

Supporting Information

Why different Ligands Can Control Stereochemistry Selectivity of Ni-Catalyzed Suzuki-Miyaura Cross-Coupling of Benzylic Carbamates with Arylboronic Esters: A Mechanistic Study

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I. CARTESIAN COORDINATES AND ELECTRONIC ENERGIES FOR ALL OF THE CALCULATED STRUCTURES.....	S2-S36
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I. Cartesian coordinates and electronic energies for all of the calculated structures

P1				P	4.250180	-1.117945	-0.443085
SCF done:	-295.498618			C	5.239570	-1.752481	1.038255
Ni	1.624349	-0.000500	-0.000309	H	4.753382	-2.648350	1.434785
P	-0.499738	-0.000133	-0.000617	H	6.271791	-1.988705	0.753706
C	-1.353082	-0.311263	1.657284	H	5.244825	-0.989946	1.822817
H	-1.053913	0.463120	2.369208	C	4.649151	-2.458526	-1.717011
H	-2.443983	-0.302184	1.544615	H	4.251782	-2.162007	-2.692434
H	-1.035759	-1.280906	2.050873	H	5.730899	-2.617216	-1.799359
C	-1.352918	1.592048	-0.557916	H	4.167450	-3.393598	-1.416666
H	-1.048956	1.826168	-1.582000	C	5.391042	0.267563	-1.048007
H	-2.443718	1.487734	-0.515449	H	6.420391	-0.087664	-1.176655
H	-1.040352	2.415784	0.089967	H	5.015943	0.651139	-2.001562
C	-1.356280	-1.279111	-1.097689	H	5.376767	1.085657	-0.321671
H	-2.446844	-1.193667	-1.020796				
H	-1.051223	-1.127586	-2.136886	P2b			
H	-1.047283	-2.282514	-0.791710	SCF done:	-1351.799368		
				C	-0.931574	1.506609	-1.030055
P2a				Ni	0.446579	-0.584212	0.325041
SCF done:	-1351.797501			O	-1.542315	-1.094257	0.258679
C	-4.388494	-0.290634	0.049841	C	-2.358063	-0.493821	-0.466677
C	-4.782797	-1.307043	-0.881113	O	-2.168490	0.663441	-1.119965
C	-3.782257	-1.897366	-1.700566	N	-3.597361	-0.989913	-0.680695
C	-2.466795	-1.501349	-1.606396	C	-4.661226	-0.329219	-1.454189
C	-2.066114	-0.494247	-0.685289	C	-5.912395	-1.140475	-1.080498
C	-3.020887	0.089669	0.123963	C	-5.358074	-2.549827	-0.802039
C	-5.385333	0.309612	0.869668	C	-4.015530	-2.277065	-0.105163
C	-6.706200	-0.075004	0.775295	C	0.334443	0.679182	-1.142787
C	-7.094844	-1.080808	-0.146865	C	0.502606	-0.059791	-2.386206
C	-6.152719	-1.681386	-0.955379	C	1.723242	-0.458858	-2.847663
C	-0.589161	-0.147166	-0.603475	C	2.941440	-0.119847	-2.151602
Ni	2.084642	-0.653840	-0.062258	C	2.845732	0.606326	-0.926502
O	1.761442	1.382852	-0.498919	C	1.539143	0.921897	-0.366874
C	0.658862	1.917378	-0.297777	H	-4.444895	-0.388789	-2.529661
O	-0.530920	1.284049	-0.290557	H	-4.733389	0.727857	-1.185449
N	0.526581	3.241023	-0.064530	H	-6.669041	-1.122898	-1.871098
C	-0.749145	3.952798	0.118705	H	-6.366970	-0.727697	-0.171064
C	-0.335781	5.430260	0.023123	H	-5.189024	-3.082157	-1.746627
C	1.107649	5.435989	0.559429	H	-6.026371	-3.161825	-0.188351
C	1.698680	4.126138	0.014546	H	-4.129792	-2.185939	0.983680
C	0.205170	-0.959718	0.415298	H	-3.259665	-3.044243	-0.295879
C	-0.014897	-0.735770	1.822233	H	-0.387256	-0.291454	-2.970478
C	0.305059	-1.685279	2.768344	H	1.797254	-1.021930	-3.776239
C	0.825730	-2.953913	2.380041	H	1.530840	1.706369	0.389800
C	1.064477	-3.211807	1.048493	P	1.484623	-1.824078	1.899445
C	0.829703	-2.219951	0.039804	C	2.941308	-2.844848	1.264881
H	-4.071508	-2.666106	-2.414090	H	3.660134	-2.177491	0.781277
H	-1.718340	-1.962413	-2.246974	H	3.430110	-3.383894	2.085000
H	-2.735353	0.865487	0.828396	H	2.582452	-3.562238	0.521012
H	-5.086419	1.079410	1.578176	C	2.305361	-0.904815	3.333105
H	-7.455995	0.391598	1.409338	H	1.546477	-0.354625	3.897522
H	-8.138802	-1.376559	-0.212820	H	2.822239	-1.601550	4.003577
H	-6.447250	-2.453290	-1.663441	H	3.026191	-0.188065	2.929767
H	-0.144337	-0.286770	-1.594913	C	0.513939	-3.143787	2.846224
H	-1.179511	3.716768	1.101563	H	1.155702	-3.673766	3.559726
H	-1.472294	3.653605	-0.644629	H	-0.312989	-2.669178	3.383146
H	-1.007870	6.085095	0.586466	H	0.094139	-3.860851	2.134377
H	-0.350542	5.755953	-1.024624	C	4.040691	0.996121	-0.282201
H	1.102896	5.417621	1.656581	H	3.974944	1.574989	0.637930
H	1.680967	6.312559	0.242162	C	4.214845	-0.457872	-2.657319
H	2.140197	4.259407	-0.982479	H	4.277026	-1.014722	-3.591012
H	2.463872	3.687663	0.661303	C	5.286255	0.651871	-0.796445
H	-0.462651	0.203958	2.139963	H	6.191242	0.959625	-0.277355
H	0.134049	-1.473310	3.821574	C	5.376997	-0.087059	-1.990582
H	1.025199	-3.711431	3.134147	H	6.349695	-0.356137	-2.394987
H	1.435361	-4.188326	0.740129	H	-1.071428	2.086232	-1.949402
H	0.764166	-2.567660	-0.992703	C	-1.048825	2.474919	0.129851

C	-1.164876	2.056104	1.464823	H	6.527848	1.595494	0.291965
C	-1.050269	3.849747	-0.144160	H	5.275866	2.708575	0.894622
C	-1.276632	2.993244	2.494600				
H	-1.155008	0.994890	1.696884	P4c			
C	-1.150486	4.790155	0.885596	SCF done: -1351.797592			
H	-0.968593	4.189661	-1.174596	C	-3.806724	0.440628	0.351587
C	-1.266240	4.363058	2.210529	C	-4.801534	-0.540368	0.030926
H	-1.367384	2.651947	3.523149	C	-4.431277	-1.630524	-0.806981
H	-1.143223	5.851623	0.650822	C	-3.148630	-1.741644	-1.293973
H	-1.349888	5.089607	3.014977	C	-2.153471	-0.773220	-0.976754
				C	-2.491220	0.294083	-0.173250
PTS_{3c}				C	-4.169169	1.533794	1.186790
SCF done: -1351.744909				C	-5.451730	1.653581	1.681576
C	-2.333333	1.719298	0.000000	C	-6.435062	0.682906	1.362452
C	-3.395786	1.095291	-0.734005	C	-6.114365	-0.389249	0.554975
C	-3.071573	0.388415	-1.925858	C	-0.742693	-0.925395	-1.550394
C	-1.769657	0.307057	-2.359530	Ni	1.447777	-0.053015	-0.241502
C	-0.713413	0.923558	-1.630756	O	1.153394	1.736441	1.752267
C	-0.995129	1.620054	-0.474733	O	1.290237	1.658496	0.526647
C	-2.649580	2.426576	1.194072	C	0.044376	0.220371	-1.399892
C	-3.949466	2.512566	1.639805	N	1.312613	2.745763	-0.273295
C	-4.999117	1.896623	0.911171	C	1.500824	2.759560	-1.735711
C	-4.727913	1.205048	-0.248400	C	1.815086	4.233764	-2.029321
C	0.705931	0.774267	-2.145133	C	0.989777	4.985785	-0.969311
Ni	2.961876	0.784140	-0.685623	C	1.122287	4.102676	0.281031
O	1.534185	2.640336	0.708985	C	-0.022997	-2.166993	-0.982786
C	2.306098	2.542205	-0.277927	C	-0.142487	-2.543053	0.367862
O	1.608785	1.855570	-1.720765	C	0.524230	-3.670910	0.857966
N	2.957201	3.623655	-0.797840	C	1.326281	-4.440844	0.008453
C	3.767874	3.609871	-2.041175	C	1.467360	-4.069272	-1.332937
C	4.210419	5.083764	-2.170378	C	0.799296	-2.941727	-1.819956
C	2.973368	5.857407	-1.643127	H	-5.181522	-2.377151	-1.060709
C	2.498580	5.004645	-0.442286	H	-2.885666	-2.582929	-1.933410
C	1.371361	-0.547648	-1.699268	H	-1.735681	1.040677	0.052440
C	0.863119	-1.359042	-0.670900	H	-3.412139	2.275218	1.433085
C	1.538595	-2.518079	-0.282759	H	-5.713066	2.494050	2.319974
C	2.736929	-2.884649	-0.904664	H	-7.442894	0.786592	1.756942
C	3.264876	-2.079038	-1.916478	H	-6.866744	-1.136003	0.308393
C	2.591236	-0.917384	-2.315479	H	-0.864324	-1.116032	-2.633981
H	-3.871005	-0.081781	-2.489822	H	0.587464	2.420768	-2.233982
H	-1.534493	-0.232429	-3.272371	H	2.307085	2.078867	-2.024099
H	-0.195643	2.088777	0.092513	H	1.556886	4.515130	-3.055451
H	-1.840607	2.896133	1.743924	H	2.885384	4.433485	-1.884847
H	-4.178899	3.053856	2.550852	H	-0.060601	5.038703	-1.281924
H	-6.018090	1.974351	1.273669	H	1.338966	6.008825	-0.794136
H	-5.528421	0.732586	-0.809003	H	1.991290	4.382493	0.892767
H	0.675660	0.780600	-3.246087	H	0.242976	4.124816	0.931883
H	3.141653	3.300535	-2.882344	H	-0.788320	-1.966564	1.024810
H	4.605637	2.913153	-1.942070	H	0.398772	-3.960148	1.898927
H	4.470169	5.347932	-3.198763	H	1.827658	-5.329059	0.385727
H	5.072796	5.273782	-1.521330	H	2.084199	-4.664429	-2.002341
H	2.197044	5.870192	-2.415641	H	0.898051	-2.663338	-2.867416
H	3.205920	6.886052	-1.355276	P	3.317894	-0.518998	1.003037
H	2.972289	5.327553	0.491368	C	2.942178	-0.976314	2.784711
H	1.414684	5.008853	-0.306067	H	2.374488	-1.910312	2.804797
H	-0.069603	-1.078070	-0.197417	H	3.867910	-1.096120	3.357976
H	1.122435	-3.142263	0.500816	H	2.331015	-0.177178	3.211662
H	3.247397	-3.795451	-0.611521	C	4.408944	-1.934165	0.413160
H	4.186593	-2.362016	-2.413695	H	4.809747	-1.696630	-0.576702
H	2.967803	-0.327058	-3.146285	H	5.238437	-2.098184	1.109792
P	4.453789	0.391948	0.943002	H	3.809347	-2.844924	0.336626
C	3.543746	0.545875	2.601506	C	4.551844	0.885560	1.200203
H	2.986979	-0.377844	2.785098	H	5.399557	0.564395	1.815155
H	4.239291	0.730605	3.425507	H	4.913965	1.197824	0.216575
H	2.832372	1.368800	2.486096	H	4.049250	1.728796	1.680279
C	5.483729	-1.188855	1.162680				
H	6.182985	-1.283537	0.326978	PTS_{3a}			
H	6.040749	-1.157876	2.103839	SCF done: -1351.778490			
H	4.811980	-2.050450	1.156833	C	-3.695371	-0.775915	0.551859
C	5.774774	1.751939	1.070087	C	-4.558096	-1.336031	-0.448064
H	6.256187	1.746404	2.052432	C	-3.983818	-1.751854	-1.679939

