SUPPLEMENTARY INFORMATION

Mono- and dinuclear Ni(I) products formed upon bromide abstraction from the Ni(I) ring-expanded NHC complex [Ni(6-Mes)(PPh_3)Br]

William J. M. Blackaby, Sara Sabater, Rebecca C. Poulten, Michael J. Page, Andrea Folli, Vera Krewald, Mary F. Mahon, Damien Murphy, Emma Richards and Michael K. Whittlesey

Department of Chemistry, University of Bath, Claverton Down, Bath BA2 7AY, UK and School of Chemistry, Cardiff University, Park Place, Cardiff CF10 3AT, UK

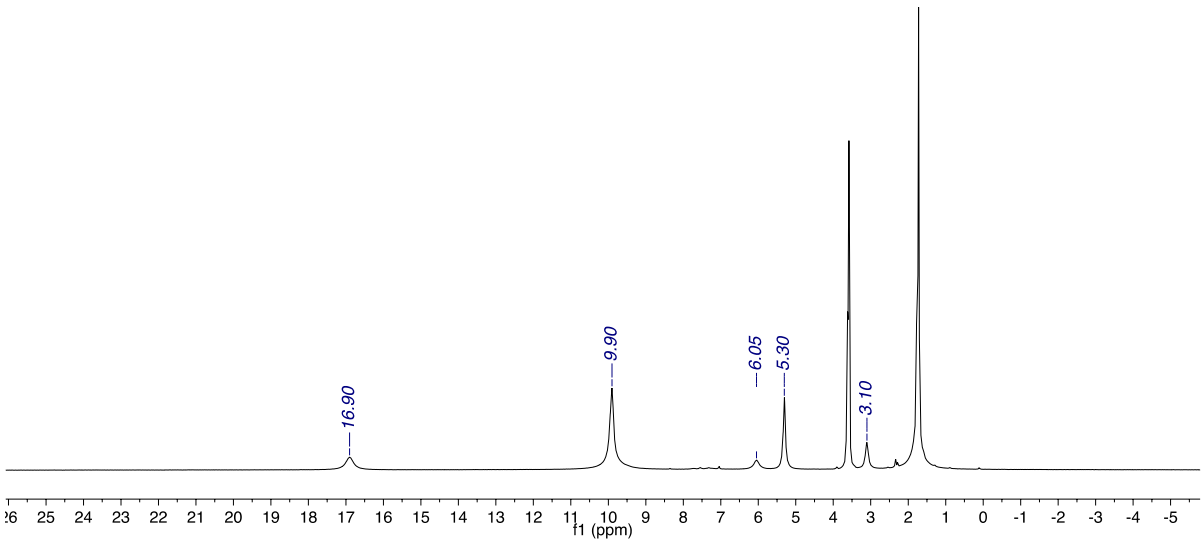

Figure S1. ^{1}H NMR spectrum (500 MHz, THF-d_8, 298 K) of [Ni(6-Mes)(PPh_3)(THF)][PF_6] (**2**).

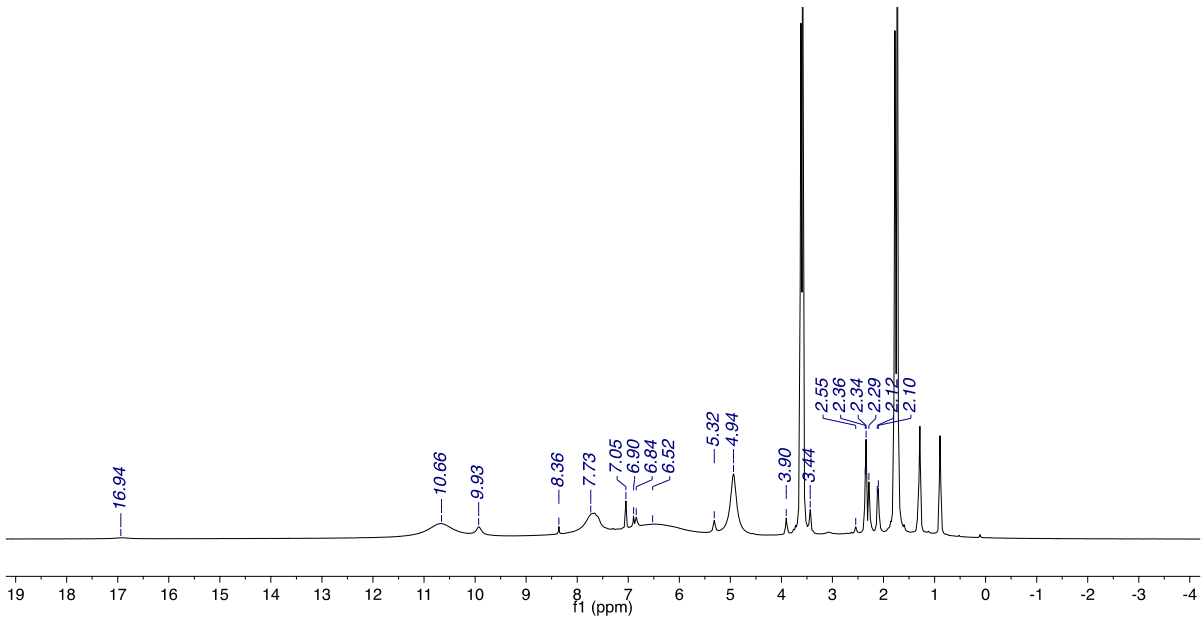

Figure S2. ^{1}H NMR spectrum (500 MHz, THF-d_8, 298 K) of [Ni(6-Mes)(PPh_3)(CO)][PF_6] (**5**).

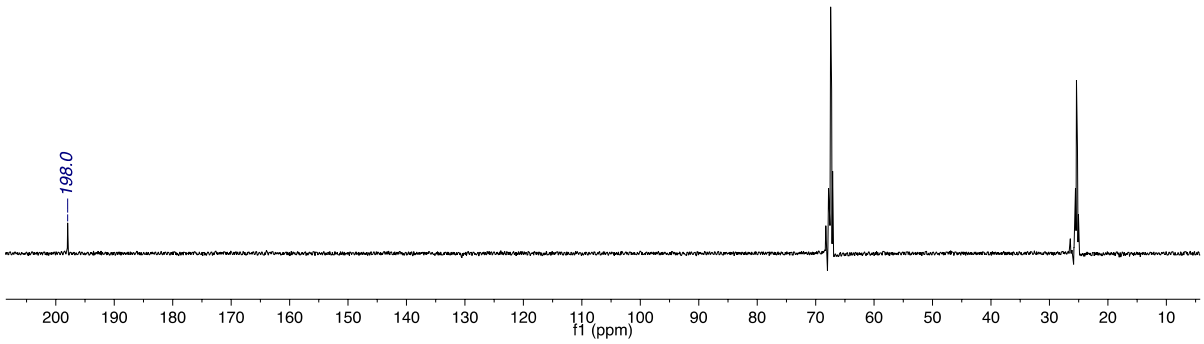

Figure S3. $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, 298 K) recorded ca. < 5 min after the addition of 13CO (1 atm) to a THF-d_8 solution of [Ni(6-Mes)(PPh_3)(CO)][PF_6] (**5**).

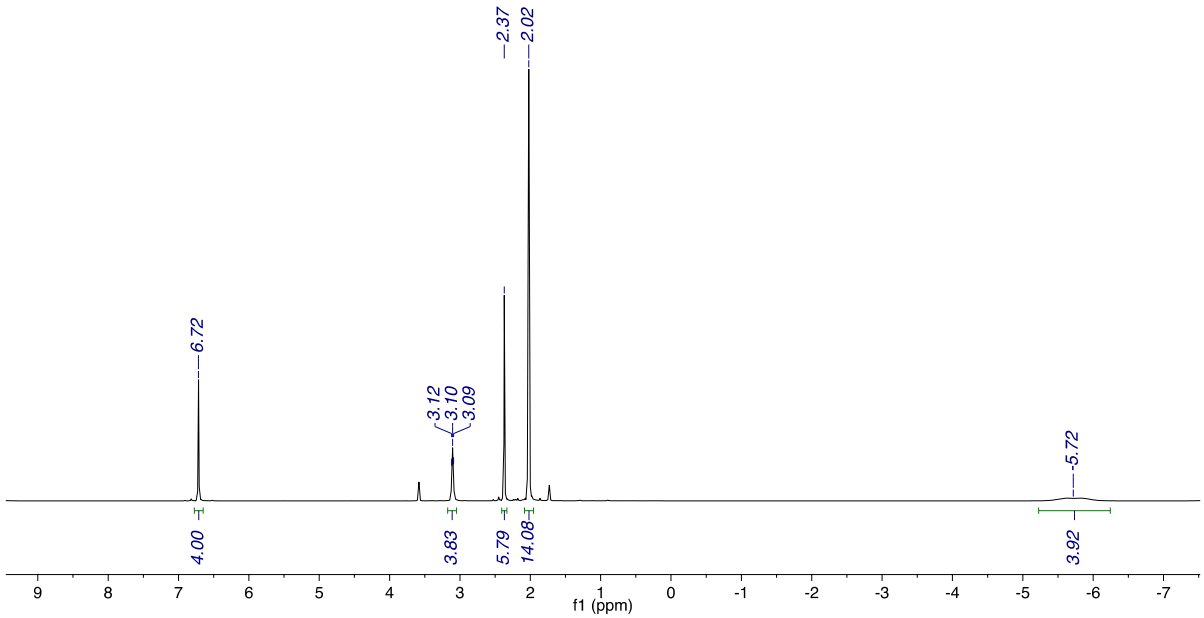

Figure S4. ^{1}H NMR spectrum (500 MHz, THF-d_8, 298 K) of [Ni(6-Mes)(BH_4)]$_2$ (**6**).

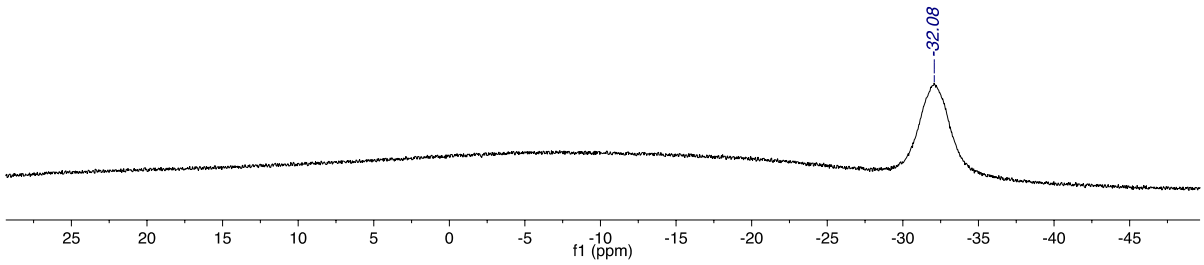

Figure S5. ^{11}B NMR spectrum (128 MHz, THF-d_8, 298 K) of [Ni(6-Mes)(BH_4)]$_2$ (**6**).

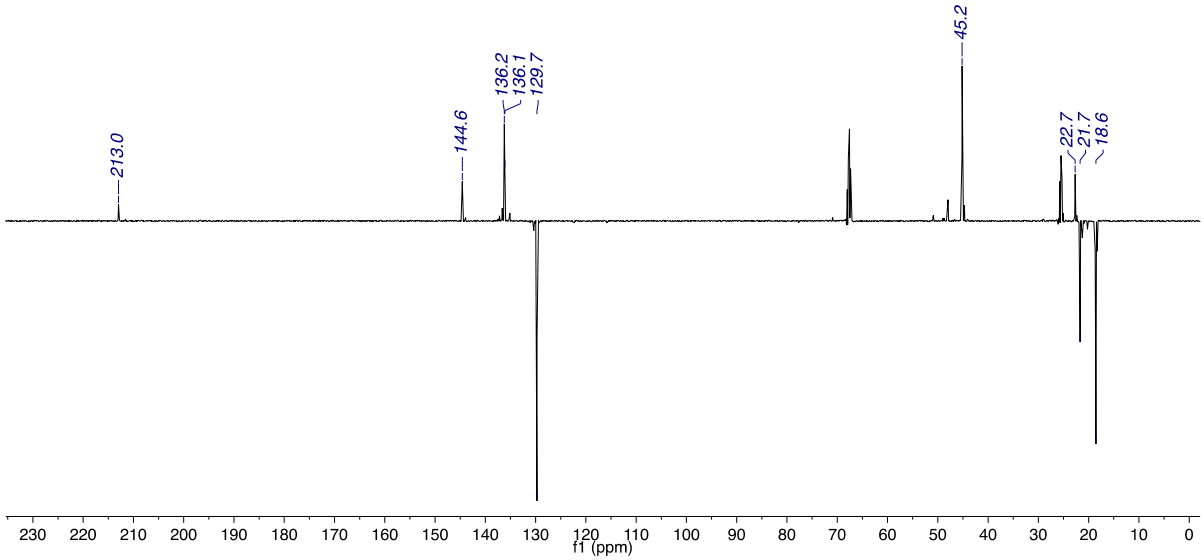

Figure S6. $^{13}C\{^{1}H\}$ PENDANT NMR spectrum (102 MHz, THF-d_8, 298 K) of [Ni(6-Mes)$(BH_4)]_2$ (**6**).

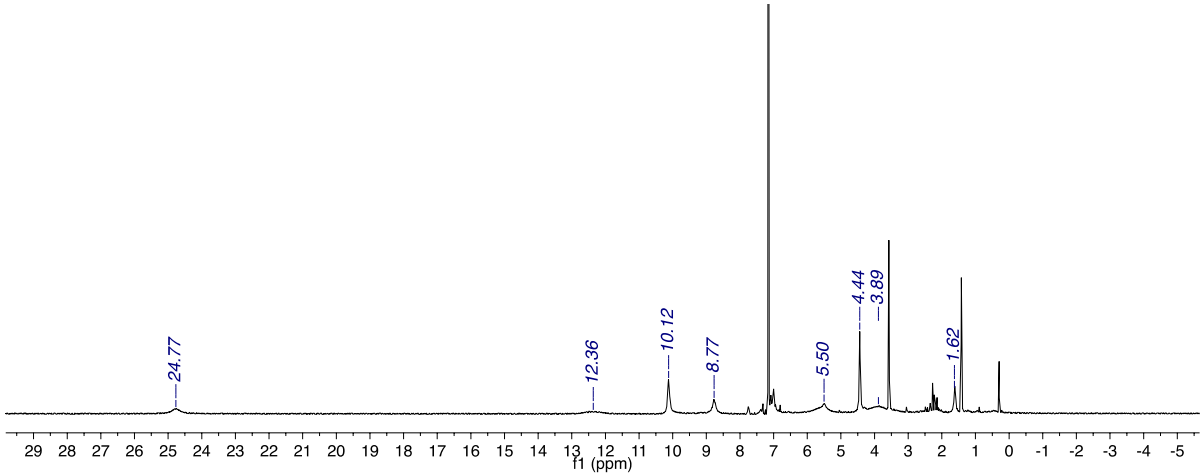

Figure S7. ^{1}H NMR spectrum (500 MHz, C_6D_6, 298 K) of Ni(6-Mes)$(PPh_3)(NCBH_3)$ (**7**).

