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Experimental and theoretical investigation of octahedral and square-planar isothiocyanato complexes of Ni(II) with acylhydrazones of 2-(diphenylphosphino)benzaldehyde

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Table S1. Selected average bond lengths (Å) for DFT energy-minimized structures of **1** and **2** and comparison to available crystallographic data.

Molecule	Method	Ni1-P1	Ni1-N2	Ni1-N4	Ni1-O1	Ni1-N5	Ni1-N6
1	S12g Vacuo	2.28	2.13	1.94	2.32	2.19	2.19
	S12g Cosmo	2.31	2.10	2.00	2.33	2.08	2.11
	X-ray [29]	2.37	2.09	2.03	2.15	2.01	2.01
2	S12g Vacuo	2.14	1.87	1.82	2.01	-	-
	S12g Cosmo	2.16	1.87	1.84	1.98	-	-
	X-ray [26]	2.15	1.86	1.86	1.90	-	-

Table S2. The energy difference between the product and the sum of the reactants for the structures optimized in COMSO (Scheme 4b from the Manuscript).

Side chain	Deprotonated ligand	Protonated ligand
	ΔE_{cosmo}	ΔE_{cosmo}
$-CH_2N(CH_3)_3$ (**L3**)	-10.88	-18.96
–OEt (**L1**)	-5.29	-17.48
–NHPh (**L2**)	-3.52	-16.18

Coordinates of optimized structures

Protonated ligand

Square-planar R=$CH_2N(CH_3)_3$
VACUO

Ni	0.986786	0.594406	0.281176
P	-1.050153	-0.069004	0.094004
O	3.095893	1.179074	-0.131661
C	5.284292	0.124223	0.094533
N	1.744797	-1.114674	0.206729
N	3.139870	-1.049716	0.204876
N	0.535581	2.297304	0.646006
S	-1.191435	4.312649	1.506925
C	-0.074684	-2.769541	0.243049
C	-1.188271	-1.899005	0.186287
C	-2.472660	-2.443809	0.182542
H	-3.338397	-1.784884	0.149892
C	-2.667178	-3.823851	0.220630
H	-3.679332	-4.223507	0.210779
C	-1.574327	-4.687303	0.277259
H	-1.723466	-5.764745	0.314049
C	-0.293735	-4.165597	0.292198
H	0.562751	-4.837845	0.342084
C	1.290976	-2.347798	0.248952
H	2.029612	-3.154646	0.290371
C	3.749701	0.140548	0.016606
N	6.073746	-0.355548	-1.128184
C	5.749994	0.496412	-2.329263
C	5.806163	-1.802247	-1.453965
C	7.544529	-0.219639	-0.798207
H	8.125060	-0.534882	-1.669729
H	7.781857	-0.862177	0.054361
H	7.767985	0.822654	-0.559499
C	-2.181358	0.528863	1.361711
C	-3.442087	1.055877	1.067829
H	-3.763840	1.176697	0.035039
C	-4.283425	1.415475	2.117809
H	-5.266224	1.827467	1.898850
C	-3.870680	1.253491	3.437874
H	-4.534335	1.538348	4.252541
C	-2.607606	0.734646	3.725809
H	-2.282659	0.614714	4.757800
C	-1.758075	0.374545	2.691251
H	-0.766062	-0.022234	2.909860
C	-1.487360	0.386373	-1.605115
C	-1.759423	1.726789	-1.924799
H	-1.832267	2.480142	-1.143367
C	-1.913470	2.094056	-3.255480
H	-2.125060	3.132524	-3.502687
C	-1.782767	1.144551	-4.269629
H	-1.890827	1.443471	-5.311344
C	-1.507803	-0.184439	-3.954201
H	-1.410685	-0.928407	-4.743378
C	-1.358487	-0.569256	-2.627289
H	-1.141093	-1.609407	-2.390701
C	-0.240425	3.135567	1.028171
H	3.646955	-1.888678	0.466639
H	5.594475	1.156042	0.279389
H	5.616394	-0.496862	0.935551
H	6.348392	0.142525	-3.173460
H	5.996751	1.536672	-2.102555
H	4.684671	0.404414	-2.556667
H	6.469037	-2.100395	-2.271103
H	4.768034	-1.922766	-1.770218
H	6.027177	-2.416731	-0.575065

Square-planar R=$CH_2N(CH_3)_3$
COSMO

Ni	0.746187	0.467575	-0.076954
P	-1.319013	-0.159760	-0.176882
S	-1.039231	4.661886	-0.666247
N	1.367531	-1.208432	0.454686
N	2.698271	-1.097968	0.835680
N	5.794260	-0.740662	0.264587
N	0.254256	2.193937	-0.385093
O	2.705554	0.991691	0.037373
C	-2.143325	0.389888	-1.689374
C	-2.929029	1.547105	-1.721406
H	-3.124530	2.108757	-0.811299
C	-3.456884	1.978996	-2.934621
H	-4.073101	2.875253	-2.959887
C	-3.193426	1.272958	-4.107795
H	-3.604413	1.620014	-5.054379
C	-2.396756	0.126946	-4.076000
H	-2.183355	-0.422944	-4.990528
C	-1.869031	-0.317594	-2.871005
H	-1.244012	-1.209099	-2.848493
C	-2.209208	0.351431	1.328740
C	-3.610191	0.356515	1.371432
H	-4.195213	0.168476	0.473275
C	-4.257878	0.597578	2.579262

H	-5.345496	0.602724	2.610262
C	-3.518787	0.820109	3.741877
H	-4.031535	0.996456	4.686212
C	-2.125444	0.815319	3.699089
H	-1.545628	0.987710	4.603975
C	-1.466194	0.584938	2.495229
H	-0.376910	0.579689	2.468537
C	-1.483857	-1.988676	-0.192939
C	-2.709301	-2.547044	-0.558060
H	-3.515042	-1.911996	-0.918308
C	-2.920377	-3.923069	-0.466331
H	-3.883851	-4.333404	-0.759812
C	-1.911661	-4.762045	0.000226
H	-2.078567	-5.833942	0.078541
C	-0.686299	-4.224455	0.361629
H	0.112822	-4.871256	0.718424
C	-0.450319	-2.838551	0.259106
C	0.873440	-2.406334	0.600243
H	1.540516	-3.175653	0.991277
C	3.335850	0.041402	0.560049
C	4.792239	0.160816	0.970607
H	5.094333	1.191068	0.779172
H	4.877441	-0.040863	2.043483
C	7.160467	-0.342340	0.767059
H	7.200598	-0.515526	1.844357
H	7.327237	0.711468	0.540151
H	7.899593	-0.963388	0.257710
C	5.588632	-2.199445	0.577962
H	4.686404	-2.556053	0.079715
H	5.535129	-2.329904	1.661551
H	6.443570	-2.751202	0.183215
C	5.724656	-0.534697	-1.223017
H	6.479258	-1.171528	-1.688838
H	5.923718	0.515916	-1.441707
H	4.730230	-0.821696	-1.572986
C	-0.323543	3.225555	-0.505040
H	3.103146	-1.852054	1.379614

Square-planar R=*NHPh*
VACUO

Ni	-0.457484	-0.121877	-0.144937
P	1.692071	0.053250	-0.067092
S	0.874199	-4.355042	-0.988686
O	-2.557463	-0.219712	-0.087179
N	-4.253950	1.297448	0.495500
N	-2.072748	1.915788	0.516276
N	-0.756556	1.699806	0.174282
N	-0.350213	-1.906122	-0.439015
C	-6.614618	1.497503	0.696095
H	-6.451150	2.530239	1.013255
C	-7.904712	0.999170	0.614704
H	-8.745007	1.643381	0.868117
C	-8.111351	-0.316510	0.208056
H	-9.123166	-0.711290	0.141573
C	-7.019903	-1.120556	-0.110104
H	-7.181457	-2.148522	-0.426969
C	-5.715855	-0.636603	-0.033076
H	-4.863452	-1.263887	-0.279053
C	-5.522882	0.680725	0.374981
C	-2.982959	0.898245	0.267755
C	-0.019717	2.779506	0.171662
H	-0.524047	3.725908	0.389760
C	1.385358	2.886841	-0.102963
C	1.910226	4.194196	-0.177910
H	1.245613	5.044065	-0.023993
C	3.249915	4.411811	-0.448370
H	3.635347	5.428439	-0.503396
C	4.095327	3.323852	-0.653833
H	5.150160	3.482551	-0.870012
C	3.596425	2.026416	-0.578401
H	4.272283	1.188112	-0.732091
C	2.249555	1.788622	-0.294120
C	2.258532	-0.398457	1.603514
C	2.634206	0.602054	2.513353
H	2.671980	1.645898	2.208077
C	2.967342	0.261223	3.819373
H	3.259579	1.043332	4.518681
C	2.926709	-1.069242	4.227672
H	3.183480	-1.330865	5.253424
C	2.551867	-2.064617	3.325245
H	2.515016	-3.105105	3.642695
C	2.209429	-1.738437	2.018425
H	1.903554	-2.522368	1.328097
C	2.573438	-0.845681	-1.367269
C	3.708942	-1.619229	-1.120510
H	4.070475	-1.759520	-0.103876
C	4.377240	-2.203789	-2.193617
H	5.262034	-2.809268	-2.006997
C	3.917459	-2.018856	-3.493881
H	4.444890	-2.479876	-4.327539
C	2.776629	-1.252990	-3.735137
H	2.410510	-1.113400	-4.750789
C	2.101541	-0.667420	-2.675094
H	1.205096	-0.073730	-2.857178
C	0.208574	-2.937016	-0.688691