H	3.308052	4.181353	-0.387551	H	2.378230	-3.118458	1.235630
H	1.942148	6.461047	-1.155240	C	-0.127932	-3.105106	-1.741235
H	1.978216	5.968835	0.545823	H	0.314913	-4.033010	-2.120176
H	-0.217972	5.338325	-1.499919	H	-1.010141	-3.335165	-1.140580
H	-0.439465	6.063401	0.101584	H	-0.428699	-2.468763	-2.577378
H	0.005446	3.948324	1.216623	C	4.238080	-0.550184	1.400817
H	-0.747329	3.333996	-0.260574	H	3.824795	-1.156031	2.204417
H	-0.960421	-2.874154	0.357751	C	5.313998	1.037428	-0.637226
H	0.375473	-4.927625	0.680796	H	5.731858	1.665717	-1.421118
H	2.276528	-5.440630	-0.840539	C	5.562756	-0.709543	1.019003
H	2.905236	-3.812962	-2.622461	H	6.186875	-1.444542	1.520846
H	1.600158	-1.734434	-2.924729	C	6.103431	0.082190	-0.013977
P	2.768013	-0.864545	1.376530	H	7.140699	-0.047086	-0.311217
C	2.817283	-2.312733	2.586628	C	-2.343691	3.574193	-1.487098
H	2.774616	-3.254761	2.032547	H	-2.465456	3.694085	-2.561094
H	3.733895	-2.287108	3.186632	C	-3.192287	4.253700	-0.606274
H	1.950786	-2.262229	3.253146	H	-3.966849	4.913047	-0.989817
C	4.428335	-1.015257	0.507672				
H	4.519445	-0.162720	-0.169613				
H	5.249299	-1.018133	1.233602				
H	4.452891	-1.942214	-0.072853				
C	3.044811	0.597935	2.523347				
H	3.903888	0.413354	3.178062				
H	3.228806	1.483870	1.912206				
H	2.149399	0.763832	3.128727				

P4b

SCF done: -1351.842149

C	-3.044125	4.064199	0.770897
C	-2.048614	3.214936	1.257948
C	-1.173444	2.538566	0.386775
C	-1.352240	2.722875	-0.997985
C	-0.133470	1.659101	0.956887
Ni	0.300507	-0.166149	0.146673
O	-1.493302	-0.505706	-0.414621
C	-2.085955	-1.340939	0.398713
O	-1.509245	-1.966412	1.319623
N	-3.427272	-1.522628	0.165239
C	-4.254030	-2.377420	1.020457
C	-5.621713	-2.356182	0.318274
C	-5.660235	-0.964514	-0.340556
C	-4.209619	-0.751333	-0.806598
C	1.248402	1.645328	0.582680
C	1.851983	2.455614	-0.455627
C	3.141831	2.249279	-0.843528
C	3.964430	1.220449	-0.260176
C	3.407606	0.397464	0.761522
C	2.023099	0.579120	1.134989
H	-3.703087	4.577329	1.467211
H	-1.940266	3.073578	2.331309
H	-0.737425	2.162266	-1.695550
H	-0.339104	1.335311	1.979085
H	-4.314690	-1.966456	2.039514
H	-3.824411	-3.381147	1.102120
H	-6.451330	-2.529959	1.012002
H	-5.660602	-3.137443	-0.452440
H	-5.928157	-0.204437	0.404932
H	-6.380711	-0.894408	-1.162767
H	-4.056210	-1.137302	-1.826313
H	-3.902455	0.298253	-0.804227
H	1.270173	3.261737	-0.890184
H	3.586471	2.890926	-1.601848
H	1.698650	0.125266	2.073102
P	1.109674	-2.185291	-0.669741
C	2.644531	-2.195328	-1.763614
H	3.491249	-1.767483	-1.221354
H	2.889694	-3.218404	-2.070437
H	2.456870	-1.588609	-2.654620
C	1.525135	-3.462523	0.644500
H	0.651417	-3.564934	1.292932
H	1.772113	-4.425204	0.183171

P4d

SCF done: -1351.798367

C	-0.752226	1.510092	-1.233584
Ni	-0.639577	-0.611852	0.413729
O	-1.805609	-0.340366	2.821322
C	-2.040078	-0.713821	1.666855
O	-1.589144	0.531264	-0.684758
N	-3.249236	-1.175472	1.284370
C	-3.636828	-1.603944	-0.071853
C	-5.167029	-1.483505	-0.045265
C	-5.524361	-1.827740	1.412603
C	-4.390971	-1.180517	2.224328
C	0.705572	1.006496	-1.230071
C	1.134692	0.146779	-2.286223
C	2.417608	-0.350916	-2.328253
C	3.359427	-0.030486	-1.309436
C	2.939100	0.818257	-0.232734
C	1.605127	1.317224	-0.222934
H	-3.332828	-2.648756	-0.240331
H	-3.155848	-0.966270	-0.814251
H	-5.650305	-2.141968	-0.774700
H	-5.460536	-0.451354	-0.274154
H	-5.517320	-2.916525	1.554041
H	-6.510572	-1.460110	1.714761
H	-4.627439	-0.149594	2.517866
H	-4.134847	-1.730434	3.136045
H	0.426243	-0.102786	-3.073020
H	2.730828	-0.991064	-3.150775
H	1.305667	1.990513	0.576698
P	0.596670	-2.144123	1.594539
C	1.968815	-3.062006	0.690082
H	2.699221	-2.347966	0.302037
H	2.469665	-3.760224	1.369632
H	1.542474	-3.618145	-0.149951
C	1.480652	-1.411696	3.080191
H	0.737949	-0.893595	3.692350
H	1.972053	-2.197648	3.664018
H	2.228606	-0.692828	2.735092
C	-0.376846	-3.558554	2.361246
H	0.294222	-4.225898	2.913005
H	-1.123493	-3.144869	3.043048
H	-0.885308	-4.123927	1.575045
C	3.877037	1.151875	0.784218
H	3.560306	1.806367	1.593566
C	4.696285	-0.514923	-1.323034
H	5.013887	-1.155139	-2.143610
C	5.167356	0.664277	0.744651
H	5.874191	0.929656	1.526679
C	5.581056	-0.178288	-0.318740
H	6.600824	-0.553911	-0.342333
H	-1.029481	1.633818	-2.297182
C	-0.903244	2.888471	-0.583135
C	-1.488689	3.037930	0.678999

C	-0.460021	4.034334	-1.261318
C	-1.617390	4.306543	1.256677
H	-1.851784	2.157575	1.198649
C	-0.587094	5.301585	-0.688682
H	-0.010887	3.932987	-2.248614
C	-1.166671	5.441826	0.577945
H	-2.074935	4.404954	2.238611
H	-0.240268	6.178667	-1.230547
H	-1.271264	6.427197	1.025945

File

SCF done: -1351.795679

C	-0.920707	0.045629	0.294446
Ni	1.455039	-1.734988	-0.116384
O	-2.351907	0.186615	0.015018
C	-3.216211	-0.187889	1.003350
O	-2.875190	-0.618548	2.100951
N	-4.503588	-0.021169	0.612228
C	-5.617702	-0.398959	1.492032
C	-6.826827	-0.387428	0.543575
C	-6.457303	0.689583	-0.493026
C	-4.944986	0.493684	-0.692783
C	-0.254128	1.355484	-0.074446
C	-0.632436	2.077311	-1.241361
C	-0.001843	3.254795	-1.579160
C	1.040886	3.787506	-0.771769
C	1.418152	3.074499	0.413164
C	0.745988	1.863191	0.730898
H	-5.729180	0.333618	2.303816
H	-5.427418	-1.373817	1.949955
H	-7.764812	-0.177336	1.067285
H	-6.927096	-1.363923	0.052816
H	-6.654227	1.688698	-0.083888
H	-7.014633	0.596293	-1.430656
H	-4.730771	-0.235921	-1.485952
H	-4.422473	1.421788	-0.942015
H	-1.437575	1.694284	-1.860945
H	-0.301776	3.796851	-2.473770
H	1.034104	1.328581	1.633809
P	3.577425	-1.914581	0.490599
C	4.517381	-3.500236	0.065617
H	4.504404	-3.648018	-1.018126
H	5.555717	-3.446766	0.413663
H	4.019015	-4.353087	0.535600
C	4.767550	-0.614862	-0.196057
H	4.418472	0.381848	0.088297
H	5.783158	-0.771039	0.186657
H	4.777092	-0.676127	-1.288191
C	3.950523	-1.779418	2.339993
H	5.027905	-1.854421	2.528850
H	3.582941	-0.819675	2.714264
H	3.430091	-2.579409	2.874292
C	2.448394	3.608745	1.236564
H	2.728281	3.071509	2.140448
C	1.711657	5.000996	-1.088286
H	1.422558	5.540209	-1.988051
C	3.081587	4.787543	0.902528
H	3.867246	5.184116	1.540681
C	2.710289	5.490572	-0.272511
H	3.215250	6.419237	-0.526047
H	-0.823944	-0.120623	1.368676
C	-0.414129	-1.192211	-0.430411
C	0.103970	-1.176870	-1.762965
C	-0.620370	-2.474377	0.172130
C	0.239631	-2.371970	-2.497426
H	0.297597	-0.229206	-2.255527
C	-0.479871	-3.657892	-0.576831
H	-1.010219	-2.521479	1.185243
C	-0.083149	-3.607810	-1.920659
H	0.598615	-2.324948	-3.522732
H	-0.685957	-4.614000	-0.101997

