

Supporting Information for:

Synthesis and Electronic Properties of a Pentafluoroethyl-Derivatized Nickel Pincer Complex

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Full description of reference 17:

(17) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09 for Windows, Revision C.01*; Gaussian, Inc., Wallingford, CT, 2009.

Table S1: Optimized Cartesian coordinates for [LNi-Cl] (**6**):

Row	Symbol	X	Y	Z
1	Ni	16.1725119	1.5248304	-2.2635694
2	Cl	17.8056568	2.2323533	-3.6115884
3	N	14.8165477	0.9369325	-1.1439996
4	N	16.4350219	2.9926713	-0.9521012
5	N	15.7120205	-0.0275554	-3.4134782
6	C	16.0763270	4.2870900	-1.6038514

7	C	17.8544667	3.0328191	-0.4860222
8	C	16.8601921	-0.9818706	-3.4133735
9	C	15.4211007	0.4194872	-4.8094320
10	C	14.5100568	-0.6632015	-2.8348120
11	C	13.8712339	-1.7374894	-3.4424963
12	C	12.6928559	-2.2527910	-2.8966698
13	C	12.1614286	-1.6485023	-1.7568747
14	C	12.8060411	-0.5817196	-1.1337589
15	C	14.0311860	-0.0861570	-1.6379332
16	C	14.7208444	1.5821020	0.0734038
17	C	13.9578430	1.2186735	1.2077076
18	C	13.9665662	2.0121605	2.3531739
19	C	14.7298981	3.1779541	2.4233624
20	C	15.5348046	3.5203195	1.3338940
21	C	15.5430509	2.7238737	0.1949690
22	H	16.2102626	5.1192684	-0.9019064
23	H	15.0301340	4.2464559	-1.9137009
24	H	16.7139122	4.4282101	-2.4769877
25	H	18.0001796	3.8515951	0.2277645
26	H	18.5052947	3.1680810	-1.3482569
27	H	18.0886360	2.0859929	0.0046015
28	H	16.6325982	-1.8544204	-4.0380043
29	H	17.0411968	-1.3135537	-2.3889689
30	H	17.7430652	-0.4689585	-3.7960018
31	H	14.5667481	1.0989415	-4.7878639

32	H	15.1795742	-0.4406925	-5.4440668
33	H	16.2926573	0.9406888	-5.2017018
34	H	14.2761905	-2.1732373	-4.3514991
35	H	12.1918043	-3.0919353	-3.3688629
36	H	11.2219000	-2.0055677	-1.3425124
37	H	12.3321515	-0.1096481	-0.2853714
38	H	13.3941110	0.2971202	1.2160601
39	H	13.3678924	1.7044508	3.2068699
40	H	14.7211576	3.7983590	3.3139868
41	H	16.1629745	4.4048762	1.3888630

Table S2: Optimized Cartesian coordinates for [LNi-CF₃] (**7**):

Row	Symbol	X	Y	Z
1	Ni	11.4018999	-7.0218891	4.3872790
2	F	13.4643774	-8.4471446	3.2636566
3	F	13.7586374	-8.1885217	5.4173557
4	F	12.4357082	-9.7222106	4.6696147
5	N	10.1209203	-5.6609186	4.1504253
6	N	12.7121828	-5.4718303	4.4281399
7	N	9.8187697	-8.2397976	4.5389482
8	C	12.7768088	-8.3964377	4.4578341
9	C	12.9125370	-5.2195568	5.8904905
10	C	14.0401534	-5.6705387	3.7820063
11	C	9.8723050	-8.9620036	5.8474027
12	C	9.7834525	-9.2056458	3.3998313

13	C	12.0107083	-4.3097512	3.8325171
14	C	12.6609304	-3.1405145	3.4551543
15	C	11.9396612	-2.0850924	2.8876253
16	C	10.5666636	-2.2320238	2.6959265
17	C	9.9033130	-3.3908599	3.0950493
18	C	10.6094069	-4.4512968	3.7064531
19	C	8.8044216	-6.0167284	4.3375440
20	C	8.5967085	-7.4013855	4.5130976
21	C	7.3257422	-7.9393193	4.6811500
22	C	6.2086150	-7.1010128	4.7208914
23	C	6.3986227	-5.7220022	4.6162739
24	C	7.6679201	-5.1786805	4.4326540
25	H	11.9434281	-5.0181081	6.3499020
26	H	13.5663590	-4.3499321	6.0360504
27	H	13.3646566	-6.1024353	6.3422693
28	H	14.6759346	-4.7920014	3.9331955
29	H	13.8964044	-5.8368889	2.7142725
30	H	14.5286954	-6.5315312	4.2253404
31	H	9.0071594	-9.6261785	5.9567188
32	H	9.8508929	-8.2235328	6.6514549
33	H	10.7856895	-9.5466066	5.8994336
34	H	9.7275372	-8.6400613	2.4676871
35	H	8.9038909	-9.8563802	3.4745848
36	H	10.6854909	-9.8122818	3.4143970
37	H	13.7328316	-3.0357579	3.5835643

