

[Ni(L)]; S = 0.

46				H	-0.367184	-8.084875	7.364680
Coordinates from ORCA-job Ni				H	-1.135924	-6.928333	8.484637
N	0.119978	-4.584812	5.265377	C	1.631545	-6.533751	8.651200
N	-0.006701	-3.894228	4.104801	C	2.090447	-5.548238	9.536368
C	1.088811	-5.496495	5.175343	C	2.995817	-5.869033	10.553631
Ni	1.000046	-4.152825	2.575778	C	3.459197	-7.182168	10.689842
C	-0.914703	-2.942898	4.010430	C	3.009067	-8.172106	9.808216
N	1.375997	-6.251130	6.250287	C	2.097103	-7.850529	8.798251
S	2.026018	-5.747242	3.692579	H	1.735102	-4.521237	9.425742
H	2.111975	-6.947188	6.155374	H	3.342636	-5.091848	11.236935
C	0.664233	-6.165989	7.541382	H	4.168341	-7.434477	11.480413
H	-1.569239	-2.698690	4.847161	H	3.366291	-9.198324	9.909845
C	-0.947282	-2.274491	2.742877	H	1.747579	-8.635008	8.123136
C	-1.814129	-1.233818	2.425727	C	1.079272	-2.723232	-0.356844
C	-1.723634	-0.665880	1.150526	C	1.184755	-2.142875	-1.649912
C	-0.787950	-1.147768	0.249361	C	2.091859	-2.582752	-2.598852
C	0.088090	-2.211488	0.592234	C	2.953633	-3.651695	-2.284553
N	-0.016433	-2.751557	1.837122	C	2.889338	-4.244167	-1.037159
H	-2.534769	-0.882830	3.163394	C	1.968066	-3.807073	-0.042901
H	-2.383992	0.153363	0.864246	H	0.531867	-1.315263	-1.922138
H	-0.729081	-0.697083	-0.736603	H	2.133909	-2.102925	-3.576902
C	-0.607029	-7.024363	7.525599	H	3.673535	-4.014252	-3.021125
H	0.377808	-5.111948	7.660652	H	3.547426	-5.071985	-0.768377
H	-1.273396	-6.688444	6.719239	O	2.026124	-4.462536	1.102512

[Pd(L)]; S = 1.

46				H	-0.332482	-7.817306	7.557494
Coordinates from ORCA-job Pd				H	-0.930535	-6.543948	8.655259
N	0.405157	-4.558995	5.331779	C	1.863240	-6.501360	8.753922
N	0.222562	-3.911828	4.165579	C	2.400106	-5.576658	9.659721
C	1.312273	-5.538606	5.238726	C	3.268930	-5.994854	10.673710
Pd	1.182874	-4.310294	2.455874	C	3.617730	-7.345155	10.784072
C	-0.668952	-2.947904	4.053059	C	3.089249	-8.275037	9.880976
N	1.592695	-6.237649	6.352581	C	2.212806	-7.856088	8.875665
S	2.191427	-6.006640	3.758221	H	2.134714	-4.520836	9.568758
H	2.269672	-6.993611	6.273559	H	3.677934	-5.264302	11.373779
C	0.927018	-6.035251	7.655449	H	4.298950	-7.673106	11.571421
H	-1.278818	-2.656345	4.909645	H	3.357477	-9.329887	9.962034
C	-0.809057	-2.321270	2.759779	H	1.799278	-8.594175	8.184277
C	-1.770534	-1.351064	2.481267	C	1.061373	-2.654821	-0.465446
C	-1.855859	-0.864718	1.171667	C	1.196935	-1.843736	-1.626321
C	-0.973298	-1.315173	0.201545	C	2.077507	-2.128329	-2.655729
C	0.047982	-2.250963	0.522461	C	2.888999	-3.274409	-2.561191
N	0.065363	-2.745154	1.781701	C	2.817321	-4.077252	-1.438264
H	-2.446814	-1.010588	3.264092	C	1.935362	-3.801796	-0.350510
H	-2.627029	-0.140262	0.907225	H	0.603360	-0.934127	-1.703789
H	-1.076432	-0.955479	-0.818058	H	2.147532	-1.462790	-3.516683
C	-0.440101	-6.731612	7.689150	H	3.587331	-3.524922	-3.362646
H	0.774727	-4.952013	7.757964	H	3.451201	-4.959354	-1.336608
H	-1.078904	-6.338572	6.886589	O	2.014672	-4.664120	0.646955

[Pt(L)(L)]; S = 0.

46				N	0.207910	-3.889035	4.157587
Coordinates from ORCA-job Pt				C	1.300815	-5.526868	5.220060
N	0.379604	-4.566260	5.321621	Pt	1.179444	-4.247825	2.503906

C	-0.690277	-2.920119	4.076005	C	2.348044	-5.561590	9.613512
N	1.582915	-6.252312	6.315341	C	3.226939	-5.935175	10.635607
S	2.202179	-5.928462	3.727763	C	3.619966	-7.271104	10.767125
H	2.269979	-6.997382	6.223607	C	3.126074	-8.231038	9.876458
C	0.896816	-6.095974	7.613692	C	2.239620	-7.856696	8.862517
H	-1.297202	-2.651070	4.939037	H	2.047271	-4.516948	9.506507
C	-0.810145	-2.275061	2.796295	H	3.608427	-5.181231	11.326202
C	-1.741543	-1.280225	2.513840	H	4.308356	-7.564493	11.561710
C	-1.793119	-0.770427	1.212983	H	3.428610	-9.274966	9.974422
C	-0.908141	-1.233088	0.250782	H	1.853256	-8.618240	8.181208
C	0.074350	-2.208498	0.561275	C	1.068332	-2.649164	-0.430696
N	0.065896	-2.723293	1.819521	C	1.167872	-1.904979	-1.640198
H	-2.419400	-0.934837	3.293131	C	2.025278	-2.239836	-2.673100
H	-2.535091	-0.016428	0.948793	C	2.855436	-3.367686	-2.536956
H	-0.982955	-0.844115	-0.759830	C	2.818009	-4.105758	-1.369560
C	-0.433012	-6.861270	7.626680	C	1.961689	-3.771257	-0.283502
H	0.688069	-5.022832	7.719789	H	0.557684	-1.012719	-1.763779
H	-1.083381	-6.491912	6.822074	H	2.061005	-1.625790	-3.573330
H	-0.270661	-7.938618	7.483147	H	3.534991	-3.655841	-3.341329
H	-0.941246	-6.710362	8.589817	H	3.464665	-4.973031	-1.229188
C	1.844952	-6.516898	8.720142	O	2.096660	-4.571642	0.770058

[Ni(^tBuL)]; S = 0.

70

XYZ file generated by orca_plot on BaseName=Ni

N	0.110732	-4.556654	5.274720	H	3.428111	-9.087621	9.947732
N	-0.081767	-3.943107	4.080542	H	1.742324	-8.496066	8.233674
C	1.055128	-5.494055	5.183094	C	0.921131	-2.937214	-0.431099
Ni	0.833247	-4.313083	2.517064	C	1.109728	-2.250522	-1.653373
C	-1.007353	-3.009697	3.967324	C	2.072243	-2.616270	-2.582956
N	1.396050	-6.182702	6.286614	C	2.889785	-3.718864	-2.263735
S	1.889884	-5.868955	3.663780	C	2.787408	-4.433690	-1.073829
H	2.106986	-6.904298	6.191975	C	1.780055	-4.045286	-0.125057
C	0.771495	-5.992684	7.611378	H	0.496494	-1.375161	-1.861760
H	-1.628633	-2.719205	4.814381	C	2.225928	-1.819197	-3.887389
C	-1.115547	-2.439011	2.655827	H	3.654638	-4.016815	-2.976254
C	-2.061236	-1.491199	2.277141	C	3.737367	-5.605204	-0.765250
C	-2.068376	-1.062676	0.944850	O	1.700260	-4.761089	0.982645
C	-1.127682	-1.560448	0.056701	C	4.740490	-5.845242	-1.909053
C	-0.136647	-2.486714	0.476654	C	2.930536	-6.910434	-0.575823
N	-0.179042	-2.926765	1.762967	C	4.556212	-5.296422	0.511010
H	-2.780470	-1.118740	3.005502	C	3.359503	-2.365519	-4.772003
H	-2.817046	-0.347844	0.601295	C	2.538316	-0.343195	-3.555354
H	-1.157592	-1.241824	-0.981162	C	0.906068	-1.892978	-4.688503
C	-0.548793	-6.767074	7.715352	H	2.353357	-7.142178	-1.484762
H	0.557919	-4.918099	7.696614	H	2.236937	-6.827893	0.268800
H	-1.242785	-6.425885	6.935180	H	3.619625	-7.748759	-0.387485
H	-0.385036	-7.846937	7.594341	H	5.166944	-4.392246	0.364989
H	-1.008828	-6.591690	8.698638	H	5.235154	-6.135640	0.729436
C	1.781482	-6.372884	8.678029	H	3.901414	-5.141787	1.376405
C	2.349225	-5.383526	9.492470	H	4.235323	-6.102368	-2.852559
C	3.292370	-5.719437	10.469729	H	5.392067	-6.689100	-1.639468
C	3.685056	-7.052121	10.634832	H	5.384406	-4.970251	-2.086497
C	3.126300	-8.046198	9.823213	H	4.333924	-2.316377	-4.262297
C	2.176850	-7.708927	8.854073	H	3.431047	-1.762689	-5.688840
H	2.048476	-4.341949	9.358588	H	3.177671	-3.408307	-5.070831
H	3.724113	-4.939144	11.098726	H	0.662721	-2.935598	-4.940593
H	4.423729	-7.316408	11.393851	H	0.991919	-1.320932	-5.624971
				H	0.065116	-1.477860	-4.114246
				H	3.473100	-0.263561	-2.980253

H 1.734921 0.115359 -2.960617

H 2.648994 0.240840 -4.481741

[Pd(^tBuL)]; S = 0.

70

XYZ file generated by orca_plot on BaseName=Pd

N 0.246949 -4.564173 5.398545
N 0.057220 -4.015923 4.183531
C 1.145568 -5.556394 5.379231
Pd 1.008757 -4.560111 2.506404
C -0.838818 -3.069015 3.990488
N 1.426807 -6.166667 6.543946
S 2.012230 -6.154648 3.937616
H 2.102003 -6.927814 6.521797
C 0.789441 -5.842629 7.836244
H -1.449349 -2.706420 4.819122
C -0.989765 -2.564720 2.643835
C -1.983457 -1.662459 2.266862
C -2.082773 -1.319629 0.912914
C -1.178088 -1.830905 -0.005867
C -0.117216 -2.680041 0.412451
N -0.094311 -3.046625 1.714456
H -2.675418 -1.267853 3.009561
H -2.883807 -0.661277 0.574422
H -1.291645 -1.588224 -1.059018
C -0.610151 -6.464182 7.934202
H 0.693173 -4.748268 7.868925
H -1.241327 -6.093973 7.115207
H -0.558485 -7.560448 7.876100
H -1.074146 -6.186471 8.891532
C 1.716691 -6.284688 8.952126
C 2.306214 -5.334854 9.796939
C 3.165564 -5.733637 10.826771
C 3.451949 -7.090082 11.013955
C 2.871209 -8.045212 10.171445
C 2.004621 -7.644990 9.150284
H 2.089590 -4.274830 9.645416
H 3.615977 -4.983633 11.479095
H 4.125247 -7.403381 11.813974
H 3.090791 -9.105046 10.312606

H 1.549871 -8.401595 8.506478
C 0.942358 -3.105828 -0.517484
C 1.104489 -2.323881 -1.686551
C 2.054409 -2.593118 -2.660432
C 2.899532 -3.697444 -2.440032
C 2.833225 -4.501999 -1.306420
C 1.829031 -4.228501 -0.309439
H 0.481258 -1.438646 -1.803935
C 2.175836 -1.685337 -3.894333
H 3.659962 -3.921405 -3.183008
C 3.824768 -5.664019 -1.107734
O 1.782351 -5.064783 0.711879
C 4.833217 -5.761630 -2.267564
C 3.067866 -7.010663 -1.038425
C 4.637324 -5.446378 0.191090
C 3.271809 -2.164932 -4.861529
C 2.521107 -0.248904 -3.442537
C 0.831010 -1.670401 -4.655269
H 2.499624 -7.182527 -1.966084
H 2.371587 -7.025990 -0.191756
H 3.787488 -7.836429 -0.921311
H 5.205982 -4.505182 0.135112
H 5.355217 -6.271009 0.324610
H 3.980032 -5.407591 1.067575
H 4.338617 -5.955318 -3.231796
H 5.518985 -6.598988 -2.072221
H 5.440973 -4.848970 -2.365710
H 4.265333 -2.158125 -4.388290
H 3.311758 -1.493626 -5.731733
H 3.072346 -3.181610 -5.231590
H 0.561306 -2.683096 -4.989034
H 0.899136 -1.020303 -5.541206
H 0.014682 -1.294079 -4.021609
H 3.475673 -0.232187 -2.895623
H 1.744431 0.162068 -2.780749
H 2.609610 0.415575 -4.316080

[Pt(^tBuL)]; S = 0.

70

XYZ file generated by orca_plot on BaseName=Pt

N 0.247093 -4.563409 5.394965
N 0.077845 -3.970268 4.184922
C 1.179353 -5.517975 5.366744
Pt 1.076860 -4.421845 2.571462
C -0.840115 -3.029153 4.023615
N 1.454020 -6.168552 6.510172
S 2.104981 -6.006902 3.914696
H 2.151853 -6.908294 6.476510
C 0.754272 -5.930369 7.788810
H -1.464549 -2.713882 4.858000
C -0.959554 -2.485110 2.696777
C -1.925165 -1.557344 2.317858
C -1.981271 -1.171370 0.974791
C -1.060439 -1.674145 0.067636

C -0.030635 -2.561474 0.476633
N -0.048111 -2.971844 1.772600
H -2.629950 -1.175329 3.055052
H -2.757254 -0.484994 0.634411
H -1.143532 -1.389290 -0.976702
C -0.609516 -6.633242 7.810989
H 0.592641 -4.845292 7.852811
H -1.230080 -6.268180 6.981509
H -0.493860 -7.721774 7.715270
H -1.123829 -6.418402 8.758759
C 1.665058 -6.353403 8.925053
C 2.189092 -5.393258 9.800899
C 3.032068 -5.771873 10.851168
C 3.367928 -7.118051 11.028568
C 2.853374 -8.082995 10.155163
C 2.002776 -7.703233 9.112990

H	1.932837	-4.341024	9.657970	C	2.445819	-0.294329	-3.586196
H	3.430412	-5.014076	11.527835	C	0.743893	-1.809196	-4.661714
H	4.027905	-7.415742	11.845333	H	2.454955	-7.154023	-1.710389
H	3.111614	-9.134915	10.288810	H	2.456599	-6.884418	0.054125
H	1.599276	-8.467769	8.445092	H	3.803242	-7.765255	-0.717969
C	1.021416	-3.005407	-0.454697	H	5.351134	-4.400381	0.002596
C	1.141275	-2.282283	-1.668369	H	5.506489	-6.154158	0.275128
C	2.049589	-2.600714	-2.664525	H	4.207861	-5.237476	1.086388
C	2.896967	-3.700624	-2.432386	H	4.200768	-6.046518	-3.187426
C	2.878885	-4.444114	-1.257286	H	5.451180	-6.655818	-2.083826
C	1.938951	-4.093918	-0.227143	H	5.398737	-4.926220	-2.479479
H	0.509871	-1.408486	-1.814547	H	4.192821	-2.230954	-4.481193
C	2.113693	-1.758500	-3.948048	H	3.192246	-1.640372	-5.825207
H	3.615008	-3.971362	-3.201053	H	2.988548	-3.305268	-5.241575
C	3.863727	-5.612043	-1.052498	H	0.481581	-2.843904	-4.926723
O	2.001938	-4.839922	0.870712	H	0.770302	-1.210695	-5.585070
C	4.775166	-5.810701	-2.278488	H	-0.057032	-1.409897	-4.022465
C	3.090340	-6.934264	-0.838202	H	3.418347	-0.230388	-3.075434
C	4.783992	-5.330939	0.159270	H	1.685004	0.139062	-2.920440
C	3.186137	-2.270692	-4.924162	H	2.490598	0.322876	-4.496501

[Pt(^tBuL)]⁺; S = 1/2.

70

XYZ file generated by orca_plot on BaseName=Pt

N	0.171571	-4.592994	5.383234	H	1.658368	-8.488032	8.452251
N	0.022875	-3.987089	4.185005	C	1.035602	-2.944700	-0.444578
C	1.130870	-5.517879	5.366568	C	1.168271	-2.244536	-1.648074
Pt	1.073816	-4.392005	2.583190	C	2.086344	-2.593670	-2.650141
C	-0.902348	-3.060590	4.002161	C	2.916253	-3.706002	-2.424924
N	1.409829	-6.190966	6.483828	C	2.889977	-4.439876	-1.247166
S	2.112078	-5.934252	3.908576	C	1.954993	-4.041116	-0.213574
H	2.142373	-6.898090	6.445587	H	0.544592	-1.371385	-1.820368
C	0.709497	-5.990465	7.774759	C	2.148790	-1.766489	-3.931949
H	-1.557757	-2.768899	4.821763	H	3.619550	-3.992688	-3.200240
C	-0.993156	-2.490505	2.684755	C	3.841284	-5.624912	-1.031440
C	-1.949601	-1.552199	2.311933	O	2.033830	-4.733520	0.894975
C	-1.971920	-1.120514	0.983500	C	4.716610	-5.874919	-2.274070
C	-1.031713	-1.598447	0.083099	C	3.031307	-6.918976	-0.768940
C	-0.023971	-2.507091	0.487641	C	4.795772	-5.335646	0.154298
N	-0.060484	-2.957656	1.767962	C	3.220334	-2.278987	-4.907106
H	-2.669613	-1.191260	3.044618	C	2.472150	-0.298194	-3.567032
H	-2.733817	-0.416669	0.648832	C	0.769800	-1.829132	-4.633719
H	-1.087098	-1.275220	-0.951542	H	2.355088	-7.129900	-1.610943
C	-0.611712	-6.768403	7.799090	H	2.437914	-6.851525	0.149035
H	0.492361	-4.915399	7.836977	H	3.727634	-7.765197	-0.671606
H	-1.262155	-6.434832	6.979168	H	5.370059	-4.414924	-0.027067
H	-0.437568	-7.848139	7.696881	H	5.509026	-6.167397	0.253720
H	-1.125602	-6.586292	8.753261	H	4.253686	-5.228941	1.099895
C	1.658031	-6.363727	8.896909	H	4.113988	-6.110716	-3.163923
C	2.165141	-5.368930	9.743489	H	5.367809	-6.737296	-2.076143
C	3.044226	-5.699058	10.780067	H	5.365586	-5.016917	-2.504275
C	3.432911	-7.029010	10.970866	H	4.227518	-2.236328	-4.466371
C	2.935429	-8.027337	10.125600	H	3.223166	-1.646980	-5.805803
C	2.048583	-7.697252	9.097024	H	3.021832	-3.311799	-5.228285
H	1.866707	-4.329468	9.590274	H	0.509311	-2.865060	-4.892711
H	3.428619	-4.916373	11.435848	H	0.801068	-1.236416	-5.559221
H	4.120830	-7.288519	11.777353	H	-0.030864	-1.421983	-3.999863
H	3.234357	-9.066528	10.271377	H	3.444267	-0.225826	-3.058186
				H	1.707548	0.139423	-2.909354
				H	2.513389	0.306539	-4.484373

[Pt(^tBuL)]⁻; S = 1/2.

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XYZ file generated by orca_plot on BaseName=Pt

N	0.418424	-4.457995	5.439911	H	1.754095	-8.434748	8.475117
N	0.197461	-3.896570	4.212075	C	1.002398	-3.041110	-0.479933
C	1.338784	-5.398131	5.422194	C	1.135802	-2.292972	-1.673109
Pt	1.123951	-4.408841	2.570310	C	2.041283	-2.596584	-2.681270
C	-0.772730	-2.967596	4.032467	C	2.873409	-3.711688	-2.476943
N	1.717097	-6.001181	6.603490	C	2.842398	-4.479742	-1.315795
S	2.206651	-5.936221	3.941769	C	1.907433	-4.144294	-0.272714
H	2.217749	-6.880336	6.485538	H	0.510080	-1.410039	-1.791417
C	0.858828	-5.918844	7.798814	C	2.117215	-1.718315	-3.939962
H	-1.384250	-2.649372	4.875506	H	3.590585	-3.974064	-3.250037
C	-0.940577	-2.483133	2.720137	C	3.815786	-5.660274	-1.131469
C	-1.936941	-1.567311	2.302223	O	1.957463	-4.907284	0.808470
C	-2.026009	-1.229908	0.965037	C	4.730194	-5.849146	-2.356550
C	-1.103706	-1.752107	0.033670	C	3.029218	-6.977622	-0.938804
C	-0.063064	-2.605061	0.457777	C	4.732161	-5.410111	0.089885
N	-0.035821	-2.993145	1.761885	C	3.176195	-2.221290	-4.935714
H	-2.631789	-1.166446	3.040964	C	2.479371	-0.271189	-3.539158
H	-2.813840	-0.557022	0.620675	C	0.746084	-1.717746	-4.652630
H	-1.204900	-1.494963	-1.016256	H	2.396986	-7.180029	-1.817930
C	-0.440115	-6.724262	7.642278	H	2.390478	-6.923672	-0.050055
H	0.597856	-4.856661	7.907113	H	3.731346	-7.819070	-0.821989
H	-0.995455	-6.358529	6.767757	H	5.317667	-4.488473	-0.053477
H	-0.228164	-7.794422	7.501447	H	5.438586	-6.248057	0.206076
H	-1.071733	-6.610010	8.535557	H	4.144095	-5.313093	1.009541
C	1.674187	-6.335440	9.008609	H	4.156405	-6.061651	-3.271904
C	2.072147	-5.380842	9.955071	H	5.396693	-6.705245	-2.174245
C	2.836321	-5.749846	11.067457	H	5.363444	-4.967667	-2.540839
C	3.218886	-7.084058	11.242644	H	4.184765	-2.213220	-4.495422
C	2.829873	-8.044695	10.301781	H	3.190765	-1.566631	-5.819845
C	2.058570	-7.672647	9.196268	H	2.958803	-3.243694	-5.279055
H	1.780322	-4.337365	9.815343	H	0.463971	-2.738099	-4.951423
H	3.135955	-4.993963	11.795817	H	0.780260	-1.088471	-5.556029
H	3.816783	-7.375140	12.108237	H	-0.045293	-1.327168	-3.996505
H	3.124903	-9.087636	10.431421	H	3.455060	-0.242010	-3.031035
				H	1.730283	0.154767	-2.855562
				H	2.532305	0.373323	-4.430877