H	0.009003	-4.522899	-2.499662
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TS_{5e}

SCF done: -1351.7625643

C	0.082152	-0.513921	0.327622
Ni	-1.807965	-1.584274	0.243769
O	2.280975	-0.175911	0.543526
C	2.845644	-0.502372	-0.573035
O	2.289949	-1.108992	-1.531580
N	4.177161	-0.146012	-0.693095
C	4.995493	-0.525375	-1.844788
C	6.432168	-0.267751	-1.357354
C	6.263201	0.880607	-0.344729
C	4.934085	0.542261	0.352173
C	-0.261994	0.861937	0.700773
C	-0.220033	1.331844	2.050028
C	-0.536144	2.633596	2.356429
C	-0.908410	3.562627	1.343532
C	-0.911682	3.118192	-0.020273
C	-0.577313	1.770513	-0.303185
H	4.750644	0.092789	-2.722912
H	4.812405	-1.568057	-2.124579
H	7.118854	-0.026013	-2.176412
H	6.820379	-1.159843	-0.847793
H	6.174444	1.837714	-0.875840
H	7.099220	0.964717	0.358684
H	5.092426	-0.112313	1.224029
H	4.394426	1.426804	0.706248
H	0.120429	0.661733	2.832168
H	-0.482038	2.977611	3.387202
H	-0.550385	1.447480	-1.341908
P	-3.075582	-1.212531	-1.587862
C	-4.333709	-2.546461	-2.030487
H	-5.046633	-2.667483	-1.209833
H	-4.875152	-2.275611	-2.943614
H	-3.815766	-3.497199	-2.185145
C	-4.141484	0.340879	-1.590628
H	-3.507390	1.215109	-1.421032
H	-4.667659	0.447516	-2.545702
H	-4.872064	0.282345	-0.778645
C	-2.115021	-1.045571	-3.199426
H	-2.798847	-0.861367	-4.035383
H	-1.402811	-0.220610	-3.120407
H	-1.550044	-1.963659	-3.381553
C	-1.246720	4.048986	-1.044734
H	-1.234547	3.715896	-2.080558
C	-1.248171	4.911723	1.628597
H	-1.241540	5.246751	2.663675
C	-1.573828	5.352509	-0.735869
H	-1.825844	6.053331	-1.527632
C	-1.577070	5.788100	0.614089
H	-1.834382	6.818369	0.846069
H	0.426051	-0.679167	-0.690720
C	-0.014516	-1.699563	1.161274
C	-1.006870	-1.791620	2.190419
C	0.689347	-2.887726	0.790993
C	-1.241310	-3.032098	2.834162
H	-1.481924	-0.899519	2.589641
C	0.452419	-4.079620	1.449638
H	1.425768	-2.807107	-0.004051
C	-0.519873	-4.159221	2.473430
H	-1.978616	-3.083595	3.631358
H	1.015308	-4.967354	1.172581
H	-0.697646	-5.105188	2.978660

F_{2e}

SCF done: -1351.370389

C	1.007048	-1.025458	-0.305018
Ni	-1.838807	-0.230426	-0.211888
O	2.378353	-0.583899	-0.070436
C	3.031584	-0.012479	-1.125286

H	6.289215	2.280519	-0.257728	H	1.099442	-0.346214	0.794375
H	7.198105	1.151000	0.761350	H	2.897805	-0.103535	2.448812
H	5.189341	-0.116233	1.301690	H	5.199819	-0.620045	3.210587
H	4.481657	1.495527	1.140666	H	6.663572	-2.116087	1.853506
H	-0.030795	0.572547	2.808480	H	5.829500	-3.086458	-0.265080
H	-1.118852	2.713667	3.328995	H	-0.190440	-0.987136	-2.527525
H	-0.252911	1.490255	-1.408365	H	2.344327	3.591569	0.693187
P	-3.034376	-1.785761	-1.206463	H	0.879180	4.410759	1.245483
C	-3.950359	-2.857712	0.041717	H	2.727234	5.796314	-0.271128
H	-4.689196	-2.250648	0.572839	H	0.992581	6.061504	-0.516808
H	-4.456231	-3.687227	-0.464206	H	2.800727	4.160437	-2.105262
H	-3.232859	-3.252232	0.765814	H	1.728608	5.404094	-2.771623
C	-4.406223	-1.353216	-2.427514	H	-0.254159	4.093416	-2.255913
H	-3.976465	-0.840236	-3.292600	H	0.881438	2.772263	-2.560704
H	-4.919782	-2.260722	-2.763631	H	-2.239986	-2.225054	-3.070166
H	-5.128189	-0.685124	-1.949178	H	-4.279226	-3.378602	-2.287781
C	-2.040129	-3.061345	-2.170020	H	-4.558476	-3.960587	0.120636
H	-2.695931	-3.856503	-2.541606	H	-2.796619	-3.336755	1.754462
H	-1.542040	-2.573543	-3.012403	H	-0.690828	-2.281181	0.972176
H	-1.274989	-3.490211	-1.517383	P	-2.915181	0.738169	1.137803
C	-1.682791	3.795395	-1.127037	C	-4.692852	0.108260	1.116693
H	-1.501366	3.523324	-2.164435	H	-4.708531	-0.968837	1.301871
C	-2.120117	4.501764	1.550632	H	-5.290889	0.618051	1.880324
H	-2.278213	4.780352	2.590283	H	-5.132391	0.295578	0.132258
C	-2.296841	4.996841	-0.815931	C	-2.459919	0.607216	2.957520
H	-2.602662	5.672805	-1.610181	H	-1.465809	1.044725	3.075352
C	-2.522145	5.350214	0.532272	H	-3.187210	1.140315	3.580124
H	-3.003016	6.295491	0.770028	H	-2.430517	-0.444699	3.257489
H	0.643383	-0.585993	-0.792181	C	-3.180702	2.585945	0.923419
C	0.199432	-1.791184	0.961315	H	-3.958524	2.940385	1.608952
C	-0.620207	-2.032335	2.081916	H	-2.240121	3.097933	1.134182
C	0.996485	-2.852022	0.477531	H	-3.476273	2.793650	-0.108545
C	-0.626364	-3.280969	2.709173				
H	-1.276269	-1.252860	2.455465	#5			
C	0.985053	-4.096731	1.102274	SCF done: -1953.224626			
H	1.642012	-2.662564	-0.375782	C	-4.695204	-0.594279	0.576363
C	0.176852	-4.317503	2.225281	C	-5.374847	0.053098	-0.506596
H	-1.262576	-3.442831	3.576201	C	-4.678569	0.210249	-1.736411
H	1.617024	-4.895153	0.721140	C	-3.390581	-0.249464	-1.886185
H	0.174427	-5.286961	2.717362	C	-2.697697	-0.910994	-0.824814
				C	-3.366451	-1.058276	0.382053
				C	-5.378534	-0.749656	1.815986
#4e				C	-6.669063	-0.290672	1.976558
SCF done: -1351.829563				C	-7.340454	0.348153	0.902269
C	3.028488	-1.311730	0.656815	C	-6.704699	0.514942	-0.310753
C	3.873802	-2.161532	-0.127254	Ni	-0.111684	-0.211594	-0.024963
C	3.357991	-2.685172	-1.345583	C	1.738637	-2.999710	1.347330
C	2.076821	-2.391846	-1.754226	C	1.477699	-0.606690	3.000518
C	1.213417	-1.564096	-0.970822	C	-0.762137	-2.431248	2.741076
C	1.706616	-1.032426	0.208048	P	0.553584	-1.587323	1.693499
C	3.538792	-0.760724	1.865548	O	0.848010	1.785888	0.392240
C	4.821465	-1.047237	2.285165	N	-0.491046	3.461303	-0.537444
C	5.654771	-1.896483	1.512670	C	-0.085479	2.194877	-0.455989
C	5.190528	-2.438526	0.331757	O	-0.662107	1.286660	-1.144332
C	-0.173380	-1.312664	-1.485181	C	-1.523507	3.859720	-1.515017
Ni	-1.343444	-0.206130	-0.333035	C	-1.798189	5.331165	-1.166793
O	-0.626723	1.441675	-0.957283	C	-0.467823	5.812615	-0.560475
C	0.024272	2.121967	-0.050526	C	0.013058	4.602643	0.250297
O	0.101103	1.814031	1.163580	C	-1.296385	-1.387849	-1.075173
N	0.634224	3.259914	-0.516209	C	-1.016162	-2.858174	-1.092202
C	1.441790	4.120299	0.352297	C	0.097854	-3.319106	-1.828332
C	1.790258	5.308121	-0.559537	C	0.400202	-4.676161	-1.927333
C	1.841395	4.674514	-1.962378	C	-0.406077	-5.626635	-1.288942
C	0.697241	3.646492	-1.929241	C	-1.522243	-5.193979	-0.568576
C	-1.303364	-2.141695	-1.111937	C	-1.825522	-3.831878	-0.475491
C	-2.364795	-2.464437	-2.016955	C	5.188837	-1.212337	-0.128165
C	-3.502519	-3.108915	-1.576267	C	5.418354	-0.242300	0.857286
C	-3.665883	-3.433736	-0.206724	C	4.534410	0.827613	1.000347
C	-2.687155	-3.081172	0.703151	C	3.384330	0.976218	0.197346
C	-1.515551	-2.407878	0.274041	C	3.193953	-0.009959	-0.784797
H	3.993735	-3.324016	-1.955730	B	2.464384	2.311366	0.226713
H	1.702400	-2.802976	-2.689464				