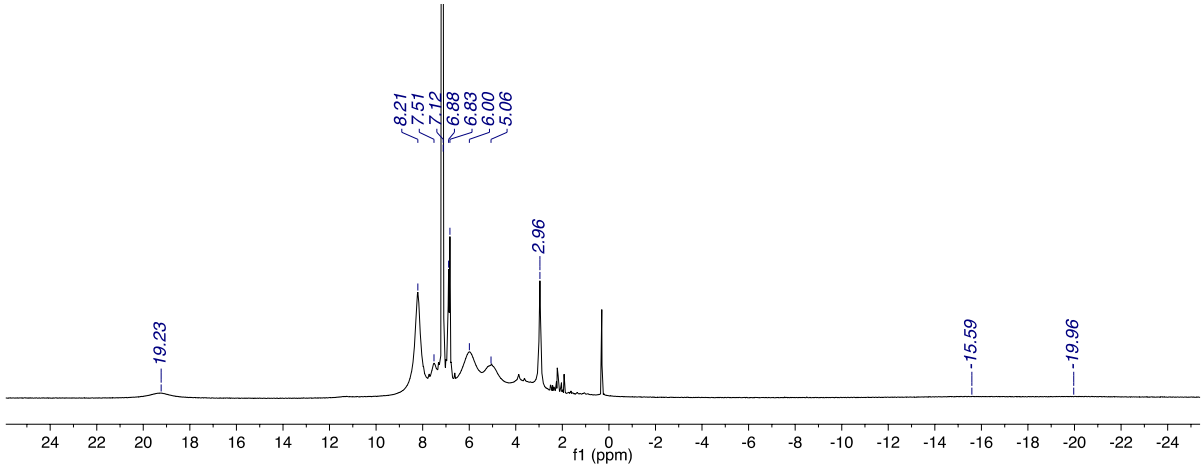

Figure S8. ^{1}H NMR spectrum (500 MHz, C_6D_6, 298 K) of Ni(6-Mes)$(PPh_3)(NPh_2)$ (**8**).

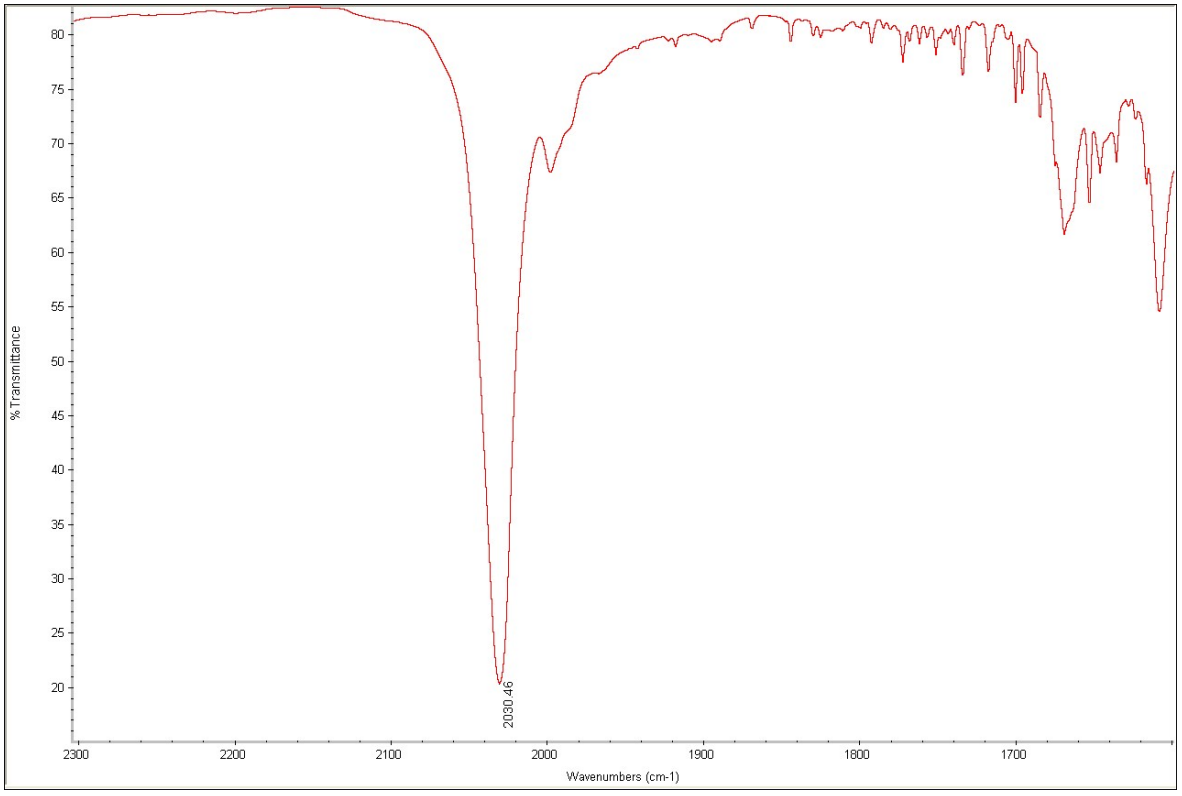

Figure S9. FTIR spectrum (KBr) of [Ni(6-Mes)(PPh_3)(CO)][PF_6] (**5**).

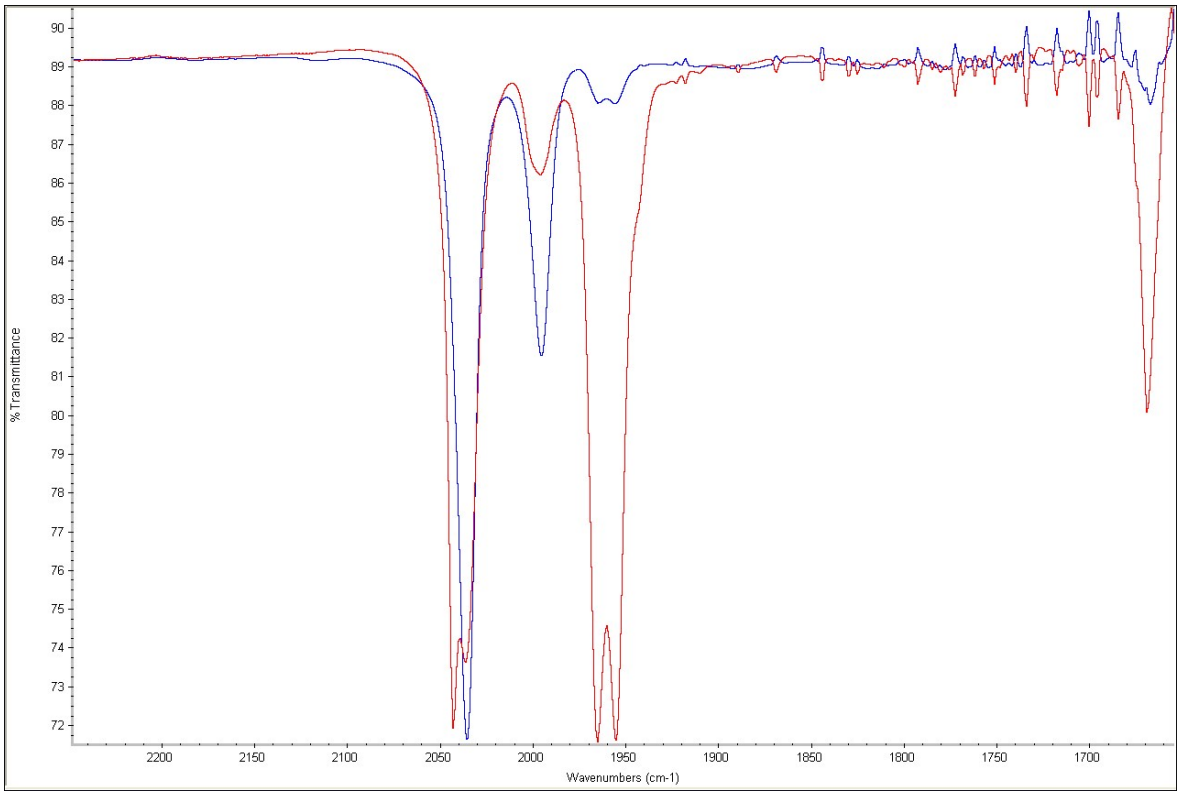

Figure S10. FTIR spectra (THF) of [Ni(6-Mes)(PPh_3)(CO)][PF_6] (**5**) (blue) and a THF sample of **2** recorded 60 mins after the addition of 1 atm CO (red).

Crystal structure refinement of [Ni(6-Mes)(η²-$C_6H_3Me_3$)][$B(C_6F_5)_4$]

Analysing the crystal structure of [Ni(6-Mes)(η²-$C_6H_3Me_3$)][$B(C_6F_5)_4$] was nothing short of excruciating, and it involved three data collections, some 350 refinements and approximately 10 data integrations. The issue appears to be that the compound is undergoing a phase transition. This is not first order in nature, as was discovered by collecting datasets at more than one temperature. Left to its own devices, the data reduction software defaulted to the monoclinic space group C2/c with the resulting dataset bearing an R_{int} value of approximately 16%. Additionally, the C2/c unit cell parameters were accompanied by higher esd values than one might expect, given the clarity of the diffraction pattern and access to a state-of-the-art diffractometer. The unrestrained unit cell parameters for this monoclinic setting were: a = 31.8867(14), b = 10.4000(4), c = 29.4479(9) Å, a = 90.291(3), b = 92.448(3), g = 89.639(3)°. On balance, it appears that the high R_{int} value for monoclinic symmetry results, in part, from trying to restrain angles of 90.29° and 89.64° to ideal values of 90°. Obviously, integrating the raw data in space group C2/c caused some problems, as restraining these angles resulted in a substantial fraction of diffraction maxima being designated as 'wrong' according to the software. Thus, substantial early efforts concentrated on indexing the datasets as though they resulted from a twinned crystal, but these did not meet with any success. The very best monoclinic data had an accompanying 145 systematic absence violations. By comparison, integrating the data in triclinic symmetry gave satisfactory statistics. In the first instance the arising R_{int} value was 3.93%. Solving in triclinic symmetry meant two cations and two anions per asymmetric unit. Disorder was notably prevalent in several regions, as detailed in the CIF file. It was noted that the nickel centres in the cations were disordered, and that, in one case, the disordered components did not sum to unity, suggesting the presence of mesitylene•••pyrimidinium pairs at some sites in the crystal. Despite the deficiencies in the analysis, however, the results afford credible and unambiguous evidence for the presence of the nickel containing cation.

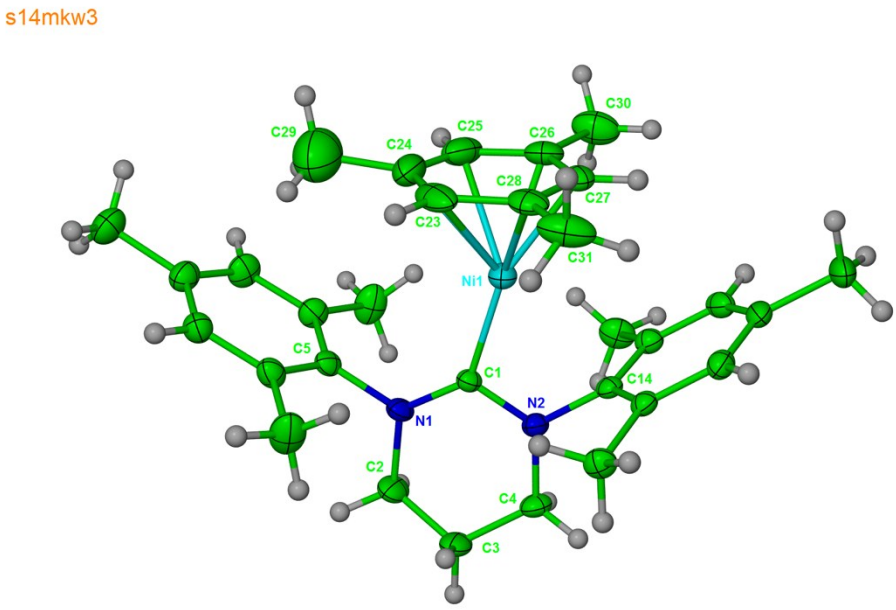

Figure S11. Molecular structure of the cation in [Ni(6-Mes)(η²-$C_6H_3Me_3$)][$B(C_6F_5)_4$].

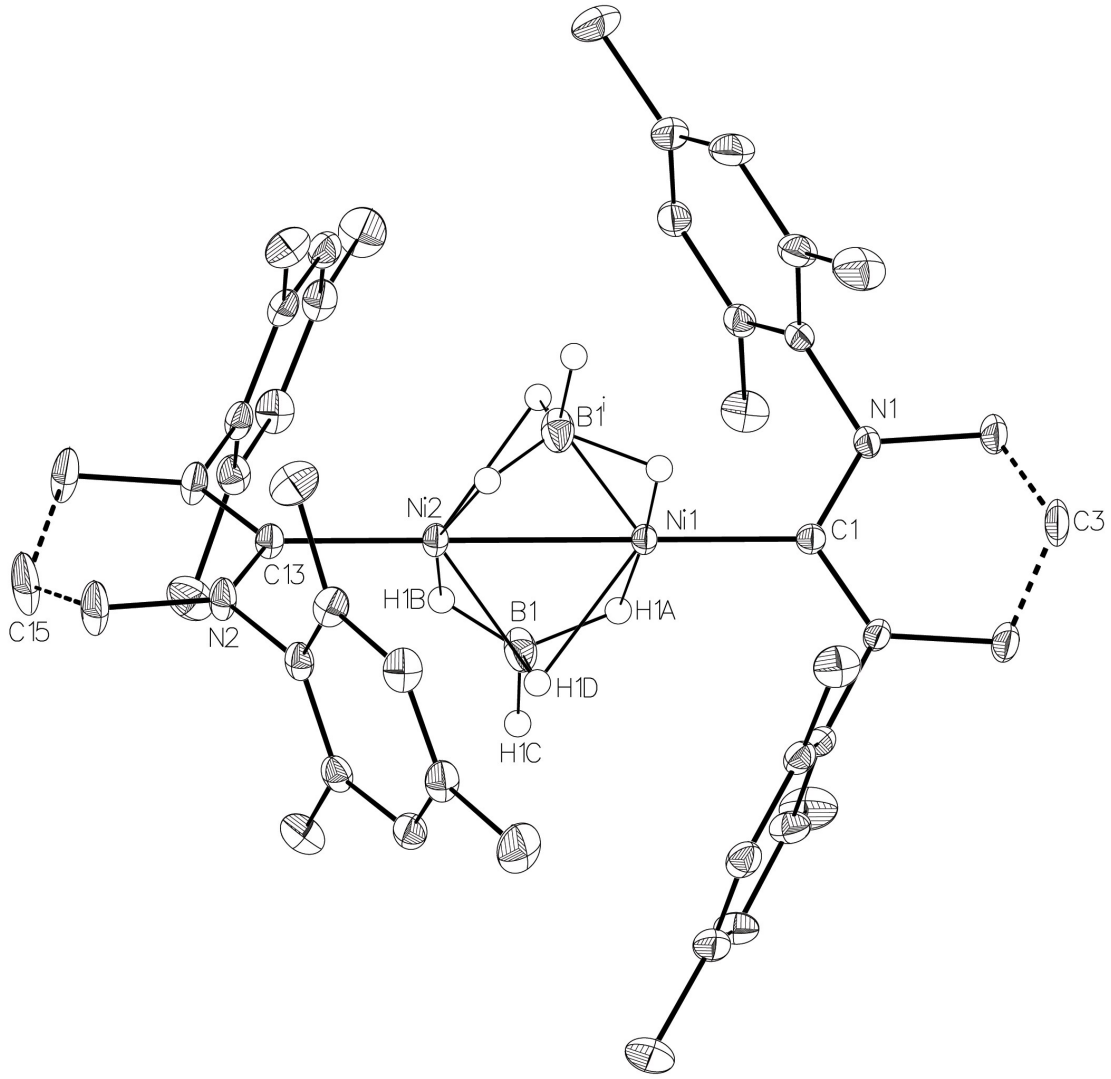

Figure S12. Molecular structure of **6a**.

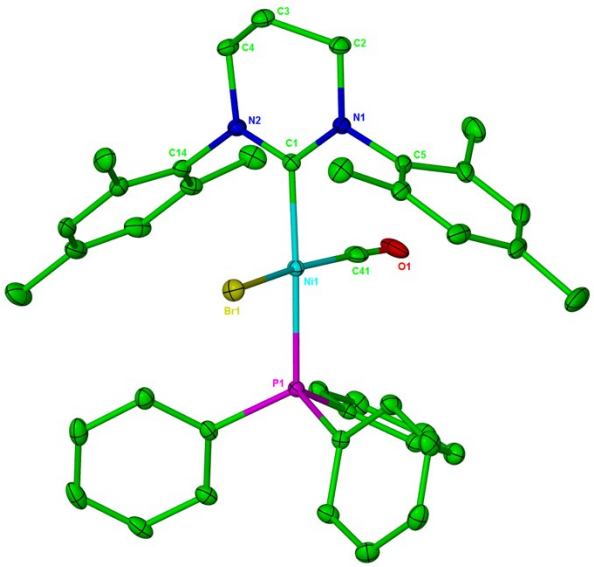

Figure S13. Molecular structure of the cation in [Ni(6-Mes)(PPh_3)(CO)Br][PF_6].

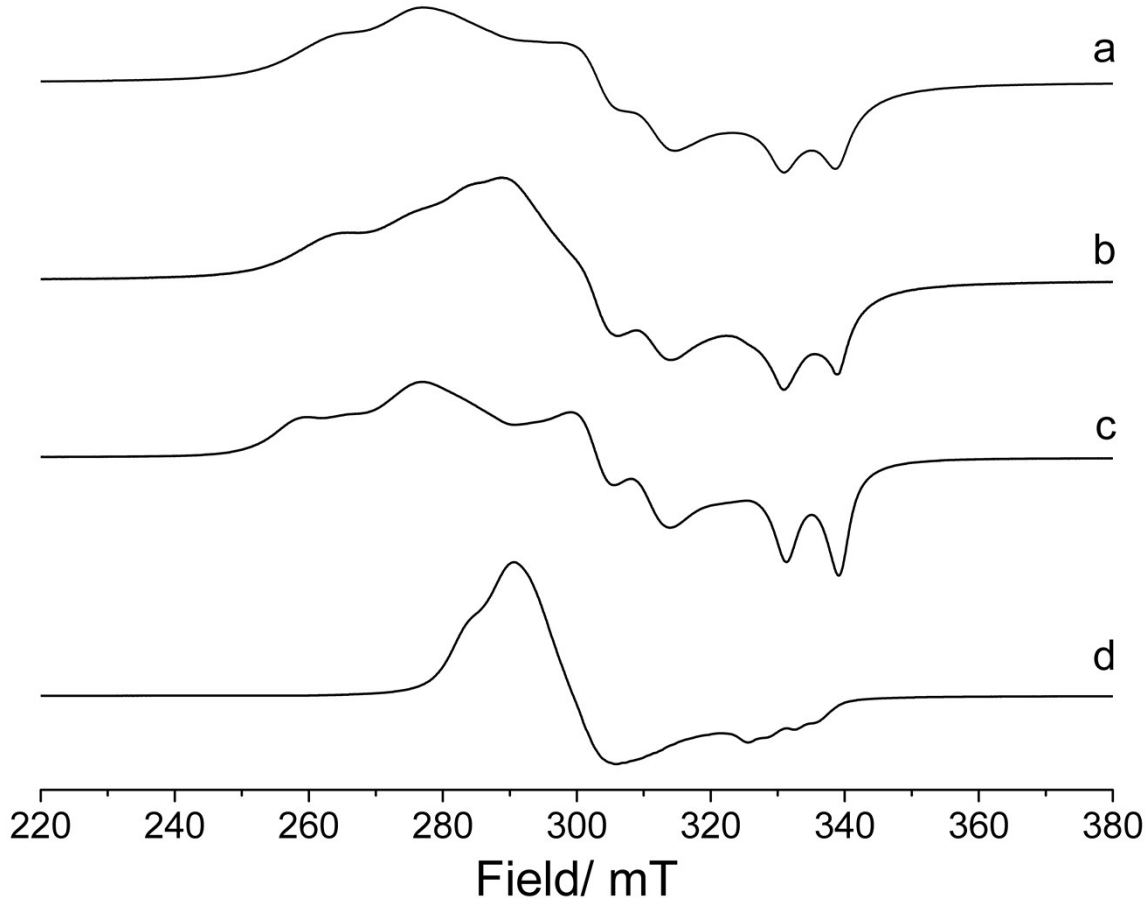

Figure S14. CW X-band EPR spectra of (a)–(c) **2** recorded on three different batches of recrystallised material. The precursor complex **1** is shown in (d) for comparative purposes.

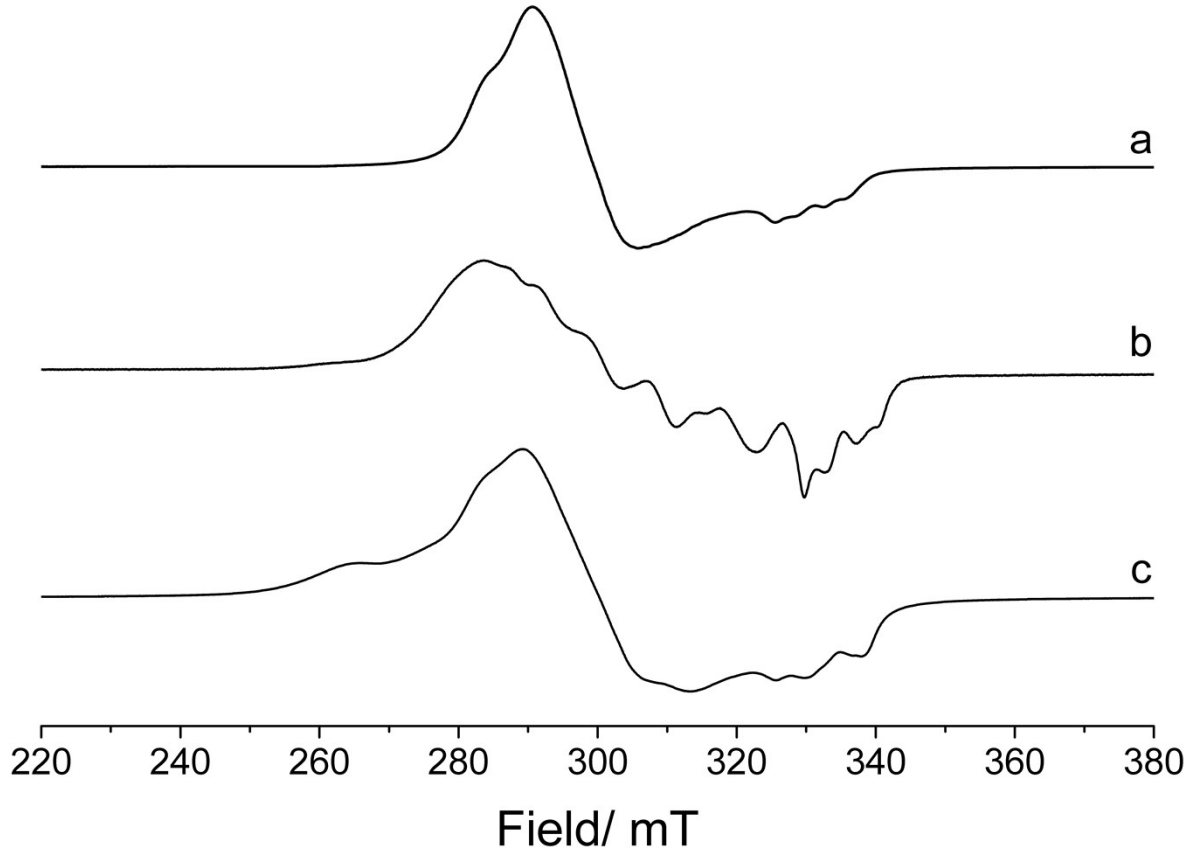

Figure S15. CW X-band EPR spectra of (a) **1**, and **3** in (b) ether/toluene and (c) THF/ toluene frozen solutions, recorded at 140 K.

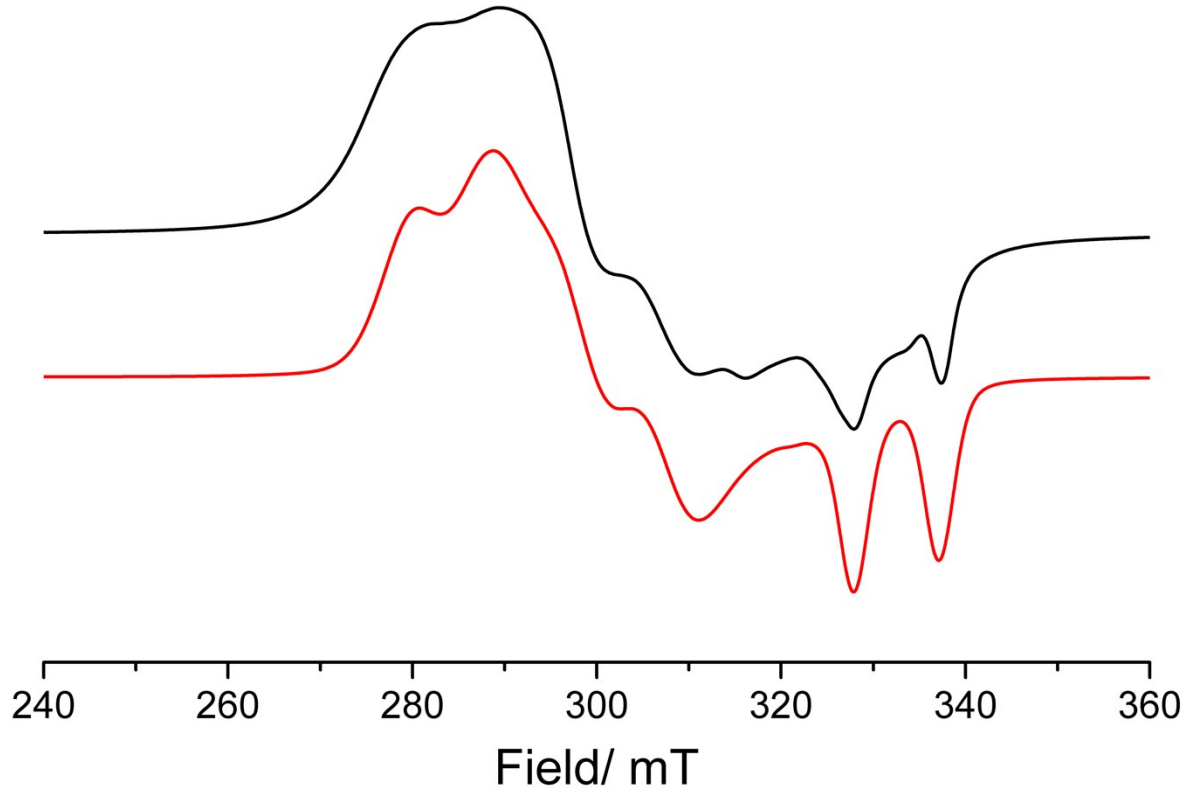

Figure S16. Experimental (black) and simulated (red) CW X-band EPR spectra of **7** recorded at 140 K, in frozen THF/toluene solution.

Table S1. Predicted magnetic coupling constant J (cm^{-1}) and Mulliken spin populations on Ni and Br atoms for $[\{Ni(6\text{-}Mes)(PPh_3)\}_2(\mu\text{-}Br)]^+$ (**3**) based on the crystal structure coordinates with optimised hydrogen atom positions using different density functionals.

		Mulliken spin population		
Density functional	J (cm^{-1})	Ni	Ni	Br
TPSSh	-97.58	-0.86	0.86	0.00
B3LYP	-76.13	-0.89	0.89	0.00
M06	-69.33	-0.93	0.93	0.00
PBE0	-64.33	-0.92	0.92	0.00

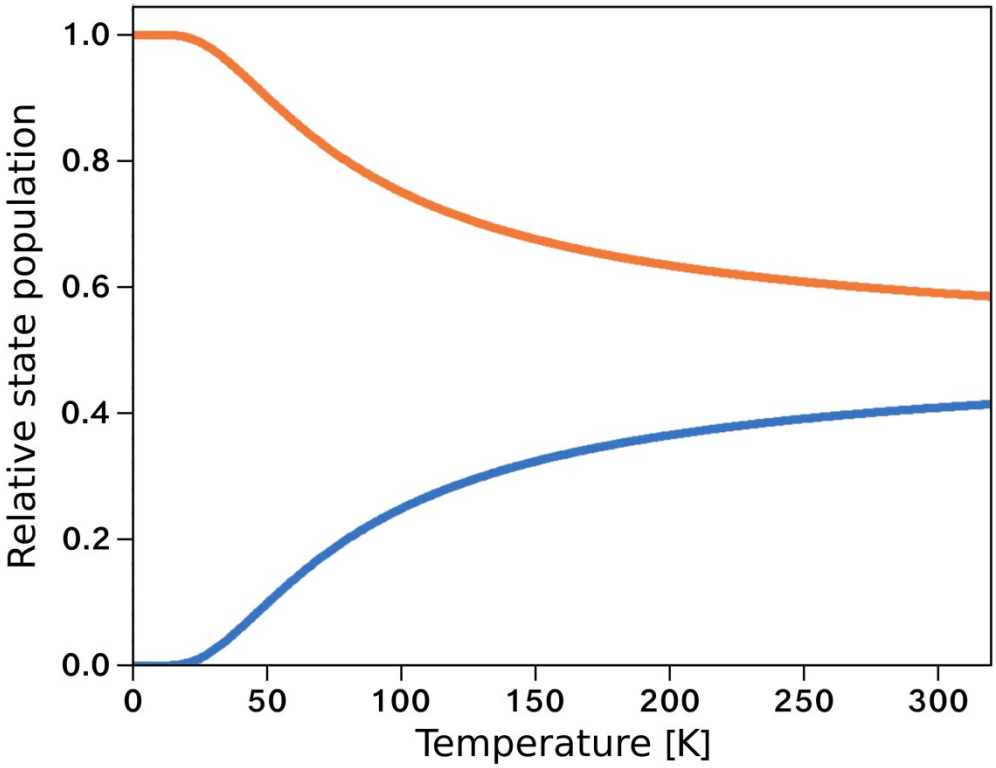

Fig S17. Boltzmann population distribution of the high-spin (S=1, ferromagnetically coupled) and broken-symmetry (S=0, antiferromagnetically coupled) states of $[\{Ni(6\text{-}Mes)(PPh_3)\}_2(\mu\text{-}Br)]^+$ (**3**) based on the crystal structure coordinates with optimised hydrogen atom positions. The energy difference between the states is taken from the B3LYP BS-DFT calculation.

Table S2. Key geometric parameters of crystal structures and fully relaxed geometries of the T- and Y-shaped complexes **1**, **2**, **5**, **7**, **8** and **8-Me**.

	Parameter	**1**	**2**	**5**	**7**	**8**	**8-Me**
Crystal structure coordinates	Distances (Å)						
	Ni-P	2.22	2.21	2.24	2.22	2.23	–
	Ni-C	1.94	1.96	1.94	1.96	1.96	–
	Ni-L	2.33	2.06	1.79	1.92	1.94	–
	Angles (°)						
	∠P-Ni-C	117.0	156.6	151.9	125.1	109.2	–
	∠C-Ni-L	133.5	103.7	106.2	132.4	142.5	–
	∠L-Ni-P	109.5	99.7	101.8	102.5	108.1	–
Fully relaxed coordinates	Distances (Å)						
	Ni-P	2.15	2.17	2.18	2.15	2.15	2.13
	Ni-C	1.88	1.92	1.91	1.90	1.88	1.88
	Ni-L	2.33	2.05	1.76	1.85	1.90	1.84
	Angles (°)						
	∠P-Ni-C	113.6	163.7	150.7	114.5	105.9	115.8
	∠C-Ni-L	136.8	97.3	106.3	144.6	149.0	135.8
	∠L-Ni-P	109.6	99.0	102.4	101.0	105.1	108.4

Table S3. Mulliken spin populations, Mulliken and Chelpg charges for the crystal structures of the T- and Y-shaped complexes **1**, **2**, **5**, **7**, **8** and **8-Me** (optimised coordinates for **8-Me**).

	1	**2**	**5**	**7**	**8**	**8-Me**
Mulliken spin populations						
Ni	0.87	0.99	0.87	0.93	0.89	0.77
L	0.08	0.02	0.06	0.00	0.03	0.15
P	0.02	-0.01	0.03	0.03	0.03	0.01
C	0.02	0.02	0.04	0.01	0.03	0.04
Mulliken charges						
Ni	0.86	0.86	0.93	0.85	0.91	0.94
L	-1.00	-0.61	0.08	-0.52	-0.73	-0.74
P	-0.27	-0.35	-0.34	-0.27	-0.32	-0.29
C	0.07	-0.06	-0.08	-0.06	-0.05	-0.06
Chelpg charges						
Ni	0.42	0.60	0.38	0.76	0.98	0.77
L	-0.67	-0.02	0.25	-0.64	-1.18	-0.01
P	-0.48	-0.61	-0.42	-0.80	-0.77	-0.69
C	-0.28	-1.08	-0.44	-0.83	-0.93	-0.95

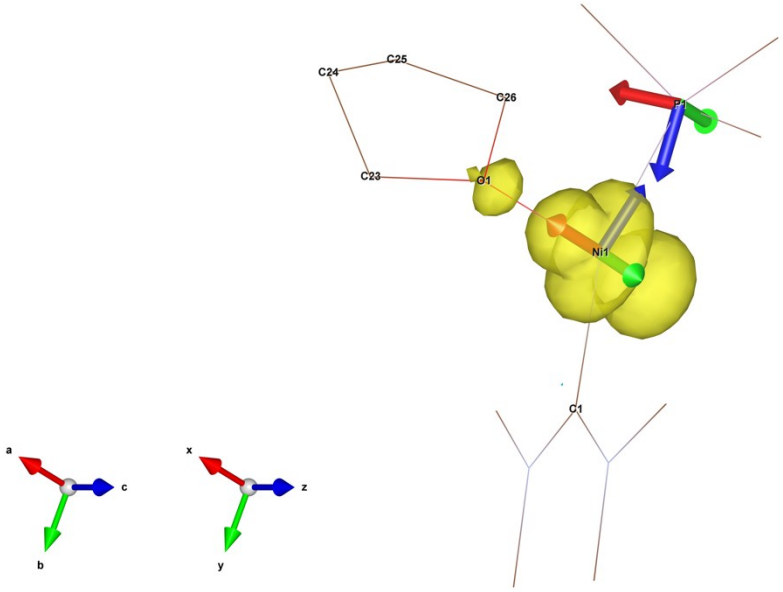

Figure S18. Spin density contour plot with **g** and **A** frames for complex **2**. The ligands are truncated for clarity.

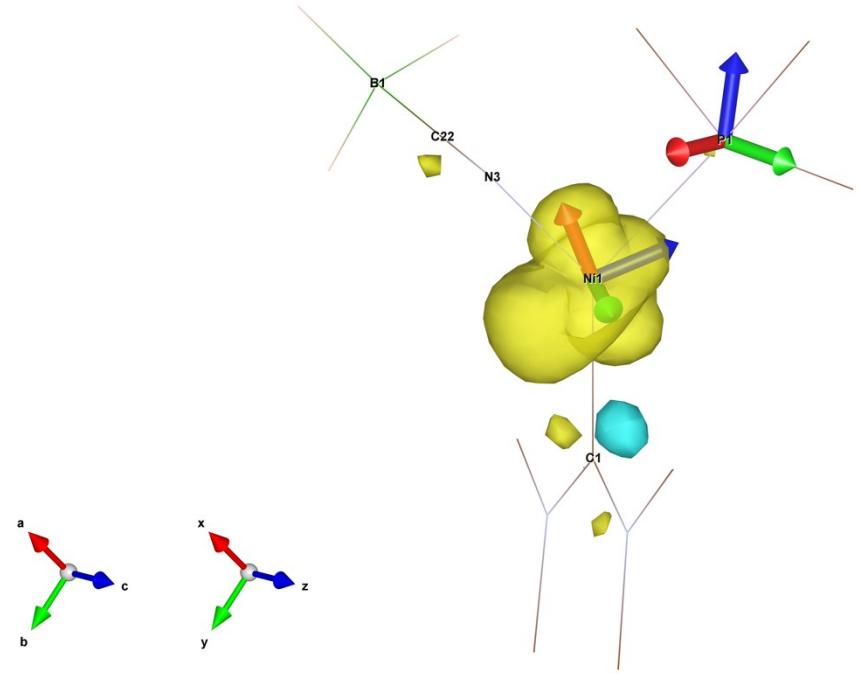

Figure S19. Spin density contour plot with **g** and **A** frames for complex **7**. The ligands are truncated for clarity.

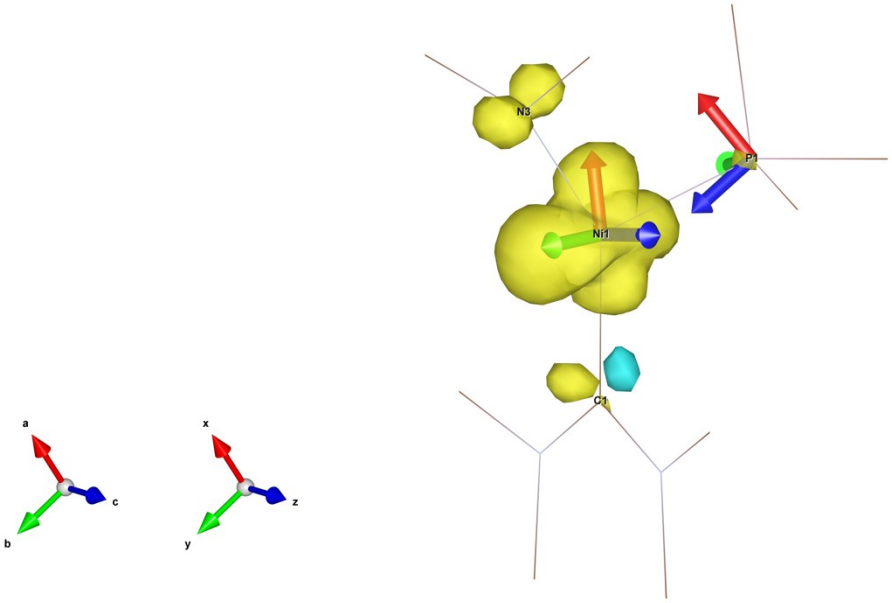

Figure S20. Spin density contour plot with **g** and **A** frames for complex **8**. The ligands are truncated for clarity.

Table S4. Anisotropy and rhombicity parameters for $[Ni(NHC)(PPh_3)X]^{0/+}$.

	Δg_3-g_1	Δg_3-g_2	Δg_2-g_1	Δg_{rel}
[Ni(6-Mes)(PPh_3)Br] **1**				
Expt	0.315	0.100	0.215	32
DFT[1]	0.230	0.033	0.197	14
[Ni(6-Mes)(PPh_3)THF][PF_6] **2**				
Expt	0.465	0.280	0.185	60
DFT	0.376	0.074	0.302	20
[Ni(6-Mes)(PPh_3)CO][PF_6] **5**				
Expt	0.150	0.064	0.086	43
DFT	0.111	0.038	0.073	34
[Ni(6-Mes)(PPh_3)($NCBH_3$)] **7**				
Expt	0.345	0.148	0.197	43
DFT	0.283	0.017	0.266	6
[Ni(6-Mes)(PPh_3)(NPh_2)] **8**				
Expt	0.240	0.140	0.100	58
DFT	0.179	0.076	0.103	42
[Ni(6-Mes)(PPh_3)(NMe_2)] **8Me**	0.098	0.046	0.052	47
DFT[2]				

[1] calculated from the crystal structure; [2] geometry optimised using the PBEO functional

Cartesian Coordinates

1. Crystal structures with relaxed hydrogen atom positions (Hopt) in Å. For **1**, **2**, **5**, **7**, and **8** the geometry is oriented such that the Ni ion is at the centre of the coordinate system, with the z-axis perpendicular to the plane containing Ni, P, $C_{carbene}$ and the coordinating ligand atom, and the x-axis along the Ni-P bond.

[Ni(6-Mes)(PPh_3)Br] (**1**, Hopt)

Br	2.333113727	0.000000000	−0.003455708
Ni	0.000000000	0.000000000	0.000000000
P	−0.741842593	−2.091190145	0.000000000
N	−1.650739759	2.081789618	−1.133720278
N	−1.923857413	1.832867747	1.128305395
C	−1.335865483	1.409682857	−0.006854387
C	−2.585395339	3.223243365	−1.200077901
H	−3.593025218	2.863109994	−1.489417705
H	−2.233980729	3.901141438	−1.996860032
C	−2.632065862	3.929895927	0.151689004
H	−1.665905331	4.441594618	0.325862037
H	−3.416216298	4.706796552	0.139391159
C	−2.889021211	2.943485947	1.217967345
H	−2.785002159	3.388457153	2.223345199
H	−3.920530060	2.544389831	1.146398004
C	−1.033539156	1.683165291	−2.378197857
C	−1.727193241	0.820827938	−3.229798522
C	−1.116980579	0.462594095	−4.425965331
H	−1.635408904	−0.245280535	−5.088677477
C	0.132518510	0.950013787	−4.798589646
C	0.766591525	1.828137641	−3.923301841
H	1.755166945	2.226415217	−4.194155026
C	0.208382586	2.213588452	−2.716824988
C	−3.085747561	0.283532149	−2.869317602
H	−3.190364621	0.164451230	−1.778357918
H	−3.262452037	−0.693161350	−3.351020075
H	−3.890989764	0.965868293	−3.203454000
C	0.790573205	0.527054584	−6.088504363
H	0.319234556	1.019669653	−6.960910001
H	0.695671103	−0.562496929	−6.246705048
H	1.863029899	0.785726318	−6.097743721
C	0.933346574	3.169291275	−1.805253092
H	1.818892443	3.594295569	−2.305809591
H	1.273836039	2.645521465	−0.892152250
H	0.283067998	4.001189186	−1.479940012
C	−1.615419906	1.128601807	2.350820684
C	−0.414524247	1.389800896	3.012754731
C	−0.125556544	0.644061713	4.158586845
H	0.825194466	0.820126489	4.680454212
C	−0.997508811	−0.330977022	4.633190458
C	−2.211643948	−0.507561986	3.981322096
H	−2.919481124	−1.260873037	4.354426047
C	−2.549839243	0.222284468	2.853771826
C	0.571984536	2.430414097	2.531381421
H	1.189255264	2.024345844	1.706602469
H	1.249202536	2.730934539	3.347989392
H	0.062594670	3.329211815	2.142259755
C	−0.627987567	−1.208326491	5.802695368
H	0.271546643	−0.837281697	6.323192151
H	−0.414712804	−2.238998069	5.459920258
H	−1.450363379	−1.277360320	6.537982811
C	−3.884569905	0.019721293	2.189789881
H	−4.315094441	−0.955489781	2.467031551
H	−3.795682955	0.049592756	1.090808702
H	−4.606171341	0.803608970	2.488457669
C	−2.414678527	−2.680146621	0.495207312
C	−3.500587491	−2.417052988	−0.335247705
H	−3.332553865	−1.923280286	−1.299612634
C	−4.791157641	−2.767697930	0.032978720
H	−5.626941515	−2.544617826	−0.642540233
C	−5.014140131	−3.410016564	1.238242200
H	−6.031636107	−3.696803152	1.533180816
C	−3.946694820	−3.677219147	2.071230360
H	−4.112144291	−4.182083171	3.032071221
C	−2.657590973	−3.316147766	1.710486978
H	−1.824925338	−3.532294571	2.390298812
C	0.340381160	−3.083034566	1.112029760
C	0.728647752	−2.492479068	2.313263544
H	0.398452811	−1.470991364	2.544759733
C	1.533200288	−3.186540148	3.209875058
H	1.825638704	−2.706784444	4.152907995

C	1.983535242	−4.453157643	2.904591501
H	2.634582431	−4.991748537	3.605492293
C	1.618529926	−5.039991230	1.705184662
H	1.976542459	−6.045321310	1.448322053
C	0.790888149	−4.359650392	0.820505303
H	0.509387682	−4.838788205	−0.125584375
C	−0.521900283	−2.878420634	−1.638754007
C	0.307110519	−2.232125693	−2.560527623
H	0.729401570	−1.251848520	−2.295718238
C	0.592671245	−2.810335138	−3.791144193
H	1.249657760	−2.285334407	−4.495683722
C	0.049822776	−4.038745982	−4.120211309
H	0.277388456	−4.500798830	−5.089779740
C	−0.803134549	−4.679299156	−3.229412446
H	−1.252000150	−5.646190846	−3.490252688
C	−1.087006975	−4.096960228	−2.003017004
H	−1.763626976	−4.611245664	−1.307326383

[Ni(6-Mes)(PPh_3)THF][PF_6] (**2**, Hopt)

Ni	0.000000000	0.000000000	0.000000000
P	−0.372211733	−2.179988461	0.000000000
O	2.060115858	0.000000000	−0.000814064
N	−0.941258005	2.476747236	−1.122577295
N	−0.393135115	2.661541621	1.092999237
C	−0.465158803	1.904218531	−0.007531161
C	−1.404145243	3.871013370	−1.206046130
H	−2.494505665	3.910811289	−1.011566686
H	−1.243182106	4.220586099	−2.239821158
C	−0.644388096	4.714457086	−0.208878555
H	−1.046455335	5.741407723	−0.189732187
H	0.418095534	4.779642565	−0.511344050
C	−0.746394785	4.089423193	1.165183998
H	−0.063177755	4.573967758	1.883096527
H	−1.771716125	4.191370755	1.573537620
C	−1.050639326	1.646508373	−2.298073812
C	−2.178409478	0.835682415	−2.461616288
C	−2.209979432	−0.036853964	−3.542509301
H	−3.077538819	−0.700292892	−3.654007641
C	−1.170742444	−0.110731681	−4.449716989
C	−0.104023258	0.769181042	−4.309601975
H	0.712403135	0.750776109	−5.044573653
C	−0.032953292	1.671902809	−3.249326253
C	−3.341133562	0.906270032	−1.501541430
H	−4.083965357	0.125602625	−1.728882804
H	−3.842806433	1.890114216	−1.549468594
H	−3.013291715	0.761810039	−0.456817908
C	−1.186526488	−1.150519744	−5.554355798
H	−0.935445049	−2.148856106	−5.146859500
H	−0.452136373	−0.917523023	−6.343834169
H	−2.185663055	−1.233159429	−6.017654013
C	1.112612726	2.650689387	−3.170835396
H	0.816121177	3.633490107	−3.585364635
H	1.980315280	2.296344480	−3.751149496
H	1.433526399	2.825828636	−2.129836697
C	0.014911641	2.051122343	2.331893269
C	1.324472868	2.227214134	2.772726906
C	1.683388861	1.696647680	4.010280697
H	2.716014952	1.828943753	4.362155689
C	0.768476608	1.020851844	4.811101894
C	−0.524904552	0.849886978	4.332724715
H	−1.258367217	0.307351508	4.944597117
C	−0.928607259	1.360535394	3.099985946
C	2.342734176	2.966765419	1.938577022
H	2.108066497	4.044808780	1.859750371
H	2.369125978	2.567384404	0.908716977
H	3.350541383	2.874946270	2.375192227
C	1.164307204	0.497036563	6.170108752
H	2.121884378	−0.053046486	6.128298101
H	0.394762634	−0.176397573	6.584358978
H	1.302312107	1.327669504	6.888356553
C	−2.351136168	1.173732611	2.624772151
H	−2.972295772	0.710277006	3.407950303
H	−2.378443034	0.518102293	1.732894950
H	−2.817676132	2.129562236	2.327364752
C	2.829136828	0.304633417	−1.184787922
H	3.031942845	1.393850505	−1.191220446
H	2.220413367	0.055464389	−2.070920838
C	4.085886908	−0.511113777	−1.050264015
H	4.936433345	−0.059974667	−1.589361571
H	3.921466294	−1.521643832	−1.472910866
C	4.286937317	−0.593670636	0.439418919

H	4.928305824	−1.434966751	0.751845438
H	4.740019515	0.338771271	0.826991335
C	2.879091100	−0.740232212	0.936553660
H	2.545778977	−1.798226162	0.929871261
H	2.695616947	−0.322629765	1.942384459
C	0.665395757	−3.054106153	−1.213583647
C	0.803682678	−2.425697887	−2.455732492
H	0.292661107	−1.469968401	−2.642074339
C	1.576150527	−3.002818620	−3.447267976
H	1.674657264	−2.498993937	−4.417318937
C	2.244392823	−4.189462288	−3.207901993
H	2.868519785	−4.636568829	−3.991924473
C	2.113781053	−4.814239172	−1.986125746
H	2.639386377	−5.757442364	−1.789837806
C	1.333546147	−4.249589441	−0.986095980
H	1.256996038	−4.751829997	−0.014740110
C	−0.231887969	−3.026000265	1.606055340
C	0.118566152	−2.253701727	2.710325721
H	0.331147364	−1.184069886	2.575406127
C	0.158515295	−2.820852319	3.979826989
H	0.421424703	−2.195608993	4.841936017
C	−0.143179805	−4.153237974	4.147236340
H	−0.115707558	−4.603342963	5.147757569
C	−0.488680948	−4.932767442	3.050004429
H	−0.736516738	−5.993042186	3.186416411
C	−0.545399904	−4.373372984	1.784103563
H	−0.866365960	−4.985034478	0.931276784
C	−2.092291560	−2.553201891	−0.501841132
C	−3.100239916	−2.176605186	0.388624135
H	−2.830472296	−1.800667281	1.385169380
C	−4.426362913	−2.271607144	0.032109978
H	−5.204777179	−1.970014020	0.744152792
C	−4.769626423	−2.717780588	−1.227983122
H	−5.827094395	−2.768822657	−1.518561457
C	−3.798060702	−3.117440228	−2.111814711
H	−4.065934631	−3.493289769	−3.107040037
C	−2.446725846	−3.045288178	−1.743920461
H	−1.675346019	−3.355023833	−2.459291619

[Ni(6-Mes)(PPh_3)CO][PF_6] (**5**, Hopt)

Ni	0.000000000	0.000000000	0.000000000
P	−0.456531410	−2.190330460	0.000000000
O	2.917960062	−0.023110527	0.027991471
N	−0.562533954	2.613079350	1.045115880
N	−0.896366091	2.420425821	−1.221376138
C	−0.543572364	1.865530692	−0.059756234
C	−0.984874995	4.027282825	1.086017363
H	−0.095049503	4.679947386	0.997211603
H	−1.443342111	4.214713301	2.071092425
C	−1.968234892	4.271730234	−0.047916542
H	−2.907400793	3.724659750	0.157976704
H	−2.217897219	5.344431101	−0.108524974
C	−1.382520117	3.803513612	−1.361866126
H	−2.136179386	3.814979649	−2.167618417
H	−0.545917748	4.454410367	−1.682846917
C	−0.236179734	1.954168400	2.287678744
C	1.067513596	2.042984900	2.784151680
C	1.355034040	1.381135571	3.971121827
H	2.377513419	1.432526039	4.370358716
C	0.389149871	0.668836889	4.663871298
C	−0.893018192	0.607248884	4.147959159
H	−1.669582507	0.048330642	4.687862460
C	−1.237320830	1.256122981	2.960571432
C	2.128906288	2.843561123	2.069392082
H	2.061376525	3.914740373	2.338901081
H	2.024231411	2.780485608	0.972876676
H	3.138035220	2.495583489	2.345127161
C	0.722207082	0.009864569	5.990533010
H	1.800956632	−0.206537801	6.074777987
H	0.162843373	−0.932502052	6.123761446
H	0.450495314	0.675644724	6.831971141
C	−2.661023087	1.237655550	2.455079455
H	−3.078286096	2.258784283	2.386527606
H	−3.307820014	0.648613596	3.125095196
H	−2.730067351	0.799150626	1.442359024
C	−0.888799546	1.576831413	−2.401083631
C	−2.027063016	0.820857654	−2.681791597
C	−2.000008058	0.029464186	−3.830049068
H	−2.884129912	−0.578540782	−4.066051351
C	−0.915709046	0.012699059	−4.685875381
C	0.190195842	0.780047197	−4.377555306

H	1.062313916	0.768879587	−5.045520117
C	0.237182188	1.573702610	−3.230576472
C	−3.250814165	0.861561521	−1.796705995
H	−3.038263816	0.428305643	−0.801261421
H	−4.072421232	0.277688060	−2.240575850
H	−3.605254047	1.894058865	−1.629961292
C	−0.930060656	−0.844953861	−5.939564722
H	−0.204351729	−0.478992829	−6.685263826
H	−1.932214345	−0.864405715	−6.401983136
H	−0.661151570	−1.891231168	−5.696801801
C	1.471746552	2.372146012	−2.913700761
H	1.297059315	3.457584340	−3.036265474
H	2.304153711	2.087742511	−3.577117985
H	1.793720107	2.220738807	−1.868030617
C	1.786094678	0.000000000	−0.001561590
C	−0.078118216	−3.021872980	1.566100317
C	−0.505082042	−4.320380784	1.855465867
H	−1.158574616	−4.858542795	1.156872882
C	−0.100083238	−4.928075316	3.034424689
H	−0.433267504	−5.951827664	3.248141381
C	0.700164608	−4.265342329	3.927111381
H	1.013691782	−4.760929522	4.854954608
C	1.101864083	−2.971731620	3.669447638
H	1.725966096	−2.424865542	4.385856609
C	0.704865881	−2.351805544	2.489801015
H	1.010463471	−1.314609772	2.295162028
C	−2.211256617	−2.518334394	−0.347321111
C	−3.148812045	−2.201945298	0.639131908
H	−2.807946482	−1.899718507	1.638938483
C	−4.497558846	−2.247521394	0.360688169
H	−5.219590681	−1.987126963	1.144959445
C	−4.938223958	−2.615208973	−0.894706483
H	−6.013372533	−2.642308352	−1.112665922
C	−4.029734846	−2.956838076	−1.863807752
H	−4.369607108	−3.264066347	−2.860922961
C	−2.659753772	−2.904509670	−1.600430409
H	−1.943389579	−3.156139864	−2.392112314
C	0.496402429	−3.020646267	−1.307212263
C	0.781923211	−2.281911754	−2.450135604
H	0.405415643	−1.251703700	−2.535500972
C	1.541199971	−2.812931500	−3.478901857
H	1.758400882	−2.209485546	−4.368350744
C	2.033411229	−4.101138317	−3.352152854
H	2.648574905	−4.528683206	−4.154866312
C	1.760781735	−4.844731257	−2.234748959
H	2.155107424	−5.864069605	−2.137788629
C	0.991220989	−4.311573560	−1.201786269
H	0.799055532	−4.913777740	−0.305912343

[Ni(6-Mes)(PPh_3)($NCBH_3$)] (**7**, Hopt)

Ni	0.000000000	0.000000000	0.000000000
P	−0.479500456	−2.167712356	0.000000000
N	−1.354140238	2.168686031	1.157879613
N	−2.043298371	1.894727840	−1.009760656
N	1.924023274	0.000000000	0.006058639
C	−1.319344695	1.445563721	0.022350405
C	−2.110099406	3.409397682	1.353848125
H	−2.980931867	3.166933886	2.000412541
H	−1.482882552	4.103704783	1.940567241
C	−2.887195861	3.110161191	−0.981280434
H	−2.794808916	3.612372282	−1.959508251
H	−3.942855571	2.776051348	−0.902488464
C	−0.536385396	1.681961692	2.242288149
C	−1.111170360	0.852976441	3.208458351
C	−0.279258799	0.313794774	4.176491861
H	−0.710509361	−0.363061048	4.927526860
C	1.087910198	0.576720886	4.200639276
C	1.605037068	1.449736652	3.267866893
H	2.678344347	1.681763216	3.277361008
C	0.807817013	2.035773529	2.286750336
C	−2.589641457	0.550896137	3.204871486
H	−3.181161960	1.430684111	3.520403204
H	−2.826322833	−0.274031676	3.896919304
H	−2.940459744	0.270477710	2.195861263
C	1.988966977	−0.098834517	5.205915559
H	1.610559836	0.020805156	6.237793522
H	3.015165614	0.302843563	5.163831706
H	2.043134591	−1.186126416	5.008929263
C	1.404608443	3.026027279	1.332913752
H	1.109520000	2.826597160	0.287999324
H	2.504996259	3.004604909	1.383918588

H	1.071971266	4.055338915	1.568729874
C	−2.091552842	1.095299716	−2.208794617
C	−1.218610596	1.372454065	−3.255666951
C	−1.289870013	0.565963692	−4.396000653
H	−0.601163950	0.767401342	−5.228017862
C	−2.193016930	−0.477064034	−4.493053509
C	−3.067778909	−0.698168192	−3.440169033
H	−3.807209467	−1.507551635	−3.511566921
C	−3.047652737	0.086562343	−2.297061633
C	−0.211181624	2.491853476	−3.171290842
H	0.501746538	2.318503134	−2.343115576
H	−0.692329948	3.467122117	−2.973232597
H	0.364302269	2.576792974	−4.107308794
C	−2.222249162	−1.368630761	−5.710629197
H	−1.691419902	−0.911813463	−6.563264176
H	−3.257168605	−1.594369534	−6.023995715
H	−1.729928511	−2.336076676	−5.492484229
C	−4.061502889	−0.116919303	−1.205811478
H	−4.715036056	0.766720880	−1.090312992
H	−3.571055790	−0.289244890	−0.230989504
H	−4.699933542	−0.988684009	−1.416976234
C	3.016266427	0.173827301	0.284003717
C	0.329380367	−3.178390745	1.303083031
C	−0.085687633	−4.479875945	1.585333744
H	−0.952926257	−4.903743402	1.063520606
C	0.577113916	−5.239270963	2.530472772
H	0.237681106	−6.262905588	2.735141241
C	1.650338865	−4.714956484	3.215607179
H	2.175046909	−5.321964211	3.964598544
C	2.060156007	−3.420740177	2.965196715
H	2.907751196	−2.992475772	3.514947492
C	1.395376632	−2.646860951	2.022273583
H	1.708916531	−1.612693895	1.840046791
C	0.102010732	−2.922944205	−1.572471440
C	0.368314268	−4.275139966	−1.746206623
H	0.249324288	−4.974551352	−0.909985328
C	0.816381375	−4.756259837	−2.969743433
H	1.037354363	−5.825653460	−3.079606013
C	0.982806306	−3.897133041	−4.040828458
H	1.338505324	−4.281210996	−5.005449258
C	0.695988051	−2.557029977	−3.888962777
H	0.817625293	−1.862259605	−4.729447324
C	0.269899980	−2.069434967	−2.661335449
H	0.054369160	−0.998806306	−2.535410449
C	−2.202019129	−2.754428482	0.152375484
C	−2.839337739	−2.579897014	1.381413568
H	−2.285377352	−2.135325333	2.218394780
C	−4.161807230	−2.964140041	1.552905531
H	−4.651282616	−2.817290498	2.523837335
C	−4.849484510	−3.531621325	0.497941381
H	−5.895772654	−3.836682772	0.630834579
C	−4.229767223	−3.723418877	−0.710245310
H	−4.775204718	−4.181220933	−1.545484215
C	−2.908091289	−3.334005436	−0.891943413
H	−2.423109007	−3.482089450	−1.864273166
C	−2.511335336	3.986525727	0.106251880
H	−1.662703834	4.605142389	−0.259301392
H	−3.318361209	4.723255965	0.277539777
B	4.513628690	0.424506360	0.722990796
H	4.639031391	1.613960827	0.994442419
H	4.728847883	−0.265627707	1.713567819
H	5.262756691	0.109562714	−0.195592943

[Ni(6-Mes)(PPh_3)(NPh_2)] (**8**, Hopt)

Ni	0.000000000	0.000000000	0.000000000
P	−0.695014838	−2.122778106	0.000000000
N	−2.103723418	1.525958042	1.305708627
N	−2.159316914	1.729217347	−0.975639568
N	1.935039741	0.000000000	−0.002217489
C	−1.555316530	1.189567514	0.111349685
C	−3.268954246	2.410156172	1.500377850
H	−2.920431954	3.444731465	1.704277603
H	−3.801017693	2.067995226	2.405001922
C	−4.154535980	2.368028325	0.285194370
H	−4.974812566	3.101561551	0.375125794
H	−4.611678285	1.365119019	0.182547091
C	−3.304180500	2.665244240	−0.928489336
H	−3.873657264	2.545306456	−1.865066669
H	−2.929081802	3.710004057	−0.906659661
C	−1.583939260	1.614972829	−2.294074083
C	−2.232244389	0.842998119	−3.264850882
C	−1.720901427	0.836390025	−4.562116969

H	−2.221572619	0.217270037	−5.320300513
C	−0.618011426	1.593944120	−4.921490080
C	−0.022705171	2.382671090	−3.944201816
H	0.843902431	3.004818126	−4.207448066
C	−0.485744053	2.416000100	−2.633293669
C	−3.484430041	0.069905923	−2.958435596
H	−3.594479048	−0.110566575	−1.878793735
H	−3.479130807	−0.913662751	−3.458453365
H	−4.384857572	0.611815467	−3.308353492
C	−0.087174532	1.576480573	−6.335591327
H	0.061574302	2.601151699	−6.722582704
H	−0.772110250	1.046118237	−7.018852567
H	0.895302233	1.068786517	−6.386455606
C	0.201877840	3.277449522	−1.612974258
H	−0.514551567	3.792606490	−0.950808595
H	0.838938043	4.034166302	−2.099914219
H	0.847441302	2.654603505	−0.964301687
C	−1.420244374	1.255854614	2.544155410
C	−0.346794734	2.077493513	2.921970695
C	0.196869140	1.909764931	4.191312852
H	1.042683040	2.545798289	4.489258205
C	−0.298696257	0.972254345	5.086448114
C	−1.366685022	0.189183303	4.691499324
H	−1.766093817	−0.567443017	5.380961305
C	−1.952881780	0.316837881	3.431878953
C	0.234896829	3.111727540	1.995467471
H	0.825002958	2.621567437	1.197676697
H	0.896256286	3.803977077	2.542132615
H	−0.546978033	3.703180324	1.487432278
C	0.316850243	0.843851345	6.459715803
H	0.115313054	1.742438881	7.073352288
H	1.415175937	0.735282905	6.398211437
H	−0.081417507	−0.030290370	7.003117978
C	−3.124189400	−0.549742719	3.058330685
H	−2.936295756	−1.601811729	3.332874505
H	−3.316217636	−0.505577900	1.975333286
H	−4.046460004	−0.230422018	3.581021222
C	2.770670206	0.200585186	−1.084567827
C	2.218674007	0.461677889	−2.357153118
H	1.124583611	0.482050909	−2.446342790
C	3.019628844	0.675452655	−3.464489310
H	2.538004586	0.869644816	−4.433008855
C	4.405601961	0.628425680	−3.372424719
H	5.036917932	0.786500442	−4.255593450
C	4.965667149	0.395715990	−2.124179088
H	6.059201400	0.376773757	−2.012380495
C	4.180662743	0.200255907	−1.001488345
H	4.661996095	0.037068742	−0.030585762
C	2.533397859	−0.606796390	1.130986453
C	3.178385956	−1.850945067	1.042863205
H	3.244954083	−2.340812235	0.064635354
C	3.707656798	−2.457871646	2.162023492
H	4.194742386	−3.437220557	2.061655961
C	3.604800510	−1.857068104	3.409912694
H	4.018497092	−2.348698532	4.299800066
C	2.969261779	−0.635741784	3.513900025
H	2.872565771	−0.142429793	4.490431629
C	2.447290637	−0.008118512	2.385488084
H	1.940700454	0.956841885	2.472517652
C	−2.193917261	−2.654045000	−0.924116179
C	−2.121978244	−3.405471536	−2.091825037
H	−1.145943894	−3.707835731	−2.489708779
C	−3.285043502	−3.803357501	−2.750281495
H	−3.203040743	−4.403726384	−3.665915967
C	−4.524316821	−3.467262586	−2.250678751
H	−5.437447600	−3.794125421	−2.764451650
C	−4.609740790	−2.699209078	−1.096203411
H	−5.589245039	−2.413883896	−0.691264936
C	−3.453113370	−2.289582028	−0.447877010
H	−3.529797776	−1.686148411	0.464557133
C	−0.984168513	−2.875998134	1.655336766
C	−1.928162975	−3.874321243	1.910084213
H	−2.561295385	−4.249654715	1.097258200
C	−2.084370320	−4.385752452	3.191270175
H	−2.841396885	−5.158758433	3.377454512
C	−1.284396707	−3.928111479	4.227018180
H	−1.409553054	−4.332785450	5.239833244
C	−0.321730645	−2.965932268	3.974386481
H	0.323274195	−2.596771124	4.781405643
C	−0.178246213	−2.436558329	2.702853440
H	0.564379875	−1.649497393	2.523720108
C	0.592031787	−3.243821909	−0.674797544

C	1.294399794	−2.828035019	−1.802125416
H	1.054816805	−1.863353632	−2.266660022
C	2.329136061	−3.597823741	−2.313315975
H	2.881334800	−3.239349441	−3.191406054
C	2.681297452	−4.788117036	−1.702147012
H	3.512598663	−5.385594575	−2.098447880
C	1.988242869	−5.215034830	−0.586117397
H	2.261134041	−6.156135324	−0.091097218
C	0.944679296	−4.451181618	−0.075549372
H	0.413684474	−4.791992103	0.821016265

[{Ni(6-Mes)(PPh_3)}$_2$(μ-Br)][$BAr^F{}_4$] (**3**, Hopt)

Br	−0.25639706659486	0.00543203944881	−0.00574864097335
Ni	−0.00141445582272	−0.00161719124827	2.36085612130032
Ni	−0.00015296700479	0.00006943559962	−2.36057605176897
P	1.60561820226017	−1.34949015931619	3.07948509144203
P	−0.05791551870586	2.05894002135374	−3.18549806491182
N	−2.34469704371215	0.72476629815857	3.85379734669628
N	−0.74048071042127	2.35773468891002	3.84469062741378
N	1.29330508165085	−2.17594567071556	−3.70999845413701
N	−0.97876641229647	−2.33616786811904	−3.73844827556246
C	−1.09323658933377	1.10305449381915	3.51892334015391
C	−3.35665812248876	1.59420589371584	4.47501178959584
H	−3.35528603985156	1.45012856464811	5.57420078584473
H	−4.34663925442599	1.27703734513996	4.10434502514930
C	−3.05814119173005	3.02726770221971	4.11375054341008
H	−3.21356066625557	3.17488081559075	3.02780945794020
H	−3.74832097937584	3.70801478939576	4.64123809170919
C	−1.63356900776029	3.34855528900485	4.46914605206826
H	−1.33443159127124	4.34521201274926	4.10070085675720
H	−1.48751072365952	3.34753071596356	5.56778226775179
C	−2.71503784431101	−0.65502943185401	3.62171055781586
C	−2.42899877749845	−1.58821900618814	4.61983031913298
C	−2.76939134334439	−2.91310378305709	4.37132598046750
H	−2.52864082279405	−3.66441311687222	5.13755855064567
C	−3.40648726236367	−3.31437335448839	3.21196100280536
C	−3.72448829242042	−2.33244751096454	2.27329095657953
H	−4.25470528127871	−2.62377739739589	1.35648035547970
C	−3.39034545329017	−0.99344948405029	2.45222617967079
C	−1.79358652423983	−1.17554099039215	5.91790027659825
H	−1.65785916434021	−2.04074711326211	6.58542073773870
H	−2.40490493353677	−0.42341129470674	6.44810974882180
H	−0.79894196182430	−0.72444861093662	5.74769910604186
C	−3.75838511178547	−4.75356266573628	2.96186435131927
H	−4.44074242247969	−5.14454284203365	3.73974050452001
H	−2.85608407107684	−5.39327494612063	2.98037698505685
H	−4.24837937643913	−4.88679621096277	1.98271413925072
C	−3.76172709508605	0.03689874783316	1.41676505947862
H	−2.92918371505758	0.73289303149341	1.21726591001044
H	−4.62794123677818	0.64319294753166	1.74434172654215
H	−4.02646442650560	−0.44141664519712	0.46064728920884
C	0.62058274353316	2.77520614659956	3.60919385930095
C	0.96260011977858	3.38668912176957	2.40589981386342
C	2.28127199338704	3.79906328993846	2.24046223773833
H	2.55386845251434	4.28167916620071	1.29084975204108
C	3.24806745733654	3.62700264790768	3.20772544406468
C	2.86717841303406	3.02923377538064	4.40270790557343
H	3.60716389026184	2.89546141114225	5.20416385482391
C	1.55701791696668	2.62008599526105	4.62810590089623
C	−0.06911153084324	3.62141305287974	1.32600318167102
H	−0.92272025151476	4.21947409586244	1.69279281565749
H	−0.48237406142534	2.66932607523513	0.94631875969116
H	0.37462737901835	4.15093382985632	0.46800278116198
C	4.66463394783550	4.09580684707505	3.00861153254400
H	4.95915322724232	4.82469364595823	3.78600831443210
H	4.79964369985589	4.57495295139238	2.02384190877158
H	5.37302739971121	3.24874274580168	3.07295180340712
C	1.15184331596998	2.06749859609513	5.97159435855196
H	0.47114366336721	2.75913614815515	6.50132066685622
H	2.03044336292630	1.90591213597652	6.61647822852413
H	0.62114709513809	1.10435384018356	5.87029339630934
C	3.28225198690384	−0.76758259210531	2.65821947485231
C	3.39513297094063	0.29139713283958	1.77272067357444
H	2.48716425376319	0.76668481992618	1.37684233116589
C	4.65233977203949	0.76293769806986	1.40744730163122
H	4.71580092044609	1.60856401643173	0.71108298217873
C	5.78686227630997	0.20444692793698	1.90667089152039
H	6.77191484043022	0.59148237472194	1.61661434651247
C	5.69003657461469	−0.85337580942627	2.79220757513313
H	6.59651168736614	−1.31192677499596	3.20743370774962

C	4.45371699930904	−1.33672181511111	3.16103879363406
H	4.39298046534716	−2.16029184520502	3.88409458158613
C	1.75524318235157	−1.83279885513262	4.83463492069472
C	2.48423440295055	−1.03474282530723	5.71103301420497
H	3.02773817018059	−0.16069563347618	5.33120470818242
C	2.53289213214323	−1.34103332060946	7.06336922244611
H	3.11947221263358	−0.70469693586252	7.73841056789390
C	1.84257991180813	−2.42285096113576	7.55347875747042
H	1.87731656848465	−2.65625198165944	8.62555331265901
C	1.12221067383286	−3.21542243301585	6.70120930174913
H	0.57397786242593	−4.08666779071269	7.08196230454079
C	1.07666893962391	−2.92697155395630	5.33889250005151
H	0.49274349142394	−3.57014871783107	4.66876312468994
C	1.44262078858161	−2.98221186272160	2.25098235191068
C	2.51721546138488	−3.79814895035463	1.95413070709632
H	3.53831629493046	−3.48964719668332	2.20604658652903
C	2.31224794738232	−5.00890590124033	1.30906347836895
H	3.17269027947959	−5.64427342702867	1.06355050694410
C	1.03510565590906	−5.41171515003231	0.98235433371580
H	0.87609684200925	−6.37283250356014	0.47630817496333
C	−0.04139954080083	−4.60443099595901	1.28242328515410
H	−1.05953717338189	−4.91438507165323	1.01548347357517
C	0.16137242483265	−3.38531328608906	1.89828152967472
H	−0.69125290146455	−2.72343864877470	2.10989923317084
C	0.10994682540928	−1.61167504512610	−3.42636663216043
C	1.49418477874537	−3.53101919920422	−4.24497558033701
H	2.42771931076134	−3.92779577869712	−3.80979623586428
H	1.63395349709506	−3.48632110847328	−5.34322854782390
C	0.30281851462913	−4.38777500650060	−3.88579096845279
H	0.27886632403854	−4.55018388551569	−2.79124991336315
H	0.38388685258856	−5.37756594555233	−4.36687938533494
C	−0.96592148615256	−3.69018877279421	−4.31968441431625
H	−1.03230611492653	−3.62813455903965	−5.42437621800061
H	−1.86770359916413	−4.21781475271273	−3.96509296712701
C	2.47778713864406	−1.39868761209570	−3.45784435683704
C	3.07990935604620	−1.45145815344869	−2.20103327452770
C	4.19967915858262	−0.68222620177835	−1.97978461506731
H	4.67070238906884	−0.70763255582205	−0.98783464140739
C	4.74509776134653	0.11875474988457	−2.96962080714038
C	4.15427252694558	0.12061361759578	−4.21924038499442
H	4.59273479638006	0.73015412512688	−5.02247372418385
C	3.04095156240355	−0.64310200463603	−4.49816261739229
C	2.53778913281226	−2.35079329030559	−1.10791059249645
H	3.13297136384806	−2.23898641589200	−0.18896773274594
H	2.56205330779823	−3.41594400892122	−1.40122956580343
H	1.49169992900862	−2.10653641083931	−0.85290817457236
C	5.96791619962335	0.95604113436120	−2.68917533619525
H	6.73907967447347	0.82424919865183	−3.46967088480907
H	6.41646376899995	0.70215444322881	−1.71385067222178
H	5.70853717977482	2.03214219318075	−2.66962301279816
C	2.46327157123228	−0.71793340742371	−5.87843420197072
H	2.69500254036604	−1.69005598684292	−6.35332441412943
H	2.87737322301126	0.06801186375046	−6.53172687133552
H	1.36407408559849	−0.61734126615523	−5.87080244308846
C	−2.27081282533774	−1.73102077030742	−3.54066082772700
C	−2.78756993563333	−0.91484696266028	−4.55252037783088
C	−4.02831838423076	−0.34138554261897	−4.36358514866710
H	−4.43355291589245	0.30851732921037	−5.15210300191605
C	−4.77253870905244	−0.55870749227469	−3.21369746064917
C	−4.23477373755982	−1.39425852262266	−2.24120419838606
H	−4.82155044244952	−1.59827776998877	−1.33438592980524
C	−2.98760008567686	−1.98675326166038	−2.37021471349022
C	−2.01448086960970	−0.69705436636263	−5.82289028837536
H	−1.03752153091937	−0.22432696213189	−5.61511508060384
H	−2.56240003474483	−0.03738875552550	−6.51433757052659
H	−1.80935110746576	−1.64917122752866	−6.34456180961180
C	−6.12420126847554	0.09244641582747	−3.02993164576574
H	−6.57440480585308	−0.17665852604906	−2.05952782588350
H	−6.82707258549617	−0.20881922580254	−3.82873914235267
H	−6.04066558348232	1.19430648777985	−3.07471075768281
C	−2.43558812281043	−2.89254657654029	−1.30372485621657
H	−1.59702290714717	−2.40604410143132	−0.77008077103541
H	−2.04677665686768	−3.83848070224221	−1.71900418885520
H	−3.20561680357674	−3.13831490308189	−0.55548243484484
C	−1.40389727943219	2.96020960035326	−2.32464580359720
C	−2.56035469446619	2.25239242196425	−2.01729876016174
H	−2.63968847185870	1.19438495072748	−2.30468234673974
C	−3.60014637681788	2.86271523984069	−1.34144216231809
H	−4.50428655432990	2.28469918602243	−1.11185110265233
C	−3.48986118256087	4.17117367439910	−0.94144260073034
H	−4.30866849947358	4.65261564420587	−0.39131593331280
C	−2.33611814537312	4.88056944743605	−1.22246784431462

H	−2.23673546140980	5.92336275526090	−0.89510297899789
C	−1.29867846799966	4.28163725050454	−1.91574131350375
H	−0.38818316241246	4.85476780441198	−2.12675779964298
C	−0.38622730178239	2.39723526187055	−4.95530025673384
C	0.61993024598594	2.14300569778385	−5.87615165220039
H	1.61074346462099	1.83533308854263	−5.51877929595455
C	0.39321155673090	2.28423507541145	−7.23244593384965
H	1.20468999753810	2.07775139439740	−7.94190239299942
C	−0.84985450593017	2.67462155248677	−7.69047253561966
H	−1.02941114240798	2.77784454073734	−8.76834087160483
C	−1.84899011106208	2.95024141510057	−6.79480427237841
H	−2.83646452893612	3.27604708990478	−7.14588889502595
C	−1.62596625935008	2.80947417985177	−5.42839509469214
H	−2.43808923077897	3.02098743961426	−4.72196229922365
C	1.41721986303297	3.08592898189030	−2.86434125457305
C	2.29386371846437	2.69923057439727	−1.85478052989963
H	2.12791418648275	1.74838095121158	−1.32973041547878
C	3.36662341258746	3.51225175748125	−1.51627348269563
H	4.04972145175226	3.19438965946682	−0.71852377230793
C	3.57944542202821	4.69458971681492	−2.17307130498433
H	4.42923290942360	5.33264023655992	−1.89833026151791
C	2.72478604918412	5.08117802128057	−3.18473887979946
H	2.89085896974911	6.02398801404034	−3.72101515684231
C	1.66012483130751	4.27289165029499	−3.53544916329267
H	0.99043980223168	4.58682876918304	−4.34669220145568

2. Fully optimised structures (opt) in Å. For **1**, **2**, **5**, **7**, and **8** the geometry is oriented such that the Ni ion is at the centre of the coordinate system, with the z-axis perpendicular to the plane containing Ni, P, $C_{carbene}$ and the coordinating ligand atom, and the x-axis along the Ni-P bond.

[Ni(6-Mes)(PPh_3)Br] (**1**, opt)

Br	2.329706687	0.000000000	−0.003473176
Ni	0.000000000	0.000000000	0.000000000
P	−0.719906198	−2.025159954	0.000000000
N	−1.602228416	1.958627230	−1.131081843
N	−2.067960473	1.651459817	1.122406693
C	−1.372976363	1.287453874	0.020770424
C	−2.547592860	3.079760053	−1.270813908
H	−3.526723133	2.702687314	−1.629401254
H	−2.153228618	3.762552009	−2.042977782
C	−2.692591338	3.785702644	0.074867479
H	−1.742976079	4.292701458	0.328339824
H	−3.481139429	4.555264162	0.019817609
C	−3.036215865	2.765882661	1.157597178
H	−2.989428862	3.220089102	2.162356949
H	−4.063889512	2.379787737	1.012912713
C	−0.780525483	1.597449383	−2.259453846
C	−1.238868870	0.639740998	−3.188901921
C	−0.400343794	0.311812643	−4.273381983
H	−0.737415981	−0.449679003	−4.989044246
C	0.862547049	0.904653875	−4.442487388
C	1.276420948	1.876864623	−3.506316693
H	2.258755325	2.354692752	−3.623346937
C	0.471100775	2.246306248	−2.417184533
C	−2.578360703	−0.033400751	−3.037702160
H	−2.979034308	0.096072648	−2.020042350
H	−2.489382549	−1.114131421	−3.247186781
H	−3.318675801	0.380647540	−3.748359559
C	1.771692033	0.494918908	−5.578268691
H	2.169824798	1.374572598	−6.116369618
H	1.245905899	−0.146750262	−6.305722108
H	2.644780104	−0.070084801	−5.199013341
C	0.930231224	3.281402820	−1.421065161
H	1.917044170	3.685013637	−1.701226809
H	1.015490116	2.837345615	−0.413054979
H	0.220031441	4.125572449	−1.348973015
C	−1.808502969	0.932440085	2.341710994
C	−0.621084048	1.194331389	3.066889283
C	−0.379280873	0.442157415	4.233739317
H	0.545175320	0.626272697	4.798165174
C	−1.278824990	−0.543555336	4.686603195
C	−2.471808333	−0.738104003	3.964320122
H	−3.193719339	−1.491965536	4.305978123
C	−2.764503934	−0.002318035	2.800737954
C	0.370412630	2.235582311	2.609812251
H	1.032713041	1.820146653	1.824960801

H	1.005567380	2.566355059	3.448737063
H	−0.131580005	3.117165810	2.175606819
C	−0.957895980	−1.398908109	5.889808731
H	−0.193671719	−0.927884152	6.531713862
H	−0.561273226	−2.381717629	5.568824991
H	−1.856351274	−1.595384406	6.501413154
C	−4.070626855	−0.195550918	2.075586160
H	−4.500885872	−1.184461420	2.297193511
H	−3.939476776	−0.115413239	0.984351211
H	−4.810164924	0.569472494	2.380645186
C	−2.379529739	−2.649315915	0.473540137
C	−3.466950418	−2.469294721	−0.410729851
H	−3.310391509	−1.955328885	−1.364438223
C	−4.739519279	−2.967632259	−0.093932196
H	−5.568007376	−2.829281103	−0.799787174
C	−4.950775684	−3.641906606	1.123320607
H	−5.944824624	−4.032864533	1.373030143
C	−3.878806043	−3.808302159	2.018172234
H	−4.033140379	−4.328239233	2.971983360
C	−2.601501705	−3.318737389	1.695634514
H	−1.772705730	−3.464916728	2.396297270
C	0.354036752	−2.982653696	1.137676457
C	0.682871822	−2.370582753	2.365856396
H	0.314959804	−1.359379496	2.576634720
C	1.478901510	−3.045802358	3.303702116
H	1.728481578	−2.560640626	4.255658199
C	1.970649335	−4.332687776	3.012979107
H	2.603404167	−4.857587472	3.739624061
C	1.656678023	−4.940151914	1.783473996
H	2.043886264	−5.940057068	1.549820801
C	0.846525582	−4.270522534	0.848977418
H	0.603861899	−4.749770759	−0.107083298
C	−0.457082834	−2.836915649	−1.625897169
C	0.492835346	−2.258541526	−2.494719892
H	1.004369041	−1.336409385	−2.189006448
C	0.769021857	−2.849169745	−3.738188889
H	1.506923943	−2.387990027	−4.405639048
C	0.089565654	−4.014754452	−4.133868176
H	0.298249836	−4.469907502	−5.110198363
C	−0.863549313	−4.593995964	−3.274918296
H	−1.396293402	−5.504485652	−3.577199265
C	−1.133481819	−4.011498081	−2.025456667
H	−1.874314097	−4.470713269	−1.360674695

[Ni(6-Mes)(PPh_3)THF][PF_6] (**2**, opt)

Ni	0.000000000	0.000000000	0.000000000
P	−0.339897533	−2.141945774	0.000000000
O	2.054444403	0.000000000	−0.002388224
N	−0.946543888	2.415893842	−1.010077170
N	0.195531628	2.726996208	0.985570672
C	−0.243188658	1.901209166	0.019285890
C	−1.267100057	3.843855493	−1.178320812
H	−2.284375709	4.044527435	−0.788515064
H	−1.276160572	4.069767899	−2.258058855
C	−0.222735911	4.681226145	−0.443059621
H	−0.522628096	5.742378697	−0.440548500
H	0.747869820	4.608185225	−0.968353985
C	−0.064226657	4.180910615	0.990830713
H	0.778090461	4.679329631	1.498026522
H	−0.975402079	4.385230600	1.587070807
C	−1.384176886	1.453012689	−1.991409210
C	−2.550880255	0.695015105	−1.727518023
C	−2.907476912	−0.312467445	−2.643015205
H	−3.789864270	−0.930124597	−2.432862341
C	−2.151357787	−0.558504890	−3.805342648
C	−1.028191511	0.256671651	−4.061533006
H	−0.438168853	0.088391367	−4.973015022
C	−0.625969227	1.271688335	−3.172860894
C	−3.376327433	0.958462815	−0.492275758
H	−4.293676892	0.349638494	−0.496806378
H	−3.659961922	2.023238294	−0.415173255
H	−2.812067101	0.714079242	0.426322504
C	−2.506481988	−1.691320482	−4.738040481
H	−1.848906804	−2.563479323	−4.555854147
H	−2.377797264	−1.402341799	−5.796114877
H	−3.545314837	−2.028900110	−4.587327636
C	0.571691855	2.139556034	−3.470285288
H	0.263395930	3.097874407	−3.930726294
H	1.258343841	1.641926018	−4.175094109
H	1.129980387	2.388463078	−2.552318733
C	0.917834312	2.154187202	2.091416152

C	2.322644820	2.310490097	2.143862769
C	3.016653498	1.723929357	3.219292930
H	4.109989107	1.823155413	3.259625185
C	2.351737370	0.996775808	4.227801467
C	0.950731690	0.876944811	4.147321867
H	0.411643368	0.325062327	4.929193859
C	0.212450264	1.441903113	3.088434976
C	3.062415989	3.055354147	1.061461693
H	3.021997792	4.150690442	1.216524744
H	2.624734046	2.852031543	0.069443481
H	4.126217696	2.766372585	1.040513175
C	3.125191690	0.323354185	5.337391828
H	3.478871845	-0.675519478	5.015379700
H	2.500293007	0.176896179	6.235122045
H	4.017517685	0.906882451	5.623346714
C	-1.280531823	1.243021394	3.006670889
H	-1.693380877	0.928392802	3.979047170
H	-1.513684617	0.452699046	2.264132781
H	-1.805535133	2.154637248	2.673912421
C	2.657207739	0.166457490	-1.330464472
H	2.934072399	1.232294043	-1.429876232
H	1.897844811	-0.084196183	-2.089124901
C	3.870265396	-0.760648308	-1.345349504
H	4.678610537	-0.375325745	-1.988922680
H	3.578381511	-1.759862313	-1.714467831
C	4.256563371	-0.832364132	0.143081612
H	4.866774864	-1.717423580	0.390030775
H	4.813430587	0.072152280	0.450195773
C	2.892275261	-0.871578635	0.818323023
H	2.468272699	-1.892413861	0.813661180
H	2.868970573	-0.465577503	1.842302892
C	0.774075915	-2.951819497	-1.196829628
C	0.749167113	-2.448460052	-2.518034692
H	0.048521571	-1.644037633	-2.779776007
C	1.622123069	-2.961981436	-3.487868514
H	1.592786383	-2.566722331	-4.510656344
C	2.542921669	-3.970605987	-3.142772379
H	3.234011190	-4.365463351	-3.897268742
C	2.578627644	-4.465582651	-1.827527068
H	3.297803724	-5.246845155	-1.553064258
C	1.695401756	-3.961599604	-0.855410805
H	1.730657720	-4.353004535	0.167940575
C	-0.094357765	-2.998541465	1.591218809
C	0.387191683	-2.253253292	2.686364059
H	0.597943175	-1.183795441	2.561269465
C	0.583312131	-2.871864438	3.931893222
H	0.957204827	-2.284927581	4.779683957
C	0.293775623	-4.238894773	4.088180171
H	0.445401353	-4.724448827	5.060007848
C	-0.201821482	-4.984477689	3.000367558
H	-0.437405612	-6.048462403	3.125602942
C	-0.401894934	-4.366978286	1.755866719
H	-0.803453335	-4.944696853	0.913801856
C	-2.012395879	-2.702043375	-0.479878325
C	-3.084791535	-2.276573310	0.334021993
H	-2.886111696	-1.660907631	1.220841023
C	-4.401699368	-2.636200653	0.013762483
H	-5.228922383	-2.298106941	0.649720159
C	-4.659566289	-3.424716023	-1.124201956
H	-5.690010576	-3.700233404	-1.379538755
C	-3.592690318	-3.862604297	-1.927533767
H	-3.786661209	-4.484615250	-2.809740540
C	-2.271469626	-3.506234173	-1.606408710
H	-1.445973381	-3.853329970	-2.237443743

[Ni(6-Mes)(PPh_3)CO][PF_6] (**5**, opt)

Ni	0.000000000	0.000000000	0.000000000
P	-0.468370941	-2.127135328	-0.001101625
O	2.917040389	-0.038051502	-0.005080617
N	-0.857707943	2.472769224	0.931193445
N	-0.548316355	2.446400076	-1.379654473
C	-0.535295946	1.825236920	-0.195809183
C	-1.233804622	3.896247297	0.971145383
H	-0.337868129	4.502987033	1.205989913
H	-1.958885909	4.040721487	1.789390020
C	-1.832268888	4.289958585	-0.382014012
H	-2.818225337	3.803950288	-0.500572449
H	-1.992641607	5.380225937	-0.417436507
C	-0.916300919	3.868114772	-1.534592801
H	-1.422286062	3.984778771	-2.507481512
H	0.004045925	4.482470031	-1.557581212

C	−0.931626019	1.608725058	2.088425410
C	0.222973570	1.372789151	2.870619701
C	0.123414262	0.434175396	3.919023472
H	1.014939886	0.223556238	4.524407021
C	−1.077700517	−0.239357944	4.207715107
C	−2.214653430	0.046744428	3.421989768
H	−3.163694261	−0.460202703	3.643519608
C	−2.168440952	0.965616247	2.360781569
C	1.511247582	2.118187661	2.622435146
H	1.549681576	3.035953704	3.239707378
H	1.614755042	2.428558313	1.570101739
H	2.384097066	1.501552608	2.894427407
C	−1.169322664	−1.236495642	5.336085000
H	−0.193337474	−1.386706387	5.825715088
H	−1.518157429	−2.216761639	4.965393823
H	−1.892025624	−0.898885510	6.102309534
C	−3.392597651	1.269868650	1.533497090
H	−3.670182034	2.337678569	1.597787687
H	−4.256043048	0.676541881	1.874274127
H	−3.224147950	1.045926775	0.465668691
C	−0.276989705	1.615110207	−2.528296321
C	−1.321344135	0.799917673	−3.033105871
C	−1.031738845	−0.044388864	−4.119274825
H	−1.829990449	−0.684768755	−4.517049518
C	0.249787267	−0.088236316	−4.707079876
C	1.258973452	0.738618863	−4.176171824
H	2.265573114	0.707264097	−4.614176257
C	1.019602421	1.603082914	−3.087961600
C	−2.699888562	0.823584221	−2.420800996
H	−2.716796870	0.273460629	−1.461572589
H	−3.432140890	0.338694117	−3.085076637
H	−3.041566591	1.851870665	−2.211677505
C	0.520499004	−1.005800185	−5.875636864
H	1.584768013	−0.992348467	−6.164742166
H	−0.075168467	−0.707072310	−6.758507714
H	0.240326053	−2.047542539	−5.635039419
C	2.113142240	2.483579205	−2.535978828
H	2.021489237	3.517619677	−2.918967276
H	3.107523693	2.107411409	−2.827053556
H	2.070089339	2.543042390	−1.434756742
C	1.756048735	0.000000000	0.000000000
C	−0.352490060	−2.992784869	1.586084343
C	−1.236651515	−4.031537248	1.947388605
H	−2.070949782	−4.299738664	1.288588609
C	−1.040721806	−4.726621552	3.152421907
H	−1.728400846	−5.533914550	3.431923417
C	0.037646895	−4.394221734	3.992370303
H	0.189269629	−4.940912055	4.930928618
C	0.913977348	−3.352603942	3.637136576
H	1.745431829	−3.081478937	4.298336575
C	0.715204327	−2.645616278	2.442516344
H	1.386689183	−1.822354238	2.172502570
C	−2.176620353	−2.304098243	−0.586343345
C	−3.230566436	−1.919428072	0.274982798
H	−3.008864262	−1.624390762	1.308012653
C	−4.551985565	−1.916793481	−0.193087386
H	−5.367082972	−1.623916370	0.479531129
C	−4.829784611	−2.283482634	−1.524067312
H	−5.863253029	−2.272902779	−1.890682252
C	−3.782285619	−2.662980423	−2.382253313
H	−3.996456099	−2.952013442	−3.418241249
C	−2.456752617	−2.674602053	−1.918833093
H	−1.641658735	−2.965461027	−2.590972251
C	0.545173522	−3.073558889	−1.172608363
C	1.123823595	−2.377795927	−2.255401286
H	0.969072846	−1.296184017	−2.356933632
C	1.891648547	−3.070878961	−3.204107051
H	2.345492740	−2.525772783	−4.039769352
C	2.086274485	−4.457803524	−3.072141522
H	2.692482023	−4.998306678	−3.809293377
C	1.510189267	−5.152227362	−1.991671928
H	1.665727221	−6.232799980	−1.886689065
C	0.739045072	−4.464005471	−1.040873305
H	0.297576298	−5.005119778	−0.195233590

[Ni(6-Mes)(PPh_3)($NCBH_3$)] (**7**, opt)

Ni	0.000000000	0.000000000	0.000000000
P	−0.408335835	−2.110386050	0.000000000
N	−2.379908083	1.414824258	1.036278245
N	−1.611076211	1.839578244	−1.112282071
N	1.846977519	0.000000000	−0.001942319

C	−1.547270617	1.099693605	0.019295918
C	−3.243928729	2.617949007	1.028397369
H	−4.271145829	2.349812855	0.718913489
H	−3.294894613	2.994776156	2.064376227
C	−2.433825552	3.045558001	−1.288138204
H	−1.892891347	3.732877748	−1.961082121
H	−3.393980649	2.785623775	−1.777227887
C	−2.421388057	0.567488113	2.199144102
C	−3.589561409	−0.196149184	2.444782997
C	−3.605996559	−1.046236778	3.566749156
H	−4.500619702	−1.657324693	3.750452545
C	−2.514448518	−1.136419492	4.451920559
C	−1.384780272	−0.340370066	4.190950897
H	−0.525854592	−0.389157361	4.872449500
C	−1.315978592	0.522177150	3.080503757
C	−4.803083560	−0.110313618	1.547663286
H	−5.437513546	0.756691288	1.812087413
H	−5.429044175	−1.012356513	1.652395518
H	−4.523750320	−0.003163030	0.485350596
C	−2.581996795	−2.020962081	5.674129480
H	−3.185969345	−1.545385494	6.471151705
H	−1.577162164	−2.216236491	6.083464889
H	−3.052215339	−2.992332647	5.441491494
C	−0.088565005	1.366041713	2.850466343
H	0.532383253	0.939022634	2.033445429
H	0.535962457	1.411397170	3.758008708
H	−0.347143916	2.393795699	2.540833790
C	−0.774160914	1.367950556	−2.189692095
C	0.534492837	1.884188081	−2.342199896
C	1.342381851	1.334896687	−3.357546527
H	2.374737843	1.694013076	−3.462240232
C	0.873445611	0.320836223	−4.215152337
C	−0.452196034	−0.137250213	−4.056279478
H	−0.832887534	−0.928768411	−4.715858631
C	−1.296594095	0.374971311	−3.056226039
C	1.054921711	2.974158621	−1.436893640
H	0.781625320	2.790246135	−0.383298119
H	0.637539132	3.960434068	−1.716596524
H	2.153111155	3.041544574	−1.499040978
C	1.763521716	−0.258628741	−5.290171379
H	2.830608230	−0.152963283	−5.029499071
H	1.606940562	0.258755598	−6.256614110
H	1.548072736	−1.328784012	−5.455784780
C	−2.712606422	−0.114712337	−2.890097003
H	−3.441455581	0.698176326	−3.064485820
H	−2.885600890	−0.494113880	−1.868336421
H	−2.932856013	−0.932239107	−3.594297497
C	3.015269158	0.003140919	−0.105235862
C	−0.347369092	−2.818884267	1.683042173
C	−1.241912871	−3.790826717	2.174133520
H	−2.062525331	−4.152311430	1.544385937
C	−1.075396665	−4.312404356	3.468612733
H	−1.777695543	−5.067533317	3.843056145
C	−0.010835242	−3.878082623	4.276403367
H	0.118863066	−4.291520773	5.284070174
C	0.882926296	−2.905568230	3.791261129
H	1.711395256	−2.555128682	4.419123241
C	0.710548716	−2.371997757	2.506350736
H	1.399720914	−1.605968938	2.129125152
C	0.900192578	−3.040860679	−0.878978862
C	1.297267197	−4.335239921	−0.484572652
H	0.831533430	−4.807798209	0.388922614
C	2.293210658	−5.016143602	−1.204685437
H	2.602562178	−6.020868771	−0.890224423
C	2.894568375	−4.410553191	−2.323892739
H	3.676034313	−4.941563429	−2.881649903
C	2.499078201	−3.119775358	−2.720215760
H	2.972581943	−2.639356023	−3.584797565
C	1.509703064	−2.434405778	−1.997305446
H	1.212206004	−1.421316276	−2.291255709
C	−1.930338127	−2.758307302	−0.756207755
C	−3.167482697	−2.507404216	−0.121936673
H	−3.175898688	−2.005153708	0.851820012
C	−4.369320961	−2.897334663	−0.730988668
H	−5.323942280	−2.704631462	−0.226320349
C	−4.352180086	−3.528125719	−1.989573648
H	−5.292732238	−3.825797919	−2.469140947
C	−3.123776361	−3.775067756	−2.627605506
H	−3.102111433	−4.266885414	−3.608143703
C	−1.917494210	−3.396881454	−2.014789026
H	−0.964576031	−3.591752898	−2.519356215
C	−2.669573935	3.670253994	0.083869048

H	−1.712481752	4.054219278	0.483659819
H	−3.367686292	4.520419428	0.004554384
B	4.564941385	0.005393346	−0.263330539
H	5.000711063	1.099942620	0.084034509
H	5.037457876	−0.880431167	0.443080077
H	4.827726807	−0.203374046	−1.442981537

[Ni(6-Mes)(PPh_3)(NPh_2)] (**8**, opt)

Ni	0.000000000	0.000000000	0.000000000
P	−0.560057203	−2.074385002	−0.001091938
N	−2.395885255	1.203783699	1.085832293
N	−2.088807994	1.429559206	−1.209739627
N	1.897517811	0.000000000	0.000000000
C	−1.613626310	0.969327574	−0.015140210
C	−3.648235777	1.983652235	1.054492704
H	−3.429419281	3.056624949	1.239093416
H	−4.285669587	1.639137764	1.886724496
C	−4.338110340	1.802733887	−0.289895283
H	−5.235086118	2.442627332	−0.352157269
H	−4.665784540	0.752732889	−0.405415032
C	−3.357138762	2.159953359	−1.396482713
H	−3.759438064	1.895496844	−2.389847185
H	−3.156565081	3.251987224	−1.408168983
C	−1.245509645	1.408159011	−2.381351407
C	−1.543745775	0.522772989	−3.445826161
C	−0.779786434	0.608126992	−4.628855510
H	−1.000373500	−0.092340489	−5.446492265
C	0.228788489	1.570047563	−4.801064251
C	0.486269357	2.450274692	−3.732335604
H	1.280155277	3.202257898	−3.835397928
C	−0.228672537	2.391166947	−2.525153275
C	−2.671054921	−0.474018206	−3.371759388
H	−3.140126649	−0.488907701	−2.379885490
H	−2.312906282	−1.499035929	−3.573687378
H	−3.448119989	−0.245122081	−4.125070977
C	1.012445676	1.674507359	−6.088407848
H	0.748271773	2.596174437	−6.641337815
H	0.816062386	0.816147803	−6.753540862
H	2.098926719	1.715762743	−5.890192676
C	0.133634018	3.331740763	−1.407603762
H	−0.744516724	3.641136567	−0.817785133
H	0.634273511	4.233500059	−1.798076641
H	0.831007808	2.826426158	−0.712400103
C	−1.861467642	0.983416771	2.408400937
C	−0.885988945	1.885233688	2.907477351
C	−0.395277602	1.698147637	4.209578476
H	0.373860593	2.386406819	4.585982405
C	−0.866208407	0.664618560	5.041885223
C	−1.894575607	−0.154213923	4.549614520
H	−2.298888412	−0.951068895	5.187728218
C	−2.411933695	−0.014442238	3.246494535
C	−0.378769333	3.027029263	2.066782669
H	0.216363211	2.646380672	1.218666426
H	0.253317886	3.706361712	2.662344526
H	−1.204434024	3.617038873	1.630128865
C	−0.258552437	0.427421049	6.403091829
H	0.004724872	1.375360330	6.905255611
H	0.676540617	−0.159411133	6.308381751
H	−0.939123399	−0.139367888	7.061534690
C	−3.500840475	−0.957323534	2.800726986
H	−3.060833879	−1.871003122	2.362172094
H	−4.168988970	−0.516732439	2.043768647
H	−4.117013388	−1.270292937	3.660773146
C	2.673962721	−0.185816027	−1.134070029
C	2.047942604	−0.153021276	−2.410058052
H	0.965218760	0.012510364	−2.441575022
C	2.776929912	−0.355282352	−3.584740987
H	2.246965596	−0.354237493	−4.544581817
C	4.167022456	−0.577203068	−3.543269363
H	4.737204854	−0.742233347	−4.465786756
C	4.811752676	−0.564769552	−2.291058508
H	5.899351460	−0.707640481	−2.233194733
C	4.088073674	−0.366949671	−1.107416417
H	4.616445456	−0.350060775	−0.147741813
C	2.420982301	−0.353894367	1.259461030
C	3.058592312	−1.601593587	1.494321902
H	3.218755634	−2.279892665	0.650912009
C	3.425036161	−1.986864356	2.789855633
H	3.883149255	−2.972120185	2.947633014
C	3.193072761	−1.134363396	3.887550521
H	3.479346550	−1.440788114	4.901111083

C	2.591910884	0.116698287	3.662425984
H	2.410293712	0.798835390	4.501944698
C	2.216348150	0.503965574	2.366626716
H	1.744396549	1.473770745	2.186828737
C	−2.111444057	−2.648992793	−0.790444522
C	−2.190528329	−3.736159974	−1.685722123
H	−1.282381094	−4.285459499	−1.958725932
C	−3.430188253	−4.121459848	−2.226429200
H	−3.476626943	−4.965016339	−2.926789675
C	−4.607111194	−3.443244692	−1.863008216
H	−5.573422200	−3.752617056	−2.280022491
C	−4.536220499	−2.364591844	−0.961752558
H	−5.448058855	−1.824853599	−0.675276274
C	−3.296134806	−1.962617540	−0.446592507
H	−3.227839428	−1.098213630	0.219032599
C	−0.725385039	−2.818364923	1.669544071
C	−1.431513791	−4.025631844	1.875493155
H	−1.943978415	−4.507630847	1.034162751
C	−1.479361827	−4.606983543	3.151323157
H	−2.034188990	−5.541234969	3.305040764
C	−0.809109771	−3.996400443	4.229928502
H	−0.840613992	−4.455346780	5.226229696
C	−0.106037285	−2.798364729	4.026845967
H	0.415666383	−2.310311259	4.857973100
C	−0.074579743	−2.202500428	2.755492455
H	0.447418569	−1.251391377	2.609983589
C	0.703882514	−3.151858397	−0.766640579
C	0.990143594	−2.971370620	−2.138486982
H	0.397434568	−2.261346892	−2.726198142
C	2.035759237	−3.678178182	−2.748861192
H	2.258976668	−3.507394620	−3.808518775
C	2.816740387	−4.571852428	−1.994485877
H	3.646455183	−5.111839716	−2.467204738
C	2.532590565	−4.765788024	−0.631247654
H	3.136119064	−5.463050520	−0.036463095
C	1.481424470	−4.061935959	−0.019563154
H	1.275234093	−4.206953863	1.046408846

[Ni(6-Mes)(PPh_3)(NPh_2)] (**8**, opt)

Ni	0.000000000000	0.000000000000	0.000000000000
P	−0.674928977628	2.023186627239	0.088751651560
N	−1.746505601561	−1.926799524307	−1.141250307002
N	−1.888129372051	−1.765570763098	1.166357249066
N	1.840171912543	0.000000000000	0.000000000001
C	−1.344508059657	−1.309855752655	0.004422062792
C	−2.740024704804	−3.009427514194	−1.218949795560
H	−2.224999275440	−3.992712582309	−1.254451526454
H	−3.295957107790	−2.903013380442	−2.167192006141
C	−3.679473345303	−2.939154184019	−0.019037003124
H	−4.344972946620	−3.819582272718	−0.003076212666
H	−4.313491482869	−2.035873893686	−0.096446657505
C	−2.854602901711	−2.869883992906	1.262608678121
H	−3.495126919029	−2.694972470025	2.143964767407
H	−2.319607840434	−3.827767439266	1.433939720866
C	−1.494667989948	−1.103061320981	2.378264446784
C	−2.381018946811	−0.159870309661	2.951244248049
C	−1.984724874478	0.495922501752	4.131434605712
H	−2.651744890109	1.254318454932	4.563505958255
C	−0.749544011162	0.222265654971	4.752810032443
C	0.093444482777	−0.744236193709	4.168623999581
H	1.057671514871	−0.973228537587	4.642846970649
C	−0.259140263551	−1.425179017770	2.986722385656
C	−3.711793921354	0.128397957180	2.307086253911
H	−3.615547024491	0.174551252998	1.210054483185
H	−4.120803572585	1.090471487224	2.653303189590
H	−4.454171413013	−0.659031007897	2.542840934682
C	−0.345529193443	0.952683113060	6.013513358535
H	−0.937796079709	0.610715288217	6.883933100555
H	−0.514220081759	2.040766149683	5.916628985963
H	0.719845525921	0.790439944941	6.250645409393
C	0.656527416068	−2.457555184438	2.377359444637
H	0.114949680414	−3.392236173554	2.146264412835
H	1.492390314674	−2.695101938453	3.056194540579
H	1.071135347388	−2.080678126081	1.422314091461
C	−1.125252108990	−1.518638896337	−2.369743317533
C	0.158709789635	−2.018120930685	−2.704705845409
C	0.722285652019	−1.623575657385	−3.931696508713
H	1.722306699898	−1.995126003864	−4.195566779801
C	0.040956386127	−0.775943447786	−4.831063459920
C	−1.238968988807	−0.317451768320	−4.472864432347

H	−1.776904384940	0.359976785797	−5.149739680386
C	−1.839029332181	−0.672926543221	−3.249197241267
C	0.915764351533	−2.914568270985	−1.758307900472
H	1.316512238562	−2.310582292495	−0.919441307827
H	1.755594088647	−3.412491020494	−2.271244697453
H	0.263825447204	−3.687057986361	−1.314378498005
C	0.683225028558	−0.369467822532	−6.138099250407
H	0.901718755040	−1.250487136036	−6.770536935136
H	1.646337269933	0.147725578744	−5.967689201958
H	0.030929349460	0.307688379110	−6.715625294133
C	−3.199570905682	−0.143771155414	−2.872394510805
H	−3.396685650047	0.822001145400	−3.368113256160
H	−3.273858009783	−0.004840544561	−1.780800819010
H	−4.009580549735	−0.838175445970	−3.170867429030
C	−2.283841061300	2.705897855521	0.658739495802
C	−2.482623309112	3.340250106236	1.904113370788
H	−1.633713858150	3.503525487431	2.576465575977
C	−3.761379238219	3.781410378589	2.286249955147
H	−3.893524644565	4.276216895910	3.257081906067
C	−4.863713448218	3.603147194224	1.431232603683
H	−5.859856306845	3.951382871941	1.730856873116
C	−4.673707270801	2.979804268811	0.182422915136
H	−5.522341857452	2.843644937379	−0.500190854646
C	−3.399773372332	2.534240378839	−0.195042740153
H	−3.256443799732	2.058225153226	−1.172060798580
C	−0.531572353364	2.869831444791	−1.532886645367
C	−0.926959133574	4.212703481807	−1.724273930606
H	−1.358705523003	4.775762344566	−0.887440599982
C	−0.769067112089	4.824219002612	−2.977418515928
H	−1.076284915994	5.868231991845	−3.119295959106
C	−0.215872016267	4.099222934053	−4.051446795311
H	−0.092611823928	4.578498156011	−5.030930756900
C	0.170630470046	2.760722412017	−3.867956805541
H	0.588784957476	2.186938318153	−4.703136905439
C	0.009706178855	2.147914185246	−2.613799869628
H	0.284673011183	1.097536227511	−2.458699508150
C	0.532638260835	2.908833706394	1.141167625985
C	0.615957837428	2.523611741863	2.499616940107
H	−0.069588970487	1.762564916874	2.889556610493
C	1.594367939750	3.073186182276	3.339953602014
H	1.642297255488	2.761696594491	4.390904712417
C	2.528314107128	3.995007440830	2.830172145518
H	3.303461560194	4.415532202748	3.482885953962
C	2.468965872329	4.361974619396	1.474209011400
H	3.200192835141	5.070660504474	1.064559797005
C	1.475725188474	3.827341140561	0.634366997362
H	1.440308387099	4.119546720816	−0.421392183848
C	2.640700536586	0.201796813032	−1.188293625269
H	3.582380704453	−0.397157163557	−1.158955750782
H	2.084428667617	−0.093258171443	−2.094945528233
H	2.948277675674	1.269258929792	−1.310971624288
C	2.610879879804	0.262246008142	1.197466469055
H	3.501855708971	−0.407309871379	1.266509695678
H	2.992794240148	1.310189606599	1.229957273395
H	1.996464323089	0.111237806089	2.100786997991