H	-4.336733	2.244937	0.838936
H	-2.368113	2.884963	0.556902

Square-planar R=*NHPh*
COSMO

Ni	-0.447792	-0.041924	-0.039706
P	1.708293	0.105693	-0.031896
S	0.412720	-4.564135	-0.256523
O	-2.465497	-0.169815	0.015686
N	-4.231518	1.371241	0.129167
N	-2.075756	2.052643	0.149050
N	-0.735376	1.805882	0.031862
N	-0.299725	-1.856676	-0.140223
C	-6.600384	1.439101	0.247829
H	-6.509460	2.521629	0.343017
C	-7.851775	0.841493	0.246602
H	-8.740040	1.464002	0.341557
C	-7.962945	-0.543806	0.126000
H	-8.943882	-1.015164	0.124494
C	-6.808852	-1.316011	0.005834
H	-6.888351	-2.397080	-0.089605
C	-5.542661	-0.731894	0.004665
H	-4.648949	-1.341146	-0.090896
C	-5.442291	0.655833	0.125879
C	-2.937281	1.001243	0.092096
C	0.011334	2.872647	0.004415
H	-0.502645	3.833392	0.058863
C	1.443764	2.942367	-0.102484
C	1.993879	4.239684	-0.163873
H	1.325660	5.097731	-0.124994
C	3.361975	4.429100	-0.274873
H	3.767312	5.437753	-0.321836
C	4.212544	3.326077	-0.325953
H	5.288393	3.463041	-0.411737
C	3.686941	2.037695	-0.264434
H	4.364450	1.187353	-0.299598
C	2.310261	1.831980	-0.148469
C	2.373190	-0.505398	1.547492
C	2.495013	0.403823	2.610830
H	2.281337	1.461279	2.463675
C	2.894485	-0.045426	3.864623
H	2.988727	0.665435	4.683428
C	3.168553	-1.397835	4.066379
H	3.478978	-1.747806	5.049714
C	3.044703	-2.302551	3.011433
H	3.259031	-3.358057	3.167360
C	2.639051	-1.866244	1.753677
H	2.534202	-2.582684	0.942292
C	2.456573	-0.720324	-1.467295
C	3.717462	-1.324332	-1.424334
H	4.264812	-1.406003	-0.487990
C	4.277618	-1.818646	-2.600460
H	5.257983	-2.289510	-2.567871
C	3.592178	-1.703421	-3.809030
H	4.038689	-2.086742	-4.725261
C	2.333555	-1.101559	-3.849549
H	1.795366	-1.011233	-4.791323
C	1.762511	-0.610550	-2.681234
H	0.779264	-0.140218	-2.708731
C	0.021876	-2.997034	-0.192973
H	-4.374477	2.371376	0.187310
H	-2.376563	3.019765	0.181241

Square-planar R=*OEt*
VACUO

Ni	1.103910	0.285382	0.125873
P	-0.990535	-0.176404	0.075724
O	3.147888	0.697287	-0.111404
O	5.002656	-0.642850	-0.492127
N	1.673506	-1.501730	0.005245
N	3.030595	-1.558786	-0.206300
N	0.734630	2.044423	0.319808
S	-0.722587	4.375969	0.806478
C	-0.298779	-2.944551	0.287255
C	-1.316822	-1.968386	0.319673
C	-2.639261	-2.376112	0.506788
H	-3.433904	-1.633881	0.538001
C	-2.962624	-3.722528	0.650572
H	-4.001634	-4.013763	0.791585
C	-1.961393	-4.690231	0.616312
H	-2.207008	-5.744275	0.731990
C	-0.645504	-4.303755	0.435794
H	0.141033	-5.057546	0.410059
C	1.097488	-2.669127	0.102201
H	1.745005	-3.548382	0.040316
C	3.724871	-0.389382	-0.263479
C	5.938682	0.475537	-0.635137
H	5.958248	1.020026	0.315685
H	5.554512	1.139673	-1.417429
C	7.278562	-0.121625	-0.987725
H	8.012340	0.684708	-1.100044
H	7.231872	-0.673587	-1.933443
H	7.633151	-0.796947	-0.200760

C	-1.975275	0.622869	1.365634
C	-3.239527	1.165841	1.126481
H	-3.650909	1.183528	0.118963
C	-3.967493	1.684614	2.193981
H	-4.951210	2.113280	2.012783
C	-3.441543	1.660524	3.482569
H	-4.016153	2.070277	4.311782
C	-2.176182	1.122565	3.716379
H	-1.758986	1.110612	4.721862
C	-1.439699	0.605812	2.660882
H	-0.444155	0.196378	2.835405
C	-1.569765	0.187789	-1.607734
C	-1.769896	1.516632	-2.012156
H	-1.684207	2.334069	-1.298613
C	-2.066029	1.788147	-3.342341
H	-2.222886	2.819073	-3.654371
C	-2.141680	0.754050	-4.275281
H	-2.359003	0.976939	-5.319114
C	-1.934845	-0.564011	-3.875933
H	-1.992507	-1.374938	-4.600447
C	-1.647495	-0.852261	-2.546927
H	-1.483182	-1.885119	-2.244609
C	0.077170	3.021094	0.542756
H	3.489595	-2.451698	-0.342533

Square-planar R=*OEt*
COSMO

Ni	1.111943	0.234601	0.010554
P	-0.991217	-0.221969	0.027189
O	3.092762	0.654130	-0.111633
O	5.014340	-0.627943	-0.159400
N	1.677186	-1.552730	0.065674
N	3.045999	-1.600765	-0.002773
N	0.689430	2.010217	0.021654
S	-0.513241	4.533498	0.206682
C	-0.311646	-2.983799	0.249898
C	-1.332805	-2.013924	0.195097
C	-2.667646	-2.419188	0.259350
H	-3.465092	-1.680669	0.211090
C	-2.998831	-3.766411	0.382588
H	-4.045619	-4.058214	0.430142
C	-1.994063	-4.730066	0.441553
H	-2.246693	-5.783670	0.539265
C	-0.665529	-4.342090	0.375807
H	0.124350	-5.089458	0.418365
C	1.098838	-2.711870	0.173391
H	1.750524	-3.586176	0.203741
C	3.713624	-0.435495	-0.095508
C	5.890841	0.541729	-0.256080
H	5.679497	1.194457	0.597195
H	5.647113	1.067709	-1.185023
C	7.306390	0.023934	-0.244463
H	7.994249	0.873717	-0.318145
H	7.491007	-0.642896	-1.094617
H	7.523100	-0.514777	0.685158
C	-1.848471	0.544669	1.434603
C	-3.193425	0.926063	1.383130
H	-3.762586	0.839270	0.460520
C	-3.807822	1.417852	2.532082
H	-4.852988	1.717360	2.491252
C	-3.091638	1.524173	3.723399
H	-3.579083	1.908090	4.618240
C	-1.751368	1.139352	3.773543
H	-1.188778	1.219778	4.701873
C	-1.125788	0.653765	2.631377
H	-0.076261	0.360954	2.666440
C	-1.722869	0.245620	-1.570821
C	-2.254558	1.523365	-1.790759
H	-2.323663	2.243740	-0.978773
C	-2.691177	1.874518	-3.064634
H	-3.110567	2.864625	-3.232001
C	-2.587480	0.968225	-4.120045
H	-2.923542	1.252062	-5.116157
C	-2.047470	-0.299392	-3.904101
H	-1.960224	-1.009275	-4.724577
C	-1.615189	-0.664987	-2.634495
H	-1.189148	-1.654612	-2.477073
C	0.161214	3.069825	0.110131
H	3.519794	-2.496626	0.015190

Octahedral R=*$CH_2N(CH_3)_3$*
VACUO

Ni	0.538435	-0.132132	0.593131
P	-1.638540	0.091451	-0.050976
O	2.857203	-0.173554	0.774305
C	4.746088	-0.186992	-0.781275
N	1.157220	-0.015363	-1.437727
N	2.506030	-0.103860	-1.493060
N	0.308757	-0.249513	2.518679
S	-1.152656	-0.537537	4.898433
C	-0.844916	0.336236	-2.828387
C	-1.881784	0.394698	-1.869280
C	-3.181080	0.653301	-2.312625

H	-3.985606	0.710383	-1.582983
C	-3.477531	0.840714	-3.657153
H	-4.503535	1.041281	-3.962511
C	-2.461973	0.766942	-4.606432
H	-2.678979	0.903794	-5.664876
C	-1.166671	0.517842	-4.190928
H	-0.366642	0.468463	-4.929888
C	0.568093	0.143298	-2.574292
H	1.195735	0.171429	-3.476559
C	3.275605	-0.152578	-0.376339
N	5.710411	-0.219963	0.368730
C	5.504614	-1.467109	1.196978
C	5.557502	1.017166	1.222815
C	7.090255	-0.243191	-0.222658
H	7.821058	-0.267789	0.589440
H	7.235435	0.656566	-0.827041
H	7.196480	-1.134642	-0.847057
C	-2.763916	-1.339534	0.160068
C	-4.123799	-1.214592	0.462588
H	-4.548618	-0.240128	0.694852
C	-4.938194	-2.342233	0.469489
H	-5.996007	-2.239276	0.709038
C	-4.406957	-3.595040	0.168773
H	-5.050618	-4.474738	0.169536
C	-3.051103	-3.722335	-0.121309
H	-2.625223	-4.700281	-0.344204
C	-2.226549	-2.602279	-0.121682
H	-1.162242	-2.706472	-0.323810
C	-2.398055	1.557504	0.718199
C	-2.857490	1.484690	2.039015
H	-2.859552	0.538124	2.576289
C	-3.282872	2.638152	2.688116
H	-3.625094	2.569691	3.719575
C	-3.242525	3.869112	2.036997
H	-3.567070	4.772637	2.553097
C	-2.765333	3.946672	0.730721
H	-2.707906	4.907996	0.220975
C	-2.336207	2.800049	0.074415
H	-1.935564	2.879086	-0.934338
C	-0.320721	-0.379683	3.516868
N	0.974988	-2.253238	0.233945
C	1.873505	-2.835634	-0.274025
S	3.140578	-3.588540	-0.991337
C	1.923780	2.566727	-0.077943
S	3.208208	3.280543	-0.809274
N	1.014644	2.002655	0.430905
H	2.950832	-0.036140	-2.404506
H	4.917163	-1.090944	-1.379344
H	4.965482	0.716149	-1.364413
H	6.358324	1.011352	1.966922
H	4.575690	0.991005	1.695949
H	5.618071	1.899284	0.577964
H	6.305197	-1.510778	1.940109
H	5.527713	-2.337152	0.533536
H	4.525060	-1.406453	1.671692

Octahedral R=*$CH_2N(CH_3)_3$*
COSMO

Ni	0.232760	0.759699	0.444344
P	-1.595185	-0.418182	-0.341704
S	2.896999	-1.862033	3.281581
S	-2.526310	3.567370	3.166374
S	0.635794	1.992546	-4.051334
N	2.849749	-0.172040	-0.314036
H	3.552229	-0.826411	-0.635102
N	1.548204	-0.448325	-0.651869
N	5.801640	0.309144	0.410951
N	0.767506	-0.449001	2.090613
N	-0.716053	2.069969	1.614017
N	0.254951	1.958865	-1.259618
O	2.325900	1.683626	0.890905
C	5.978122	0.513727	-1.070426
H	6.074877	1.583384	-1.265522
H	5.123199	0.111768	-1.615661
H	6.883098	-0.012720	-1.379795
C	7.014212	0.884190	1.107543
H	7.075881	1.950327	0.885109
H	7.896327	0.365209	0.727807
H	6.910824	0.719776	2.181388
C	5.756618	-1.159946	0.745015
H	6.724372	-1.592422	0.485209
H	4.984909	-1.671135	0.169647
H	5.553659	-1.275753	1.811240
C	4.605354	1.081177	0.951701
H	4.581980	0.901520	2.032455
H	4.823046	2.139722	0.790802
C	3.164941	0.879443	0.477100
C	1.401785	-1.367948	-1.545738
H	2.305057	-1.826321	-1.961541
C	0.164722	-1.886904	-2.103011
C	0.361006	-2.840874	-3.125065
H	1.379179	-3.110764	-3.400567
C	-0.705067	-3.436437	-3.780399
H	-0.520960	-4.167180	-4.565287
C	-2.006060	-3.094714	-3.421345
H	-2.856936	-3.552862	-3.921824

C	-2.221301	-2.169256	-2.404631
H	-3.243572	-1.922730	-2.124113
C	-1.161441	-1.549125	-1.737921
C	-2.460829	-1.604889	0.765564
C	-1.654838	-2.521876	1.458632
H	-0.571329	-2.465093	1.376818
C	-2.235735	-3.504630	2.254449
H	-1.600605	-4.214531	2.782803
C	-3.623982	-3.577412	2.376365
H	-4.077776	-4.344380	3.002909
C	-4.427716	-2.668679	1.689702
H	-5.511973	-2.723282	1.774366
C	-3.853189	-1.687396	0.883265
H	-4.496287	-0.997610	0.341781
C	-2.845665	0.733494	-1.006311
C	-2.926394	1.033175	-2.371753
H	-2.302131	0.509849	-3.092480
C	-3.794529	2.025526	-2.818927
H	-3.846483	2.249034	-3.883624
C	-4.580031	2.735728	-1.912539
H	-5.253902	3.515155	-2.266201
C	-4.490484	2.452421	-0.549111
H	-5.088524	3.010061	0.170028
C	-3.622520	1.464900	-0.095868
H	-3.544504	1.274129	0.972634
C	1.659473	-1.044106	2.594283
C	-1.474288	2.695175	2.268425
C	0.415317	1.966117	-2.434625

Octahedral R=*NHPh*
VACUO

Ni	0.232900	-0.153900	-1.463900
P	-1.552700	-0.597900	-0.105700
S	-2.021100	3.593100	-2.981100
S	2.262600	-3.688300	-3.459200
S	3.029100	0.425900	2.246600
N	2.075300	1.894100	-0.570200
N	0.770500	1.529700	-0.317100
N	-0.768300	1.085600	-2.724300
N	0.356100	-1.844900	-2.520900
N	1.615700	-1.010900	0.264800
O	2.147800	0.424700	-2.365900
N	4.089400	1.251800	-1.423500
C	2.736400	1.111000	-1.534600
C	0.250600	2.122800	0.703200
H	0.833400	2.917300	1.182000
C	-1.013600	1.832900	1.365100
C	-1.371900	2.763200	2.363600
H	-0.717300	3.617200	2.536400
C	-2.518100	2.621700	3.125800
H	-2.761600	3.363000	3.886700
C	-3.352200	1.527900	2.910800
H	-4.259200	1.395800	3.500100
C	-3.019200	0.599900	1.933800
H	-3.679200	-0.248500	1.763200
C	-1.861000	0.719700	1.157500
C	-3.234900	-0.693400	-0.843100
C	-3.764900	0.483900	-1.390700
H	-3.192500	1.409300	-1.383200
C	-5.039200	0.485300	-1.942800
H	-5.431000	1.411100	-2.363500
C	-5.797900	-0.684300	-1.964400
H	-6.798700	-0.680800	-2.398100
C	-5.270900	-1.857400	-1.430600
H	-5.856300	-2.777000	-1.442400
C	-3.993200	-1.866800	-0.874200
H	-3.597400	-2.787600	-0.450000
C	-1.350000	-2.144400	0.857200
C	-1.351600	-2.200400	2.253500
H	-1.515500	-1.300300	2.842300
C	-1.115800	-3.407000	2.906000
H	-1.108000	-3.434400	3.995800
C	-0.872600	-4.564900	2.173000
H	-0.676100	-5.506500	2.687000
C	-0.851900	-4.509500	0.780900
H	-0.628500	-5.402600	0.198300
C	-1.079000	-3.307100	0.122000
H	-1.003400	-3.256400	-0.962800
C	-1.271000	2.153400	-2.835500
C	1.169100	-2.617400	-2.908800
C	2.214900	-0.474700	1.133400
H	2.597700	1.946700	0.320000
H	4.391900	1.875600	-0.688100
C	5.110400	0.411500	-1.901100
C	6.418100	0.762700	-1.539400
C	4.876300	-0.747500	-2.646000
C	7.486900	-0.038800	-1.910500
H	6.588800	1.661900	-0.943100
C	5.960400	-1.539600	-3.007900
H	3.865600	-1.043200	-2.909700
C	7.262900	-1.197300	-2.651200
H	8.495900	0.242300	-1.608300
H	5.763200	-2.452800	-3.567500
H	8.100100	-1.833400	-2.936700

Octahedral R=*NHPh*
COSMO

Ni	-0.275631	-0.107902	-0.375972
P	1.962523	0.105417	0.237710
S	0.889769	2.258741	-4.266144
O	-2.639215	-0.484768	-0.453053
N	-4.270406	-0.487018	1.226665
N	-2.102561	-0.656892	1.785206
N	-0.765954	-0.677718	1.604621
N	-0.055544	0.458304	-2.317002
C	-6.627589	-0.416216	1.506705
H	-6.444884	-0.358216	2.580591
C	-7.926478	-0.423093	1.020365
H	-8.758228	-0.368011	1.721454
C	-8.158559	-0.504152	-0.353183
H	-9.177424	-0.512404	-0.736434
C	-7.073883	-0.574935	-1.225615
H	-7.246042	-0.639792	-2.298508
C	-5.761162	-0.567104	-0.753654
H	-4.922074	-0.623131	-1.440299
C	-5.535930	-0.487854	0.624190
C	-2.996596	-0.540654	0.729627
C	-0.065716	-0.991178	2.645336
H	-0.607792	-1.237234	3.564597
C	1.378295	-1.121482	2.759317
C	1.802970	-1.690883	3.979312
H	1.051971	-1.953254	4.722900
C	3.140768	-1.938067	4.246634
H	3.430776	-2.384466	5.196184
C	4.102378	-1.611838	3.294378
H	5.157822	-1.797383	3.483587
C	3.708372	-1.032153	2.092952
H	4.470264	-0.768280	1.363594
C	2.364438	-0.767827	1.805656
C	3.076968	-0.666813	-0.995410
C	3.244810	-2.059643	-0.981099
H	2.809352	-2.660332	-0.185431
C	3.967818	-2.688484	-1.988873
H	4.091715	-3.770563	-1.962127
C	4.524761	-1.939679	-3.026412
H	5.085841	-2.435364	-3.817815
C	4.356686	-0.555581	-3.046454
H	4.787181	0.037645	-3.851769
C	3.635747	0.080914	-2.037826
H	3.507360	1.160774	-2.074711
C	2.560468	1.826242	0.502920
C	3.341485	2.210181	1.602115
H	3.653194	1.482267	2.347293
C	3.725079	3.541073	1.759533
H	4.328559	3.824470	2.620985
C	3.335462	4.500947	0.827147
H	3.632239	5.541116	0.958016
C	2.553198	4.126408	-0.264612
H	2.230721	4.871845	-0.989974
C	2.159073	2.801069	-0.422635
H	1.520541	2.530421	-1.259233
C	0.340640	1.214651	-3.136598
H	-4.327671	-0.467385	2.236270
S	0.450276	-4.798558	-0.080248
C	0.120320	-3.243462	-0.466154
N	-0.111353	-2.121707	-0.760581
S	-1.647286	4.492984	0.216309
C	-1.195956	2.917801	0.141269
N	-0.876764	1.784298	0.093129
H	-2.446011	-0.850931	2.719971

Octahedral R=*OEt*
VACUO

Ni	0.832461	-0.194932	0.676992
P	-1.312113	0.051893	-0.081193
O	3.248056	-0.225890	0.911588
O	4.970653	-0.181597	-0.624660
N	1.580072	-0.054505	-1.370557
N	2.924053	-0.161246	-1.381852
N	0.483511	-0.225779	2.613321
S	-0.749048	-0.076626	5.137473
C	-0.373289	0.400690	-2.804701
C	-1.457499	0.386962	-1.900181
C	-2.748369	0.597154	-2.397248
H	-3.586109	0.576943	-1.702530
C	-2.991451	0.831925	-3.743008
H	-4.010959	0.996483	-4.090319
C	-1.925346	0.849105	-4.638974
H	-2.094145	1.028940	-5.700482
C	-0.642838	0.634876	-4.169426
H	0.193662	0.651879	-4.868046
C	1.035371	0.208413	-2.506521
H	1.693918	0.322592	-3.378833
C	3.668192	-0.193173	-0.226993
C	5.949407	-0.179248	0.433717
H	5.869475	-1.120094	0.993710
H	5.727849	0.644507	1.123908
C	7.302447	-0.021808	-0.221359
H	8.087696	-0.017992	0.544210
H	7.359400	0.921329	-0.778175

H	7.501855	-0.847124	-0.915549
C	-2.493169	-1.356914	0.013273
C	-3.740223	-1.301289	0.641287
H	-4.060204	-0.394919	1.150058
C	-4.587877	-2.406695	0.607561
H	-5.558608	-2.351608	1.100834
C	-4.201716	-3.571548	-0.050664
H	-4.867686	-4.435194	-0.071626
C	-2.958508	-3.629938	-0.678470
H	-2.635090	-4.534876	-1.192316
C	-2.108319	-2.532045	-0.648325
H	-1.143827	-2.597493	-1.146339
C	-2.131360	1.489585	0.695995
C	-2.481105	1.397219	2.049555
H	-2.315329	0.476546	2.605123
C	-3.007390	2.500949	2.710563
H	-3.254255	2.413422	3.767950
C	-3.173896	3.708688	2.036232
H	-3.574108	4.578076	2.559670
C	-2.794533	3.812975	0.700474
H	-2.883010	4.763560	0.174436
C	-2.269400	2.713368	0.030892
H	-1.937845	2.825880	-0.999435
C	-0.033775	-0.165955	3.674469
N	1.089947	-2.210378	0.378073
C	1.215224	-3.082497	-0.414419
S	1.357040	-4.272337	-1.522732
C	1.198852	2.700333	-0.399021
S	1.290972	3.775453	-1.622777
N	1.139056	1.883815	0.460311
H	3.423230	-0.017972	-2.254045

Octahedral R=*OEt*
COSMO

Ni	0.817370	-0.126000	0.522674
P	-1.373511	0.096530	-0.190027
O	3.122023	-0.215680	0.830848
O	4.909606	-0.272093	-0.620907
N	1.549826	0.061021	-1.449372
N	2.899530	-0.046039	-1.456192
N	0.434487	-0.287770	2.489478
S	-0.726721	-0.290970	5.055835
C	-0.419797	0.422328	-2.897696
C	-1.519936	0.352877	-2.009542
C	-2.815842	0.457737	-2.526193
H	-3.663712	0.391399	-1.846978
C	-3.051041	0.651540	-3.882633
H	-4.073091	0.732579	-4.247348
C	-1.973376	0.736635	-4.760476
H	-2.137767	0.887212	-5.825750
C	-0.682294	0.621458	-4.270496
H	0.159090	0.675981	-4.959274
C	0.996314	0.286001	-2.592483
H	1.651344	0.377918	-3.464898
C	3.612671	-0.184036	-0.296625
C	5.857302	-0.398706	0.479119
H	5.631083	-1.322343	1.024101
H	5.717156	0.452456	1.154943
C	7.239558	-0.420147	-0.123878
H	7.977313	-0.515745	0.681017
H	7.445889	0.506865	-0.671570
H	7.361945	-1.269905	-0.805665
C	-2.472455	-1.355844	0.057748
C	-3.556214	-1.386916	0.941611
H	-3.841933	-0.501555	1.502729
C	-4.296847	-2.558355	1.100457
H	-5.139460	-2.567312	1.790297
C	-3.969321	-3.704764	0.379731
H	-4.548895	-4.618163	0.508726
C	-2.897329	-3.675247	-0.514107
H	-2.635393	-4.561893	-1.090330
C	-2.152895	-2.511936	-0.672978
H	-1.319038	-2.505095	-1.372176
C	-2.173775	1.561436	0.560453
C	-2.420567	1.559967	1.941668
H	-2.206317	0.678507	2.540461
C	-2.923820	2.696141	2.566841
H	-3.117572	2.675109	3.638488
C	-3.161006	3.856818	1.829986
H	-3.546052	4.749150	2.322301
C	-2.891276	3.872657	0.463063
H	-3.057819	4.777975	-0.119130
C	-2.397558	2.734791	-0.170363
H	-2.177426	2.773481	-1.234689
C	-0.046410	-0.294253	3.568001
N	1.009306	-2.167794	0.229512
C	1.205054	-3.119701	-0.444322
S	1.449899	-4.444023	-1.373530
C	1.226496	2.906842	-0.126875
S	1.439461	4.236041	-1.054307
N	1.080601	1.944364	0.548527
H	3.401829	0.005218	-2.337342

Derotonated ligand

Square-planar R=$CH_2N(CH_3)_3$
VACUO

Ni	0.788639	-0.586898	-0.035432
P	-1.243113	0.090053	0.039240
S	-1.422936	-4.561856	0.366220
N	1.549045	1.099955	-0.319269
N	2.943424	1.105206	-0.284744
N	5.818593	0.917846	-0.190078
N	0.211216	-2.304413	0.151845
O	2.711089	-1.166798	0.091270
C	-1.846232	0.044095	1.760264
C	-2.305568	-1.152741	2.328550
H	-2.382636	-2.060348	1.733315
C	-2.661284	-1.180474	3.672789
H	-3.021862	-2.110403	4.109023
C	-2.544448	-0.035526	4.459046
H	-2.818178	-0.067318	5.513053
C	-2.074228	1.149749	3.899146
H	-1.978922	2.047266	4.508770
C	-1.722657	1.193857	2.554976
H	-1.356913	2.125777	2.126819
C	-2.370916	-0.783375	-1.085534
C	-3.711686	-1.028017	-0.777968
H	-4.107699	-0.775716	0.203876
C	-4.540811	-1.599722	-1.738431
H	-5.584171	-1.795293	-1.497376
C	-4.039970	-1.925031	-2.995961
H	-4.693865	-2.373228	-3.742696
C	-2.700624	-1.686123	-3.299301
H	-2.303588	-1.947938	-4.278759
C	-1.864027	-1.121457	-2.346673
H	-0.811651	-0.947053	-2.573035
C	-1.427844	1.851871	-0.451895
C	-2.714452	2.380013	-0.570646
H	-3.577802	1.740957	-0.398808
C	-2.916111	3.715834	-0.903367
H	-3.929195	4.104579	-0.988012
C	-1.821587	4.548647	-1.127596
H	-1.970080	5.594592	-1.390852
C	-0.540306	4.039565	-1.017056
H	0.316725	4.689418	-1.192626
C	-0.314309	2.687869	-0.678318
C	1.061435	2.282358	-0.580856
H	1.806799	3.062484	-0.744066
C	3.395499	-0.102607	-0.070783
C	4.904873	-0.291823	0.008734
H	5.146395	-0.706890	0.993943
H	5.198599	-1.031896	-0.744181
C	7.239428	0.437941	-0.068920
H	7.431925	-0.315349	-0.836695
H	7.390384	0.008371	0.924477
H	7.909843	1.290273	-0.209490
C	5.634311	1.525788	-1.557879
H	4.605979	1.880940	-1.634179
H	5.834224	0.759322	-2.311684
H	6.347474	2.348220	-1.664957
C	5.580631	1.970855	0.863475
H	6.301631	2.778457	0.707472
H	5.733146	1.521380	1.848574
H	4.555950	2.329396	0.760889
C	-0.510584	-3.252413	0.231776

Square-planar R=$CH_2N(CH_3)_3$
COSMO

Ni	0.789933	-0.536788	0.062806
P	-1.252282	0.154997	0.082365
S	-1.150393	-4.672941	0.824306
N	1.553446	1.124766	-0.340435
N	2.944078	1.098329	-0.401202
N	5.824294	0.835262	-0.460990
N	0.192139	-2.244917	0.406703
O	2.676537	-1.142531	0.082038
C	-2.008183	-0.001335	1.736149
C	-2.641170	-1.186135	2.136195
H	-2.748779	-2.018326	1.443980
C	-3.141256	-1.297094	3.430702
H	-3.641697	-2.215116	3.733260
C	-3.001777	-0.243129	4.333661
H	-3.393743	-0.337030	5.345404
C	-2.357376	0.930402	3.942364
H	-2.240792	1.755480	4.642763
C	-1.859888	1.054218	2.648934
H	-1.359046	1.974552	2.352977
C	-2.287724	-0.701158	-1.154303
C	-3.669057	-0.865591	-0.996768
H	-4.166920	-0.553567	-0.081748
C	-4.415551	-1.435340	-2.025430
H	-5.488669	-1.564219	-1.897790
C	-3.795149	-1.833416	-3.208879
H	-4.385390	-2.275633	-4.010234
C	-2.419027	-1.667468	-3.367842

H	-1.930002	-1.976753	-4.289855
C	-1.664131	-1.106105	-2.342966
H	-0.587846	-0.981575	-2.464681
C	-1.427539	1.930320	-0.331929
C	-2.708587	2.485128	-0.368910
H	-3.576407	1.868267	-0.146038
C	-2.896543	3.828304	-0.683844
H	-3.903460	4.239679	-0.706334
C	-1.795419	4.634733	-0.968210
H	-1.934288	5.684738	-1.218099
C	-0.518492	4.097685	-0.931283
H	0.342842	4.726266	-1.149501
C	-0.306740	2.739709	-0.611979
C	1.068003	2.307106	-0.592473
H	1.813417	3.071020	-0.813385
C	3.399482	-0.097516	-0.166888
C	4.895494	-0.335054	-0.184122
H	5.185224	-0.745864	0.788236
H	5.112751	-1.092314	-0.944426
C	7.230406	0.298491	-0.394857
H	7.347176	-0.479872	-1.150699
H	7.407016	-0.108093	0.602569
H	7.918615	1.122434	-0.593028
C	5.604774	1.411496	-1.835900
H	4.603455	1.837064	-1.881165
H	5.721458	0.610928	-2.570066
H	6.359929	2.183430	-1.999351
C	5.687566	1.922308	0.573799
H	6.445868	2.679912	0.364226
H	5.855936	1.485071	1.560423
H	4.687780	2.348357	0.504093
C	-0.386307	-3.264823	0.577137

Square-planar R=*NHPh*
VACUO

Ni	-0.513649	0.014773	0.019561
P	1.622963	-0.120933	0.011581
S	0.568570	4.329338	1.183374
O	-2.498507	0.138705	-0.002414
N	-4.247264	-1.334593	-0.503073
N	-2.154190	-2.088010	-0.594909
N	-0.845924	-1.797013	-0.405402
N	-0.344232	1.794205	0.424915
C	-6.622134	-1.361905	-0.512101
H	-6.564073	-2.405540	-0.827670
C	-7.855778	-0.760352	-0.326182
H	-8.762796	-1.338655	-0.498157
C	-7.928840	0.570301	0.080393
H	-8.897179	1.044627	0.228801
C	-6.751540	1.283989	0.292784
H	-6.799681	2.324565	0.609466
C	-5.503576	0.696559	0.110801
H	-4.586368	1.253426	0.277455
C	-5.436386	-0.640449	-0.295449
C	-2.924098	-1.020573	-0.346304
C	-0.047807	-2.830074	-0.556626
H	-0.562468	-3.758086	-0.806812
C	1.376543	-2.913102	-0.390945
C	1.950364	-4.199706	-0.526776
H	1.298045	-5.040397	-0.760761
C	3.306712	-4.412443	-0.361814
H	3.713618	-5.417277	-0.469771
C	4.148372	-3.343991	-0.050059
H	5.216733	-3.501245	0.088383
C	3.610945	-2.070008	0.080431
H	4.271228	-1.237686	0.315458
C	2.243304	-1.838250	-0.092252
C	2.381772	0.698834	-1.439700
C	2.756222	-0.073683	-2.548004
H	2.647673	-1.156606	-2.526254
C	3.281324	0.540317	-3.679873
H	3.573047	-0.069970	-4.533825
C	3.431040	1.923853	-3.719139
H	3.843631	2.402181	-4.607227
C	3.050024	2.694844	-2.622487
H	3.157370	3.778209	-2.649000
C	2.517321	2.093103	-1.487555
H	2.215710	2.712733	-0.645511
C	2.393275	0.519579	1.538535
C	3.623822	1.180395	1.560525
H	4.143155	1.409909	0.632265
C	4.186540	1.548658	2.779746
H	5.143079	2.069160	2.793247
C	3.529553	1.260635	3.972311
H	3.973466	1.553660	4.923213
C	2.299237	0.605998	3.950823
H	1.777446	0.386026	4.881002
C	1.728603	0.240227	2.738860
H	0.759349	-0.259001	2.716188
C	0.055205	2.862576	0.762099
H	-4.353343	-2.302537	-0.772372

Square-planar R=*NHPh*
COSMO

Ni	-0.492929	-0.018190	-0.003662
P	1.658480	-0.153410	-0.017815
S	0.265005	4.470420	0.863062
O	-2.467023	0.116842	-0.035895
N	-4.249012	-1.397780	-0.127595
N	-2.155163	-2.184581	-0.185150
N	-0.827469	-1.866319	-0.167304
N	-0.332932	1.796661	0.257684
C	-6.619228	-1.347907	-0.242661
H	-6.588395	-2.436725	-0.294785
C	-7.834561	-0.681814	-0.273035
H	-8.755330	-1.258433	-0.349435
C	-7.873543	0.711930	-0.209208
H	-8.826847	1.236313	-0.234786
C	-6.677486	1.420977	-0.111773
H	-6.695047	2.508389	-0.060914
C	-5.446963	0.767834	-0.079973
H	-4.521131	1.330021	-0.005631
C	-5.412359	-0.631404	-0.146524
C	-2.916761	-1.091924	-0.111902
C	-0.033962	-2.905507	-0.244769
H	-0.546827	-3.865057	-0.306229
C	1.405101	-2.960835	-0.276931
C	1.971034	-4.252043	-0.390427
H	1.306032	-5.112986	-0.432036
C	3.342023	-4.437993	-0.455253
H	3.747446	-5.444391	-0.543703
C	4.199777	-3.337727	-0.407660
H	5.278229	-3.471893	-0.462313
C	3.666663	-2.058796	-0.289430
H	4.341728	-1.205962	-0.255044
C	2.284221	-1.857522	-0.218370
C	2.413333	0.776674	-1.397135
C	2.607363	0.130278	-2.626939
H	2.359265	-0.923360	-2.742392
C	3.132322	0.833163	-3.706743
H	3.286321	0.321852	-4.655377
C	3.459738	2.181777	-3.570701
H	3.874550	2.728742	-4.416240
C	3.256091	2.829789	-2.352533
H	3.509913	3.882598	-2.242345
C	2.726698	2.136020	-1.267979
H	2.569521	2.651775	-0.323309
C	2.396167	0.410411	1.559508
C	3.704041	0.904760	1.639271
H	4.298523	1.056752	0.741142
C	4.253591	1.204920	2.883328
H	5.269496	1.591609	2.939510
C	3.511409	1.005783	4.046904
H	3.948702	1.237233	5.017209
C	2.209055	0.512118	3.969694
H	1.625701	0.355212	4.875305
C	1.648948	0.217704	2.729772
H	0.629774	-0.165005	2.669959
C	-0.071238	2.920723	0.520352
H	-4.402413	-2.395471	-0.191031

Square-planar R=*OEt*
VACUO

Ni	1.209010	-0.230784	-0.042651
P	-0.879216	0.210640	-0.120700
O	3.142800	-0.651593	0.094167
O	5.035703	0.464109	0.753814
N	1.788294	1.473445	0.534016
N	3.119470	1.565143	0.797327
N	0.798998	-1.926269	-0.617748
S	-0.441288	-4.176029	-1.730113
C	-0.253164	2.894203	0.534045
C	-1.255197	1.983459	0.133285
C	-2.570649	2.424677	-0.033337
H	-3.338116	1.719534	-0.345300
C	-2.922495	3.747915	0.198816
H	-3.954112	4.068315	0.063451
C	-1.944742	4.655534	0.605625
H	-2.205288	5.696685	0.791894
C	-0.637425	4.234957	0.767034
H	0.124429	4.948642	1.078530
C	1.140660	2.596492	0.726640
H	1.771915	3.420848	1.059312
C	3.714340	0.408134	0.525988
C	5.797365	-0.738646	0.521377
H	5.694897	-1.032165	-0.531495
H	5.387136	-1.549606	1.137012
C	7.229143	-0.419196	0.884403
H	7.859507	-1.301934	0.726384
H	7.307181	-0.120746	1.936335
H	7.615574	0.398469	0.264776
C	-1.667828	-0.171861	-1.724149
C	-2.993956	-0.598062	-1.836207
H	-3.587159	-0.796470	-0.945885
C	-3.558793	-0.773069	-3.096285
H	-4.591260	-1.109892	-3.179094

C	-2.808851	-0.526664	-4.242367
H	-3.255315	-0.667994	-5.226192
C	-1.484182	-0.108272	-4.132139
H	-0.890516	0.076422	-5.026185
C	-0.911742	0.064744	-2.878330
H	0.128848	0.377571	-2.787781
C	-1.810812	-0.624765	1.216828
C	-2.167605	-1.975986	1.110226
H	-1.941370	-2.543560	0.209661
C	-2.820177	-2.600646	2.167674
H	-3.099840	-3.649111	2.075018
C	-3.104804	-1.898257	3.337244
H	-3.612888	-2.395387	4.163415
C	-2.735865	-0.560639	3.450903
H	-2.950474	-0.005508	4.363259
C	-2.090984	0.077277	2.396952
H	-1.810428	1.124702	2.493566
C	0.261692	-2.869031	-1.106137

Square-planar R=*OEt*
COSMO

Ni	1.177189	-0.206559	-0.049943
P	-0.919992	0.258524	-0.131904
O	3.097647	-0.662552	0.110657
O	5.017304	0.444826	0.719325
N	1.769422	1.503404	0.477544
N	3.119752	1.580137	0.718992
N	0.760873	-1.910527	-0.609126
S	-0.248937	-4.371158	-1.503312
C	-0.260093	2.938280	0.501124
C	-1.281920	2.024264	0.165148
C	-2.606829	2.462362	0.078463
H	-3.397256	1.757478	-0.170190
C	-2.938777	3.792447	0.312697
H	-3.976853	4.110450	0.240922
C	-1.937163	4.705807	0.641882
H	-2.185104	5.749322	0.826617
C	-0.620891	4.283693	0.733668
H	0.159772	4.996348	0.993709
C	1.142253	2.635561	0.647223
H	1.779003	3.469874	0.940771
C	3.694019	0.407559	0.495278
C	5.770379	-0.779098	0.515496
H	5.662518	-1.089285	-0.530770
H	5.350778	-1.563144	1.156881
C	7.206592	-0.475179	0.866572
H	7.812437	-1.377221	0.724485
H	7.297896	-0.159859	1.912677
H	7.610363	0.315647	0.223327
C	-1.685214	-0.108576	-1.750214
C	-3.038937	-0.440024	-1.883193
H	-3.670810	-0.566038	-1.007299
C	-3.586681	-0.610368	-3.152365
H	-4.639302	-0.870283	-3.248569
C	-2.795293	-0.446051	-4.288061
H	-3.229734	-0.578107	-5.278005
C	-1.446185	-0.114980	-4.157191
H	-0.823190	0.012409	-5.040718
C	-0.889381	0.051302	-2.893029
H	0.166352	0.303206	-2.791446
C	-1.832868	-0.630680	1.179383
C	-2.332182	-1.923245	0.968181
H	-2.236448	-2.401673	-0.004242
C	-2.964260	-2.597877	2.009072
H	-3.362001	-3.596315	1.835692
C	-3.086877	-2.001958	3.264200
H	-3.581235	-2.535461	4.074854
C	-2.575196	-0.722935	3.481473
H	-2.664375	-0.252331	4.459017
C	-1.948553	-0.037423	2.445414
H	-1.555034	0.961674	2.625554
C	0.326604	-2.944100	-0.990345