C	4.171874	-0.558858	-1.413181	H	-3.002074	-0.091420	1.202312
C	4.556942	0.806461	-1.622422	H	-4.389110	3.188191	-1.492690
C	3.891394	1.809011	-0.865189	H	-4.132603	1.533106	-2.108948
C	2.904904	1.479965	0.036162	H	-3.184702	2.887076	-2.781602
C	2.493705	0.126505	0.261834	H	0.362237	1.072403	-3.782316
C	3.147805	-0.855344	-0.475846	H	0.352705	-0.014278	-2.364168
C	4.834371	-1.574228	-2.161922	H	1.083075	1.601287	-2.237033
C	5.823621	-1.256643	-3.068749	H	-1.864191	-0.965476	-2.854374
C	6.201829	0.095572	-3.273478	C	-4.476043	-1.061850	0.001223
C	5.580079	1.102032	-2.563234	H	-5.205828	-1.058600	0.804725
Ni	-0.321765	-0.439312	0.164610	O	-5.991826	-2.152681	-1.590811
C	-1.798692	-3.625965	0.357160	C	-7.015032	-2.199079	-0.605351
C	0.164887	-3.262905	-1.793742	H	-7.870309	-2.675620	-1.088134
C	0.998926	-3.816838	0.924029	H	-6.707117	-2.795562	0.263673
P	-0.197733	-2.716623	-0.027775	H	-7.297073	-1.191049	-0.274116
O	-0.592136	1.595130	0.054814				
N	-0.715825	3.545908	1.257233				
C	-0.968692	2.223417	1.244772	P7			
O	-1.411528	1.583249	2.186443	SCF done: -1953.227222			
C	-1.037361	4.348674	2.448936	C	3.161699	1.881847	-1.605092
C	-0.384569	5.703625	2.142445	C	2.979435	3.156386	-0.971393
C	-0.478679	5.802957	0.609232	C	2.470729	3.172182	0.356068
C	-0.221737	4.363222	0.133095	C	2.161585	2.002129	1.011181
C	1.394611	-0.144696	1.236038	C	2.324582	0.714520	0.403512
C	1.662529	-1.022487	2.424156	C	2.823650	0.699194	-0.897122
C	0.641898	-1.176864	3.389606	C	3.672451	1.853812	-2.935591
C	0.833129	-1.946277	4.536471	C	3.984691	3.019779	-3.603173
C	2.058683	-2.586690	4.765356	C	3.804115	4.278319	-2.972565
C	3.088774	-2.422681	3.836512	C	3.312507	4.339630	-1.684229
C	2.894615	-1.649895	2.686277	Ni	0.153949	-1.116137	0.249515
C	-4.787392	-1.595773	-1.257664	C	0.149395	-4.486558	-0.430077
C	-3.823510	-1.560493	-2.277843	C	0.462962	-2.822051	-2.818841
C	-2.567880	-1.009920	-2.024806	C	2.717017	-3.374860	-1.132913
C	-2.197224	-0.471584	-0.769005	P	0.909288	-2.858081	-0.988492
C	-3.204049	-0.519706	0.222306	O	-1.232325	1.957119	0.149762
B	-1.531970	1.556077	-1.077557	N	-1.634648	2.062623	2.405125
O	-2.673812	2.304943	-0.845599	C	-1.208888	1.342823	1.354734
C	-3.641495	2.483864	-1.869902	O	-0.737954	0.204353	1.493822
O	-0.997940	1.572597	-2.355241	C	-1.558191	1.523694	3.775763
C	0.266661	1.030801	-2.692877	C	-1.763003	2.766167	4.653824
H	4.180963	2.849454	-1.002406	C	-2.665094	3.668424	3.792908
H	2.421714	2.266197	0.611075	C	-2.146189	3.445902	2.362996
H	2.876105	-1.899054	-0.344518	C	1.932830	-0.512030	1.154590
H	4.549106	-2.612709	-2.003971	C	2.991700	-1.499585	1.527025
H	6.319881	-2.044336	-3.630354	C	2.653603	-2.559250	2.401731
H	6.983756	0.334266	-3.989822	C	3.591551	-3.503326	2.815978
H	5.868420	2.140508	-2.714390	C	4.919336	-3.425402	2.372629
H	-1.652971	-4.699526	0.194453	C	5.282026	-2.373215	1.527652
H	-2.603795	-3.259984	-0.280165	C	4.338037	-1.426558	1.116317
H	-2.065501	-3.451608	1.403019	C	-4.341087	-2.018953	-1.262209
H	1.134573	-2.865006	-2.105221	C	-3.469794	-1.303525	-2.093347
H	-0.608924	-2.881508	-2.461807	C	-2.151252	-1.071145	-1.688776
H	0.185223	-4.356637	-1.848951	C	-1.637298	-1.534315	-0.460218
H	0.816415	-4.854923	0.624945	C	-2.543972	-2.241356	0.346652
H	0.834822	-3.710493	1.997661	B	-2.340288	2.139209	-0.681910
H	2.035155	-3.556569	0.707806	O	-3.583286	1.951753	-0.164969
H	-0.647338	3.862249	3.347104	C	-4.754055	2.034868	-0.983213
H	-2.127090	4.432789	2.559108	O	-2.138792	2.574299	-1.950332
H	0.666334	5.695078	2.458536	C	-0.830205	2.796024	-2.489665
H	-0.882896	6.530170	2.658571	H	2.340376	4.130538	0.856628
H	0.233146	6.513222	0.176786	H	1.794762	2.042903	2.034898
H	-1.487631	6.116926	0.314225	H	2.956196	-0.252397	-1.406885
H	-0.755983	4.123573	-0.787988	H	3.816137	0.889691	-3.420016
H	0.847604	4.174624	-0.028677	H	4.374500	2.978034	-4.617465
H	1.045725	0.808823	1.641185	H	4.057401	5.190948	-3.506221
H	-0.306880	-0.668738	3.231549	H	3.176388	5.301935	-1.193667
H	0.025422	-2.041668	5.259190	H	0.480276	-5.297893	-1.087709
H	2.209722	-3.187858	5.658538	H	-0.939109	-4.406124	-0.453917
H	4.055622	-2.891684	4.007487	H	0.473412	-4.698537	0.592909
H	3.720223	-1.523439	1.992258	H	0.914966	-1.942848	-3.287908
H	-4.085271	-1.953746	-3.257092	H	-0.619666	-2.771490	-2.939094
				H	0.848304	-3.725367	-3.303904

H	2.780527	-4.215005	-1.833466	H	4.270495	0.087118	0.801832
H	3.107979	-3.678935	-0.161792	H	4.470699	-1.632320	0.395471
H	3.324095	-2.547698	-1.506938	H	1.204655	-0.343307	3.631042
H	-0.597344	1.026735	3.931200	H	2.187765	0.906850	2.842390
H	-2.349893	0.777880	3.924624	H	2.972553	-0.322545	3.883632
H	-0.800010	3.258504	4.838528	H	3.261923	-2.984041	3.197365
H	-2.203661	2.518493	5.624303	H	2.682285	-3.695906	1.662688
H	-2.626164	4.722483	4.084537	H	1.514420	-3.192671	2.900577
H	-3.708609	3.337801	3.865033	H	-0.134586	-0.120897	-2.373075
H	-2.931796	3.544126	1.611787	H	0.996556	-1.897007	-3.397179
H	-1.330739	4.138134	2.114545	H	1.953710	-4.167691	-3.331431
H	1.441147	-0.217243	2.087459	H	1.489226	-5.681982	-1.399520
H	1.626202	-2.632965	2.755833	H	0.047827	-4.881651	0.460786
H	3.288322	-4.303103	3.489010	H	-0.998274	-2.656319	0.362278
H	5.653895	-4.160861	2.690875	H	0.340675	4.114150	1.105467
H	6.311800	-2.280326	1.187861	H	2.932709	0.826209	-1.541962
H	4.656274	-0.612207	0.471933	H	-0.294031	1.730037	1.171965
H	-3.838274	-0.940749	-3.050486	C	2.711271	2.880740	-0.988074
H	-2.222445	-2.618104	1.318225	H	3.543925	3.185853	-1.614393
H	-5.607748	2.152263	-0.310920	O	2.246980	5.165773	-0.208812
H	-4.868911	1.112087	-1.559112	C	3.310577	5.662075	-1.002384
H	-4.697613	2.889294	-1.665340	H	3.332200	6.741006	-0.834255
H	-0.928318	2.797327	-3.577733	H	4.274975	5.228513	-0.701645
H	-0.133198	2.013554	-2.178088	H	3.143251	5.463859	-2.070367
H	-0.445407	3.766412	-2.159408				
H	-1.510143	-0.513231	-2.371456				
C	-3.875103	-2.490515	-0.029782	P₉			
H	-4.525385	-3.043076	0.641831	SCF done: -2057.322346			
O	-5.621940	-2.195785	-1.737767	C	-1.616737	3.685060	0.363820
C	-6.534570	-2.936007	-0.945139	C	-0.826837	3.963698	-0.801067
H	-7.468716	-2.963792	-1.510426	C	-0.976137	3.106062	-1.930104
H	-6.180974	-3.962772	-0.776475	C	-1.848556	2.042860	-1.900101
H	-6.711566	-2.451974	0.025639	C	-2.652446	1.748669	-0.749549
				C	-2.512541	2.578700	0.354997
				C	-1.481217	4.537648	1.497179
				C	-0.608534	5.606013	1.479227
				C	0.174073	5.875246	0.327429
				C	0.065916	5.069355	-0.787600
				Ni	-2.617032	-1.087264	-0.548737
				C	-2.595854	-3.583047	-2.867128
				C	-5.052622	-3.404385	-1.251539
				C	-4.650928	-1.579430	-3.523961
				P	-3.741795	-2.333200	-2.064861
				O	-1.592334	-2.662321	0.145166
				N	-0.175316	-2.340222	1.916402
				C	-1.020579	-1.873441	0.987572
				O	-1.308208	-0.606852	0.904667
				C	0.484278	-1.506846	2.941261
				C	1.014471	-2.551296	3.935841
				C	1.333672	-3.762164	3.039528
				C	0.188447	-3.764029	2.013692
				C	-3.602730	0.597380	-0.841179
				C	-4.742985	0.507613	0.132119
				C	-6.070140	0.613907	-0.329449
				C	-7.159709	0.492898	0.537346
				C	-6.950295	0.263900	1.900175
				C	-5.640526	0.157746	2.380267
				C	-4.553472	0.274136	1.511055
				C	7.873746	-0.817354	-0.467785
				C	7.150777	-1.247545	0.651887
				C	5.816779	-0.866003	0.805226
				C	5.145471	-0.048718	-0.126165
				C	5.903673	0.356698	-1.236920
				B	3.577858	0.383623	0.000560
				O	3.321490	1.787331	-0.438282
				C	4.001748	2.824977	0.220723
				O	2.655187	-0.383727	-0.865176
				C	2.786077	-1.782493	-0.919000
				H	-0.384871	3.302941	-2.821943
				H	-1.944163	1.405031	-2.776557
				H	-3.116779	2.408935	1.240919
				H	-2.083776	4.334013	2.379838

