543	3.3941505222	-0.7814611277
H	1.0	8.0943964435	4.6944927583	0.4657468571
H	1.0	6.9064851505	3.3636153697	0.5119700411

Electronic Energy (Hartrees): -2016.5315603372

Total Gibbs Energy Correction (kJ mol⁻¹): +848.473