38	H	12.4517476	-1.1769732	2.5852576
39	H	9.9969553	-1.4380325	2.2194386
40	H	8.8475399	-3.4924550	2.8847506
41	H	7.1931606	-9.0115348	4.7945277
42	H	5.2156596	-7.5192978	4.8525391
43	H	5.5456751	-5.0513410	4.6851346
44	H	7.7819319	-4.1035694	4.4042034

Table S3: Optimized Cartesian coordinates for [LNi-Cl]⁺ (**9**):

Row	Symbol	X	Y	Z
1	Ni	16.1756623	1.5276904	-2.2680653
2	Cl	17.7654580	2.2187416	-3.5822087
3	N	14.8267014	0.9436529	-1.1548825
4	N	16.4197014	3.0150769	-0.9708924
5	N	15.7373021	-0.0450776	-3.4037537
6	C	15.9941972	4.2985476	-1.6221510
7	C	17.8478452	3.1215415	-0.5155486
8	C	16.8760107	-1.0206506	-3.3387265
9	C	15.4881666	0.3545746	-4.8306492
10	C	14.5125942	-0.6427827	-2.8453289
11	C	13.8534323	-1.7103565	-3.4373213
12	C	12.6469379	-2.1666626	-2.8932932
13	C	12.0926360	-1.5286359	-1.7773580
14	C	12.7580416	-0.4772665	-1.1615044
15	C	14.0120436	-0.0506253	-1.6608292

16	C	14.7542054	1.5553467	0.0816733
17	C	14.0258290	1.1249914	1.2166164
18	C	14.0359118	1.8924629	2.3734919
19	C	14.7657584	3.0856378	2.4307681
20	C	15.5433282	3.4877200	1.3382755
21	C	15.5615381	2.7133040	0.1873266
22	H	16.1018529	5.1324453	-0.9204335
23	H	14.9488578	4.2163681	-1.9265649
24	H	16.6212959	4.4653008	-2.4974845
25	H	17.9578147	3.9474779	0.1934424
26	H	18.4781690	3.2927092	-1.3852425
27	H	18.1372728	2.1867387	-0.0319093
28	H	16.6488154	-1.9075553	-3.9397353
29	H	17.0330565	-1.3194382	-2.3003675
30	H	17.7713775	-0.5316278	-3.7214991
31	H	14.6512296	1.0545740	-4.8626774
32	H	15.2498245	-0.5265769	-5.4336392
33	H	16.3827929	0.8372599	-5.2170740
34	H	14.2508334	-2.1864654	-4.3272021
35	H	12.1277200	-2.9967024	-3.3613132
36	H	11.1286663	-1.8473435	-1.3939191
37	H	12.2876142	0.0419207	-0.3382717
38	H	13.5050082	0.1777547	1.2102946
39	H	13.4809132	1.5543021	3.2426637
40	H	14.7580445	3.6874049	3.3337713

41 H 16.1376345 4.3922297 1.4105133

Table S4: Optimized Cartesian coordinates for [LNi-Me]:

Row	Symbol	X	Y	Z
1	Ni	11.3892924	-6.9893052	4.4351998
2	N	10.0908971	-5.6297142	4.1584618
3	N	12.7069254	-5.4779602	4.3944962
4	N	9.8268084	-8.2245166	4.5728669
5	C	12.7464981	-8.3791676	4.6004723
6	C	13.0870203	-5.2257383	5.8152874
7	C	13.9281009	-5.7565013	3.5936602
8	C	9.8456310	-8.9210996	5.8910606
9	C	9.8612611	-9.2171904	3.4625692
10	C	11.9946712	-4.2897161	3.8660045
11	C	12.6565650	-3.1148936	3.5295762
12	C	11.9475982	-2.0273789	3.0101940
13	C	10.5709521	-2.1531270	2.8231713
14	C	9.8952198	-3.3175852	3.1813001
15	C	10.5865875	-4.4149798	3.7499141
16	C	8.7796721	-6.0128767	4.3021863
17	C	8.5931991	-7.4055815	4.4844542
18	C	7.3281152	-7.9682029	4.6098012
19	C	6.1898803	-7.1574200	4.5992438
20	C	6.3537441	-5.7755380	4.4900658
21	C	7.6163265	-5.2050192	4.3487501