Octahedral R=*$CH_2N(CH_3)_3$*
VACUO

Ni	0.536800	0.217900	-0.841000
P	-1.402100	-0.264700	0.262100
S	-1.545300	4.307200	-1.837300
S	-0.342700	-3.715700	-3.342800
S	3.297500	-2.576300	2.226000
N	2.247300	2.292800	0.324600
N	0.993500	1.789100	0.498700
N	5.089700	0.994700	0.366700
N	-0.355200	1.753200	-1.925500
N	0.355400	-1.225700	-2.226200
N	1.712700	-1.055000	0.452900
O	2.498700	0.892600	-1.559100
C	5.064600	-0.381800	-0.247100
H	5.659300	-0.356800	-1.164800
H	4.028900	-0.643600	-0.474100
H	5.469300	-1.093900	0.477800
C	6.505500	1.442300	0.536700
H	6.979900	1.523100	-0.445100
H	7.038000	0.709800	1.150500

H	6.513100	2.417200	1.033300
C	4.445300	0.942700	1.730400
H	5.051200	0.285000	2.359900
H	3.440900	0.531400	1.637900
H	4.396100	1.958600	2.130500
C	4.382700	1.995900	-0.565400
H	4.545500	2.987000	-0.131600
H	4.881000	1.906500	-1.535700
C	2.896300	1.694400	-0.673700
C	0.295100	2.395600	1.404000
H	0.762400	3.270300	1.871100
C	-1.036100	2.077700	1.889600
C	-1.522800	2.975800	2.865900
H	-0.882600	3.805100	3.167200
C	-2.776900	2.846300	3.433700
H	-3.112000	3.565600	4.181500
C	-3.608500	1.802900	3.033100
H	-4.604400	1.687500	3.459900
C	-3.154600	0.906600	2.075100
H	-3.805000	0.094900	1.754400
C	-1.883500	1.010500	1.501300
C	-2.890100	-0.346000	-0.806500
C	-3.497400	0.856700	-1.195800
H	-3.146900	1.809400	-0.803400
C	-4.539500	0.845700	-2.114500
H	-4.990600	1.791500	-2.414900
C	-4.980300	-0.357300	-2.662900
H	-5.789000	-0.361600	-3.395400
C	-4.367000	-1.550800	-2.291100
H	-4.685000	-2.495000	-2.732600
C	-3.326200	-1.549900	-1.367100
H	-2.846100	-2.490400	-1.107600
C	-1.343500	-1.831300	1.223400
C	-1.560500	-1.900000	2.604300
H	-1.853300	-1.013600	3.162800
C	-1.377600	-3.099600	3.287600
H	-1.536700	-3.130400	4.366200
C	-0.977400	-4.244000	2.605100
H	-0.817700	-5.177600	3.146200
C	-0.751900	-4.180600	1.232300
H	-0.410300	-5.058900	0.685600
C	-0.920400	-2.984800	0.545900
H	-0.683000	-2.948500	-0.513500
C	-0.848200	2.829900	-1.892900
C	0.067700	-2.265400	-2.710000
C	2.345000	-1.717000	1.200300

Octahedral R=*$CH_2N(CH_3)_3$*
COSMO

Ni	0.577800	0.351000	-0.543700
P	-1.462400	-0.192000	0.442400
S	-1.699100	4.183000	-2.437200
S	-0.082500	-3.669100	-2.957100
S	3.341200	-3.373700	0.707400
N	2.314500	2.187000	0.911800
N	1.014600	1.755400	0.929100
N	5.373400	1.036800	0.021700
N	-0.307200	1.859900	-1.660000
N	0.418500	-1.039700	-2.079400
N	1.723900	-1.079700	0.478400
O	2.485100	1.121800	-1.155600
C	5.268700	-0.015000	-1.045300
H	5.462900	0.449400	-2.014200
H	4.266000	-0.440400	-1.028700
H	6.018400	-0.780800	-0.837000
C	6.763400	1.597200	0.011900
H	6.953400	2.051700	-0.962100
H	7.467200	0.781800	0.188800
H	6.848200	2.346400	0.800700
C	5.099700	0.416800	1.359600
H	5.839300	-0.367600	1.531500
H	4.094500	-0.007700	1.353700
H	5.180900	1.188600	2.127500
C	4.411900	2.190100	-0.230200
H	4.627900	2.942800	0.529300
H	4.653900	2.583500	-1.221000
C	2.954500	1.782900	-0.181900
C	0.269500	2.323200	1.823400
H	0.751600	3.085900	2.441500
C	-1.147300	2.131500	2.084900
C	-1.685300	3.077500	2.984800
H	-1.018400	3.825200	3.409600
C	-3.028600	3.093600	3.327100
H	-3.403100	3.847400	4.016400
C	-3.887200	2.142600	2.781300
H	-4.944400	2.134100	3.036400
C	-3.377900	1.188300	1.907500
H	-4.052000	0.440800	1.496900
C	-2.026900	1.156500	1.546300
C	-2.858900	-0.416700	-0.724800
C	-3.444200	0.714100	-1.313700
H	-3.131400	1.711600	-1.015000
C	-4.432700	0.574900	-2.283200

H	-4.877700	1.465100	-2.724900
C	-4.848600	-0.694700	-2.687800
H	-5.620900	-0.802900	-3.447800
C	-4.266900	-1.822600	-2.111300
H	-4.582700	-2.818800	-2.416700
C	-3.277600	-1.686700	-1.138600
H	-2.836600	-2.582100	-0.708600
C	-1.478500	-1.694700	1.492500
C	-1.987900	-1.718700	2.796700
H	-2.415400	-0.822800	3.240200
C	-1.952900	-2.894300	3.546000
H	-2.351200	-2.894700	4.559200
C	-1.414000	-4.059500	3.002400
H	-1.389200	-4.976400	3.589300
C	-0.897800	-4.040800	1.706400
H	-0.464500	-4.941800	1.275600
C	-0.917700	-2.865800	0.960600
H	-0.485700	-2.862000	-0.036300
C	-0.883900	2.841400	-1.978700
C	0.207900	-2.144200	-2.452200
C	2.395400	-2.048700	0.565700

Octahedral R=*NHPh*
VACUO

Ni	0.491900	-0.153100	0.411600
P	-1.787900	-0.107100	0.076400
S	-0.758000	0.420600	4.995400
O	2.699200	-0.185900	0.322800
N	4.281700	-0.013000	-1.382400
N	2.157900	-0.100600	-1.979700
N	0.868800	-0.178400	-1.672500
N	0.334600	-0.127800	2.453000
C	6.638700	0.231700	-1.602200
H	6.506700	0.176900	-2.686000
C	7.904700	0.394200	-1.064400
H	8.762400	0.463000	-1.735400
C	8.076600	0.474500	0.317900
H	9.070000	0.608400	0.742500
C	6.952600	0.384600	1.140600
H	7.068900	0.450800	2.222700
C	5.674700	0.219300	0.621400
H	4.798100	0.156200	1.260400
C	5.501800	0.139400	-0.771900
C	2.973700	-0.101200	-0.892300
C	0.066700	-0.261400	-2.700200
H	0.557900	-0.254900	-3.680100
C	-1.363500	-0.438200	-2.735000
C	-1.899400	-0.628900	-4.035100
H	-1.209600	-0.597200	-4.879100
C	-3.239800	-0.873300	-4.267200
H	-3.593600	-1.016700	-5.291300
C	-4.127100	-0.948700	-3.193300
H	-5.184800	-1.156300	-3.353000
C	-3.636200	-0.751600	-1.909600
H	-4.324800	-0.805100	-1.068500
C	-2.287100	-0.478100	-1.654500
C	-2.749000	-1.342800	1.042500
C	-2.809100	-2.663900	0.573700
H	-2.347700	-2.937900	-0.372900
C	-3.449100	-3.645200	1.321400
H	-3.474200	-4.667300	0.939800
C	-4.022100	-3.328400	2.552400
H	-4.514600	-4.102900	3.142800
C	-3.939200	-2.024500	3.035600
H	-4.353100	-1.770200	4.012200
C	-3.302100	-1.035100	2.290600
H	-3.224900	-0.028900	2.699400
C	-2.618200	1.503100	0.427000
C	-3.511700	2.126100	-0.451900
H	-3.760300	1.665700	-1.404700
C	-4.082300	3.354200	-0.124800
H	-4.772200	3.828500	-0.826500
C	-3.764400	3.979000	1.078000
H	-4.207100	4.945500	1.327000
C	-2.856000	3.376800	1.946000
H	-2.573400	3.866900	2.877000
C	-2.277200	2.154700	1.621900
H	-1.541800	1.719500	2.291400
C	-0.110300	0.090600	3.524100
H	4.271700	0.024600	-2.392300
S	0.097700	-4.724600	-1.049900
C	0.341500	-3.279800	-0.308100
N	0.494800	-2.246700	0.244800
S	1.113800	4.575100	-0.501200
C	0.862200	3.022300	-0.034300
N	0.682400	1.908600	0.315300

Octahedral R=*NHPh*
COSMO

Ni	0.471665	-0.152844	0.240430
P	-1.841014	-0.104910	-0.041875
S	-0.578000	0.957182	4.747433
O	2.665444	-0.230120	0.151700
N	4.235831	0.159871	-1.531554
N	2.107257	-0.019265	-2.131915
N	0.815592	-0.192556	-1.801996

N	0.388200	-0.051430	2.297225
C	6.592961	0.354129	-1.773237
H	6.425096	0.487007	-2.842935
C	7.881822	0.371587	-1.262817
H	8.720610	0.520791	-1.941937
C	8.099591	0.198593	0.106116
H	9.111050	0.211309	0.508321
C	7.002387	0.009453	0.946074
H	7.158299	-0.126313	2.015528
C	5.699746	-0.009886	0.450428
H	4.850315	-0.156155	1.110384
C	5.483006	0.162433	-0.925748
C	2.946309	-0.044576	-1.065023
C	0.005083	-0.350600	-2.810260
H	0.469044	-0.336031	-3.801223
C	-1.419687	-0.626148	-2.816146
C	-1.935439	-0.953803	-4.094518
H	-1.254315	-0.942393	-4.944588
C	-3.260196	-1.302381	-4.295519
H	-3.607750	-1.553722	-5.296744
C	-4.139713	-1.335953	-3.213724
H	-5.184112	-1.611081	-3.349131
C	-3.667490	-0.996983	-1.952046
H	-4.360116	-1.006426	-1.113319
C	-2.332941	-0.635171	-1.727866
C	-2.736754	-1.263117	1.074174
C	-2.811911	-2.623224	0.738492
H	-2.436484	-2.973988	-0.220452
C	-3.360980	-3.540386	1.629460
H	-3.413443	-4.592190	1.349602
C	-3.834206	-3.118435	2.872449
H	-4.258224	-3.838761	3.571496
C	-3.757666	-1.769109	3.213891
H	-4.121162	-1.426427	4.181967
C	-3.212339	-0.846584	2.323189
H	-3.152961	0.198327	2.619024
C	-2.680850	1.523355	0.185159
C	-3.603826	2.043327	-0.732455
H	-3.868009	1.486823	-1.628466
C	-4.196887	3.285312	-0.511277
H	-4.911760	3.673188	-1.236217
C	-3.880374	4.023610	0.627691
H	-4.346130	4.993955	0.798047
C	-2.951963	3.519825	1.538151
H	-2.681036	4.096462	2.421572
C	-2.347689	2.285664	1.315189
H	-1.601172	1.925060	2.018025
C	-0.010643	0.368107	3.327166
H	4.249715	0.280206	-2.535686
S	0.054271	-4.707984	-1.141283
C	0.303623	-3.276151	-0.381777
N	0.477568	-2.252863	0.184085
S	1.169341	4.393198	1.556101
C	0.920418	2.963531	0.788342
N	0.742643	1.942446	0.223139

Octahedral R=*OEt*
VACUO

Ni	1.004899	0.112383	-0.417751
P	-1.217835	-0.090186	0.198798
O	3.167501	0.178306	-0.646541
O	4.990898	0.291319	0.729774
N	1.702313	-0.043140	1.578189
N	3.028760	0.063467	1.705127
N	0.605323	0.226359	-2.418360
S	-0.488250	0.203186	-5.020444
C	-0.347967	-0.431223	2.929383
C	-1.423695	-0.428273	2.001558
C	-2.731255	-0.625710	2.459008
H	-3.543002	-0.605409	1.733004
C	-3.028186	-0.846554	3.795632
H	-4.060246	-1.000791	4.111610
C	-1.982217	-0.855344	4.720198
H	-2.182633	-1.019944	5.780524
C	-0.685784	-0.650511	4.291196
H	0.125159	-0.656410	5.020054
C	1.063491	-0.240794	2.696096
H	1.692582	-0.293151	3.591253
C	3.634522	0.177442	0.509928
C	5.780301	0.458408	-0.445337
H	5.465198	1.363976	-0.983909
H	5.628087	-0.391335	-1.126622
C	7.222018	0.554215	0.011248
H	7.890124	0.684775	-0.850042
H	7.518727	-0.355621	0.548653
H	7.356392	1.406783	0.689242
C	-2.406493	1.319914	0.058642
C	-3.630647	1.264110	-0.615198
H	-3.937297	0.351691	-1.121224
C	-4.473833	2.373287	-0.638826
H	-5.424614	2.311221	-1.171528
C	-4.107275	3.551545	0.006898
H	-4.765639	4.422176	-0.023707
C	-2.889591	3.613043	0.683404
H	-2.570439	4.529345	1.180049
C	-2.048753	2.507042	0.713938

H	-1.102475	2.575959	1.244293
C	-2.064675	-1.491141	-0.629379
C	-2.355919	-1.375731	-1.996318
H	-2.120964	-0.462283	-2.538201
C	-2.917336	-2.444404	-2.685471
H	-3.117729	-2.335998	-3.751599
C	-3.173240	-3.647426	-2.028911
H	-3.596237	-4.492514	-2.576208
C	-2.846978	-3.779910	-0.682055
H	-2.989013	-4.731693	-0.169338
C	-2.291227	-2.711840	0.015203
H	-2.000324	-2.848719	1.054168
C	0.160168	0.220033	-3.509818
N	1.103493	2.191235	-0.154852
C	1.126162	3.272753	0.316504
S	1.114514	4.776107	0.980807
C	1.014832	-3.046197	0.166781
S	0.895981	-4.517978	0.882584
N	1.097765	-1.990409	-0.359225

Octahedral R=*OEt*
COSMO

Ni	0.909421	0.139294	-0.404581
P	-1.316518	-0.099835	0.212547
O	3.055840	0.248825	-0.705338
O	4.924740	0.171686	0.622411
N	1.632784	-0.110678	1.531332
N	2.981394	-0.059012	1.625398
N	0.511183	0.386366	-2.411335
S	-0.666795	0.392457	-4.974695
C	-0.411395	-0.410505	2.925112
C	-1.505853	-0.321533	2.026579
C	-2.814209	-0.387666	2.523119
H	-3.646528	-0.307917	1.825735
C	-3.082648	-0.560749	3.874116
H	-4.112230	-0.611630	4.223324
C	-2.016121	-0.666230	4.767020
H	-2.199496	-0.801965	5.831860
C	-0.716128	-0.592441	4.296688
H	0.110051	-0.665259	5.002618
C	1.012906	-0.319382	2.652786
H	1.649513	-0.431326	3.535844
C	3.571245	0.127817	0.434719
C	5.740511	0.363017	-0.553373
H	5.473961	1.316557	-1.027356
H	5.535355	-0.441571	-1.271116
C	7.182964	0.349785	-0.103511
H	7.838481	0.491917	-0.970512
H	7.439110	-0.606561	0.368232
H	7.380019	1.156781	0.612571
C	-2.447670	1.323022	-0.102766
C	-3.461264	1.330043	-1.067012
H	-3.680531	0.439865	-1.650067
C	-4.220346	2.480323	-1.284036
H	-5.007291	2.466300	-2.037267
C	-3.981371	3.635283	-0.542904
H	-4.574524	4.532522	-0.717322
C	-2.980285	3.632017	0.429928
H	-2.787387	4.524675	1.024114
C	-2.219691	2.488337	0.646773
H	-1.442250	2.503232	1.408087
C	-2.110941	-1.580181	-0.528158
C	-2.289592	-1.626315	-1.919381
H	-2.013853	-0.777529	-2.539143
C	-2.807779	-2.764582	-2.528936
H	-2.949624	-2.775799	-3.609226
C	-3.125839	-3.888044	-1.765308
H	-3.524342	-4.782107	-2.243994
C	-2.921723	-3.860806	-0.387271
H	-3.151629	-4.736579	0.218350
C	-2.414344	-2.718467	0.228405
H	-2.251550	-2.723378	1.303685
C	0.026992	0.395269	-3.487950
N	0.985827	2.205464	-0.045404
C	1.130303	3.163774	0.629402
S	1.301816	4.504928	1.559892
C	1.254667	-2.972634	0.014531
S	1.464871	-4.393859	0.806111
N	1.111827	-1.955072	-0.571342