P₈							
SCF done: -1297.386291							
C	-3.671569	0.097553	0.543907				
C	-4.430116	0.826321	-0.428850				
C	-3.841319	1.050585	-1.703425				
C	-2.587375	0.569092	-1.999305				
C	-1.816140	-0.176691	-1.052013				
C	-2.375955	-0.376991	0.203622				
C	-4.241902	-0.117246	1.830782				
C	-5.499951	0.357285	2.137961				
C	-6.251097	1.073373	1.170805				
C	-5.724078	1.301912	-0.083624				
Ni	0.888704	-0.809475	-0.061956				
C	4.174067	-0.932737	1.182498				
C	2.170849	-0.138600	3.160098				
C	2.474797	-2.950998	2.435771				
P	2.375929	-1.239909	1.648134				
C	-0.472649	-0.655619	-1.485295				
C	-0.058606	-2.062354	-1.509794				
C	0.794288	-2.547513	-2.549521				
C	1.332379	-3.820639	-2.508986				
C	1.072948	-4.678162	-1.416890				
C	0.273479	-4.227838	-0.378648				
C	-0.277831	-2.927327	-0.402195				
C	1.986710	3.814539	-0.240572				
C	0.907209	3.378014	0.540365				
C	0.565812	2.024650	0.572883				
C	1.286002	1.054467	-0.153062				
C	2.351140	1.521551	-0.937010				
H	-4.399490	1.612597	-2.449700				
H	-2.161019	0.754581	-2.982425				
H	-1.809754	-0.878954	0.983471				
H	-3.666967	-0.667093	2.573646				
H	-5.921353	0.183065	3.124968				
H	-7.242034	1.442325	1.422869				
H	-6.294997	1.853455	-0.827948				
H	4.826532	-1.066117	2.052428				

H	-0.517611	6.247624	2.351953	C	-4.753808	-0.354024	1.166774
H	0.861167	6.717109	0.327056	C	-4.111649	-1.512253	1.641010
H	0.667051	5.268808	-1.671934	C	-3.033063	-2.045026	0.943437
H	-3.164013	-4.295958	-3.474029	C	-2.537219	-1.469348	-0.252185
H	-2.053591	-4.108284	-2.077401	C	-3.201235	-0.303773	-0.686828
H	-1.871474	-3.060656	-3.498364	B	-1.539953	-2.306022	-1.289093
H	-5.833556	-2.764099	-0.832442	O	-2.180812	-2.502638	-2.576526
H	-4.587792	-3.970698	-0.440133	C	-3.093669	-3.566022	-2.733388
H	-5.492392	-4.096104	-1.978358	O	-1.058259	-3.544612	-0.728257
H	-5.098340	-2.367605	-4.138419	C	-0.014256	-3.546944	0.211810
H	-3.951890	-1.001150	-4.134855	H	4.209459	-2.796708	-1.769807
H	-5.440986	-0.914717	-3.165351	H	2.399151	-1.326353	-2.527230
H	-0.237488	-0.814170	3.385478	H	2.688609	0.957713	1.105874
H	1.308414	-0.935693	2.495336	H	4.349189	0.351062	2.820058
H	0.236666	-2.813232	4.664933	H	6.169870	-1.128110	3.598687
H	1.886396	-2.186042	4.486937	H	6.947066	-3.022577	-2.173980
H	1.393512	-4.704838	3.592707	H	5.898854	-3.432333	-0.030734
H	2.291507	-3.606490	2.529523	H	-2.099215	3.556582	1.855244
H	0.483071	-4.151059	1.034145	H	-2.821179	2.552277	0.564444
H	-0.673514	-4.348735	2.362734	H	-1.471604	3.654903	0.184274
H	-3.997682	0.581863	-1.861483	H	-0.725422	0.006121	3.175452
H	-6.248607	0.814317	-1.384624	H	-2.354946	0.266036	2.524062
H	-8.171196	0.586761	0.148580	H	-1.617429	1.497552	3.591272
H	-7.794394	0.171005	2.578674	H	0.296593	3.246090	2.868568
H	-5.462776	-0.024366	3.437735	H	1.279580	3.145980	1.381437
H	-3.543684	0.165255	1.896904	H	1.402103	1.873909	2.627192
H	7.648388	-1.879595	1.383422	H	1.023999	0.453600	-2.299156
H	5.430228	0.985316	-1.989392	H	-0.483789	2.510212	-2.338062
H	3.741755	2.884754	1.294363	H	-0.318531	4.954005	-2.640888
H	3.722177	3.779942	-0.244519	H	1.707733	6.182232	-1.853088
H	5.095321	2.716519	0.149502	H	3.573655	4.904777	-0.803856
H	2.704628	-2.247630	0.078039	H	3.416580	2.466379	-0.528859
H	3.750257	-2.087175	-1.353147	H	-4.496227	-1.986076	2.540652
H	1.981419	-2.182084	-1.551277	H	-2.918118	0.139457	-1.640878
H	5.277335	-1.232648	1.678092	H	-3.429254	-3.575519	-3.777473
C	7.244483	-0.008654	-1.422256	H	-3.978887	-3.440369	-2.087388
H	7.777390	0.339547	-2.301689	H	-2.630100	-4.533319	-2.497330
O	9.182638	-1.238622	-0.540494	H	0.086992	-4.563512	0.612743
C	9.953016	-0.839882	-1.660433	H	-0.204597	-2.865357	1.060948
H	10.940901	-1.284124	-1.518748	H	0.944323	-3.253707	-0.239681
H	9.519354	-1.209572	-2.600232	H	-2.585919	-2.969479	1.299815
H	10.050881	0.253502	-1.714624	C	-4.291471	0.260148	-0.002272
K	0.737993	1.157740	0.228298	H	-4.788720	1.134515	-0.410501
O	3.050331	0.199411	1.413237	O	-5.816155	0.084277	1.910829
H	3.707119	0.465830	2.071333	C	-6.583224	1.176744	1.424771

P10

SCF done: -1628.457708

C	4.062377	-0.686620	0.935714
C	4.512772	-1.774306	0.118447
C	3.881447	-1.972346	-1.140203
C	2.869057	-1.144689	-1.565099
C	2.406798	-0.047934	-0.771074
C	3.015193	0.147093	0.462937
C	4.686596	-0.476260	2.198542
C	5.702889	-1.301085	2.632334
C	6.145549	-2.378296	1.822014
C	5.561802	-2.607083	0.592980
Ni	-0.368577	0.117313	-0.437018
C	-1.894356	2.989110	0.941059
C	-1.423774	0.761314	2.803489
C	0.725374	2.568104	2.122962
P	-0.669966	1.608995	1.303882
O	-0.372949	-1.358513	-1.641770
C	1.296024	0.800478	-1.298201
C	1.433911	2.293485	-1.370759
C	0.401205	3.035953	-1.984397
C	0.493419	4.416112	-2.156744
C	1.630686	5.106446	-1.718766
C	2.672178	4.389148	-1.126802
C	2.577484	3.003269	-0.957950

PTS11

SCF done: -1628.452182

C	4.066285	-0.867607	0.762954
C	4.497981	-1.859257	-0.178042
C	3.861085	-1.893759	-1.448855
C	2.861296	-1.004064	-1.767859
C	2.410374	-0.003065	-0.848418
C	3.030334	0.030958	0.396361
C	4.697770	-0.819626	2.039213
C	5.701448	-1.706364	2.368121
C	6.126019	-2.687106	1.434723
C	5.535074	-2.758395	0.189822
Ni	-0.399456	0.115474	-0.471280
C	-2.110825	2.036261	1.942174
C	-0.123580	0.119630	2.938779
C	0.669744	2.720293	1.911584
P	-0.455637	1.270734	1.485437
O	-0.412264	-1.174505	-1.954616
C	1.298111	0.909698	-1.253082
C	1.493412	2.398007	-1.200596
C	0.437120	3.236093	-1.619836

C	0.566936	4.623980	-1.650543	O	-0.754131	-1.112749	-1.536535
C	1.768979	5.228703	-1.260603	C	1.277781	0.854688	-1.150272
C	2.833756	4.417499	-0.861971	C	1.769618	2.265676	-1.269986
C	2.699710	3.025079	-0.837007	C	0.899224	3.250275	-1.791875
C	-4.967181	-0.380015	0.958943	C	1.296037	4.576445	-1.957816
C	-4.064823	-1.260105	1.578765	C	2.592290	4.976165	-1.606691
C	-2.785120	-1.424375	1.053749	C	3.477206	4.016810	-1.107885
C	-2.326466	-0.741489	-0.099722	C	3.075460	2.686502	-0.947229
C	-3.272172	0.129744	-0.685433	C	-5.151705	-0.467892	0.657663
B	-1.496790	-2.024529	-1.456947	C	-4.191490	-1.127343	1.437776
O	-2.484575	-2.174278	-2.437701	C	-2.836896	-0.821270	1.288287
C	-3.543325	-3.098214	-2.249795	C	-2.370818	0.140205	0.366626
O	-1.129088	-3.158927	-0.731791	C	-3.364003	0.783255	-0.391478
C	0.077592	-3.216049	0.003600	B	-1.294114	-2.394138	-1.334427
H	4.179375	-2.638021	-2.176406	O	-2.239717	-2.780614	-2.236734
H	2.392540	-1.055982	-2.746718	C	-2.873736	-4.057208	-2.143146
H	2.722650	0.766799	1.133869	O	-0.873192	-3.220767	-0.350959
H	4.377148	-0.065202	2.755416	C	0.151324	-2.909810	0.596008
H	6.173706	-1.655143	3.346119	H	3.667896	-3.018787	-2.207975
H	6.918620	-3.380390	1.704258	H	2.090954	-1.205423	-2.716571
H	5.857900	-3.507738	-0.530214	H	2.693066	0.470848	1.193745
H	-2.038765	2.491724	2.935851	H	4.266600	-0.599604	2.769185
H	-2.891740	1.275608	1.940496	H	5.853733	-2.418210	3.296756
H	-2.363307	2.808161	1.209969	H	6.348676	-4.187981	1.607940
H	0.868825	-0.325997	2.828840	H	5.246795	-4.130107	-0.609217
H	-0.871154	-0.675767	2.950809	H	-1.594567	4.121590	2.068410
H	-0.171485	0.678124	3.879833	H	-2.620292	3.067414	1.047319
H	0.452309	3.034083	2.938457	H	-1.298439	4.014911	0.311706
H	0.483419	3.550683	1.227882	H	-0.279691	0.570001	3.465535
H	1.720830	2.442267	1.833796	H	-1.969709	0.984695	3.098161
H	1.015080	0.672397	-2.285231	H	-0.905449	2.184341	3.894119
H	-0.503497	2.779933	-1.924862	H	0.896109	3.639060	2.776904
H	-0.269539	5.236199	-1.980783	H	1.532646	3.514198	1.111471
H	1.874539	6.310383	-1.280164	H	1.902754	2.248659	2.300776
H	3.782206	4.867029	-0.575795	H	0.835749	0.603650	-2.125445
H	3.551402	2.418412	-0.544971	H	-0.111085	2.956550	-2.074651
H	-4.396284	-1.815058	2.452797	H	0.594365	5.301037	-2.366320
H	-3.011159	0.665962	-1.598154	H	2.906532	6.009011	-1.732938
H	-4.113656	-3.141702	-3.183135	H	4.495199	4.300023	-0.848013
H	-4.209109	-2.769338	-1.440136	H	3.792328	1.962357	-0.572446
H	-3.160558	-4.097376	-2.010071	H	-4.525032	-1.876652	2.151799
H	0.114652	-4.187743	0.506559	H	-3.085084	1.545914	-1.121338
H	0.125372	-2.422532	0.765670	H	-3.545249	-4.144959	-3.000478
H	0.953149	-3.113534	-0.647845	H	-3.451081	-4.131916	-1.215804
H	-2.134054	-2.151507	1.534845	H	-2.133353	-4.863826	-2.170859
C	-4.566704	0.320424	-0.188392	H	0.007226	-3.572276	1.453075
H	-5.245372	0.995759	-0.699391	H	0.087718	-1.866512	0.921660
O	-6.202518	-0.286120	1.535075	H	1.135884	-3.085969	0.155507
C	-7.177244	0.552515	0.928174	H	-2.130723	-1.363019	1.916841
H	-8.074962	0.454527	1.541234	C	-4.735125	0.497742	-0.264757
H	-6.854070	1.601902	0.920112	H	-5.450844	1.028458	-0.885053
H	-7.397924	0.229705	-0.097563	O	-6.458382	-0.835329	0.871389
H	-0.673931	-0.804644	-2.813750	C	-7.467842	-0.207488	0.097808
				H	-8.411990	-0.649486	0.422692
				H	-7.494412	0.876791	0.274156
				H	-7.327224	-0.396409	-0.975422
				H	-1.214944	-0.704913	-2.288997
P12							
SCF done: -1628.469156							
C	3.826077	-1.310198	0.766776				
C	4.112639	-2.330158	-0.200377				
C	3.455142	-2.257639	-1.459210				
C	2.570507	-1.240640	-1.741250				
C	2.263169	-0.210762	-0.794977				
C	2.903825	-0.282106	0.438087				
C	4.478086	-1.372439	2.032583				
C	5.364457	-2.387387	2.326213				
C	5.646559	-3.394032	1.366544				
C	5.032168	-3.362033	0.131457				
Ni	-0.499986	0.480534	-0.166354				
C	-1.611570	3.456593	1.198122				
C	-0.952964	1.375414	3.157041				
C	1.139310	2.952082	1.958661				
P	-0.425291	2.024485	1.471354				
P13							
SCF done: -1297.386291							
C	-3.671569	0.097553	0.543907				
C	-4.430116	0.826321	-0.428850				
C	-3.841319	1.050585	-1.703425				
C	-2.587375	0.569092	-1.999305				
C	-1.816140	-0.176691	-1.052013				
C	-2.375955	-0.376991	0.203622				
C	-4.241902	-0.117246	1.830782				
C	-5.499951	0.357285	2.137961				
C	-6.251097	1.073373	1.170805				
C	-5.724078	1.301912	-0.083624				
Ni	0.888704	-0.809475	-0.061956				

C	4.174067	-0.932737	1.182498	C	-0.310330	-3.987671	-0.887666
C	2.170849	-0.138600	3.160098	C	-0.611667	-2.619312	-0.709106
C	2.474797	-2.950998	2.435771	C	2.629714	3.168584	-0.354347
P	2.375929	-1.239909	1.648134	C	1.410129	3.078992	0.333796
C	-0.472649	-0.655619	-1.485295	C	0.622308	1.935002	0.233784
C	-0.058606	-2.062354	-1.509794	C	1.022532	0.822854	-0.542465
C	0.794288	-2.547513	-2.549521	C	2.231058	0.956911	-1.258896
C	1.332379	-3.820639	-2.508986	H	-4.403188	1.825713	-2.529276
C	1.072948	-4.678162	-1.416890	H	-2.119413	1.073417	-3.045484
C	0.273479	-4.227838	-0.378648	H	-1.614877	-0.316196	0.990313
C	-0.277831	-2.927327	-0.402195	H	-3.474247	-0.092026	-2.613364
C	1.986710	3.814539	-0.240572	H	-5.770819	0.656279	3.144260
C	0.907209	3.378014	0.540365	H	-7.179440	1.732590	1.389008
C	0.565812	2.024650	0.572883	H	-6.283885	2.061281	-0.894995
C	1.286002	1.054467	-0.153062	H	4.312102	-1.241463	2.820016
C	2.351140	1.521551	-0.937010	H	4.044081	-0.162631	1.417465
H	-4.399490	1.612597	-2.449700	H	4.191192	-1.914517	1.168783
H	-2.161019	0.754581	-2.982425	H	0.567371	-0.195359	3.751950
H	-1.809754	-0.878954	0.983471	H	1.747257	0.926430	3.043528
H	-3.666967	-0.667093	2.573646	H	2.275222	-0.267197	4.267581
H	-5.921353	0.183065	3.124968	H	2.464820	-2.957965	3.839937
H	-7.242034	1.442325	1.422869	H	2.119996	-3.770892	2.285102
H	-6.294997	1.853455	-0.827948	H	0.784244	-3.124437	3.256835
H	4.826532	-1.066117	2.052428	H	-0.066089	0.310402	-2.410353
H	4.270495	0.087118	0.801832	H	1.168461	-1.392058	-3.365364
H	4.470699	-1.632320	0.395471	H	1.690558	-3.780792	-3.626904
H	1.204655	-0.343307	3.631042	H	0.738614	-5.468756	-2.048383
H	2.187765	0.906850	2.842390	H	-0.752142	-4.713309	-0.208008
H	2.972553	-0.322545	3.883632	H	-1.393066	-2.350996	-0.004757
H	3.261923	-2.984041	3.197365	H	1.093073	3.921871	0.942774
H	2.682285	-3.695906	1.662688	H	2.563364	0.151128	-1.910850
H	1.514420	-3.192671	2.900577	H	-0.320358	1.908838	0.772208
H	-0.134586	-0.120897	-2.373075	C	3.038792	2.097006	-1.158752
H	0.996556	-1.897007	-3.397179	H	3.967697	2.137396	-1.718794
H	1.953710	-4.167691	-3.331431	O	3.332450	4.336385	-0.186424
H	1.489226	-5.681982	-1.399520	C	4.556334	4.492745	-0.885628
H	0.047827	-4.881651	0.460786	H	4.931867	5.481282	-0.613615
H	-0.998274	-2.656319	0.362278	H	5.290354	3.730792	-0.588321
H	0.340675	4.114150	1.105467	H	4.406324	4.446844	-1.973120
H	2.932709	0.826209	-1.541962				
H	-0.294031	1.730037	1.171965	P15			
C	2.711271	2.880740	-0.988074	SCF done: -1297.391515			
H	3.543925	3.185853	-1.614393	C	4.039338	0.065276	-0.778046
O	2.246980	5.165773	-0.208812	C	4.805624	-1.060671	-0.336062
C	3.310577	5.662075	-1.002384	C	4.298424	-1.838361	0.743194
H	3.332200	6.741006	-0.834255	C	3.102775	-1.519857	1.343599
H	4.274975	5.228513	-0.701645	C	2.328607	-0.401367	0.912013
H	3.143251	5.463859	-2.070367	C	2.806881	0.366711	-0.129573
				C	4.537911	0.853784	-1.851383
				C	5.736249	0.543368	-2.461290
				C	6.493049	-0.572789	-2.023604
				C	6.036064	-1.355904	-0.983203
				Ni	-1.969624	-1.318196	-0.418994
				C	-5.301004	-0.225882	-0.012145
				C	-4.034283	0.774331	-2.429158
				C	-4.837638	-2.011875	-2.264275
				P	-3.943241	-0.697232	-1.241010
				C	1.009982	-0.116125	1.646366
				C	0.014891	-1.272668	1.494702
				C	-0.680860	-1.727692	2.612429
				C	-1.564049	-2.827840	2.528516
				C	-1.764440	-3.475720	1.318689
				C	-1.077080	-3.042713	0.150205
				C	-0.169921	-1.938038	0.242306
				C	-0.527093	3.878352	0.805188
				C	0.304288	3.638708	1.909048
				C	0.770088	2.352081	2.160874
				C	0.425980	1.265248	1.337987
				C	-0.411648	1.522627	0.250784
				H	4.873203	-2.694655	1.090451
				H	2.729589	-2.132323	2.161567

PTS₁₄							
SCF done: -1297.355143							
C	-3.546503	0.549163	0.543301				
C	-4.356579	1.170493	-0.462609				
C	-3.800791	1.347885	-1.759371				
C	-2.522246	0.926292	-2.045826				
C	-1.706510	0.293003	-1.061413				
C	-2.230218	0.128388	0.209955				
C	-4.088920	0.377936	1.848211				
C	-5.369772	0.795527	2.143435				
C	-6.171110	1.407618	1.145617				
C	-5.672788	1.590603	-0.127532				
Ni	0.840502	-1.031758	0.093248				
C	3.817194	-1.142169	1.847225				
C	1.604452	-0.090527	3.418952				
C	1.821734	-2.956965	2.952250				
P	1.945731	-1.316097	2.023437				
C	-0.334883	-0.164315	-1.468542				
C	-0.093713	-1.641514	-1.614718				
C	0.764521	-2.111290	-2.655697				
C	1.054308	-3.458301	-2.805680				
C	0.516503	-4.412950	-1.917615				

H	2.245474	1.231364	-0.472136	H	-6.999305	0.988400	-0.962238
H	3.957126	1.711151	-2.185091	C	-2.393759	-2.534679	0.378048
H	6.105069	1.155335	-3.280661	H	-1.541202	-2.596808	-0.309164
H	7.435883	-0.808754	-2.510612	H	-1.997207	-2.655516	1.394145
H	6.614967	-2.212539	-0.643937	H	-3.060346	-3.380236	0.179166
H	-6.233821	0.020245	-0.532848	C	0.771217	0.020027	2.267973
H	-4.972872	0.635960	0.576167	H	1.193029	0.907200	2.756252
H	-5.474633	-1.062268	0.670928	H	1.189047	-0.864588	2.764425
H	-3.378608	0.591905	-3.285611	C	-0.771238	0.023383	2.267938
H	-3.691928	1.677238	-1.915098	H	-1.193094	-0.857067	2.768226
H	-5.060360	0.928590	-2.783269	H	-1.189045	0.914660	2.752322
H	-5.806372	-1.640650	-2.618923	Ni	0.000013	-0.004860	-1.750745
H	-4.992529	-2.903558	-1.650202				
H	-4.216206	-2.286539	-3.121390				
H	1.268317	-0.092446	2.714000	#2b			
H	-0.530094	-1.236533	3.571936	SCF done: -2150.978762			
H	-2.079819	-3.169168	3.422987	C	0.653338	-0.179043	3.018665
H	-2.422848	-4.339786	1.262472	C	0.201846	1.052763	3.591895
H	-1.063550	-3.687715	-0.726737	C	-0.938754	1.704860	3.011630
H	0.538324	-1.752262	-0.563305	C	-1.602685	1.160756	1.944864
H	0.572339	4.470607	2.553911	C	-1.205390	-0.099092	1.359527
H	-0.720406	0.703330	-0.401583	C	-0.048931	-0.741157	1.883431
H	1.422442	2.187760	3.016611	C	1.763835	-0.832682	3.605519
C	-0.886762	2.811132	-0.026482	C	2.418273	-0.290616	4.701401
H	-1.530052	2.962366	-0.886847	C	1.980573	0.930056	5.256867
O	-0.934268	5.174300	0.631551	C	0.888682	1.585170	4.708059
C	-1.766948	5.479254	-0.476923	C	-2.243702	-0.806154	0.502209
H	-1.953198	6.553523	-0.423028	Ni	0.423618	0.421329	0.307893
H	-1.270919	5.242261	-1.427824	O	-2.656687	-1.507619	-2.115425
H	-2.722816	4.940913	-0.419871	C	-1.949461	-2.227196	-1.414182
				O	-1.623714	-1.967447	-0.118566
#1				N	-1.384538	-3.385980	-1.836086
SCF done: -1094.690893				C	-0.567824	-4.289385	-1.010447
N	1.096845	0.012524	0.829251	C	-0.089134	-5.344657	-2.022380
N	-1.096843	0.011261	0.829245	C	-1.220353	-5.384312	-3.066411
C	0.000005	0.006119	0.017098	C	-1.651170	-3.913772	-3.180129
C	-2.459125	0.005504	0.384312	C	-3.475528	-1.274130	1.270517
C	-3.130185	1.226461	0.191492	C	-3.368129	-1.881532	2.530201
C	-3.124509	-1.224276	0.206191	C	-4.507513	-2.331916	3.200103
C	-4.481187	1.195341	-0.179285	C	-5.772025	-2.176997	2.620865
C	-4.472725	-1.206237	-0.164535	C	-5.888488	-1.569323	1.367869
C	-5.171503	-0.007369	-0.359779	C	-4.745715	-1.121794	0.697353
H	-5.003281	2.137655	-0.335810	H	-1.266868	2.653333	3.431995
H	-4.989387	-2.153794	-0.310214	H	-2.471758	1.670177	1.533649
C	2.459127	0.005767	0.384329	H	0.167904	-1.772514	1.614441
C	3.131631	1.226389	0.194491	H	2.103440	-1.773387	3.176638
C	3.123058	-1.224368	0.203200	H	3.270716	-0.808285	5.135138
C	4.482592	1.194630	-0.176369	H	2.495129	1.352008	6.116692
C	4.471295	-1.206964	-0.167493	H	0.540942	2.522840	5.138054
C	5.171489	-0.008447	-0.359805	H	-2.568485	-0.138484	-0.299422
H	5.005782	2.136715	-0.330596	H	-1.177942	-4.736936	-0.214048
H	4.986849	-2.154763	-0.315507	H	0.254793	-3.746069	-0.536629
C	2.412183	2.544863	0.351464	H	0.098502	-6.314777	-1.551112
H	3.085905	3.382266	0.142352	H	0.845645	-5.014602	-2.493226
H	1.559903	2.606438	-0.336182	H	-2.055543	-5.990644	-2.693448
H	2.017233	2.681319	1.366199	H	-0.905219	-5.802534	-4.027757
C	6.632759	-0.023387	-0.749727	H	-1.056590	-3.373157	-3.930466
H	7.255299	-0.443481	0.051369	H	-2.706065	-3.782269	-3.436826
H	6.801931	-0.635804	-1.644233	H	-2.390237	-1.991541	2.990887
H	7.000229	0.986507	-0.960778	H	-4.409508	-2.797623	4.177853
C	2.390818	-2.534362	0.371735	H	-6.659222	-2.523693	3.145282
H	1.993856	-2.657190	1.387427	H	-6.867160	-1.443535	0.910796
H	1.538391	-2.593864	-0.315893	H	-4.834773	-0.662319	-0.284030
H	3.056527	-3.380179	0.171023	N	0.893446	2.379992	-1.818386
C	-2.409227	2.544497	0.345124	N	2.642315	1.133341	-1.439197
H	-1.557101	2.603437	-0.342964	C	1.356020	1.353814	-1.059845
H	-3.082082	3.382150	0.134229	C	3.499888	0.117438	-0.902098
H	-2.013814	2.682935	1.359404	C	4.313585	0.415315	0.208655
C	-6.632770	-0.021531	-0.749744	C	3.551478	-1.143323	-1.524138
H	-6.802454	-0.635039	-1.643410	C	5.185169	-0.572839	0.679182
H	-7.255731	-0.439947	0.051898	C	4.439365	-2.101370	-1.017396
				C	5.265324	-1.836495	0.080247

H	5.814261	-0.350065	1.539462	C	3.494027	-2.570387	2.754576
H	4.485557	-3.078850	-1.494716	H	4.310469	-2.141778	3.333729
C	-0.402419	2.987132	-1.707481	C	2.490984	-4.445121	1.608484
C	-0.596045	4.022090	-0.767124	H	2.526727	-5.483348	1.286130
C	-1.436605	2.586095	-2.570438	C	3.564262	-3.893016	2.326230
C	-1.847026	4.641088	-0.705345	H	4.437044	-4.498231	2.559708
C	-2.674165	3.241818	-2.473053	C	-2.632445	-0.529080	2.515899
C	-2.900964	4.266301	-1.551542	C	-3.157295	-1.061158	1.327479
H	-2.004224	5.436863	0.021341	C	-3.314507	-0.767088	3.720400
H	-3.479967	2.934051	-3.137170	C	-4.320982	-1.830730	1.352037
C	0.509468	4.435168	0.175487	H	-2.666696	-0.850415	0.382424
H	0.192619	5.277731	0.798886	C	-4.472998	-1.547042	3.747008
H	0.787878	3.605562	0.835726	H	-2.928952	-0.344268	4.645613
H	1.416653	4.740386	-0.360844	C	-4.980072	-2.082851	2.560356
C	-4.240443	4.963790	-1.467351	H	-4.713335	-2.231651	0.421465
H	-4.147768	6.034705	-1.690485	H	-4.981369	-1.726943	4.691015
H	-4.958533	4.536334	-2.175042	H	-5.885407	-2.684825	2.574672
H	-4.671925	4.880682	-0.461625	H	-1.330841	0.877184	3.469932
C	-1.271494	1.454899	-3.558771	Ni	0.187057	0.065841	0.216879
H	-0.238629	1.350486	-3.903540	C	0.758547	-0.307009	-1.574246
H	-1.566606	0.498994	-3.107318	N	1.992669	-0.060942	-2.079798
H	-1.911440	1.612272	-4.434309	N	0.004242	-0.789803	-2.596292
C	4.228919	1.755985	0.898560	C	3.124054	0.456270	-1.361704
H	3.229326	1.913586	1.319942	C	2.134058	-0.394365	-3.513829
H	4.955514	1.819578	1.714659	C	-1.390721	-1.118489	-2.548288
H	4.423559	2.587184	0.209386	C	0.717449	-0.856966	-3.891056
C	6.207078	-2.888965	0.621648	C	4.081844	-0.436614	-0.846722
H	5.830712	-3.313447	1.562224	C	3.300819	1.850310	-1.267862
H	6.333082	-3.715738	-0.085786	H	2.885497	-1.180163	-3.651673
H	7.198627	-2.470078	0.831214	H	2.459902	0.486308	-4.079303
C	2.654844	-1.472829	-2.694636	C	-1.776187	-2.461058	-2.386228
H	1.598740	-1.349509	-2.427376	C	-2.349971	-0.105633	-2.756490
H	2.845788	-0.822105	-3.557421	H	0.237502	-0.196987	-4.624208
H	2.810282	-2.506311	-3.021683	H	0.695268	-1.876545	-4.291791
C	1.895850	2.937759	-2.752049	C	5.204545	0.094069	-0.198945
H	2.091788	3.991417	-2.518236	C	3.926849	-1.931080	-0.995226
H	1.530027	2.887283	-3.784350	C	4.439784	2.332334	-0.612933
C	3.120591	2.037422	-2.506993	C	2.293236	2.809612	-1.855154
H	3.408690	1.465037	-3.397017	C	-3.142297	-2.773878	-2.428699
H	4.000638	2.598952	-2.171452	C	-0.751002	-3.550233	-2.175071