22	H	12.1845290	-4.9994431	6.3855103
23	H	13.7772621	-4.3743782	5.8838055
24	H	13.5637110	-6.1167065	6.2277524
25	H	14.6411793	-4.9260427	3.6531691
26	H	13.6422123	-5.9086806	2.5514032
27	H	14.4081247	-6.6569098	3.9717189
28	H	8.9921185	-9.6034917	5.9858711
29	H	9.7889238	-8.1718941	6.6829008
30	H	10.7699678	-9.4867413	5.9947871
31	H	9.8083073	-8.6817225	2.5128944
32	H	9.0127059	-9.9102207	3.5292758
33	H	10.7928304	-9.7817877	3.5082311
34	H	13.7320150	-3.0345090	3.6565655
35	H	12.4676659	-1.1130440	2.7418057
36	H	10.0068300	-1.3338261	2.3837493
37	H	8.8372682	-3.3927463	2.9727923
38	H	7.2164484	-9.0425544	4.7289874
39	H	5.2023319	-7.5976500	4.6964318
40	H	5.4842183	-5.1232443	4.5217312
41	H	7.7030974	-4.1277387	4.3197228
42	H	13.5394318	-8.1287527	5.3230389
43	H	12.3805638	-9.3694942	4.9025864
44	H	13.2437815	-8.5296001	3.6278117

Table S6: Total energies of all optimized structures (a.u.)

[LNi-Cl] (**6**): -2754.38184332

[LNi-CF₃] (**7**): -2631.75949400

[LNi-Cl]⁺ (**9**): -2754.16044407

[LNi-Me]: -2334.02099085

NMR Data for complex 8:

Figure S1: ¹H NMR spectrum in C₆D₆:

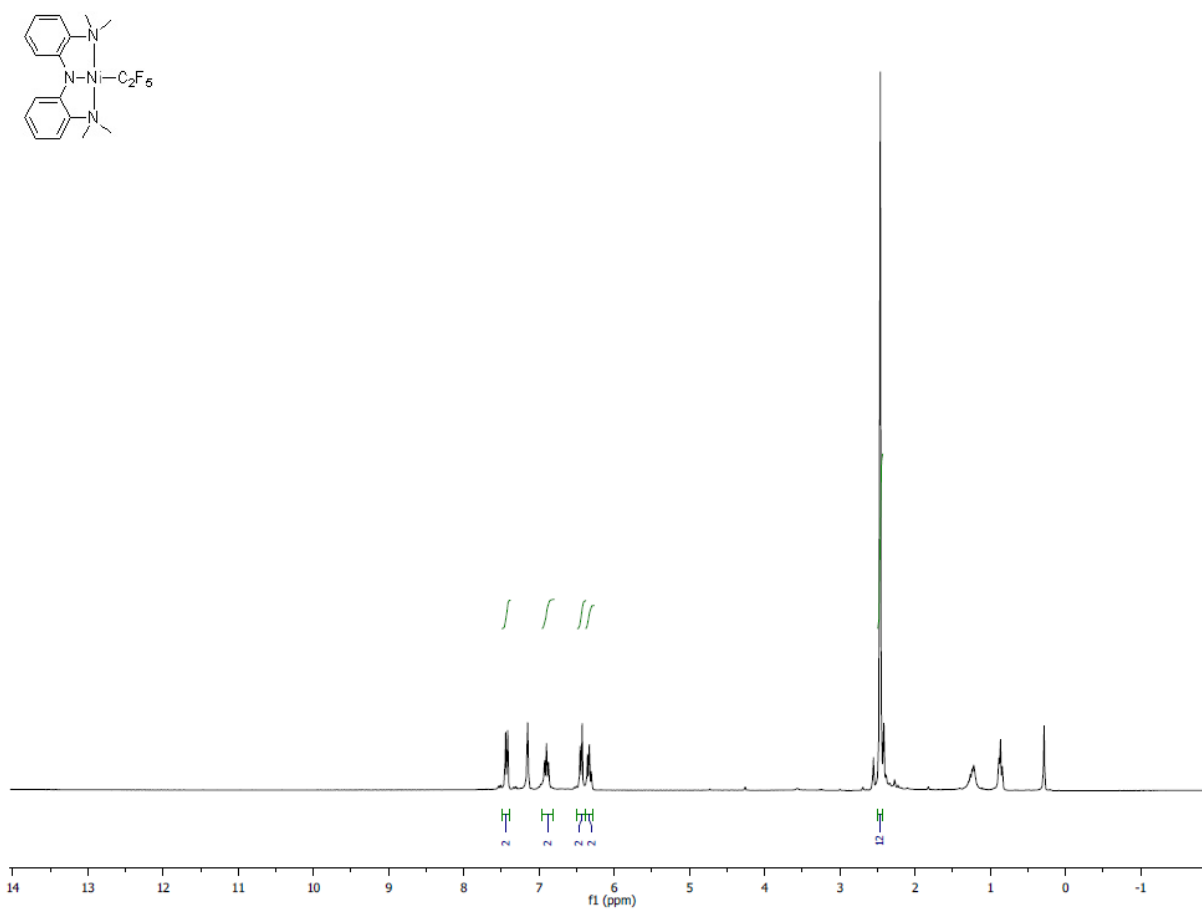


Figure S2: $^{13}\text{C}\{^1\text{H}\}$ NMR in THF

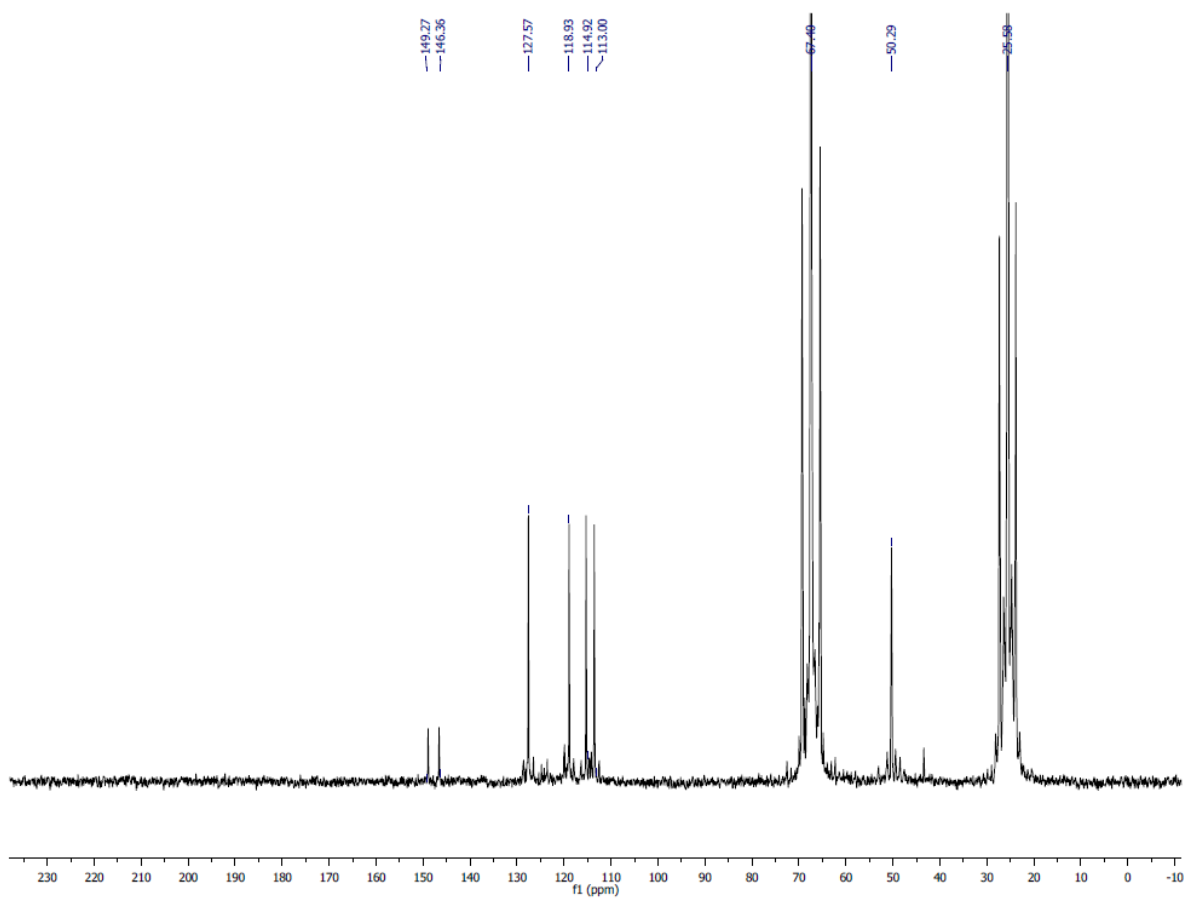


Figure S3: ^{19}F NMR in C_6D_6 in the presence of trifluorotoluene as an internal standard:

