Oxidative Addition of 2-Substituted Azoliums to Group-10 Metal Zero Complexes – A DFT Study

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Supporting Information

1. Metal Zero DMPE Reactants

NiDMPE
B3lyp/lanl2dz:6-31G(d) 5D optimized geometry
Energy = -1090.289859 a.u.
Enthalpy Correction = 0.22586 a.u.
B3lyp/l2aug:6-311+G(2d,p) 5D
Single point energy = -2429.44628244 a.u.

Atom	x-coord	y-coord	z-coord
Ni	0.000002	-1.345386	0.000000
P	-1.659149	-0.024133	-0.013069
P	1.659148	-0.024132	0.013069
C	0.690829	1.567043	0.343782
H	1.273227	2.449420	0.042347
H	0.562992	1.627829	1.432508
C	-0.690832	1.567041	-0.343788
H	-0.562995	1.627822	-1.432513
H	-1.273231	2.449419	-0.042358
C	3.070236	0.200832	1.212673
H	2.702660	0.077463	2.236480
H	3.824386	-0.572216	1.031203
H	3.545472	1.186071	1.120915
C	2.535072	0.400463	-1.578517
H	1.808787	0.458766	-2.395254
H	3.074975	1.353602	-1.511298
H	3.248387	-0.393547	-1.823200
C	-3.070242	0.200829	-1.212667
H	-3.824389	-0.572222	-1.031198
H	-3.545480	1.186066	-1.120907
H	-2.702668	0.077464	-2.236477
C	-2.535068	0.400463	1.578520
H	-1.808781	0.458763	2.395254
H	-3.074970	1.353604	1.511302
H	-3.248385	-0.393545	1.823204

PdDMPE
B3lyp/lanl2dz:6-31G(d) optimized geometry
Energy = -1047.770289 a.u.
Enthalpy Correction = 0.225845 a.u.
B3lyp/l2aug:6-311+G(2d,p) 5D
Single point energy = -1047.924437 a.u.

Atom	x-coord	y-coord	z-coord
Pd	0.000003	-1.305717	0.000000
P	1.737509	0.223577	0.016351
P	-1.737511	0.223574	-0.016351
C	-0.683201	1.754038	-0.359225
H	-1.244999	2.661364	-0.094541
H	-0.530518	1.783350	-1.446113
C	0.683196	1.754038	0.359226
H	0.530513	1.783349	1.446115
H	1.244994	2.661365	0.094543
C	-3.145847	0.552817	-1.194113

H	-2.799641	0.415794	-2.223578
H	-3.944622	-0.173033	-1.009641
H	-3.555920	1.565599	-1.086790
C	-2.548103	0.703856	1.590861
H	-1.803119	0.705026	2.392540
H	-3.019272	1.693888	1.537434
H	-3.310972	-0.038428	1.847479
C	3.145844	0.552819	1.194114
H	3.944621	-0.173029	1.009641
H	3.555916	1.565602	1.086793
H	2.799636	0.415794	2.223579
C	2.548101	0.703862	-1.590861
H	1.803116	0.705034	-2.392539
H	3.019270	1.693894	-1.537432
H	3.310968	-0.038422	-1.847481

PtDMPE

B3lyp/lanl2dz:6-31G(d) optimized geometry
Energy = -1040.183859 a.u.
Enthalpy Correction = 0.226077 a.u.
B3lyp/l2aug:6-311+G(2d,p) 5D
Single point energy = -1040.342997 a.u.

Atom	x-coord	y-coord	z-coord
Pt	0.000050	-0.984306	-0.000002
P	1.733931	0.450638	0.006990
P	-1.734006	0.450557	-0.006991
C	-0.697167	2.003404	-0.337677
H	-1.257198	2.899624	-0.035370
H	-0.579165	2.056297	-1.427550
C	0.697025	2.003445	0.337651
H	0.579022	2.056354	1.427523
H	1.257011	2.899686	0.035324
C	-3.108520	0.705816	-1.235208
H	-2.721874	0.552228	-2.247240
H	-3.891418	-0.037848	-1.055462
H	-3.547346	1.709560	-1.165410
C	-2.596603	0.885594	1.580571
H	-1.868962	0.896752	2.397371
H	-3.092193	1.863038	1.523130
H	-3.344377	0.119284	1.807979
C	3.108408	0.705932	1.235232
H	3.891332	-0.037709	1.055498
H	3.547206	1.709690	1.165444
H	2.721748	0.552330	2.247256
C	2.596541	0.885690	-1.580557
H	1.868913	0.896829	-2.397368
H	3.092107	1.863146	-1.523108
H	3.344336	0.119397	-1.807951

2. 2-Substitued Azolium Reactants

NN2H$^+$
B3lyp/6-31G(d) optimized geometry
Energy = -305.230760 a.u.
Enthalpy Correction = 0.14935 a.u.
B3lyp/6-311+G(2d,p) 5D
Single point energy = -305.314267 a.u.

Atom	x-coord	y-coord	z-coord
C	-2.483062	-0.553259	0.000006
N	-1.089152	-0.084146	-0.000007
C	0.000000	-0.861886	-0.000013
N	1.089152	-0.084146	0.000007
C	2.483062	-0.553259	0.000007
C	-0.681601	1.237538	0.000006
C	0.681602	1.237538	-0.000011
H	2.489923	-1.643503	0.000055
H	2.989241	-0.185425	0.894752
H	2.989213	-0.185502	-0.894786
H	-2.989249	-0.185422	-0.894734
H	-2.989207	-0.185505	0.894807
H	-2.489922	-1.643503	-0.000046
H	-1.387299	2.054192	0.000014
H	1.387298	2.054191	-0.000014
H	0.000000	-1.941517	-0.000018

NN2Me$^+$
B3lyp/6-31G(d) optimized geometry
Energy = -344.557658 a.u.
Enthalpy Correction = 0.178892 a.u.
B3lyp/6-311+G(2d,p) 5D
Single point energy = -344.651859 a.u.

Atom	x-coord	y-coord	z-coord
C	-2.485444	0.226158	-0.002168
N	-1.090672	-0.238929	-0.003349
C	0.003738	0.548029	-0.006064
N	1.082227	-0.260787	0.000706
C	2.480548	0.189372	-0.004310
C	-0.696167	-1.565730	0.002454
C	0.663357	-1.579333	0.004563
H	2.659915	0.862838	0.836387
H	2.709944	0.696241	-0.944836
H	3.122127	-0.685666	0.096638
H	-2.681283	0.828113	0.887580
H	-3.134641	-0.648968	0.009493
H	-2.688981	0.808316	-0.903604
H	-1.410728	-2.373836	0.004131
H	1.362146	-2.401204	0.007566
C	0.032929	2.036412	0.005365
H	-0.938700	2.448061	-0.273572
H	0.289170	2.418187	1.001665
H	0.776381	2.416487	-0.701987

NN2Ph$^+$
B3lyp/6-31G(d) optimized geometry
Energy = -536.298526 a.u.
Enthalpy Correction = 0.235177 a.u.
B3lyp/6-311+G(2d,p) 5D
Single point energy = -536.441747 a.u.

Atom	x-coord	y-coord	z-coord
C	-1.142588	2.447864	0.472369
N	-1.571888	1.071736	0.188896
C	-0.767243	0.000021	-0.000012
N	-1.571835	-1.071754	-0.188873
C	-1.142497	-2.447844	-0.472466
C	-2.892749	0.669534	0.116343
C	-2.892709	-0.669621	-0.116287
H	-0.117002	-2.434756	-0.839242
H	-1.798109	-2.865740	-1.238211
H	-1.202648	-3.055004	0.434057
H	-1.797966	2.865696	1.238355
H	-1.203136	3.055024	-0.434127
H	-0.116967	2.434847	0.838787
H	-3.708651	1.364802	0.239292
H	-3.708588	-1.364922	-0.239212
C	0.702357	0.000032	0.000000
C	1.407160	0.816026	-0.902367
C	2.800377	0.811776	-0.898947
C	3.496507	0.000008	0.000017
C	2.800340	-0.811768	0.898979
C	1.407147	-0.816006	0.902384
H	0.868767	1.431665	-1.617406
H	3.341419	1.436911	-1.602319
H	4.582222	0.000000	0.000038
H	3.341389	-1.436909	1.602341
H	0.868716	-1.431630	1.617399

NO2H$^+$
B3lyp/6-31G(d) optimized geometry
Energy = -285.741980 a.u.
Enthalpy Correction = 0.106414 a.u.
B3lyp/6-311+G(2d,p) 5D
Single point energy = -285.823229 a.u.

Atom	x-coord	y-coord	z-coord
N	-0.627053	0.009845	-0.000001
C	0.139894	-1.062229	-0.000024
O	1.410649	-0.725576	-0.000002
C	1.474032	0.648154	-0.000010
C	0.212018	1.128382	0.000005
H	2.457256	1.091462	0.000189
H	-0.171429	2.137502	-0.000166
C	-2.102222	0.034420	0.000020
H	-2.447064	0.553395	-0.896210
H	-2.447083	0.553342	0.896282
H	-2.471752	-0.991178	-0.000029

H	-0.158077	-2.101191	0.000015

NO2Me$^+$

B3lyp/6-31G(d) optimized geometry
Energy = -235.076746 a.u.
Enthalpy Correction = 0.135841 a.u.
B3lyp/6-311+G(2d,p) 5D
Single point energy = -325.169081 a.u.

Atom	x-coord	y-coord	z-coord
N	-0.177969	0.689186	-0.000007
C	-0.299551	-0.633431	0.000006
O	0.906703	-1.179744	-0.000008
C	1.841928	-0.169646	-0.000014
C	1.185664	1.005796	0.000029
H	2.879163	-0.463763	-0.000010
H	1.539850	2.025299	0.000024
C	-1.269256	1.677333	-0.000010
H	-1.188529	2.297441	-0.895147
H	-1.188568	2.297397	0.895161
H	-2.226358	1.157305	-0.000043
C	-1.516914	-1.479312	0.000007
H	-2.128300	-1.287654	0.889078
H	-2.128391	-1.287536	-0.888974
H	-1.217925	-2.529281	-0.000076

NS2H$^+$

B3lyp/6-31G(d) optimized geometry
Energy = -608.725313 a.u.
Enthalpy Correction = 0.103407 a.u.
B3lyp/6-311+G(2d,p) 5D
Single point energy = -608.813379 a.u.

Atom	x-coord	y-coord	z-coord
N	0.928766	-0.029000	-0.000015
C	0.054561	-1.029300	0.000014
S	-1.556918	-0.492209	0.000000
C	-1.021232	1.156396	-0.000018
C	0.333953	1.224453	0.000025
H	-1.727429	1.975756	-0.000007
H	0.955242	2.110176	0.000014
C	2.396816	-0.212461	-0.000005
H	2.812441	0.253339	0.895806
H	2.812483	0.253490	-0.895717
H	2.622347	-1.278384	-0.000092
H	0.349654	-2.070562	0.000002

NS2Me$^+$

B3lyp/6-31G(d) optimized geometry
Energy = -648.053832 a.u.
Enthalpy Correction = 0.132854 a.u.
B3lyp/6-311+G(2d,p) 5D
Single point energy = -648.152864 a.u.

Atom	x-coord	y-coord	z-coord

N	-0.707532	-0.586022	-0.000237
C	-0.225043	0.662497	-0.000070
S	1.487218	0.657810	0.000097
C	1.525156	-1.073872	0.000018
C	0.267661	-1.575723	-0.000130
H	2.458934	-1.619062	0.000046
H	-0.029768	-2.615329	-0.000201
C	-2.153400	-0.892766	0.000219
H	-2.617551	-0.479870	0.898425
H	-2.276451	-1.974847	-0.006002
H	-2.620253	-0.469508	-0.891677
C	-1.064865	1.894998	-0.000068
H	-1.709314	1.926992	0.886663
H	-0.438708	2.789262	0.001671
H	-1.706717	1.928743	-0.888641

3. Precursor Complexes

Ni_NN2Me+_PC
B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1434.87415640 a.u.
Enthalpy Correction = 0.404891 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -2774.12741365

Atom	X-Coord	Y-Coord	Z-Coord
Ni	0.193125	-0.565928	-0.119044
P	0.256686	1.636381	0.091069
P	2.488518	-0.716354	-0.037356
C	-1.151872	-2.363977	-0.453035
H	-1.443598	-2.715361	-1.444181
H	-0.020706	-2.349985	-0.469797
H	-1.401957	-3.126518	0.287879
C	-1.817794	-1.038685	-0.136749
N	-2.644241	-0.403069	-1.073197
C	-2.324220	-0.288382	-2.482012
H	-1.386773	0.265624	-2.626808
H	-2.223352	-1.276825	-2.941028
H	-3.136473	0.237634	-2.986755
N	-2.455639	-0.821844	1.092236
C	-1.939317	-1.241657	2.382940
H	-1.125101	-0.591637	2.727465
H	-2.751680	-1.213264	3.112698
H	-1.569034	-2.268748	2.327817
C	-3.560481	0.394700	-0.400444
H	-4.254271	1.028751	-0.930984
C	-3.445720	0.139785	0.925088
H	-4.019478	0.511853	1.759949
C	2.990963	1.018781	0.448134
H	4.035549	1.211426	0.175076
H	2.932846	1.074855	1.542544

C	2.057633	2.063669	-0.187827
H	2.213723	2.101257	-1.273392
H	2.271402	3.067854	0.198856
C	-0.605495	2.887482	-0.968185
H	-0.269381	3.904065	-0.733500
H	-0.405440	2.686903	-2.025317
H	-1.684848	2.823849	-0.802731
C	-0.053540	2.305453	1.792963
H	0.499988	1.723836	2.536348
H	0.254353	3.354959	1.865184
H	-1.119535	2.235479	2.029086
C	3.342900	-0.956381	-1.664909
H	2.923151	-0.281105	-2.417034
H	4.419926	-0.771355	-1.583918
H	3.188046	-1.982786	-2.012630
C	3.513237	-1.765219	1.093490
H	3.412648	-2.817844	0.810174
H	4.572976	-1.490195	1.047802
H	3.162865	-1.656172	2.124730

Ni_NN2Ph+_PC

B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1626.62787325 a.u.
Enthalpy Correction = 0.462311 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -2965.93324628

Atom	X-Coord	Y-Coord	Z-Coord
Ni	0.462091	-0.169722	0.018800
P	1.161829	1.974818	0.298496
P	2.527315	-0.746615	-0.641422
C	-2.418408	-0.067762	-0.184995
N	-3.080546	-0.361826	-1.343585
C	-3.059560	-1.622516	-2.088936
H	-2.258680	-1.628011	-2.833503
H	-2.926647	-2.456666	-1.400357
H	-4.019606	-1.728296	-2.596832
N	-2.905668	1.141760	0.225371
C	-2.495135	1.882767	1.411702
H	-1.442344	1.671174	1.607649
H	-2.630735	2.948652	1.218797
H	-3.095812	1.600128	2.280542
C	-3.935637	0.682304	-1.670914
H	-4.545514	0.657371	-2.560043
C	-3.832870	1.610883	-0.692147
H	-4.334468	2.556465	-0.559321
C	3.622776	0.723224	-0.278862
H	4.542476	0.691002	-0.875282
H	3.921289	0.651831	0.774631
C	2.845608	2.026036	-0.524908
H	2.667725	2.163512	-1.599254
H	3.412890	2.899390	-0.180484
C	-0.327010	-3.195552	1.818985
C	-1.049615	-2.207444	2.558564

C	-1.602557	-1.122684	1.935721
C	-1.434742	-0.891218	0.508903
C	-0.582085	-1.842126	-0.206841
C	-0.131516	-3.026950	0.477109
H	0.032987	-4.086890	2.323805
H	-1.215882	-2.351333	3.622296
H	-2.234633	-0.456635	2.513093
H	-0.634943	-1.896613	-1.292150
H	0.376507	-3.792541	-0.104477
C	2.804669	-1.031925	-2.451954
H	2.433363	-0.177967	-3.027299
H	3.866799	-1.177670	-2.678615
H	2.252444	-1.920467	-2.774689
C	3.448983	-2.153905	0.124500
H	2.952593	-3.097224	-0.121699
H	4.485193	-2.196873	-0.228248
H	3.445166	-2.048487	1.213714
C	0.399990	3.517357	-0.401219
H	-0.530388	3.758933	0.121106
H	1.078287	4.372881	-0.307508
H	0.167456	3.367062	-1.460279
C	1.567628	2.506881	2.030418
H	2.163502	1.734777	2.526690
H	2.126383	3.449334	2.040369
H	0.649275	2.638570	2.611587

Ni_NO2Me+_PC

B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1415.41941410 a.u.
Enthalpy Correction = 0.362190 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -2754.67131726

Atom	X-Coord	Y-Coord	Z-Coord
Ni	0.104248	-0.607776	-0.094010
P	0.122467	1.603974	0.049113
P	2.428314	-0.683405	0.000300
C	-1.788888	-1.051953	-0.316250
O	-2.328799	-0.585632	-1.514550
N	-2.752290	-0.767928	0.669360
C	-2.531286	-0.943161	2.091294
H	-1.802058	-0.220849	2.483827
H	-3.479831	-0.816121	2.617203
H	-2.164932	-1.953876	2.295021
C	-3.435581	0.183456	-1.206925
H	-3.936550	0.665157	-2.030642
C	-3.695716	0.092774	0.107226
H	-4.496292	0.520508	0.691737
C	2.869386	1.076624	0.441298
H	3.910761	1.294738	0.176634
H	2.791844	1.165028	1.532248
C	1.910629	2.065229	-0.244329
H	2.067679	2.056934	-1.330243
H	2.093972	3.091966	0.095438

C	-0.779461	2.680847	-1.148527
H	-0.429063	3.716978	-1.083269
H	-0.623446	2.313754	-2.167127
H	-1.850989	2.649928	-0.934977
C	-0.249421	2.389206	1.682871
H	0.329201	1.906108	2.476096
H	-0.006704	3.457765	1.667503
H	-1.311896	2.274781	1.917137
C	3.319768	-0.970259	-1.596093
H	2.909149	-0.327681	-2.380977
H	4.392174	-0.769821	-1.495931
H	3.183760	-2.010062	-1.909893
C	3.410041	-1.687704	1.202163
H	3.326405	-2.749453	0.949156
H	4.468787	-1.406999	1.187247
H	3.019443	-1.547490	2.214867
C	-1.156272	-2.437932	-0.404272
H	-0.033396	-2.459699	-0.302136
H	-1.522588	-3.093594	0.387779
H	-1.358874	-2.871022	-1.385473

Ni_NS2H+_PC
B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1699.08709941 a.u.
Enthalpy Correction = 0.327940 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -3038.33735980

Atom	X-Coord	Y-Coord	Z-Coord
Ni	0.058508	-0.401613	-0.004592
P	0.796826	1.695211	0.098093
P	2.185821	-1.171594	-0.097203
C	-1.803782	-0.534388	-0.098747
S	-2.691084	-0.235020	-1.595313
N	-2.716892	-0.603041	0.922771
C	-2.291593	-0.859197	2.297687
H	-1.517528	-1.633427	2.294388
H	-1.885711	0.048942	2.754103
H	-3.144273	-1.209965	2.881698
C	-4.226188	-0.186580	-0.752969
H	-5.155328	-0.014052	-1.276843
C	-4.046049	-0.397411	0.565592
H	-4.805432	-0.422583	1.335898
C	3.246411	0.326916	0.255653
H	4.265240	0.183214	-0.122726
H	3.320422	0.420088	1.346422
C	2.608784	1.593329	-0.346086
H	2.666518	1.564015	-1.441262
H	3.139774	2.496299	-0.021922
C	0.124857	3.005764	-1.009685
H	0.691651	3.938025	-0.913553
H	0.163049	2.669862	-2.050308
H	-0.921637	3.199153	-0.754423
C	0.788758	2.496003	1.763915

H	1.262473	1.842403	2.502646
H	1.320972	3.453446	1.743672
H	-0.243443	2.675365	2.080247
C	2.743005	-1.722416	-1.771363
H	2.505793	-0.960233	-2.519891
H	3.821724	-1.913091	-1.786704
H	2.216336	-2.640721	-2.048281
C	2.864411	-2.473518	1.020763
H	2.379215	-3.429645	0.801730
H	3.945701	-2.587538	0.888799
H	2.658182	-2.217399	2.064488
H	-1.037732	-1.580628	-0.125900

Ni_NS2Me+_PC
B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1738.42738572 a.u.
Enthalpy Correction = 0.360756 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -3077.68780070

Atom	X-Coord	Y-Coord	Z-Coord
C	-2.921093	-1.077836	-1.286114
N	-2.811515	0.055911	-0.523385
C	-1.937685	-0.053038	0.588381
S	-1.517109	-1.848956	0.738293
C	-2.307954	-2.182727	-0.800317
Ni	-0.024065	-0.243089	0.246604
C	-2.331423	0.692187	1.849196
C	-3.625011	1.244731	-0.754051
P	0.790217	1.807101	-0.101201
C	1.122657	2.776099	1.438340
P	2.069905	-1.114713	-0.051094
C	2.892529	-2.242979	1.155785
C	2.492052	1.543509	-0.827867
C	3.207184	0.363667	-0.145594
C	0.043787	3.066810	-1.227836
C	2.329227	-1.970944	-1.669870
H	-4.380777	1.371883	0.028615
H	-2.996736	2.140383	-0.791104
H	-4.134048	1.140522	-1.713607
H	-2.302630	-3.175163	-1.225983
H	-3.503272	-1.036972	-2.199179
H	4.135966	0.111597	-0.670651
H	3.483756	0.628652	0.882508
H	2.351682	1.336890	-1.896276
H	3.084716	2.463174	-0.754005
H	0.726057	3.909604	-1.383960
H	-0.189014	2.614196	-2.196350
H	-0.884903	3.449496	-0.793335
H	1.673486	2.163648	2.158214
H	1.703067	3.679466	1.220635
H	0.176634	3.069768	1.903261
H	1.990182	-1.333997	-2.492678
H	3.384544	-2.220909	-1.824235

H	1.740871	-2.893481	-1.694847
H	2.346265	-3.190432	1.199571
H	3.930167	-2.447698	0.871198
H	2.877601	-1.796864	2.154923
H	-3.341476	0.428522	2.189741
H	-1.631595	0.469629	2.658918
H	-2.299836	1.773799	1.678813

Pd_NN2H+_PC
B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1353.03250764 a.u.
Enthalpy Correction = 0.374832 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -1353.27692008

Atom	X-Coord	Y-Coord	Z-Coord
Pd	0.003351	-0.448272	0.020231
P	0.762521	1.818386	-0.035778
P	2.320653	-1.141873	0.023455
H	-1.422071	-1.647349	0.049016
C	-2.123710	-0.691391	0.014022
N	-2.922744	-0.519371	-1.088349
C	-2.461781	-0.674362	-2.461920
H	-1.722718	-1.478810	-2.502251
H	-3.310774	-0.932720	-3.097770
H	-1.999472	0.250098	-2.821627
N	-2.936718	-0.455665	1.094404
C	-2.494383	-0.532206	2.480728
H	-1.747587	-1.325060	2.574046
H	-2.046762	0.414948	2.797389
H	-3.349772	-0.765578	3.117762
C	-4.175731	-0.086358	-0.697299
H	-4.950980	0.143963	-1.411676
C	-4.184370	-0.046321	0.662908
H	-4.968397	0.225369	1.352746
C	3.237873	0.465158	0.311913
H	4.289469	0.363077	0.016555
H	3.228440	0.644462	1.394514
C	2.586064	1.649120	-0.426268
H	2.665868	1.509076	-1.511822
H	3.107230	2.584950	-0.187831
C	0.216068	3.113087	-1.240204
H	-0.819655	3.396438	-1.028273
H	0.844873	4.008926	-1.181818
H	0.260588	2.714681	-2.258475
C	0.771689	2.754244	1.563166
H	1.185179	2.130861	2.361669
H	1.365724	3.671952	1.483845
H	-0.253036	3.022256	1.838450
C	3.035538	-1.750971	-1.572320
H	2.757601	-1.079345	-2.390330
H	4.128269	-1.818706	-1.522521
H	2.629872	-2.741850	-1.798711
C	3.095126	-2.275612	1.262216

H	2.723663	-3.292960	1.105244
H	4.187667	-2.281492	1.177974
H	2.816966	-1.965466	2.274076

Pd_NN2Me+_PC

B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1392.34266981 a.u.
Enthalpy Correction = 0.405986 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -1392.59558823

Atom	X-Coord	Y-Coord	Z-Coord
Pd	0.318621	-0.409426	-0.214685
P	0.761572	1.866907	0.129495
P	2.577012	-1.073046	-0.046939
C	-1.974638	-2.161030	-0.654577
H	-2.115999	-2.320254	-1.724553
H	-0.865529	-2.058392	-0.478664
H	-2.275363	-3.071422	-0.126141
C	-2.749942	-0.990200	-0.181418
N	-3.331314	-0.037665	-0.947790
C	-3.152108	0.109170	-2.391927
H	-2.102137	0.329739	-2.610018
H	-3.459350	-0.802291	-2.909452
H	-3.777348	0.934238	-2.733571
N	-3.080678	-0.725839	1.104554
C	-2.597042	-1.475006	2.265113
H	-1.509778	-1.377649	2.338002
H	-3.062742	-1.061998	3.160098
H	-2.871835	-2.529028	2.178300
C	-3.977269	0.871710	-0.127554
H	-4.503461	1.724333	-0.526685
C	-3.822426	0.441632	1.152227
H	-4.187776	0.847328	2.082382
C	3.281401	0.552410	0.584124
H	4.367641	0.574614	0.425049
H	3.122179	0.559059	1.670078
C	2.633966	1.799707	-0.051077
H	2.842164	1.822710	-1.128449
H	3.076240	2.710058	0.375181
C	0.377870	3.362207	-0.905517
H	0.996023	4.222933	-0.623487
H	0.550979	3.134850	-1.962100
H	-0.675661	3.633714	-0.783375
C	0.572936	2.566324	1.840584
H	0.896497	1.829814	2.582425
H	1.162706	3.481826	1.968769
H	-0.479836	2.798111	2.031548
C	3.543960	-1.342661	-1.607680
H	3.262003	-0.595916	-2.356216
H	4.624409	-1.281103	-1.431043
H	3.309237	-2.330584	-2.016407
C	3.392971	-2.282701	1.099522
H	3.188623	-3.302137	0.757145

H	4.478825	-2.137148	1.142784
H	2.979848	-2.174594	2.107280

Pd_NN2Ph+_PC

B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1584.08851965 a.u.
Enthalpy Correction = 0.462609 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -1584.39545597

Atom	X-Coord	Y-Coord	Z-Coord
Pd	-0.411230	-0.160252	0.008370
P	-1.450247	1.991249	0.363266
P	-2.590123	-0.961285	-0.661217
C	2.619038	0.104156	-0.209994
N	2.952095	1.350183	0.235637
C	2.423651	2.010853	1.425003
H	1.392644	1.678967	1.576302
H	3.025091	1.777007	2.306968
H	2.444601	3.089186	1.255559
N	3.282449	-0.065571	-1.390427
C	3.376964	-1.289097	-2.189667
H	2.555545	-1.352407	-2.908589
H	4.324661	-1.267225	-2.730032
H	3.359986	-2.159906	-1.534157
C	3.785982	1.965570	-0.683616
H	4.161936	2.964553	-0.528844
C	3.986601	1.089724	-1.697014
H	4.574428	1.173319	-2.597366
C	-3.644079	0.578467	-0.786365
H	-4.709837	0.322350	-0.734159
H	-3.466744	1.003050	-1.782752
C	-3.284495	1.605901	0.300181
H	-3.556950	1.218486	1.290196
H	-3.852857	2.533551	0.155810
C	-1.388090	3.073910	1.870859
H	-2.147364	3.863707	1.834247
H	-1.551197	2.467783	2.767636
H	-0.403866	3.545810	1.954578
C	-1.271552	3.242189	-0.996364
H	-1.425613	2.761128	-1.967090
H	-1.987811	4.065018	-0.888564
H	-0.258054	3.656092	-0.987517
C	-3.463199	-1.956726	0.634111
H	-3.439112	-1.423693	1.589506
H	-4.505630	-2.158215	0.362152
H	-2.940727	-2.908128	0.774164
C	-3.039248	-1.869126	-2.213071
H	-2.578623	-2.862243	-2.203337
H	-4.124121	-1.988338	-2.314936
H	-2.658428	-1.326991	-3.084347
C	1.791464	-0.877833	0.485425
C	2.050563	-1.132755	1.881955
C	1.579945	-2.263902	2.499131

C	0.843150	-3.238542	1.770355
C	0.577371	-3.039783	0.438334
C	0.989492	-1.845849	-0.234895
H	2.677850	-0.447157	2.441696
H	1.811281	-2.436478	3.545997
H	0.519033	-4.148866	2.265478
H	0.047335	-3.794758	-0.136306
H	0.991518	-1.858704	-1.320702

Pd_NO2H+_PC
B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1333.56405655 a.u.
Enthalpy Correction = 0.332279 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -1333.80631303

Atom	X-Coord	Y-Coord	Z-Coord
Pd	0.043164	-0.546015	-0.191689
P	-0.404855	1.745063	0.159838
P	-2.359229	-0.945024	-0.076547
C	-3.063539	0.788241	-0.135098
H	-4.094962	0.792346	0.237836
H	-3.107667	1.075745	-1.193032
C	-2.206929	1.796361	0.653898
H	-2.245826	1.571298	1.727096
H	-2.596280	2.814335	0.527919
C	-3.345297	-1.837637	-1.358298
H	-3.087074	-1.461860	-2.352934
H	-3.102225	-2.904167	-1.325181
H	-4.421961	-1.715130	-1.196634
C	-3.026541	-1.628926	1.507883
H	-2.599309	-1.091803	2.360107
H	-4.118917	-1.552652	1.548689
H	-2.742304	-2.681958	1.597522
C	0.411831	2.810243	1.429074
H	1.466761	2.944135	1.170900
H	-0.064160	3.795767	1.485810
H	0.354965	2.331288	2.411192
C	-0.329418	2.782470	-1.367061
H	-0.877548	2.295607	-2.178667
H	-0.753985	3.777672	-1.192099
H	0.712148	2.889919	-1.684293
N	3.009914	-0.828927	0.621454
C	2.089001	-0.826426	-0.397182
O	2.738274	-0.364224	-1.509128
C	4.004095	0.028577	-1.140862
C	4.187241	-0.245278	0.164673
H	4.629467	0.448593	-1.911476
H	5.042257	-0.095132	0.805624
C	2.724071	-1.249983	1.984657
H	2.275828	-0.433358	2.560201
H	3.650850	-1.571500	2.463722
H	2.023916	-2.090128	1.959262
H	1.489035	-1.812466	-0.580489

Pd_NO2Me+_PC
B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1372.87847766 a.u.
Enthalpy Correction = 0.362360 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -1373.13096594

Atom	X-Coord	Y-Coord	Z-Coord
Pd	-0.088822	-0.644105	-0.067924
P	-0.171596	1.710614	0.058764
P	-2.552356	-0.673337	-0.005685
C	-2.949671	1.139828	-0.236332
H	-3.974245	1.347933	0.095971
H	-2.919041	1.339967	-1.314661
C	-1.956343	2.053206	0.504303
H	-2.044567	1.908793	1.588552
H	-2.183454	3.108322	0.305254
C	-3.674848	-1.492924	-1.226027
H	-3.353925	-1.253672	-2.244488
H	-3.620814	-2.578842	-1.100027
H	-4.715290	-1.175180	-1.094669
C	-3.356051	-1.070903	1.614230
H	-2.852802	-0.533804	2.424139
H	-4.418178	-0.800925	1.612289
H	-3.265025	-2.142809	1.815883
C	0.734277	2.825736	1.225968
H	1.799025	2.830309	0.976221
H	0.353128	3.851852	1.165347
H	0.619762	2.467156	2.253373
C	0.032864	2.574819	-1.563175
H	-0.542471	2.061842	-2.339034
H	-0.297837	3.617902	-1.500868
H	1.086227	2.551790	-1.855506
N	2.938014	-0.564684	0.663148
C	2.052019	-1.082031	-0.279303
O	2.471366	-0.598465	-1.504531
C	3.382941	0.407174	-1.268393
C	3.672049	0.443986	0.045140
H	3.758696	0.937527	-2.128047
H	4.366221	1.062937	0.592984
C	2.793002	-0.720972	2.100016
H	1.940141	-0.141260	2.476239
H	3.709307	-0.381360	2.586364
H	2.641929	-1.774135	2.350817
C	1.612308	-2.533258	-0.269245
H	2.008227	-3.056806	0.602979
H	0.504752	-2.685001	-0.243718
H	1.953042	-3.020322	-1.185982

Pd_NS2H+_PC
B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1656.56496584 a.u.

Enthalpy Correction = 0.331187 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -1656.81571766

Atom	X-Coord	Y-Coord	Z-Coord
C	-3.505479	-0.624909	1.016093
N	-3.132930	0.410267	0.199417
C	-2.173636	0.067255	-0.763618
S	-2.013077	-1.728990	-0.772400
C	-3.018054	-1.840538	0.667652
C	-3.598723	1.783043	0.340206
Pd	-0.130358	-0.254294	-0.237392
P	0.932212	1.852854	-0.029810
C	0.733765	2.748284	1.576030
P	2.047043	-1.253149	0.178165
C	2.937729	-1.947704	-1.285361
C	3.111125	0.194385	0.697716
C	2.760705	1.469674	-0.090299
C	2.362601	-2.511020	1.493008
C	0.738471	3.191298	-1.286730
H	3.333458	2.327343	0.283789
H	3.023913	1.348202	-1.148583
H	2.936591	0.350454	1.769682
H	4.174208	-0.048333	0.580699
H	0.918235	2.788088	-2.287919
H	-0.282263	3.584534	-1.255167
H	1.437761	4.014574	-1.103047
H	0.930891	2.069739	2.411189
H	1.417414	3.602381	1.639936
H	-0.293731	3.111530	1.673218
H	1.872755	-3.451332	1.221350
H	3.434307	-2.697383	1.623221
H	1.940778	-2.170006	2.443290
H	2.937317	-1.223215	-2.105328
H	3.973002	-2.206587	-1.036997
H	2.421602	-2.847804	-1.633446
H	-3.205870	-2.792773	1.140872
H	-4.170565	-0.425206	1.847439
H	-2.813193	2.421344	0.762393
H	-4.467803	1.802995	0.999826
H	-3.893515	2.178927	-0.636852
H	-2.268934	0.577855	-1.720525

Pd_NS2Me+_PC
B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1695.88151871 a.u.
Enthalpy Correction = 0.360750 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -1696.14351832

Atom	X-Coord	Y-Coord	Z-Coord
Pd	0.036393	-0.281652	0.178015

P	-0.950395	1.863746	-0.086931
P	-2.206216	-1.195182	-0.088225
C	-3.225703	0.269371	-0.645855
H	-4.293428	0.081945	-0.479366
H	-3.083624	0.363074	-1.729863
C	-2.789711	1.564840	0.061812
H	-3.014547	1.506278	1.134215
H	-3.340498	2.427528	-0.333002
C	-2.664265	-2.517051	-1.294823
H	-2.288300	-2.259510	-2.289692
H	-2.202812	-3.462036	-0.991298
H	-3.749673	-2.656486	-1.347451
C	-3.048989	-1.742641	1.464189
H	-2.955766	-0.971286	2.234652
H	-4.111001	-1.950303	1.292344
H	-2.567121	-2.650702	1.839588
C	-0.673449	3.286668	1.058872
H	0.356420	3.644970	0.965690
H	-1.353404	4.115949	0.833871
H	-0.832532	2.968332	2.093461
C	-0.778513	2.637047	-1.758483
H	-1.037032	1.911260	-2.535177
H	-1.426202	3.515297	-1.859480
H	0.259422	2.943940	-1.918990
N	3.000107	0.232305	-0.481505
C	2.138790	-0.053459	0.596782
S	1.859039	-1.852000	0.580828
C	2.713392	-2.007645	-0.944861
C	3.230583	-0.817625	-1.332485
H	2.789965	-2.960010	-1.447953
H	3.813454	-0.645790	-2.229155
C	3.569852	1.561071	-0.674100
H	2.774894	2.312458	-0.742405
H	4.139765	1.568726	-1.604280
H	4.241327	1.825975	0.148511
C	2.420442	0.631718	1.919303
H	2.259844	1.710787	1.834159
H	1.743620	0.260479	2.692269
H	3.452373	0.458756	2.253167

Pt_NN2Me+_PC

B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1384.75788338 a.u.
Enthalpy Correction = 0.406276 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -1385.01586518

Atom	X-Coord	Y-Coord	Z-Coord
Pt	0.372270	-0.244440	-0.088900
P	0.958519	1.949489	0.102609
P	2.444076	-1.187831	-0.048999
C	-2.207739	-2.044986	-0.568352
H	-2.352149	-2.264533	-1.627269
H	-1.115245	-1.832398	-0.417041

H	-2.436130	-2.945763	0.009687
C	-3.048672	-0.905407	-0.136491
N	-3.682232	-0.015915	-0.931906
C	-3.574963	0.044022	-2.391251
H	-2.549579	0.298544	-2.675181
H	-3.859886	-0.913250	-2.832945
H	-4.255631	0.814729	-2.753208
N	-3.330813	-0.572865	1.141843
C	-2.750549	-1.220939	2.320702
H	-1.668408	-1.055975	2.329856
H	-3.199302	-0.780433	3.211182
H	-2.965586	-2.291943	2.307302
C	-4.343722	0.909458	-0.141678
H	-4.918772	1.715737	-0.568661
C	-4.123783	0.560975	1.153604
H	-4.468950	1.006208	2.073296
C	3.371664	0.385475	0.427542
H	4.433624	0.284506	0.167829
H	3.317256	0.448487	1.521563
C	2.801102	1.679544	-0.202755
H	2.923623	1.648098	-1.292648
H	3.367135	2.548999	0.156904
C	0.608078	3.376559	-1.028957
H	1.316998	4.199002	-0.875692
H	0.668056	3.042565	-2.069054
H	-0.405894	3.745767	-0.845053
C	0.930960	2.762147	1.768226
H	1.245142	2.045097	2.532407
H	1.595528	3.633640	1.798985
H	-0.087629	3.085568	2.004541
C	3.248434	-1.684490	-1.640983
H	3.008472	-0.953917	-2.418942
H	4.337402	-1.752887	-1.533985
H	2.860841	-2.657109	-1.959165
C	3.151023	-2.413025	1.146820
H	2.798368	-3.416614	0.889629
H	4.247417	-2.406842	1.128956
H	2.807632	-2.178324	2.158667

Pt_NN2Ph+_PC

B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1576.51091915 a.u.
Enthalpy Correction = 0.462533 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -1576.82667377

Atom	X-Coord	Y-Coord	Z-Coord
Pt	0.399878	-0.140282	-0.005139
P	1.493472	1.931666	0.340597
P	2.468940	-0.974835	-0.721771
C	-2.669275	0.176454	-0.223630
N	-3.427086	-0.195717	-1.294269
C	-3.576084	-1.539250	-1.860093
H	-2.833827	-1.720205	-2.642060

H	-3.471589	-2.285259	-1.072873
H	-4.575830	-1.612881	-2.291342
N	-2.990146	1.476925	0.029776
C	-2.419028	2.313761	1.078260
H	-1.381833	2.006698	1.235466
H	-2.457099	3.353972	0.749141
H	-2.980894	2.212236	2.010492
C	-4.180915	0.885195	-1.729571
H	-4.843239	0.809835	-2.577356
C	-3.914531	1.922313	-0.900884
H	-4.298356	2.930096	-0.883196
C	3.742766	0.303161	-0.237978
H	4.666855	0.163099	-0.811769
H	3.987980	0.122884	0.816150
C	3.194517	1.727588	-0.422593
H	3.088663	1.955947	-1.490897
H	3.885847	2.469307	-0.004515
C	-0.968457	-2.985449	2.041206
C	-1.589356	-1.864461	2.689206
C	-1.978413	-0.766637	1.982245
C	-1.737165	-0.653952	0.543598
C	-1.004281	-1.766482	-0.093365
C	-0.716819	-2.945430	0.703509
H	-0.735816	-3.873837	2.620755
H	-1.799475	-1.914703	3.753754
H	-2.525465	0.023082	2.487876
H	-1.136261	-1.940728	-1.158472
H	-0.293952	-3.809124	0.195739
C	2.720605	-1.186856	-2.540429
H	2.443242	-0.266568	-3.062802
H	3.761914	-1.435534	-2.774552
H	2.073676	-1.990153	-2.906483
C	3.141423	-2.541217	-0.017562
H	2.521612	-3.382484	-0.342063
H	4.174184	-2.716627	-0.338663
H	3.104595	-2.495422	1.074693
C	0.984588	3.568661	-0.362049
H	0.077697	3.927004	0.133700
H	1.772071	4.318932	-0.228660
H	0.772967	3.460520	-1.430172
C	1.878860	2.355003	2.101063
H	2.295472	1.478537	2.605812
H	2.590850	3.185065	2.170602
H	0.959345	2.632967	2.625955

Pt_NO2Me+_PC

B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1365.29728818 a.u.
Enthalpy Correction = 0.362028 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -1365.55832308

Atom	X-Coord	Y-Coord	Z-Coord
Pt	-0.092641	-0.488755	-0.093274

P	-0.185103	1.773532	0.065038
P	-2.516685	-0.568680	0.037508
C	-2.960971	1.232744	-0.192188
H	-3.975597	1.425902	0.175893
H	-2.970912	1.422222	-1.272534
C	-1.955166	2.167188	0.505786
H	-2.035688	2.068241	1.595369
H	-2.164869	3.216122	0.263239
C	-3.599483	-1.437574	-1.178494
H	-3.292261	-1.180998	-2.196686
H	-3.493633	-2.519605	-1.052629
H	-4.652548	-1.168211	-1.041425
C	-3.261133	-1.005938	1.670508
H	-2.767535	-0.443179	2.468525
H	-4.335215	-0.790691	1.688985
H	-3.110379	-2.071775	1.867688
C	0.794361	2.750177	1.281584
H	1.851982	2.711549	1.008790
H	0.460861	3.794612	1.287225
H	0.673066	2.331327	2.284425
C	0.109311	2.618050	-1.544391
H	-0.547730	2.198313	-2.311085
H	-0.075847	3.694729	-1.457385
H	1.143240	2.449473	-1.856407
N	2.902023	-0.630216	0.726117
C	2.004259	-0.895785	-0.334366
O	2.569070	-0.275160	-1.454813
C	3.551708	0.585613	-1.004615
C	3.755639	0.390122	0.308647
H	4.042680	1.193888	-1.746894
H	4.472110	0.842445	0.977950
C	2.606344	-0.931480	2.112935
H	3.508552	-0.780267	2.709760
H	2.303841	-1.978127	2.214356
H	1.798352	-0.297609	2.505502
C	1.572184	-2.348465	-0.594680
H	2.066942	-3.030672	0.100115
H	0.477048	-2.562648	-0.476576
H	1.807336	-2.610063	-1.627690

Pt_NS2Me+_PC

B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1688.27277359 a.u.
Enthalpy Correction = 0.359501 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -1688.53979021

Atom	X-Coord	Y-Coord	Z-Coord
Pt	-0.203817	-0.495486	-0.003207
P	-0.297985	1.778371	0.078967
P	-2.621675	-0.538674	-0.063123
C	-3.055816	1.262793	-0.303172
H	-4.085663	1.453426	0.020987
H	-3.018376	1.459285	-1.381671

C	-2.079372	2.190449	0.443005
H	-2.210032	2.091795	1.527696
H	-2.269302	3.240834	0.191072
C	-3.606662	-1.400748	-1.363319
H	-3.223383	-1.136268	-2.353196
H	-3.508800	-2.483470	-1.237512
H	-4.667399	-1.133127	-1.303788
C	-3.473958	-1.000446	1.508584
H	-3.033570	-0.451659	2.346382
H	-4.546470	-0.782440	1.458774
H	-3.338426	-2.069778	1.698153
C	0.650212	2.782581	1.297203
H	1.715497	2.724609	1.059616
H	0.329301	3.830199	1.258584
H	0.491324	2.397270	2.308091
C	0.057844	2.565564	-1.544435
H	-0.594086	2.143009	-2.314008
H	-0.097154	3.648919	-1.490985
H	1.093217	2.358386	-1.828079
N	2.767642	-0.508110	0.944508
C	1.902403	-0.951974	-0.090906
S	2.656624	-0.416191	-1.653094
C	3.700123	0.707564	-0.785364
C	3.635335	0.496846	0.544067
H	4.356022	1.384957	-1.312618
H	4.224252	1.002589	1.299569
C	2.404689	-0.694095	2.340497
H	3.215943	-0.327752	2.972495
H	2.257975	-1.755141	2.563019
H	1.475666	-0.157550	2.583120
C	1.431515	-2.413827	-0.060845
H	0.325062	-2.553542	0.126395
H	1.618372	-2.921004	-1.008867
H	1.905310	-2.963470	0.755340

4. Transition Structures

Ni_NN2Me+_TS
B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1434.86736012 a.u.
Enthalpy Correction = 0.402978 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -2774.12107239

Atom	X-Coord	Y-Coord	Z-Coord
Ni	-0.106292	-0.455342	0.011742
P	-0.539052	1.718594	0.003681
P	-2.383812	-0.909955	-0.008605
C	1.088585	-2.232302	0.008565
H	0.534997	-2.541772	0.901489
H	0.551612	-2.550695	-0.890639
H	2.046839	-2.757277	0.021426
C	1.767319	-0.641738	0.006659

N	2.588669	-0.368617	1.099501
C	2.199126	-0.556740	2.485942
H	1.172068	-0.209570	2.630056
H	2.267587	-1.608769	2.789783
H	2.860269	0.032453	3.125423
N	2.580012	-0.375431	-1.095473
C	2.194563	-0.601873	-2.478232
H	1.153012	-0.304446	-2.624160
H	2.825089	0.008383	-3.129096
H	2.311573	-1.653953	-2.767102
C	3.861236	0.001251	0.672361
H	4.640031	0.266579	1.370595
C	3.856282	-0.003581	-0.680179
H	4.629905	0.256614	-1.386060
C	-3.147840	0.751194	-0.405849
H	-4.208075	0.769279	-0.126406
H	-3.103720	0.871666	-1.495778
C	-2.378589	1.891692	0.286743
H	-2.539316	1.852819	1.371512
H	-2.735878	2.871267	-0.052989
C	0.204063	2.887522	1.226474
H	-0.196526	3.900197	1.106892
H	-0.001098	2.544025	2.245117
H	1.289452	2.919567	1.088660
C	-0.254795	2.591872	-1.602540
H	-0.786553	2.081207	-2.411201
H	-0.595223	3.632236	-1.556400
H	0.814031	2.580421	-1.837899
C	-3.161672	-1.348848	1.614846
H	-2.832439	-0.654401	2.394205
H	-4.255296	-1.322340	1.555659
H	-2.851611	-2.356362	1.910537
C	-3.246313	-2.055891	-1.177439
H	-2.962261	-3.089524	-0.954726
H	-4.335373	-1.968775	-1.099130
H	-2.946504	-1.835883	-2.206973

Ni_NN2Ph+_TS

B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1626.60779847 a.u.
Enthalpy Correction = 0.459766 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -2965.91368357

Atom	X-Coord	Y-Coord	Z-Coord
Ni	-0.275062	-0.033067	0.012493
P	-2.021701	-1.381798	-0.358432
P	-1.723552	1.731540	0.297081
C	1.327643	-1.035693	0.122625
N	2.009383	-1.863414	-0.766013
C	2.043610	-1.710291	-2.208005
H	1.034981	-1.525976	-2.588487
H	2.695703	-0.880448	-2.504326
H	2.421919	-2.634742	-2.648640

N	1.635102	-1.577851	1.372735
C	0.973080	-1.228632	2.621816
H	0.473142	-0.264820	2.505684
H	0.219842	-1.978571	2.889893
H	1.708808	-1.162668	3.429568
C	2.724336	-2.835514	-0.079896
H	3.339738	-3.555912	-0.596380
C	2.481548	-2.669045	1.240918
H	2.822627	-3.233509	2.095241
C	-3.427373	0.959426	0.332258
H	-4.202142	1.693626	0.081533
H	-3.614510	0.640028	1.365463
C	-3.489534	-0.251761	-0.617779
H	-3.450553	0.084110	-1.661932
H	-4.429886	-0.802962	-0.495946
C	3.069728	3.061218	-0.549777
C	3.078355	2.479826	0.722616
C	2.365180	1.309681	0.968528
C	1.617152	0.685000	-0.051839
C	1.648232	1.268255	-1.340680
C	2.350100	2.451543	-1.579052
H	3.632467	3.970345	-0.739316
H	3.649279	2.938231	1.525417
H	2.409777	0.871100	1.959823
H	1.091449	0.818964	-2.157749
H	2.341318	2.890202	-2.573222
C	-1.816505	2.921749	-1.116914
H	-1.983231	2.381392	-2.054130
H	-2.623042	3.649749	-0.977808
H	-0.864511	3.454529	-1.203043
C	-1.728310	2.857546	1.763512
H	-0.794929	3.428908	1.782850
H	-2.570313	3.557729	1.735158
H	-1.787278	2.271421	2.686226
C	-2.117533	-2.533090	-1.802641
H	-1.363720	-3.319493	-1.695550
H	-3.105007	-3.002027	-1.876581
H	-1.915429	-1.987987	-2.730000
C	-2.561903	-2.470988	1.038368
H	-2.683960	-1.883543	1.953472
H	-3.510251	-2.969590	0.809084
H	-1.799965	-3.234856	1.222762

Ni_NO2Me+_TS

B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1415.41231799 a.u.
Enthalpy Correction = 0.360486 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -2754.66458817

Atom	X-Coord	Y-Coord	Z-Coord
Ni	0.010443	-0.465935	-0.073780
P	0.440076	1.705732	0.019906
P	2.283928	-0.905513	0.002096

C	-1.808144	-0.604964	-0.245002
O	-2.403456	-0.369011	-1.462946
N	-2.799762	-0.418816	0.701479
C	-2.651590	-0.679106	2.124211
H	-1.623607	-0.463071	2.423535
H	-3.323354	-0.025438	2.686206
H	-2.885114	-1.722488	2.370341
C	-3.756045	-0.135529	-1.263787
H	-4.352063	0.053651	-2.141136
C	-4.014060	-0.171525	0.051083
H	-4.934996	-0.023482	0.593973
C	3.049504	0.747202	0.420858
H	4.109321	0.769259	0.141071
H	3.005339	0.855665	1.511928
C	2.276712	1.891474	-0.261298
H	2.436546	1.864437	-1.346368
H	2.627212	2.869676	0.088728
C	-0.333204	2.841709	-1.208093
H	0.063451	3.858476	-1.115849
H	-0.147827	2.474593	-2.221891
H	-1.415738	2.867289	-1.050348
C	0.136233	2.550386	1.634543
H	0.661702	2.029385	2.440535
H	0.473916	3.592078	1.605234
H	-0.934647	2.533861	1.859742
C	3.063050	-1.349267	-1.615949
H	2.755092	-0.642550	-2.392719
H	4.156134	-1.348101	-1.545703
H	2.732222	-2.347218	-1.920967
C	3.092414	-2.075470	1.181008
H	2.792725	-3.101253	0.943577
H	4.184130	-2.008887	1.125372
H	2.774794	-1.856294	2.205184
C	-1.095912	-2.252048	-0.281553
H	-0.503490	-2.508451	-1.165902
H	-0.652234	-2.664273	0.630394
H	-2.079713	-2.707350	-0.412033

Ni_NS2H+_TS

B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1699.08710850 a.u.
Enthalpy Correction = 0.326309 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -3038.33752007

Atom	X-Coord	Y-Coord	Z-Coord
Ni	0.045095	-0.384026	0.010370
P	0.848616	1.696414	0.100837
P	2.149065	-1.202438	-0.098872
C	-1.813901	-0.475281	-0.087968
S	-2.686782	-0.176609	-1.587610
N	-2.733744	-0.571825	0.919057
C	-2.320987	-0.831795	2.298235
H	-1.523743	-1.581610	2.296237

H	-1.951356	0.083184	2.770970
H	-3.171357	-1.215412	2.864676
C	-4.235399	-0.185840	-0.770324
H	-5.162037	-0.036166	-1.305578
C	-4.066303	-0.404630	0.548262
H	-4.833122	-0.460354	1.309414
C	3.261591	0.264173	0.224412
H	4.268309	0.087751	-0.172198
H	3.359250	0.361814	1.312902
C	2.649525	1.544696	-0.373416
H	2.688571	1.509051	-1.469251
H	3.209638	2.434435	-0.061940
C	0.197361	3.034394	-0.986149
H	0.797035	3.946578	-0.897349
H	0.201842	2.703770	-2.029143
H	-0.836207	3.261547	-0.707152
C	0.891827	2.485080	1.771684
H	1.350905	1.809744	2.499900
H	1.457646	3.422964	1.750597
H	-0.128865	2.699103	2.103187
C	2.654553	-1.778603	-1.780322
H	2.418801	-1.016427	-2.529268
H	3.727686	-1.995551	-1.817757
H	2.099472	-2.685743	-2.037780
C	2.804185	-2.520125	1.013662
H	2.280557	-3.459626	0.812111
H	3.877603	-2.673262	0.859109
H	2.629965	-2.250046	2.059682
H	-0.998465	-1.566536	-0.111316

Ni_NS2Me+_TS

B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1738.38518597 a.u.
Enthalpy Correction = 0.357782 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -3077.64340335

Atom	X-Coord	Y-Coord	Z-Coord
Ni	0.138835	-0.455458	0.053973
P	0.614056	1.717441	0.005114
P	2.409490	-0.919818	-0.025216
C	-1.690040	-0.590135	-0.029514
S	-2.493468	-0.426333	-1.612277
N	-2.633404	-0.305624	0.939875
C	-2.330363	-0.416517	2.364605
H	-2.384474	-1.457772	2.704727
H	-1.326226	-0.030246	2.553615
H	-3.049701	0.176443	2.933729
C	-4.053320	-0.104846	-0.861849
H	-4.941825	0.064861	-1.452422
C	-3.932487	-0.084547	0.476524
H	-4.716679	0.100263	1.199338
C	3.228717	0.730239	0.281080
H	4.269149	0.722558	-0.064288

H	3.254017	0.880845	1.367738
C	2.431926	1.860068	-0.397419
H	2.524020	1.788117	-1.488275
H	2.818280	2.845007	-0.109363
C	-0.221333	2.805273	-1.223495
H	0.184864	3.821871	-1.194816
H	-0.096347	2.396908	-2.230690
H	-1.293318	2.843624	-1.007373
C	0.427308	2.645843	1.591627
H	0.977255	2.145247	2.394158
H	0.798421	3.671755	1.492810
H	-0.629785	2.681690	1.872464
C	3.041388	-1.423424	-1.688659
H	2.680989	-0.731966	-2.456462
H	4.136451	-1.441985	-1.711080
H	2.667944	-2.422375	-1.935538
C	3.288305	-2.073355	1.118255
H	2.946197	-3.097927	0.940136
H	4.372533	-2.036440	0.968558
H	3.064208	-1.815204	2.157999
C	-0.929232	-2.258271	0.133916
H	-0.486729	-2.657661	-0.783854
H	-0.333320	-2.526493	1.014638
H	-1.912380	-2.713911	0.251404

Pd_NN2H+_TS

B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1353.03051056 a.u.
Enthalpy Correction = 0.371400 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -1353.27782794

Atom	X-Coord	Y-Coord	Z-Coord
Pd	-0.054454	-0.368916	0.024407
P	1.005378	1.803483	-0.055515
P	2.173656	-1.272023	0.040177
H	-1.264959	-1.542014	0.076990
C	-2.130626	-0.421820	0.013036
N	-2.947170	-0.379544	-1.080880
C	-2.481502	-0.497217	-2.457396
H	-1.582147	-1.117196	-2.472834
H	-3.258331	-0.970281	-3.061812
H	-2.244839	0.487241	-2.872302
N	-2.962651	-0.274898	1.086206
C	-2.515799	-0.260127	2.473986
H	-1.628546	-0.891148	2.565273
H	-2.265640	0.757013	2.790794
H	-3.308849	-0.655813	3.111892
C	-4.261831	-0.168941	-0.694014
H	-5.064975	-0.090357	-1.410280
C	-4.271519	-0.103313	0.662141
H	-5.084789	0.043543	1.355873
C	3.307624	0.192071	0.307356
H	4.330431	-0.053975	-0.003228

H	3.339444	0.376096	1.388752
C	2.803741	1.446117	-0.430507
H	2.879897	1.303200	-1.515974
H	3.422230	2.316965	-0.180444
C	0.587405	3.131755	-1.270729
H	-0.417735	3.512705	-1.064891
H	1.298060	3.964016	-1.215893
H	0.597129	2.722492	-2.285433
C	1.083580	2.732263	1.543358
H	1.438535	2.076129	2.343833
H	1.751355	3.598008	1.469505
H	0.082010	3.081753	1.812301
C	2.766887	-1.992589	-1.556250
H	2.583086	-1.293164	-2.377458
H	3.837310	-2.223228	-1.516140
H	2.213255	-2.912548	-1.767272
C	2.764232	-2.499435	1.286632
H	2.234464	-3.446000	1.142562
H	3.841251	-2.678028	1.193950
H	2.547325	-2.138677	2.296619

Pd_NN2Me+_TS

B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1392.31868499 a.u.
Enthalpy Correction = 0.403217 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -1392.57562860

Atom	X-Coord	Y-Coord	Z-Coord
Pd	-0.037705	-0.424412	-0.005424
P	-0.769198	1.841491	0.012649
P	-2.450819	-1.010761	-0.010766
C	1.366530	-2.266116	-0.028270
H	0.874216	-2.667847	0.860414
H	0.893133	-2.641098	-0.938516
H	2.401165	-2.615004	-0.021700
C	1.997676	-0.509260	-0.001608
N	2.791624	-0.237734	1.093710
C	2.399108	-0.455682	2.478337
H	1.326530	-0.278436	2.579112
H	2.630800	-1.476816	2.803154
H	2.935581	0.248718	3.118325
N	2.796205	-0.213000	-1.087477
C	2.412596	-0.403945	-2.478798
H	1.331570	-0.284089	-2.570190
H	2.905296	0.351315	-3.096013
H	2.699823	-1.398850	-2.838684
C	4.061006	0.162045	0.686846
H	4.828256	0.430980	1.396290
C	4.063871	0.177493	-0.666582
H	4.833897	0.462846	-1.366557
C	-3.295906	0.621537	-0.363396
H	-4.356196	0.573645	-0.086657
H	-3.257911	0.772059	-1.449779

C	-2.604049	1.791546	0.360142
H	-2.716881	1.684610	1.446456
H	-3.067077	2.747152	0.084652
C	-0.141169	3.072717	1.238947
H	-0.680841	4.023630	1.166908
H	-0.253603	2.676605	2.252794
H	0.922603	3.257237	1.059613
C	-0.657378	2.770245	-1.583678
H	-1.125512	2.194631	-2.387856
H	-1.149958	3.746518	-1.511467
H	0.394160	2.924311	-1.845166
C	-3.205637	-1.533272	1.597724
H	-2.910332	-0.843555	2.394457
H	-4.299389	-1.562470	1.539262
H	-2.841210	-2.530086	1.865765
C	-3.257020	-2.157465	-1.218049
H	-2.927174	-3.183014	-1.023490
H	-4.349597	-2.121300	-1.145537
H	-2.959226	-1.893617	-2.237629

Pd_NN2Ph+_TS

B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1584.05759279 a.u.
Enthalpy Correction = 0.460179 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -1584.36763681

Atom	X-Coord	Y-Coord	Z-Coord
Pd	-0.264250	-0.032855	0.022642
P	-2.176555	-1.467108	-0.205936
P	-1.910271	1.796271	0.168768
C	1.524357	-1.056416	0.047939
N	2.157208	-1.771097	-0.953182
C	2.068793	-1.510432	-2.380410
H	1.051741	-1.205156	-2.635819
H	2.772527	-0.728059	-2.684332
H	2.304083	-2.431320	-2.918073
N	1.917139	-1.696982	1.212905
C	1.341649	-1.490641	2.536330
H	0.685014	-0.620269	2.509930
H	0.746594	-2.362531	2.829765
H	2.133888	-1.334787	3.275225
C	2.948836	-2.775257	-0.412542
H	3.542229	-3.426901	-1.035041
C	2.794778	-2.733769	0.930872
H	3.211197	-3.356232	1.707853
C	-3.574130	0.946710	0.290000
H	-4.379658	1.631613	-0.001570
H	-3.733461	0.703136	1.348189
C	-3.620697	-0.334734	-0.563088
H	-3.568538	-0.081821	-1.629784
H	-4.565956	-0.869955	-0.408995
C	3.345332	3.105400	-0.235837
C	3.206250	2.463182	0.997646

C	2.426980	1.313701	1.112235
C	1.765188	0.769796	-0.007141
C	1.923220	1.427163	-1.248758
C	2.696278	2.584449	-1.356343
H	3.958329	3.997468	-0.322853
H	3.710381	2.856623	1.876092
H	2.353962	0.834879	2.082028
H	1.413808	1.060151	-2.132673
H	2.789108	3.078164	-2.319986
C	-2.088114	2.859186	-1.336505
H	-2.227318	2.234586	-2.224509
H	-2.938500	3.544318	-1.247208
H	-1.174033	3.444464	-1.477045
C	-1.976593	3.037014	1.538320
H	-1.089512	3.676348	1.490303
H	-2.870417	3.667074	1.471335
H	-1.973223	2.524849	2.505503
C	-2.330081	-2.755398	-1.523028
H	-1.589299	-3.542824	-1.352445
H	-3.328606	-3.206724	-1.529289
H	-2.136318	-2.309991	-2.503618
C	-2.728771	-2.384285	1.305025
H	-2.787659	-1.703813	2.159875
H	-3.709380	-2.849050	1.152119
H	-2.003167	-3.167836	1.544661

Pd_NO2H+_TS

B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1333.56162683 a.u.
Enthalpy Correction = 0.328486 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -1333.80646374

Atom	X-Coord	Y-Coord	Z-Coord
Pd	0.144476	-0.390307	-0.111046
P	-0.828404	1.786679	0.104484
P	-2.117010	-1.220415	-0.067831
C	-3.199701	0.292820	-0.252958
H	-4.223572	0.074992	0.074100
H	-3.248596	0.517489	-1.325729
C	-2.628072	1.497745	0.516654
H	-2.682366	1.319804	1.598095
H	-3.213510	2.402576	0.312253
C	-2.761169	-2.378011	-1.350949
H	-2.541287	-1.986173	-2.348459
H	-2.262463	-3.346573	-1.248979
H	-3.842537	-2.522505	-1.251383
C	-2.686269	-1.982942	1.516035
H	-2.466059	-1.318686	2.357173
H	-3.762485	-2.186673	1.493653
H	-2.150956	-2.923202	1.679398
C	-0.293266	3.046596	1.342562
H	0.733333	3.357438	1.125680
H	-0.941657	3.929389	1.316613

H	-0.317632	2.617063	2.348562
C	-0.881363	2.742731	-1.475084
H	-1.303326	2.125938	-2.274014
H	-1.482828	3.652343	-1.367754
H	0.135429	3.020793	-1.768061
N	3.138034	-0.511850	0.657548
C	2.169506	-0.444215	-0.289724
O	2.793626	-0.182493	-1.462843
C	4.148519	-0.063411	-1.235968
C	4.381574	-0.261949	0.072496
H	4.771039	0.150419	-2.089058
H	5.296999	-0.253343	0.643303
C	2.898212	-0.779933	2.070947
H	2.865187	0.153501	2.640780
H	3.694022	-1.419211	2.459521
H	1.939033	-1.293390	2.167807
H	1.336473	-1.585531	-0.369349

Pd_NO2Me+_TS

B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1372.85948315 a.u.
Enthalpy Correction = 0.360409 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -1373.11409611

Atom	X-Coord	Y-Coord	Z-Coord
Pd	0.049437	-0.434109	-0.092843
P	-0.651575	1.820553	0.036926
P	-2.353633	-0.985016	-0.001279
C	-3.206785	0.654509	-0.285062
H	-4.253626	0.604683	0.037806
H	-3.215909	0.825914	-1.368723
C	-2.476188	1.805535	0.430798
H	-2.564841	1.693293	1.518696
H	-2.925253	2.772293	0.172463
C	-3.189097	-2.115494	-1.199323
H	-2.934397	-1.825603	-2.223324
H	-2.838451	-3.140046	-1.039330
H	-4.277999	-2.094841	-1.082155
C	-3.018941	-1.543867	1.631782
H	-2.680570	-0.871240	2.425846
H	-4.114222	-1.572624	1.630639
H	-2.640920	-2.546067	1.857204
C	0.050800	3.017501	1.253030
H	1.117207	3.158532	1.051739
H	-0.451226	3.989245	1.189243
H	-0.059118	2.626845	2.269161
C	-0.537690	2.728973	-1.566092
H	-1.033795	2.158536	-2.356663
H	-0.998051	3.720737	-1.494529
H	0.514133	2.842688	-1.845333
N	2.979321	-0.316770	0.730146
C	2.034744	-0.494290	-0.246333
O	2.643959	-0.180029	-1.426393

C	3.974257	0.118479	-1.182225
C	4.197186	0.035195	0.137615
H	4.580950	0.376235	-2.034413
H	5.090653	0.205344	0.718279
C	2.788063	-0.586065	2.148435
H	3.222511	0.223457	2.741314
H	3.258513	-1.533405	2.434241
H	1.717395	-0.637061	2.352470
C	1.386515	-2.280119	-0.388047
H	1.027731	-2.787870	0.510000
H	0.816013	-2.563040	-1.276083
H	2.423163	-2.574574	-0.559865

Pd_NS2H+_TS

B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1656.53657447 a.u.
Enthalpy Correction = 0.325709 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -1656.78836134

Atom	X-Coord	Y-Coord	Z-Coord
Pd	0.000162	-0.376036	-0.049582
P	-2.240344	-1.236033	-0.139195
P	-1.027000	1.784177	0.156011
C	-2.842688	1.458777	0.457638
H	-3.431505	2.356141	0.231846
H	-2.957649	1.263450	1.531303
C	-3.345668	0.255457	-0.360644
H	-3.341399	0.496437	-1.431011
H	-4.380575	0.010038	-0.093261
C	-0.579432	3.011386	1.459965
H	-0.645662	2.547945	2.448895
H	0.450947	3.346311	1.305716
H	-1.241937	3.883459	1.429682
C	-1.005621	2.790897	-1.392776
H	-1.373928	2.196172	-2.233933
H	-1.624874	3.689025	-1.289865
H	0.021630	3.092699	-1.618795
C	-2.784540	-2.387998	-1.472352
H	-2.266706	-3.345117	-1.358388
H	-3.865529	-2.561465	-1.433835
H	-2.521836	-1.974089	-2.450413
C	-2.873997	-2.036418	1.400772
H	-2.709600	-1.382103	2.262181
H	-3.943366	-2.260797	1.320882
H	-2.328526	-2.968624	1.576118
N	2.922781	-0.536664	0.905501
C	2.045006	-0.405893	-0.122398
S	2.944815	0.004472	-1.561522
C	4.465769	-0.004905	-0.702343
C	4.262388	-0.309446	0.595661
H	5.403874	0.205562	-1.195832
H	5.004156	-0.390433	1.378824
C	2.477572	-0.870632	2.261686

H	2.126271	0.026584	2.779050
H	3.308748	-1.311894	2.814496
H	1.659060	-1.591958	2.197080
H	1.171884	-1.574107	-0.247650

Pd_NS2Me+_TS

B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1695.83175366 a.u.
Enthalpy Correction = 0.357832 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -1696.09407684

Atom	X-Coord	Y-Coord	Z-Coord
Pd	-0.095012	-0.445672	-0.004146
P	-0.765223	1.819645	0.076573
P	-2.504892	-0.948348	-0.066977
C	-3.315677	0.703521	-0.402530
H	-4.380069	0.670175	-0.140642
H	-3.259940	0.872001	-1.485241
C	-2.610602	1.845520	0.352077
H	-2.768361	1.741453	1.432898
H	-3.023942	2.819008	0.061537
C	-3.271720	-2.063732	-1.323746
H	-2.947857	-1.771780	-2.327380
H	-2.943591	-3.092941	-1.147187
H	-4.365716	-2.031277	-1.277044
C	-3.289636	-1.505868	1.512543
H	-3.012716	-0.834564	2.331157
H	-4.381510	-1.533884	1.427873
H	-2.930658	-2.508666	1.764935
C	-0.109986	3.001027	1.333014
H	0.969228	3.118937	1.194880
H	-0.585991	3.983496	1.240172
H	-0.288401	2.613548	2.340625
C	-0.515242	2.710506	-1.518854
H	-1.010052	2.170256	-2.331237
H	-0.910307	3.731308	-1.472768
H	0.554488	2.751064	-1.746508
N	2.788128	-0.329937	0.952744
C	1.905147	-0.526876	-0.078474
S	2.744001	-0.130064	-1.585075
C	4.254034	0.181520	-0.743845
C	4.087213	0.025182	0.581668
H	5.150626	0.472276	-1.271847
H	4.831679	0.158068	1.355622
C	2.426035	-0.611936	2.341821
H	1.434645	-0.203459	2.548437
H	3.154004	-0.140303	3.004390
H	2.418802	-1.691229	2.531571
C	1.206630	-2.325375	-0.170197
H	0.583889	-2.790550	0.600431
H	0.887368	-2.608172	-1.175180
H	2.228569	-2.673650	-0.021591

Pt_NN2Me+_TS
B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1384.74424969 a.u.
Enthalpy Correction = 0.403224 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -1385.00725150

Atom	X-Coord	Y-Coord	Z-Coord
Pt	-0.095595	-0.362065	-0.018924
P	-0.672277	1.856862	0.041962
P	-2.468792	-0.872530	-0.016542
C	1.517856	-2.201750	-0.095329
H	1.039574	-2.640735	0.783322
H	1.026556	-2.555860	-1.004842
H	2.548811	-2.569947	-0.121100
C	1.962926	-0.521487	-0.011941
N	2.753046	-0.240973	1.108999
C	2.373829	-0.540286	2.478527
H	1.318361	-0.298156	2.626506
H	2.538227	-1.596615	2.727255
H	2.973851	0.072492	3.155489
N	2.771740	-0.135493	-1.087993
C	2.416027	-0.303393	-2.485913
H	1.369590	-0.024369	-2.635036
H	3.045055	0.352063	-3.092836
H	2.563251	-1.337085	-2.824069
C	4.013148	0.198881	0.717081
H	4.770922	0.465025	1.437807
C	4.024644	0.263443	-0.634417
H	4.794505	0.596128	-1.313496
C	-3.267911	0.794726	-0.312591
H	-4.315752	0.780978	0.009774
H	-3.270176	0.957538	-1.397636
C	-2.503510	1.929749	0.394833
H	-2.615591	1.843507	1.482825
H	-2.904906	2.909221	0.107920
C	0.080154	2.973632	1.299523
H	-0.347704	3.980629	1.238575
H	-0.090178	2.573016	2.303069
H	1.159454	3.035010	1.130474
C	-0.459704	2.782837	-1.538985
H	-0.968603	2.258039	-2.352455
H	-0.863550	3.798253	-1.457070
H	0.605040	2.843289	-1.783489
C	-3.210912	-1.436024	1.580151
H	-2.881629	-0.785788	2.396075
H	-4.305611	-1.431466	1.536568
H	-2.870409	-2.452249	1.801992
C	-3.291555	-1.957656	-1.264347
H	-2.986346	-2.996116	-1.101883
H	-4.383148	-1.896665	-1.193880
H	-2.980649	-1.664832	-2.271687

Pt_NN2Ph+_TS
B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1576.48628091 a.u.
Enthalpy Correction = 0.460328 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -1576.80290605

Atom	X-Coord	Y-Coord	Z-Coord
Pt	-0.265327	-0.009851	0.013161
P	-2.027540	-1.491647	-0.239857
P	-1.931784	1.730921	0.190316
C	1.586803	-0.948926	0.061400
N	2.220998	-1.731395	-0.916110
C	2.158849	-1.518637	-2.346997
H	1.133820	-1.275941	-2.642611
H	2.826959	-0.708815	-2.666123
H	2.460259	-2.439926	-2.850490
N	1.977604	-1.563141	1.268582
C	1.287650	-1.413487	2.541972
H	0.868214	-0.410000	2.627326
H	0.464869	-2.133570	2.632330
H	1.997664	-1.578973	3.357812
C	2.991892	-2.722646	-0.323163
H	3.592492	-3.397996	-0.912914
C	2.827477	-2.632603	1.014806
H	3.231763	-3.236286	1.812899
C	-3.560993	0.819415	0.316076
H	-4.393980	1.471811	0.028707
H	-3.703496	0.567185	1.374402
C	-3.556611	-0.461367	-0.540324
H	-3.554816	-0.203839	-1.606921
H	-4.457593	-1.058977	-0.356369
C	3.216493	3.210555	-0.301358
C	3.201547	2.548427	0.932054
C	2.543980	1.332209	1.070168
C	1.875342	0.730555	-0.022371
C	1.918382	1.410616	-1.266937
C	2.571395	2.636871	-1.397247
H	3.739097	4.156604	-0.406998
H	3.716274	2.979406	1.786203
H	2.582851	0.824483	2.027147
H	1.412240	0.997402	-2.131446
H	2.576577	3.140884	-2.359694
C	-2.146385	2.820661	-1.286835
H	-2.272913	2.209881	-2.185957
H	-3.013908	3.480520	-1.176483
H	-1.247949	3.431568	-1.418323
C	-1.999297	2.921608	1.600152
H	-1.132844	3.588453	1.553269
H	-2.913199	3.525341	1.574271
H	-1.957457	2.375033	2.547099
C	-2.035765	-2.699001	-1.633721
H	-1.206338	-3.402045	-1.511635
H	-2.976473	-3.259936	-1.667421
H	-1.901886	-2.168544	-2.580979

C	-2.467840	-2.533231	1.221277
H	-2.577373	-1.904926	2.109789
H	-3.404278	-3.075170	1.047207
H	-1.670967	-3.258702	1.411491

Pt_NO2Me+_TS

B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1365.29042241 a.u.
Enthalpy Correction = 0.360433 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -1365.55270873

Atom	X-Coord	Y-Coord	Z-Coord
Pt	-0.007675	-0.359221	-0.085868
P	-0.610980	1.839923	0.036949
P	-2.379379	-0.871589	0.021121
C	-3.214137	0.786724	-0.199393
H	-4.240963	0.755164	0.182845
H	-3.280086	0.968592	-1.279195
C	-2.418255	1.914638	0.484002
H	-2.476068	1.817169	1.575150
H	-2.830791	2.897590	0.227026
C	-3.209342	-1.950796	-1.222460
H	-2.944553	-1.622489	-2.231922
H	-2.865024	-2.982190	-1.097616
H	-4.298619	-1.927124	-1.110088
C	-3.022093	-1.494094	1.636461
H	-2.669419	-0.854636	2.451006
H	-4.117277	-1.519301	1.646724
H	-2.643125	-2.505343	1.814067
C	0.232917	2.930067	1.253309
H	1.300757	2.973036	1.018936
H	-0.179682	3.944457	1.221724
H	0.114865	2.525332	2.262493
C	-0.453182	2.730723	-1.564956
H	-1.022749	2.210427	-2.339822
H	-0.813862	3.761661	-1.478761
H	0.597963	2.740095	-1.867668
N	2.938771	-0.212404	0.756035
C	1.991508	-0.477740	-0.230049
O	2.605476	-0.158271	-1.428863
C	3.938166	0.131501	-1.180701
C	4.156940	0.093258	0.141400
H	4.552194	0.366098	-2.034416
H	5.053736	0.281525	0.711704
C	2.770584	-0.505945	2.168636
H	3.412309	0.157530	2.754006
H	3.031521	-1.545864	2.404450
H	1.730586	-0.325380	2.450921
C	1.540805	-2.187775	-0.322064
H	1.194732	-2.678644	0.590784
H	0.972208	-2.518153	-1.196491
H	2.576690	-2.495665	-0.495655

Pt_NS2Me+_TS
B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1688.26379422 a.u.
Enthalpy Correction = 0.357998 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -1688.53244750

Atom	X-Coord	Y-Coord	Z-Coord
Pt	-0.125153	-0.363486	-0.023937
P	-0.719812	1.840643	0.089125
P	-2.498064	-0.842933	-0.063402
C	-3.312928	0.820437	-0.317367
H	-4.359454	0.790995	0.007089
H	-3.318360	1.010867	-1.397602
C	-2.550609	1.938375	0.418333
H	-2.679434	1.840612	1.503293
H	-2.933315	2.926490	0.136726
C	-3.251556	-1.910276	-1.364118
H	-2.936368	-1.566705	-2.353772
H	-2.906417	-2.940814	-1.234616
H	-4.345450	-1.895441	-1.308982
C	-3.237444	-1.481865	1.503253
H	-2.942630	-0.848694	2.345311
H	-4.330715	-1.512484	1.442018
H	-2.865793	-2.493137	1.695845
C	0.067322	2.903494	1.365591
H	1.149965	2.912069	1.207547
H	-0.309771	3.930249	1.305394
H	-0.136030	2.504304	2.363394
C	-0.435924	2.729983	-1.494177
H	-0.996241	2.247181	-2.299729
H	-0.742635	3.778711	-1.416138
H	0.628200	2.681230	-1.745419
N	2.760448	-0.278543	0.974854
C	1.883095	-0.490029	-0.086897
S	2.755918	-0.013958	-1.581873
C	4.266860	0.209848	-0.702017
C	4.073851	0.027347	0.614990
H	5.180710	0.485401	-1.207780
H	4.816488	0.116867	1.397567
C	2.396898	-0.617380	2.346565
H	3.106234	-0.147571	3.031266
H	2.414246	-1.702115	2.512938
H	1.393569	-0.241532	2.561223
C	1.359451	-2.217808	-0.241490
H	0.729967	-2.720578	0.502725
H	1.065654	-2.486585	-1.258335
H	2.375758	-2.582673	-0.078679

5. Products

Ni_NN2H+_PR
B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1395.59333499 a.u.
Enthalpy Correction = 0.373331 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -2734.84112251

Atom	X-Coord	Y-Coord	Z-Coord
Ni	-0.050080	-0.524467	0.031229
P	-0.683145	1.665806	-0.090212
P	-2.185017	-1.078393	0.060254
C	1.869094	-0.430217	0.029535
N	2.701190	-0.301834	1.095736
C	2.264533	-0.206457	2.484204
H	1.174996	-0.252677	2.504301
H	2.666304	-1.042390	3.063758
H	2.601028	0.735616	2.927325
N	2.697047	-0.542654	-1.041805
C	2.252849	-0.739896	-2.417300
H	1.177167	-0.920593	-2.406613
H	2.472465	0.143066	-3.025544
H	2.755055	-1.609564	-2.849453
C	4.031831	-0.332940	0.696328
H	4.847704	-0.250254	1.397902
C	4.028956	-0.483343	-0.650808
H	4.841895	-0.554526	-1.357034
C	-3.191435	0.446869	-0.336980
H	-4.222928	0.339486	0.018086
H	-3.235473	0.526837	-1.430280
C	-2.518374	1.693040	0.264079
H	-2.635763	1.700368	1.354831
H	-2.976662	2.614584	-0.113424
C	0.009610	2.984039	0.998974
H	-0.504663	3.938412	0.844786
H	-0.090349	2.692431	2.048876
H	1.073366	3.117918	0.779205
C	-0.547382	2.406157	-1.778189
H	-1.042554	1.765570	-2.514309
H	-0.999951	3.403018	-1.812406
H	0.507748	2.489045	-2.056171
C	-2.789839	-1.620379	1.715834
H	-2.575701	-0.856319	2.469115
H	-3.868490	-1.809579	1.696519
H	-2.269758	-2.538147	2.004881
C	-2.815740	-2.371858	-1.085573
H	-2.348714	-3.328761	-0.835950
H	-3.903674	-2.470212	-1.009550
H	-2.549151	-2.120926	-2.116537

H	0.178499	-1.997188	0.094505

Ni_NN2Me+_PR

B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1434.90432570 a.u.
Enthalpy Correction = 0.404817 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -2774.16161436

Atom	X-Coord	Y-Coord	Z-Coord
Ni	-0.096268	-0.521554	-0.009374
P	-0.547789	1.738121	0.015834
P	-2.314561	-0.826790	-0.007820
C	0.144697	-2.473710	-0.100061
H	-0.624586	-3.036457	0.441632
H	0.079818	-2.732869	-1.165530
H	1.119449	-2.795608	0.275316
C	1.828918	-0.361104	0.004920
N	2.648626	-0.352724	1.089211
C	2.193966	-0.433352	2.473423
H	1.122093	-0.635120	2.468440
H	2.708221	-1.249590	2.987927
H	2.390713	0.505261	3.000711
N	2.671064	-0.308393	-1.061070
C	2.252143	-0.351890	-2.458430
H	1.163850	-0.409615	-2.487569
H	2.587709	0.545895	-2.986208
H	2.669463	-1.235250	-2.950033
C	3.984088	-0.297465	0.706671
H	4.790533	-0.284930	1.423769
C	3.998384	-0.270406	-0.648430
H	4.819622	-0.232239	-1.347628
C	-3.159416	0.807997	-0.327689
H	-4.202702	0.785938	0.007802
H	-3.176317	0.955685	-1.414667
C	-2.373858	1.940615	0.354859
H	-2.505333	1.893999	1.443130
H	-2.729433	2.925942	0.031589
C	0.262147	2.885691	1.213971
H	-0.132303	3.903021	1.120221
H	0.098308	2.536205	2.238033
H	1.340354	2.908792	1.027247
C	-0.296238	2.597856	-1.601942
H	-0.841065	2.079904	-2.396988
H	-0.637978	3.637460	-1.556356
H	0.767683	2.588376	-1.858242
C	-2.984855	-1.377051	1.621146
H	-2.715187	-0.661169	2.403611
H	-4.075380	-1.473423	1.587340
H	-2.550332	-2.345889	1.884550
C	-3.080906	-1.988061	-1.212724
H	-2.676875	-2.992817	-1.060308
H	-4.168745	-2.019098	-1.092695
H	-2.843076	-1.675752	-2.234101

Ni_NN2Ph+_PR
B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1626.64074844 a.u.
Enthalpy Correction = 0.462130 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -2965.95068481

Atom	X-Coord	Y-Coord	Z-Coord
Ni	0.232359	-0.034217	0.012679
P	2.364763	0.808670	0.004523
P	1.161179	-2.073518	0.001914
C	-0.711132	1.653840	-0.001227
N	-1.127722	2.365037	-1.082091
C	-0.922166	1.970761	-2.470973
H	-0.150262	1.200784	-2.501912
H	-1.846481	1.568047	-2.894793
H	-0.597734	2.834199	-3.057962
N	-1.165407	2.359844	1.067843
C	-1.009065	1.959841	2.461795
H	-0.243277	1.185408	2.516792
H	-0.699788	2.819651	3.062272
H	-1.949628	1.561290	2.852298
C	-1.850605	3.487025	-0.694495
H	-2.269143	4.179188	-1.408848
C	-1.874239	3.483685	0.660536
H	-2.316934	4.172705	1.363277
C	3.004112	-1.894753	0.269094
H	3.542728	-2.775495	-0.099224
H	3.169131	-1.849801	1.352812
C	3.511050	-0.607409	-0.402641
H	3.508295	-0.719667	-1.494122
H	4.541344	-0.378529	-0.105933
C	-4.062199	-2.109543	-0.008717
C	-3.430744	-1.814325	1.201048
C	-2.166795	-1.212884	1.209013
C	-1.503779	-0.891494	0.012426
C	-2.153834	-1.199963	-1.194731
C	-3.417484	-1.802986	-1.207960
H	-5.043310	-2.575690	-0.016347
H	-3.920509	-2.052995	2.142246
H	-1.699390	-1.006763	2.170443
H	-1.678331	-0.976750	-2.148481
H	-3.896505	-2.031459	-2.157155
C	1.013578	-2.940780	-1.618067
H	1.451394	-2.333843	-2.416773
H	1.520306	-3.911193	-1.590473
H	-0.045455	-3.093192	-1.843745
C	0.641400	-3.338734	1.230917
H	-0.423988	-3.546506	1.104691
H	1.213014	-4.263917	1.103548
H	0.797324	-2.959494	2.245529
C	2.877397	2.158299	-1.145052
H	2.314778	3.068411	-0.914881

H	3.947389	2.373246	-1.054698
H	2.660222	1.873347	-2.179265
C	2.971855	1.412638	1.643726
H	2.840625	0.638606	2.406111
H	4.031393	1.686263	1.595835
H	2.395408	2.291482	1.948765

Ni_NO2H+_PR
B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1376.12804276 a.u.
Enthalpy Correction = 0.330734 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -2715.37245999

Atom	X-Coord	Y-Coord	Z-Coord
Ni	-0.057685	-0.495003	-0.106713
P	0.615239	1.651675	0.255896
P	2.064406	-1.085940	-0.182027
C	-1.944286	-0.289677	-0.215411
O	-2.508522	0.608214	-1.056019
N	-2.964726	-0.941199	0.366422
C	-2.832226	-2.013511	1.352118
H	-1.790714	-2.333927	1.363933
H	-3.124935	-1.653220	2.342168
H	-3.470241	-2.851973	1.062942
C	-3.879816	0.500421	-1.000727
H	-4.455614	1.152278	-1.637171
C	-4.187021	-0.458565	-0.111247
H	-5.135783	-0.845337	0.226404
C	3.097795	0.366459	0.379654
H	4.128946	0.277334	0.018346
H	3.137541	0.326778	1.475280
C	2.451503	1.682836	-0.085639
H	2.574262	1.806544	-1.168806
H	2.924169	2.549072	0.391763
C	-0.061164	3.076684	-0.696173
H	0.448202	4.008784	-0.429967
H	0.055492	2.896375	-1.768897
H	-1.129283	3.181338	-0.485457
C	0.468830	2.192710	2.015425
H	0.945267	1.463185	2.677274
H	0.934154	3.172157	2.169650
H	-0.588429	2.256754	2.290794
C	2.632634	-1.442555	-1.897681
H	2.405452	-0.598451	-2.555460
H	3.710245	-1.636888	-1.922509
H	2.099576	-2.318861	-2.277196
C	2.671017	-2.511570	0.807689
H	2.192286	-3.427369	0.449697
H	3.757607	-2.615968	0.721426
H	2.406695	-2.375955	1.860623
H	-0.286731	-1.955322	-0.329777

Ni_NO2Me+_PR
B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1415.43798506 a.u.
Enthalpy Correction = 0.361850 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -2754.69273421

Atom	X-Coord	Y-Coord	Z-Coord
Ni	-0.010788	-0.506490	-0.090355
P	0.475824	1.730167	0.184725
P	2.208398	-0.844644	-0.090387
C	-1.894364	-0.282700	-0.241344
O	-2.442637	0.282708	-1.339199
N	-2.924200	-0.654179	0.537117
C	-2.804009	-1.327292	1.829484
H	-1.747071	-1.509109	2.021005
H	-3.221936	-0.697613	2.619579
H	-3.337567	-2.280703	1.800375
C	-3.817888	0.245359	-1.245587
H	-4.381581	0.654602	-2.067896
C	-4.140565	-0.332996	-0.077332
H	-5.095285	-0.548957	0.376268
C	3.064871	0.716531	0.467247
H	4.115790	0.721278	0.155347
H	3.055664	0.718282	1.564254
C	2.312068	1.941138	-0.079038
H	2.472689	2.037689	-1.159878
H	2.668843	2.869329	0.382150
C	-0.289591	3.012012	-0.897219
H	0.126921	4.003974	-0.693186
H	-0.119161	2.759813	-1.948030
H	-1.369970	3.039395	-0.727979
C	0.188421	2.381602	1.890545
H	0.694050	1.750894	2.627994
H	0.555211	3.408923	1.989246
H	-0.883145	2.368282	2.112916
C	2.868287	-1.144653	-1.786307
H	2.576457	-0.328662	-2.454165
H	3.960248	-1.227171	-1.775338
H	2.444696	-2.071520	-2.183699
C	2.958063	-2.183257	0.924908
H	2.560189	-3.150610	0.605407
H	4.047516	-2.193967	0.817147
H	2.704225	-2.039570	1.979560
C	-0.261280	-2.452384	-0.288771
H	0.377816	-2.842681	-1.089270
H	0.030219	-2.925118	0.658074
H	-1.289674	-2.740467	-0.520764

Ni_NS2H+_PR
B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1699.10046955 a.u.
Enthalpy Correction = 0.327872 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -3038.35297229

Atom	X-Coord	Y-Coord	Z-Coord
Ni	0.086976	-0.495884	-0.069753
P	0.784901	1.639860	0.320147
P	2.206848	-1.087378	-0.247470
C	-1.811285	-0.354543	-0.108588
S	-2.637058	0.455270	-1.396734
N	-2.737718	-0.889717	0.706115
C	-2.384262	-1.654072	1.911215
H	-1.370078	-2.033905	1.787823
H	-2.439477	-1.012294	2.795344
H	-3.077444	-2.490576	2.023508
C	-4.213015	0.031979	-0.782237
H	-5.129042	0.318006	-1.279334
C	-4.073365	-0.684188	0.352951
H	-4.854862	-1.093831	0.978912
C	3.266934	0.342931	0.320902
H	4.283317	0.262257	-0.081814
H	3.348160	0.268372	1.412395
C	2.609957	1.675648	-0.077748
H	2.698711	1.836522	-1.159340
H	3.100453	2.524053	0.413574
C	0.097411	3.111201	-0.552041
H	0.624339	4.025024	-0.257952
H	0.186401	2.981128	-1.634895
H	-0.963554	3.221163	-0.308357
C	0.696078	2.118834	2.101634
H	1.174549	1.357070	2.724403
H	1.184459	3.083131	2.278587
H	-0.352488	2.193910	2.405899
C	2.703182	-1.383102	-1.997076
H	2.452610	-0.515177	-2.614059
H	3.778157	-1.578759	-2.073153
H	2.152345	-2.244286	-2.385855
C	2.854533	-2.547917	0.662729
H	2.357757	-3.450070	0.294639
H	3.935877	-2.649964	0.523646
H	2.638561	-2.449735	1.730787
H	-0.160375	-1.951455	-0.297320

Ni_NS2Me+_PR
B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1738.41069453 a.u.
Enthalpy Correction = 0.359217 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -3077.67302835

Atom	X-Coord	Y-Coord	Z-Coord
Ni	0.127027	-0.511750	-0.012919
P	0.632501	1.733408	0.165764
P	2.345544	-0.852074	-0.121246

C	-1.770671	-0.324207	-0.088315
S	-2.573565	0.070845	-1.570767
N	-2.711064	-0.538122	0.848442
C	-2.387452	-0.915699	2.231993
H	-1.318236	-1.113017	2.290560
H	-2.656585	-0.104219	2.914370
H	-2.940040	-1.818555	2.503932
C	-4.161640	-0.071543	-0.860132
H	-5.069091	0.085732	-1.425776
C	-4.042443	-0.403123	0.441702
H	-4.833904	-0.567507	1.160970
C	3.233476	0.721573	0.344570
H	4.265527	0.715082	-0.024806
H	3.285235	0.751063	1.439982
C	2.454492	1.934955	-0.189272
H	2.563010	2.009607	-1.278251
H	2.833408	2.871994	0.235020
C	-0.169988	3.024457	-0.878575
H	0.270341	4.010003	-0.694145
H	-0.053096	2.774689	-1.937518
H	-1.240470	3.068836	-0.657069
C	0.434434	2.395791	1.880608
H	0.974370	1.767727	2.595767
H	0.809546	3.422198	1.954244
H	-0.624902	2.388235	2.155414
C	2.903231	-1.203741	-1.843999
H	2.569840	-0.410996	-2.520250
H	3.994172	-1.284925	-1.896180
H	2.459511	-2.144211	-2.183870
C	3.160225	-2.162115	0.881912
H	2.741946	-3.137879	0.619259
H	4.239981	-2.178087	0.701079
H	2.978722	-1.986615	1.946651
C	-0.127531	-2.467483	-0.060266
H	0.461895	-2.914770	-0.869235
H	0.226770	-2.866042	0.898971
H	-1.167694	-2.769188	-0.203328

Pd_NN2H+_PR
B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1353.05133758 a.u.
Enthalpy Correction = 0.373474 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -1353.29944308

Atom	X-Coord	Y-Coord	Z-Coord
Pd	0.031805	-0.543985	0.029519
P	0.743444	1.788235	-0.064698
P	2.314847	-1.054223	0.036537
C	-2.039891	-0.388721	0.011713
N	-2.860491	-0.420686	-1.069118
C	-2.416012	-0.549455	-2.453362
H	-1.340696	-0.731514	-2.450373
H	-2.921299	-1.394544	-2.928548

H	-2.634969	0.364833	-3.013347
N	-2.873091	-0.294905	1.079457
C	-2.446592	-0.272975	2.475131
H	-1.362502	-0.388327	2.502267
H	-2.730257	0.673022	2.946153
H	-2.908604	-1.100957	3.019804
C	-4.192514	-0.344517	-0.682494
H	-5.002029	-0.356624	-1.396009
C	-4.200571	-0.266127	0.671045
H	-5.018539	-0.197521	1.371618
C	3.253717	0.543500	0.277166
H	4.292133	0.426950	-0.055443
H	3.284805	0.734246	1.357096
C	2.571254	1.712966	-0.453545
H	2.659077	1.585752	-1.539823
H	3.056171	2.664096	-0.203069
H	-0.253235	-2.106045	0.115171
C	2.987106	-2.186234	1.321261
H	2.704146	-1.829831	2.315951
H	2.557325	-3.182187	1.181305
H	4.078600	-2.252737	1.258113
C	2.958922	-1.746399	-1.545815
H	2.720308	-1.077690	-2.378057
H	4.044307	-1.887387	-1.498970
H	2.480273	-2.710966	-1.738033
C	0.082897	3.001093	-1.289117
H	-0.978180	3.179318	-1.088956
H	0.617263	3.955750	-1.235209
H	0.177509	2.597337	-2.301754
C	0.666399	2.720339	1.529708
H	1.146265	2.143765	2.326243
H	1.161021	3.694168	1.445501
H	-0.379501	2.878534	1.810382

Pd_NN2Me+_PR
B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1392.36031795 a.u.
Enthalpy Correction = 0.404939 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -1392.61955736

Atom	X-Coord	Y-Coord	Z-Coord
Pd	-0.065266	-0.490093	-0.011276
P	-0.666738	1.873199	0.032327
P	-2.391599	-0.860490	-0.014745
C	0.250566	-2.568317	-0.074741
H	-0.487002	-3.099994	0.534050
H	0.151274	-2.881208	-1.120039
H	1.249069	-2.825423	0.283119
C	2.007124	-0.290290	-0.001098
N	2.831296	-0.282013	1.078922
C	2.391253	-0.384364	2.467160
H	1.323202	-0.604564	2.469962
H	2.928015	-1.194320	2.968311

H	2.576141	0.554071	2.998847
N	2.839055	-0.195369	-1.070957
C	2.413303	-0.214897	-2.467235
H	1.325280	-0.283020	-2.490373
H	2.737717	0.697973	-2.975430
H	2.838987	-1.083050	-2.978372
C	4.161335	-0.181441	0.689574
H	4.971551	-0.159093	1.402148
C	4.166369	-0.127790	-0.665122
H	4.981973	-0.053141	-1.367926
C	-3.240629	0.775300	-0.316128
H	-4.288356	0.727575	0.003611
H	-3.245561	0.938181	-1.401034
C	-2.500133	1.921217	0.394891
H	-2.609755	1.826316	1.482480
H	-2.923680	2.893052	0.114572
C	0.045889	3.058158	1.256434
H	-0.430411	4.042088	1.186394
H	-0.087051	2.671191	2.271411
H	1.118393	3.173252	1.070891
C	-0.508450	2.792022	-1.564546
H	-0.999940	2.237262	-2.369400
H	-0.952251	3.791288	-1.496802
H	0.550173	2.894546	-1.822830
C	-3.086778	-1.460194	1.584948
H	-2.831330	-0.766527	2.391412
H	-4.176260	-1.559858	1.529262
H	-2.652772	-2.434934	1.827603
C	-3.118406	-2.000978	-1.262806
H	-2.711656	-3.005725	-1.115272
H	-4.209275	-2.042412	-1.175364
H	-2.850307	-1.668759	-2.270030

Pd_NN2Ph+_PR

B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1584.09379143 a.u.
Enthalpy Correction = 0.461899 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -1584.40816641

Atom	X-Coord	Y-Coord	Z-Coord
Pd	0.217460	0.004987	0.027375
P	2.414236	1.054427	0.017695
P	1.412650	-2.025973	-0.005240
C	-0.999772	1.701229	0.011798
N	-1.471376	2.369305	-1.072566
C	-1.173900	2.033140	-2.460705
H	-0.410709	1.254155	-2.468709
H	-2.072434	1.661012	-2.960938
H	-0.803073	2.915882	-2.989443
N	-1.563934	2.328098	1.075879
C	-1.393429	1.932248	2.469981
H	-0.604149	1.181760	2.519304
H	-1.112478	2.800305	3.072821

H	-2.321576	1.503328	2.858010
C	-2.328405	3.394229	-0.691840
H	-2.808294	4.042075	-1.409178
C	-2.386737	3.368045	0.662259
H	-2.928269	3.988104	1.360010
C	3.226047	-1.638500	0.234108
H	3.845468	-2.460582	-0.143711
H	3.401352	-1.580592	1.315638
C	3.607911	-0.309450	-0.440847
H	3.568530	-0.411910	-1.532683
H	4.634930	-0.022661	-0.184267
C	2.850556	2.424836	-1.140146
H	3.919081	2.661723	-1.095425
H	2.591194	2.144286	-2.165636
H	2.280932	3.321282	-0.875660
C	3.047717	1.670641	1.641751
H	2.955171	0.890928	2.403836
H	4.097380	1.975871	1.569916
H	2.452204	2.530514	1.963933
C	1.324955	-2.928820	-1.608216
H	1.691924	-2.292633	-2.419429
H	1.919041	-3.848312	-1.576571
H	0.280554	-3.179211	-1.815280
C	1.037468	-3.309835	1.255903
H	-0.004852	-3.621385	1.146211
H	1.693104	-4.179541	1.142050
H	1.164304	-2.892305	2.259266
C	-1.539631	-1.090160	0.002475
C	-2.148048	-1.431761	-1.214565
C	-3.333603	-2.176460	-1.242136
C	-3.931117	-2.591623	-0.051089
C	-3.335358	-2.258374	1.166595
C	-2.149487	-1.514208	1.192444
H	-1.704835	-1.120778	-2.158343
H	-3.788018	-2.430110	-2.196935
H	-4.850775	-3.169377	-0.071478
H	-3.791142	-2.577289	2.100969
H	-1.704851	-1.273623	2.155829

Pd_NO2H+_PR

B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1333.58457110 a.u.
Enthalpy Correction = 0.330895 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -1333.82985215

Atom	X-Coord	Y-Coord	Z-Coord
Pd	0.063619	-0.521225	-0.116194
P	-0.662091	1.769359	0.261731
P	-2.207941	-1.054037	-0.151259
C	-3.155823	0.552908	-0.250002
H	-4.198350	0.395156	0.051700
H	-3.170645	0.847117	-1.306767
C	-2.496501	1.650466	0.603179

H	-2.608014	1.421957	1.670418
H	-2.981717	2.618800	0.432224
C	-2.867434	-2.075935	-1.529336
H	-2.577898	-1.636378	-2.488058
H	-2.435231	-3.078853	-1.470581
H	-3.958992	-2.149889	-1.478659
C	-2.829969	-1.881593	1.372398
H	-2.577539	-1.287228	2.255332
H	-3.915903	-2.018310	1.328499
H	-2.350150	-2.859306	1.473195
C	-0.011949	2.808784	1.638720
H	1.045991	3.025009	1.461061
H	-0.557158	3.755591	1.716522
H	-0.096000	2.267405	2.585703
C	-0.533598	2.870944	-1.213319
H	-1.018070	2.401954	-2.074779
H	-0.996962	3.845676	-1.025759
H	0.521817	3.016408	-1.461864
N	3.135306	-0.938300	0.311142
C	2.103267	-0.235384	-0.179199
O	2.645401	0.800059	-0.857311
C	4.018763	0.730374	-0.793820
C	4.346902	-0.348136	-0.063164
H	4.579390	1.495039	-1.306138
H	5.303565	-0.754422	0.225602
C	3.034781	-2.152241	1.122262
H	3.410183	-1.956296	2.130099
H	3.621611	-2.948803	0.658309
H	1.986591	-2.445187	1.165160
H	0.336493	-2.062436	-0.419194

Pd_NO2Me+_PR

B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1372.89309490 a.u.
Enthalpy Correction = 0.362148 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -1373.14963350

Atom	X-Coord	Y-Coord	Z-Coord
Pd	0.029614	-0.469430	-0.129428
P	-0.576668	1.865211	0.190524
P	-2.290184	-0.860747	-0.057015
C	-3.154696	0.789163	-0.178693
H	-4.190445	0.702842	0.170842
H	-3.198158	1.046571	-1.244223
C	-2.398366	1.875613	0.604982
H	-2.480491	1.693062	1.683681
H	-2.830654	2.865084	0.414553
C	-3.074707	-1.898085	-1.356972
H	-2.861081	-1.479873	-2.344966
H	-2.656817	-2.908142	-1.316210
H	-4.159072	-1.955566	-1.215658
C	-2.890950	-1.595484	1.523528
H	-2.572551	-0.981130	2.370802

H	-3.983062	-1.679943	1.530090
H	-2.457491	-2.592568	1.646608
C	0.178214	2.934517	1.490766
H	1.239930	3.083110	1.270346
H	-0.310288	3.913716	1.538131
H	0.095984	2.446535	2.466715
C	-0.446107	2.891548	-1.338892
H	-0.983755	2.408876	-2.160351
H	-0.852630	3.896924	-1.183858
H	0.605303	2.971240	-1.631444
N	3.063978	-0.631718	0.568780
C	2.069035	-0.202089	-0.223031
O	2.658093	0.477089	-1.229001
C	4.026396	0.458139	-1.065031
C	4.302505	-0.228291	0.056035
H	4.621718	0.958138	-1.811350
H	5.237226	-0.470594	0.537023
C	2.891058	-1.406408	1.797386
H	3.257009	-0.831982	2.652618
H	3.444205	-2.346000	1.722782
H	1.828254	-1.614172	1.919138
C	0.331424	-2.514626	-0.534110
H	-0.266548	-3.140912	0.135922
H	0.017330	-2.679911	-1.569877
H	1.381218	-2.797168	-0.435502

Pd_NS2H+_PR

B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1656.55701774 a.u.
Enthalpy Correction = 0.328033 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -1656.80980680

Atom	X-Coord	Y-Coord	Z-Coord
Pd	-0.075992	-0.521712	-0.107925
P	-2.350079	-1.043610	-0.237371
P	-0.813101	1.755247	0.356468
C	-2.651533	1.612052	0.666754
H	-3.136830	2.588308	0.549117
H	-2.775428	1.318296	1.716617
C	-3.296429	0.567633	-0.260576
H	-3.291946	0.923299	-1.298351
H	-4.344397	0.394788	0.012592
C	-0.192021	2.739014	1.787675
H	-0.291814	2.159693	2.710411
H	0.868118	2.967030	1.639789
H	-0.743218	3.679563	1.894075
C	-0.681813	2.932559	-1.060636
H	-1.144974	2.500909	-1.952950
H	-1.166754	3.887604	-0.830873
H	0.373150	3.116982	-1.285871
C	-2.966778	-1.972885	-1.698793
H	-2.532471	-2.976625	-1.694817
H	-4.059027	-2.052420	-1.684467

H	-2.652138	-1.470213	-2.617823
C	-3.022027	-1.967359	1.207722
H	-2.798153	-1.431999	2.134888
H	-4.106079	-2.097798	1.120327
H	-2.546535	-2.950978	1.260213
N	2.898388	-0.869630	0.702032
C	1.982543	-0.326771	-0.115854
S	2.815568	0.544446	-1.353885
C	4.386498	0.141547	-0.713877
C	4.237369	-0.620993	0.389473
H	5.307130	0.471550	-1.173960
H	5.012659	-1.036554	1.019392
C	2.546508	-1.695440	1.867301
H	2.819273	-1.172837	2.788448
H	3.081176	-2.647069	1.812253
H	1.472856	-1.876182	1.843000
H	0.207013	-2.051027	-0.451108

Pd_NS2Me+_PR

B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1695.86616088 a.u.
Enthalpy Correction = 0.359332 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -1696.13020181

Atom	X-Coord	Y-Coord	Z-Coord
Pd	-0.107977	-0.481471	-0.066684
P	-0.716404	1.866864	0.180348
P	-2.431646	-0.855859	-0.101423
C	-3.283075	0.796331	-0.273423
H	-4.331938	0.718093	0.036487
H	-3.283998	1.044386	-1.342043
C	-2.551739	1.885639	0.529509
H	-2.672123	1.710208	1.605777
H	-2.973724	2.875298	0.317912
C	-3.150105	-1.894826	-1.438350
H	-2.877326	-1.484276	-2.414895
H	-2.743769	-2.907991	-1.368361
H	-4.241278	-1.943067	-1.358587
C	-3.123006	-1.584620	1.445248
H	-2.861325	-0.963882	2.307298
H	-4.213119	-1.673993	1.385211
H	-2.693826	-2.578968	1.601247
C	-0.007562	2.946184	1.498632
H	1.063953	3.082312	1.321859
H	-0.488649	3.930103	1.512548
H	-0.136811	2.472375	2.476526
C	-0.535873	2.890515	-1.346843
H	-1.039656	2.403320	-2.187030
H	-0.956064	3.892713	-1.208552
H	0.524722	2.983390	-1.600674
N	2.846417	-0.529185	0.879981
C	1.949488	-0.269703	-0.086060
S	2.810985	0.227850	-1.498692

C	4.365990	0.070369	-0.723771
C	4.192167	-0.346398	0.547702
H	5.296296	0.279336	-1.232799
H	4.951868	-0.543595	1.292479
C	2.466925	-0.986640	2.225539
H	2.736259	-0.226989	2.964779
H	2.986588	-1.920447	2.454936
H	1.390491	-1.152399	2.236387
C	0.195309	-2.545994	-0.351580
H	-0.503519	-3.136541	0.248917
H	0.028133	-2.746276	-1.415078
H	1.214689	-2.836966	-0.091160

Pt_NN2H+_PR

B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1345.50541218 a.u.
Enthalpy Correction = 0.374324 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -1345.76156844

Atom	X-Coord	Y-Coord	Z-Coord
C	-2.393752	-0.559672	-2.449693
N	-2.828228	-0.391931	-1.065645
C	-2.003987	-0.332177	0.012650
N	-2.833888	-0.211264	1.081688
C	-2.408663	-0.158786	2.477828
C	-4.158718	-0.309002	-0.674934
C	-4.162411	-0.196376	0.675649
H	-1.322715	-0.253603	2.508808
H	-2.857376	-0.986098	3.034471
H	-2.711984	0.789547	2.931465
H	-2.651976	0.324867	-3.039802
H	-2.875764	-1.439077	-2.885199
H	-1.312767	-0.703994	-2.453421
H	-4.970290	-0.341671	-1.385327
H	-4.977861	-0.112700	1.377380
H	-0.195133	-2.079815	0.120249
Pt	0.049655	-0.485441	0.028586
P	2.345649	-0.891358	0.041181
P	0.650048	1.847127	-0.089550
C	2.478529	1.872790	-0.472869
H	2.908163	2.850160	-0.223488
H	2.572423	1.748024	-1.558832
C	3.223178	0.742425	0.259225
H	3.261870	0.943839	1.336878
H	4.259949	0.667195	-0.088952
C	-0.083688	2.978971	-1.346578
H	0.026490	2.547817	-2.346089
H	-1.151194	3.108374	-1.142957
H	0.400175	3.961450	-1.326272
C	0.495955	2.802041	1.482760
H	0.999695	2.270221	2.295160
H	0.929709	3.803145	1.384720
H	-0.561444	2.900312	1.747196

C	3.028879	-1.979649	1.354518
H	2.633645	-2.990951	1.222617
H	4.122745	-2.011834	1.310358
H	2.715887	-1.616077	2.337344
C	3.012550	-1.594355	-1.524208
H	2.767942	-0.940085	-2.365955
H	4.099453	-1.717549	-1.467144
H	2.549389	-2.568514	-1.705787

Pt_NN2Me+_PR
B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1384.81387503 a.u.
Enthalpy Correction = 0.405449 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -1385.08121393

Atom	X-Coord	Y-Coord	Z-Coord
Pt	-0.067896	-0.417385	-0.006874
P	-0.605813	1.924428	-0.006435
P	-2.389795	-0.744890	0.006682
C	0.222099	-2.511543	-0.041571
H	-0.458211	-3.024668	0.647618
H	0.026909	-2.881317	-1.056155
H	1.243520	-2.790819	0.230470
C	1.980925	-0.229186	0.006982
N	2.799897	-0.183021	1.091320
C	2.362953	-0.233476	2.484392
H	1.274039	-0.286483	2.500667
H	2.774545	-1.120709	2.973618
H	2.698179	0.661491	3.016640
N	2.817865	-0.192164	-1.063951
C	2.404588	-0.259963	-2.463519
H	1.315539	-0.297151	-2.498465
H	2.762737	0.620787	-3.004499
H	2.811193	-1.161176	-2.930929
C	4.131904	-0.118975	0.702060
H	4.939033	-0.076764	1.417100
C	4.143181	-0.124893	-0.653118
H	4.962155	-0.089464	-1.354937
C	-3.213676	0.901463	-0.296522
H	-4.253124	0.879073	0.050850
H	-3.242677	1.049050	-1.383125
C	-2.430036	2.039775	0.379395
H	-2.526711	1.972491	1.470163
H	-2.825796	3.018001	0.081905
C	0.173582	3.088809	1.192963
H	-0.272038	4.087163	1.127267
H	0.050902	2.709744	2.211939
H	1.244585	3.168005	0.981579
C	-0.427670	2.806220	-1.619035
H	-0.950833	2.256023	-2.406584
H	-0.828693	3.824028	-1.564218
H	0.631328	2.859556	-1.889867
C	-3.073336	-1.336677	1.611208

H	-2.797149	-0.646220	2.413294
H	-4.164418	-1.421349	1.566901
H	-2.648626	-2.317138	1.846959
C	-3.120965	-1.880355	-1.239844
H	-2.730985	-2.890023	-1.082021
H	-4.212826	-1.903087	-1.159934
H	-2.838196	-1.556973	-2.245718

Pt_NN2Ph+_PR

B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1576.54797439 a.u.
Enthalpy Correction = 0.462463 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -1576.86953410

Atom	X-Coord	Y-Coord	Z-Coord
Pt	0.188608	-0.017033	0.016628
P	2.417152	0.887278	-0.004746
P	1.245187	-2.110664	0.008280
C	-0.865235	1.757962	0.007116
N	-1.302073	2.455006	-1.074532
C	-1.076546	2.084214	-2.468451
H	-0.395716	1.233010	-2.491449
H	-2.021705	1.801741	-2.940280
H	-0.635401	2.924816	-3.011591
N	-1.346772	2.440328	1.079037
C	-1.174704	2.055087	2.476868
H	-0.517091	1.186698	2.515814
H	-0.729619	2.880299	3.040236
H	-2.141585	1.794590	2.916048
C	-2.054740	3.554569	-0.683107
H	-2.495321	4.233730	-1.396547
C	-2.082751	3.545265	0.671594
H	-2.551957	4.215156	1.375494
C	3.075556	-1.840879	0.255048
H	3.643234	-2.703144	-0.113517
H	3.246816	-1.785328	1.337147
C	3.541453	-0.543068	-0.428374
H	3.512102	-0.655556	-1.519336
H	4.577766	-0.308312	-0.158029
C	2.888960	2.197953	-1.212964
H	3.964248	2.403341	-1.179050
H	2.617053	1.885286	-2.225680
H	2.347802	3.120523	-0.980453
C	3.082705	1.530357	1.593140
H	2.968723	0.777364	2.378617
H	4.141580	1.796004	1.503055
H	2.520455	2.420318	1.892138
C	1.091996	-3.035587	-1.574465
H	1.503897	-2.443962	-2.397469
H	1.617784	-3.994679	-1.521203
H	0.031942	-3.214242	-1.777013
C	0.757698	-3.323803	1.297198
H	-0.307270	-3.546714	1.189394

H	1.336368	-4.248830	1.205700
H	0.917799	-2.893666	2.290184
C	-1.649803	-0.988780	-0.000346
C	-2.276562	-1.326098	-1.212478
C	-3.509861	-1.987098	-1.235748
C	-4.148065	-2.327033	-0.042269
C	-3.541335	-2.002210	1.172033
C	-2.307896	-1.341566	1.190306
H	-1.802268	-1.075819	-2.159538
H	-3.970319	-2.235290	-2.189073
H	-5.105618	-2.839782	-0.058059
H	-4.026702	-2.262982	2.109513
H	-1.856841	-1.108275	2.152820

Pt_NO2H+_PR
B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1326.03859504 a.u.
Enthalpy Correction = 0.331650 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -1326.29178310

Atom	X-Coord	Y-Coord	Z-Coord
Pt	-0.047674	-0.450625	-0.098824
P	2.235011	-0.933594	-0.123168
P	0.627447	1.834966	0.267743
C	2.470124	1.868683	-0.037682
H	2.916927	2.754250	0.429277
H	2.610975	1.972016	-1.120684
C	3.146270	0.582835	0.469195
H	3.134380	0.550970	1.565641
H	4.196790	0.542835	0.157875
C	-0.034273	3.193182	-0.784145
H	0.109278	2.944468	-1.839578
H	-1.107366	3.302256	-0.604330
H	0.464143	4.143142	-0.564058
C	0.428547	2.464404	1.990084
H	0.894747	1.771474	2.696748
H	0.880145	3.455642	2.104710
H	-0.636301	2.528560	2.233841
C	2.854803	-2.309339	0.923352
H	2.421550	-3.249981	0.571721
H	3.946796	-2.376463	0.877200
H	2.544490	-2.154644	1.960644
C	2.898399	-1.283157	-1.802363
H	2.654685	-0.458618	-2.478226
H	3.984241	-1.423131	-1.774897
H	2.426773	-2.189701	-2.192177
N	-3.081364	-0.842928	0.355367
C	-2.056421	-0.161489	-0.182457
O	-2.608318	0.827712	-0.919805
C	-3.980364	0.748799	-0.847813
C	-4.297274	-0.285651	-0.051875
H	-4.548381	1.475481	-1.405156
H	-5.249792	-0.681288	0.264149

C	-2.974363	-2.003467	1.241291
H	-3.559311	-2.829030	0.828481
H	-3.350378	-1.745008	2.234731
H	-1.925701	-2.290180	1.303887
H	-0.323628	-2.024885	-0.344795

Pt_NO2Me+_PR

B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1365.34656291 a.u.
Enthalpy Correction = 0.362787 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -1365.61106776

Atom	X-Coord	Y-Coord	Z-Coord
Pt	0.018132	-0.394515	-0.121953
P	-0.544651	1.919218	0.202692
P	-2.298655	-0.760239	-0.026223
C	-3.146770	0.897262	-0.122135
H	-4.175082	0.822755	0.250443
H	-3.209157	1.159515	-1.185410
C	-2.356210	1.967874	0.649492
H	-2.422577	1.786474	1.729313
H	-2.769361	2.966487	0.465738
C	-3.085050	-1.780097	-1.335588
H	-2.865451	-1.354089	-2.318755
H	-2.673593	-2.792944	-1.301131
H	-4.169778	-1.830172	-1.195373
C	-2.874907	-1.513345	1.551428
H	-2.544979	-0.905797	2.398988
H	-3.966284	-1.601772	1.571070
H	-2.434576	-2.509410	1.655890
C	0.269002	2.932301	1.509369
H	1.328992	3.057845	1.267323
H	-0.191185	3.922690	1.591789
H	0.194390	2.419911	2.473108
C	-0.404732	2.960767	-1.312639
H	-0.971332	2.505660	-2.130169
H	-0.775623	3.976164	-1.135936
H	0.643885	3.009700	-1.620971
N	3.013162	-0.596984	0.581392
C	2.026559	-0.131144	-0.202132
O	2.625483	0.579529	-1.181416
C	3.991957	0.543323	-1.009487
C	4.255968	-0.183980	0.088161
H	4.595246	1.063815	-1.735025
H	5.186061	-0.450268	0.565436
C	2.835413	-1.407409	1.787159
H	3.212511	-0.861727	2.656246
H	3.378572	-2.349625	1.680769
H	1.771426	-1.606821	1.909525
C	0.310382	-2.453087	-0.522155
H	-0.251106	-3.086066	0.175494
H	-0.043346	-2.658726	-1.539482
H	1.361988	-2.748278	-0.470857

Pt_NS2H+_PR
B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1649.01091693 a.u.
Enthalpy Correction = 0.328736 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -1649.27158678

Atom	X-Coord	Y-Coord	Z-Coord
C	4.204463	-0.576432	0.402719
N	2.864854	-0.819743	0.713758
C	1.953886	-0.269094	-0.107030
S	2.796400	0.605297	-1.342323
C	4.361059	0.189040	-0.697034
C	2.511861	-1.651924	1.874784
Pt	-0.081049	-0.462159	-0.099979
P	-0.722515	1.816359	0.370689
C	-0.562198	2.995348	-1.039091
P	-2.371414	-0.893188	-0.206352
C	-3.050953	-1.835068	1.220339
C	-3.265737	0.745172	-0.190116
C	-2.555062	1.756945	0.725617
C	-3.004114	-1.772869	-1.688906
C	-0.008054	2.736527	1.797729
H	-2.995805	2.755209	0.620726
H	-2.666938	1.465521	1.777355
H	-3.277895	1.109445	-1.224684
H	-4.310077	0.606686	0.113338
H	-0.125378	2.150354	2.713907
H	1.060652	2.899659	1.627809
H	-0.496428	3.708141	1.927747
H	-1.070085	2.593545	-1.920850
H	-0.990942	3.971844	-0.789054
H	0.494982	3.126255	-1.289367
H	-2.586568	-2.783458	-1.711388
H	-4.097348	-1.834201	-1.673493
H	-2.681350	-1.250255	-2.593724
H	-2.811170	-1.322625	2.156228
H	-4.137232	-1.945399	1.135759
H	-2.590533	-2.826836	1.247943
H	5.284728	0.514484	-1.154231
H	4.976061	-0.998910	1.032545
H	2.809850	-1.144699	2.796624
H	3.026938	-2.613024	1.800497
H	1.434576	-1.810308	1.866407
H	0.173450	-2.022969	-0.439995

Pt_NS2Me+_PR
B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1688.31953729 a.u.
Enthalpy Correction = 0.359928 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D

Single Point Energy = -1688.59156298

Atom	X-Coord	Y-Coord	Z-Coord
Pt	-0.102163	-0.409265	-0.066522
P	-0.651865	1.920400	0.183992
P	-2.423909	-0.743070	-0.081499
C	-3.250144	0.921959	-0.227191
H	-4.292448	0.861604	0.106843
H	-3.269678	1.174620	-1.294415
C	-2.477828	1.991621	0.563722
H	-2.584199	1.819981	1.641895
H	-2.874283	2.992594	0.357095
C	-3.144635	-1.758948	-1.431410
H	-2.856776	-1.342873	-2.401038
H	-2.752179	-2.777729	-1.365533
H	-4.236732	-1.791727	-1.359174
C	-3.099429	-1.488257	1.461162
H	-2.819139	-0.880845	2.326660
H	-4.190645	-1.568320	1.413832
H	-2.674562	-2.487563	1.595454
C	0.123643	2.943781	1.506006
H	1.194411	3.048625	1.305171
H	-0.323955	3.942212	1.552635
H	0.001107	2.449884	2.474551
C	-0.453642	2.948732	-1.334930
H	-0.988974	2.487177	-2.169909
H	-0.831962	3.965012	-1.180657
H	0.605855	3.001971	-1.603941
N	2.815537	-0.485999	0.894466
C	1.928271	-0.210106	-0.078109
S	2.804913	0.284489	-1.487232
C	4.350361	0.103633	-0.700006
C	4.163694	-0.317038	0.567913
H	5.286264	0.303107	-1.202515
H	4.916809	-0.527141	1.315798
C	2.429322	-0.945010	2.238285
H	2.712276	-0.192784	2.980012
H	2.936263	-1.887300	2.460902
H	1.350576	-1.094237	2.251423
C	0.182703	-2.487432	-0.356181
H	-0.499057	-3.083797	0.260654
H	-0.009401	-2.716973	-1.411280
H	1.204483	-2.800246	-0.124234

6. Radicals

NN_2•

UB3lyp/6-31G(d) optimized geometry
Energy = -304.521248 a.u.
ROB3lyp/6-311+G(2d,p) 5D
Single point energy = -304.560221 a.u.

Atom	x-coord	y-coord	z-coord
C	2.492521	-0.608762	0.000007

N	1.101021	-0.122714	0.000007
C	0.000078	-0.859454	0.000001
N	-1.100966	-0.122896	-0.000006
C	-2.492514	-0.608750	-0.000007
C	0.680819	1.209187	-0.000033
C	-0.680930	1.209084	0.000033
H	-2.479638	-1.698421	-0.000064
H	-2.998161	-0.244565	-0.896180
H	-2.998130	-0.244657	0.896220
H	2.998321	-0.244672	0.896143
H	2.998291	-0.244757	-0.896181
H	2.479327	-1.698416	0.000059
H	1.390287	2.023568	-0.000059
H	-1.390521	2.023362	0.000060

NO_2•
UB3lyp/6-31G(d) optimized geometry
Energy = -285.029628 a.u.
ROB3lyp/6-311+G(2d,p) 5D
Single point energy = -285.107491 a.u.

Atom	x-coord	y-coord	z-coord
N	-0.641515	-0.039913	0.000003
C	0.154035	-1.079635	-0.000007
O	1.408498	-0.785641	-0.000013
C	1.475695	0.612558	0.000032
C	0.213287	1.086307	-0.000029
H	2.464489	1.043932	0.000059
H	-0.175006	2.094459	-0.000052
C	-2.120279	-0.031972	0.000011
H	-2.466499	0.483238	-0.897595
H	-2.466490	0.483225	0.897629
H	-2.470300	-1.063887	0.000005

NS_2•
UB3lyp/6-31G(d) optimized geometry
Energy = -608.020006 a.u.
ROB3lyp/6-311+G(2d,p) 5D
Single point energy = -608.105255 a.u.

Atom	x-coord	y-coord	z-coord
N	-0.949940	-0.071507	-0.000005
C	-0.047939	-1.021383	-0.000061
S	1.567122	-0.531647	0.000034
C	1.002772	1.129241	-0.000084
C	-0.351050	1.196072	0.000064
H	1.712269	1.947063	-0.000128
H	-0.979445	2.077544	0.000126
C	-2.416578	-0.297459	-0.000003
H	-2.839300	0.157275	-0.897866
H	-2.839296	0.157261	0.897867
H	-2.601826	-1.371070	-0.000011

H•
UB3lyp/6-31G(d) optimized geometry

Energy = -0.500273 a.u.
ROB3lyp/6-311+G(2d,p) 5D
Single point energy = -0.502156 a.u.

Atom	x-coord	y-coord	z-coord
H	0.000000	0.000000	0.000000

$CH_3^{\bullet}$
UB3lyp/6-31G(d) optimized geometry
Energy = -39.838292 a.u.
ROB3lyp/6-311+G(2d,p) 5D
Single point energy = -39.854608 a.u.

Atom	x-coord	y-coord	z-coord
C	0.000097	-0.000001	-0.000145
H	-0.539833	0.938313	0.000290
H	1.082787	-0.002135	0.000291
H	-0.543536	-0.936174	0.000290

$Ph^{\bullet}$
UB3lyp/6-31G(d) optimized geometry
Energy = -231.561284 a.u.
ROB3lyp/6-311+G(2d,p) 5D
Single point energy = -231.627029 a.u.

Atom	x-coord	y-coord	z-coord
C	-1.226273	-0.771918	0.000011
C	0.000204	-1.400134	0.000003
C	1.226517	-0.771641	-0.000015
C	1.214085	0.632756	0.000009
C	-0.000177	1.324702	0.000002
C	-1.214307	0.632432	-0.000012
H	-2.162662	-1.323644	0.000014
H	2.163125	-1.323002	-0.000003
H	2.154485	1.179388	0.000018
H	-0.000380	2.411277	0.000004
H	-2.154857	1.178797	-0.000014

7. Simple Organics

H_2
B3lyp/6-31G(d) optimized geometry
Energy = -1.175482 a.u.
B3lyp/6-311+G(2d,p) 5D
Single point energy = -1.17957 a.u.

Atom	x-coord	y-coord	z-coord
H	0.000000	0.000000	0.371394
H	0.000000	0.000000	-0.371394

CH_4

B3lyp/6-31G(d) optimized geometry
Energy = -40.518383 a.u.
B3lyp/6-311+G(2d,p) 5D
Single point energy = -40.534847 a.u.

Atom	x-coord	y-coord	z-coord
C	0.000003	0.000000	0.000000
H	1.082625	0.153962	-0.000977
H	-0.505967	0.968643	-0.038908
H	-0.284341	-0.595053	-0.872263
H	-0.292331	-0.527551	0.912148

Benzene
B3lyp/6-31G(d) optimized geometry
Energy = -232.248659 a.u.
B3lyp/6-311+G(2d,p) 5D
Single point energy = -232.317223 a.u.

Atom	x-coord	y-coord	z-coord
C	0.988360	-0.986572	-0.000004
C	-0.360333	-1.349161	-0.000068
C	-1.348608	-0.362659	0.000056
C	-0.988276	0.986655	-0.000009
C	0.360220	1.349188	-0.000062
C	1.348640	0.362550	0.000058
H	1.757369	-1.754386	0.000063
H	-0.640564	-2.399115	-0.000082
H	-2.398068	-0.644671	0.000156
H	-1.757474	1.754269	-0.000006
H	0.640692	2.399071	-0.000016
H	2.398038	0.644823	0.000064

8. Palladium Alkyl Complexes for ABE's

Pd_H2_DMPE
B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1048.95698095 a.u.
Enthalpy Correction = 0.241319 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -1049.12157697

Atom	X-Coord	Y-Coord	Z-Coord
Pd	0.000000	0.000000	1.361718
P	0.891029	-1.358773	-0.391044
P	-0.891029	1.358773	-0.391044
C	-0.663520	0.391268	-1.985909
H	-0.728041	1.051681	-2.860575
H	-1.508848	-0.306430	-2.049222
C	0.663520	-0.391268	-1.985909
H	1.508848	0.306430	-2.049222
H	0.728041	-1.051681	-2.860575

C	-2.662362	1.881936	-0.490974
H	-3.307566	1.004542	-0.384477
H	-2.879108	2.558387	0.341455
H	-2.893446	2.388965	-1.435182
C	0.000000	2.944485	-0.739913
H	1.071944	2.748659	-0.840264
H	-0.364927	3.433145	-1.651271
H	-0.134040	3.620872	0.109724
C	2.662362	-1.881936	-0.490974
H	2.879108	-2.558387	0.341455
H	2.893446	-2.388965	-1.435182
H	3.307566	-1.004542	-0.384477
C	0.000000	-2.944485	-0.739913
H	-1.071944	-2.748659	-0.840264
H	0.364927	-3.433145	-1.651271
H	0.134040	-3.620872	0.109724
H	-0.569644	0.810554	2.616732
H	0.569644	-0.810554	2.616732

Pd_H_C6H5_DMPE

B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1279.99981914 a.u.
Enthalpy Correction = 0.329663 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -1280.23312489

Atom	X-Coord	Y-Coord	Z-Coord
Pd	-0.058221	-0.727509	0.014362
P	-0.347080	1.663721	-0.020993
P	-2.431889	-0.814445	0.010841
C	-3.043767	0.912870	-0.402844
H	-4.098004	1.032020	-0.120711
H	-2.993225	1.005609	-1.495543
C	-2.172377	1.999770	0.256924
H	-2.329083	1.995793	1.343463
H	-2.453999	2.997705	-0.102594
C	-3.392192	-1.871029	-1.163304
H	-3.045312	-1.686746	-2.184657
H	-3.200417	-2.922887	-0.930403
H	-4.470266	-1.680418	-1.106693
C	-3.261878	-1.172212	1.627515
H	-2.865355	-0.506299	2.400249
H	-4.349860	-1.049120	1.568652
H	-3.031493	-2.199541	1.925762
C	0.491258	2.784631	1.185043
H	1.572935	2.648147	1.089809
H	0.241351	3.838816	1.019558
H	0.208177	2.502904	2.204149
C	0.008264	2.486677	-1.639779
H	-0.569670	2.003810	-2.433998
H	-0.228062	3.557049	-1.621102
H	1.069286	2.353600	-1.873186
H	0.178332	-2.309650	-0.006590
C	2.003504	-0.673926	0.017785

C	2.725221	-0.505875	1.212936
C	4.117547	-0.363716	1.213656
C	4.829151	-0.388839	0.012473
C	4.132762	-0.564249	-1.185029
C	2.740744	-0.709204	-1.179015
H	2.198442	-0.489446	2.165396
H	4.646828	-0.237183	2.156755
H	5.911363	-0.280740	0.010351
H	4.674553	-0.596224	-2.128952
H	2.226738	-0.860326	-2.126259

Pd_H_CH3_DMPE

B3lyp/lanl2dz:6-31G(d) 5D Optimised Geometry
Energy = -1088.26497176 a.u.
Enthalpy Correction = 0.272581 a.u.

B3lyp/l2aug:6-311+G(2d,p) 5D
Single Point Energy = -1088.44234324

Atom	X-Coord	Y-Coord	Z-Coord
Pd	-0.169032	-1.182074	0.008492
P	-1.378135	0.909653	-0.011383
P	1.780095	0.183687	0.006809
C	1.230362	1.952147	0.321612
H	1.999610	2.669427	0.006994
H	1.123648	2.054909	1.409377
C	-0.114101	2.251326	-0.368249
H	0.020622	2.270813	-1.457627
H	-0.493347	3.239117	-0.075491
C	3.158964	-0.028637	1.221647
H	2.751014	-0.031747	2.237155
H	3.633258	-0.999909	1.050292
H	3.916020	0.760018	1.138133
C	2.699684	0.316895	-1.596081
H	2.003343	0.579811	-2.398371
H	3.501823	1.063429	-1.554819
H	3.129328	-0.659760	-1.839254
C	-2.737204	1.312197	-1.202202
H	-3.580402	0.638184	-1.020334
H	-3.082082	2.348379	-1.106353
H	-2.387883	1.141347	-2.225260
C	-2.113155	1.459976	1.599090
H	-1.353289	1.412129	2.385221
H	-2.514006	2.479263	1.546063
H	-2.918630	0.772622	1.876435
H	0.634248	-2.559938	0.058885
C	-1.827987	-2.462122	-0.023352
H	-1.564829	-3.512973	-0.148166
H	-2.364433	-2.341520	0.927222
H	-2.487321	-2.159010	-0.846891

9. LANL2DZAUG:6-311+G(2d,p) Basis Set Implementation

Gaussian03 Basis Set and Pseudopotential genecp cards:

```
! basis set for high-level single points
-C -H -N -P -Ni 0
6-311+G(2d,p)
****
-Pd 0
S 3 1.00
           0.278700D+01 -.161024D+01
           0.196500D+01 0.184898D+01
           0.624300D+00 0.603749D+00
S 3 1.00
           0.278700D+01 0.135408D+01
           0.196500D+01 -.167809D+01
           0.624300D+00 -.855938D+00
S 1 1.00
           0.208100D+00 0.100000D+01
S 1 1.00
           0.832000D-01 0.100000D+01
S 1 1.00
           0.333000D-01 0.100000D+01
P 3 1.00
           0.599900D+01 -.103491D+00
           0.144300D+01 0.745695D+00
           0.526400D+00 0.365649D+00
P 1 1.00
           0.175500D+00 0.100000D+01
P 1 1.00
           0.585000D-01 0.100000D+01
P 1 1.00
           0.195000D-01 0.100000D+01
D 2 1.00
           0.609100D+01 0.376146D-01
           0.171900D+01 0.520048D+00
D 1 1.00
           0.605600D+00 0.100000D+01
D 1 1.00
           0.188300D+00 0.100000D+01
D 1 1.00
           0.628000D-01 0.100000D+01
F 2 1.00
           0.361217D+01 0.173786D+00
           0.129541D+01 0.597338D+00
F 1 1.00
           0.554710D+00 0.100000D+01
F 1 1.00
           0.237530D+00 0.100000D+01
****
-Pt 0
S    3 1.00
  0.2547000000D+01 -0.1473918000D+01
  0.1614000000D+01  0.1911572000D+01
  0.5167000000D+00  0.3922319000D+00
```

```
S    3 1.00
  0.2547000000D+01  0.1438817000D+01
  0.1614000000D+01 -0.2091182000D+01
  0.5167000000D+00 -0.1092132000D+01
S    1 1.00
  0.2651000000D+00  0.1000000000D+01
S    1 1.00
  0.5800000000D-01  0.1000000000D+01
S    1 1.00
  0.1270000000D-01  0.1000000000D+01
P    3 1.00
  0.2911000000D+01 -0.5247438000D+00
  0.1836000000D+01  0.9671884000D+00
  0.5982000000D+00  0.5438632000D+00
P    1 1.00
  0.6048000000D+00  0.1000000000D+01
P    1 1.00
  0.9960000000D-01  0.1000000000D+01
P    1 1.00
  0.2900000000D-01  0.1000000000D+01
P    1 1.00
  0.0844000000D-01  0.1000000000D+01
D    1 1.00
  0.1243000000D+01  0.1000000000D+01
D    1 1.00
  0.4271000000D+00  0.1000000000D+01
D    1 1.00
  0.1370000000D+00  0.1000000000D+01
D    1 1.00
  0.0439000000D+00  0.1000000000D+01
F    1 1.00
  3.9720000000D+00  0.1000000000D+01
F    1 1.00
  0.9930000000D+00  0.1000000000D+01
F    1 1.00
  0.2480000000D+00  0.1000000000D+01
****
```