TS_{3b}

SCF done: -2150.967091

C	-1.377367	0.263853	2.573606
O	-0.293953	2.022152	0.131070
C	-1.250071	2.464758	0.839292
O	-1.973688	1.780956	1.667097
N	-1.588076	3.783264	0.726188
C	-2.693868	4.406785	1.464360
C	-2.850824	5.770521	0.772085
C	-1.425618	6.089699	0.284140
C	-0.883091	4.719674	-0.155778
C	-0.092189	-0.266545	2.185827
C	1.079586	0.271747	2.873799
C	2.243094	-0.420881	2.987056
C	2.368726	-1.769835	2.474339
C	1.291101	-2.316889	1.719585
C	0.119619	-1.495521	1.402658
H	-2.434011	4.519584	2.526923
H	-3.593140	3.786671	1.409996
H	-3.259384	6.534343	1.441729
H	-3.529786	5.679124	-0.085582
H	-0.823074	6.481247	1.113844
H	-1.400552	6.827732	-0.524337
H	-1.116062	4.512793	-1.210852
H	0.199611	4.624934	-0.032410
H	0.992144	1.255871	3.332788
H	3.087282	0.011685	3.520090
H	-0.764011	-2.076239	1.139107
C	1.373886	-3.665477	1.317663
H	0.537962	-4.103497	0.775586

4b

SCF done: -2151.003332

C	3.494027	-2.570387	2.754576
H	4.310469	-2.141778	3.333729
C	2.490984	-4.445121	1.608484
H	2.526727	-5.483348	1.286130
C	3.564262	-3.893016	2.326230
H	4.437044	-4.498231	2.559708
C	-2.632445	-0.529080	2.515899
C	-3.157295	-1.061158	1.327479
C	-3.314507	-0.767088	3.720400
C	-4.320982	-1.830730	1.352037
H	-2.666696	-0.850415	0.382424
C	-4.472998	-1.547042	3.747008
H	-2.928952	-0.344268	4.645613
C	-4.980072	-2.082851	2.560356
H	-4.713335	-2.231651	0.421465
H	-4.981369	-1.726943	4.691015
H	-5.885407	-2.684825	2.574672
H	-1.330841	0.877184	3.469932
Ni	0.187057	0.065841	0.216879
C	0.758547	-0.307009	-1.574246
N	1.992669	-0.060942	-2.079798
N	0.004242	-0.789803	-2.596292
C	3.124054	0.456270	-1.361704
C	2.134058	-0.394365	-3.513829
C	-1.390721	-1.118489	-2.548288
C	0.717449	-0.856966	-3.891056
C	4.081844	-0.436614	-0.846722
C	3.300819	1.850310	-1.267862
H	2.885497	-1.180163	-3.651673
H	2.459902	0.486308	-4.079303
C	-1.776187	-2.461058	-2.386228
C	-2.349971	-0.105633	-2.756490
H	0.237502	-0.196987	-4.624208
H	0.695268	-1.876545	-4.291791
C	5.204545	0.094069	-0.198945
C	3.926849	-1.931080	-0.995226
C	4.439784	2.332334	-0.612933
C	2.293236	2.809612	-1.855154
C	-3.142297	-2.773878	-2.428699
C	-0.751002	-3.550233	-2.175071
C	-3.701038	-0.466336	-2.790335
C	-1.937554	1.336293	-2.936943
C	5.399132	1.472547	-0.064533
H	5.943211	-0.592120	0.211540
H	4.609825	-2.460509	-0.325505
H	2.910922	-2.256529	-0.757106
H	4.150866	-2.258964	-2.020376
H	4.581494	3.409035	-0.533749
H	2.117174	2.612402	-2.920593
H	1.329891	2.727856	-1.341389
H	2.649517	3.841624	-1.764723
C	-4.118925	-1.794883	-2.635231
H	-3.446244	-3.810830	-2.296732
H	-0.007232	-3.259593	-1.427763
H	-1.232114	-4.476039	-1.843032
H	-0.207322	-3.780471	-3.101690
H	-4.446915	0.311907	-2.943873
H	-1.377836	1.700943	-2.069339
H	-1.293828	1.466367	-3.816796
H	-2.817483	1.973285	-3.075241
C	6.602079	2.020802	0.669790
C	-5.586786	-2.153087	-2.703914
H	6.925478	2.980492	0.250475
H	6.373390	2.189779	1.731105
H	7.449837	1.327953	0.625317
H	-5.981012	-2.016816	-3.719696
H	-5.758169	-3.197114	-2.420629
H	-6.185773	-1.519402	-2.038322

C	0.891540	1.060422	-1.941970	H	-5.279461	-2.115694	-0.055007
O	-0.213643	1.855421	0.638636	H	-3.487357	-3.617055	0.144615
C	0.305937	3.066183	0.393344	H	-1.883876	-2.878292	0.133056
O	1.443069	3.467181	0.768731	H	-2.578457	-3.454094	1.660410
N	-0.525641	3.915477	-0.299242	H	-5.106296	1.830691	1.620886
C	-0.173956	5.343560	-0.494566	H	-2.342080	1.367545	3.662714
C	-1.539518	5.995448	-0.827052	H	-1.655874	1.938921	2.119322
C	-2.332223	4.841456	-1.500601	H	-3.194205	2.615871	2.737748
C	-1.924419	3.603958	-0.665764	C	4.895898	-1.175093	1.378810
C	0.025301	-0.024129	-2.276361	H	4.557730	-3.203734	0.739004
C	-1.318408	0.196715	-2.774210	H	0.959404	-3.337440	0.782269
C	-2.193033	-0.830256	-2.931250	H	2.457755	-4.284785	0.633741
C	-1.828341	-2.187361	-2.613760	H	1.705895	-4.053734	2.218912
C	-0.542701	-2.439490	-2.047353	H	4.906601	0.833296	2.143238
C	0.357489	-1.334433	-1.796489	H	1.421114	1.039660	3.405643
H	0.533929	5.454525	-1.324504	H	3.069855	1.683515	3.582492
H	0.291776	5.740474	0.410420	H	2.127778	1.999741	2.104653
H	-1.436408	6.872381	-1.470980	C	-6.744848	0.185488	0.186509
H	-2.043658	6.291075	0.099654	C	6.357888	-1.156847	0.974167
H	-1.992122	4.717894	-2.535075	H	-7.341935	0.710239	0.940407
H	-3.412463	5.008374	-1.496984	H	-6.701241	0.819290	-0.708469
H	-2.554631	3.507480	0.226807	H	-7.262973	-0.741003	-0.079910
H	-1.981003	2.667638	-1.222919	H	6.955570	-0.566977	1.677149
H	-1.594907	1.208982	-3.047979	H	6.770613	-2.169869	0.929916
H	-3.186042	-0.648415	-3.330066	H	6.452976	-0.702192	-0.019899
H	1.391554	-1.570366	-1.564052				
C	-0.160658	-3.781731	-1.816447				
H	0.830044	-3.982412	-1.425332				
C	-2.692090	-3.270011	-2.888130				
H	-3.667211	-3.063870	-3.317573				
C	-1.023017	-4.829201	-2.099672				
H	-0.709571	-5.851179	-1.919250				
C	-2.300844	-4.574117	-2.632869				
H	-2.968298	-5.398352	-2.855637				
C	2.378680	0.958793	-1.992902				
C	3.176936	1.837419	-1.234355				
C	3.018540	0.060093	-2.871384				
C	4.566623	1.804174	-1.348709				
H	2.702166	2.528677	-0.544325				
C	4.408367	0.029569	-2.976304				
H	2.417761	-0.591548	-3.495223				
C	5.190713	0.903594	-2.216038				
H	5.163924	2.489484	-0.757056				
H	4.879500	-0.660420	-3.668043				
H	6.271077	0.893358	-2.312509				
H	0.488708	2.064441	-2.067790				
Ni	0.149019	0.209489	-0.214606				
C	-0.239878	-0.728842	1.461005				
N	-1.419476	-0.884103	2.111076				
N	0.750196	-1.149968	2.286455				
C	-2.738480	-0.599623	1.607561				
C	-1.270132	-1.441162	3.504554				
C	2.158424	-1.142237	1.982790				
C	0.263844	-1.625736	3.627842				
C	-3.440221	-1.608098	0.927816				
C	-3.339225	0.643348	1.879675				
H	-1.816038	-2.384249	3.583018				
H	-1.666733	-0.727719	4.229949				
C	2.743738	-2.311346	1.459305				
C	2.937701	-0.005542	2.261051				
H	0.700891	-1.007639	4.415466				
H	0.551197	-2.668805	3.779300				
C	-4.737160	-1.340101	0.476031				
C	-2.810257	-2.968045	0.704493				
C	-4.638302	0.872901	1.415729				
C	-2.587199	1.709427	2.649273				
C	4.106094	-2.309114	1.155920				
C	1.916160	-3.566650	1.257280				
C	4.302666	-0.046637	1.946765				
C	2.353541	1.249253	2.875722				
C	-5.345914	-0.102674	0.703846				
				*2a			
				SCF done:	-2150.971052		
				C	-5.643006	-0.802209	-0.558416
				C	-6.177979	0.527915	-0.569650
				C	-5.309776	1.607750	-0.251069
				C	-3.987060	1.384168	0.059855
				C	-3.446080	0.068509	0.067732
				C	-4.271856	-0.995728	-0.237906
				C	-6.506694	-1.889299	-0.871987
				C	-7.832899	-1.674140	-1.182645
				C	-8.360900	-0.357234	-1.193075
				C	-7.550020	0.717171	-0.892423
				C	-1.961989	-0.094213	0.348980
				Ni	0.765739	0.269377	-0.237609
				O	0.405280	-0.989314	1.478952
				C	-0.614847	-1.691547	1.560899
				O	-1.820459	-1.369993	1.054064
				N	-0.634244	-2.883270	2.196542
				C	-1.819083	-3.740012	2.367090
				C	-1.343562	-4.785518	3.388945
				C	0.166613	-4.900235	3.109950
				C	0.583637	-3.456485	2.788336
				C	-1.080337	-0.063524	-0.896312
				C	-1.116764	-1.175528	-1.810941
				C	-0.768786	-1.039160	-3.137126
				C	-0.409910	0.235908	-3.664128
				C	-0.334212	1.323352	-2.822888
				C	-0.587154	1.201369	-1.416240
				H	-5.707452	2.620523	-0.250422
				H	-3.340147	2.224246	0.302253
				H	-3.877624	-2.007829	-0.232482
				H	-6.100112	-2.898546	-0.866706
				H	-8.479576	-2.514484	-1.422675
				H	-9.407589	-0.198660	-1.440202
				H	-7.951688	1.728459	-0.899898
				H	-1.645189	0.701952	1.031545
				H	-2.093999	-4.205720	1.410763
				H	-2.674882	-3.153601	2.712424
				H	-1.875220	-5.736648	3.285813
				H	-1.512226	-4.415661	4.408257
				H	0.341616	-5.543811	2.238615
				H	0.728979	-5.316201	3.951761
				H	0.862810	-2.900976	3.694396
				H	1.416794	-3.387309	2.083894
				H	-1.450824	-2.144667	-1.444632

H	-0.797650	-1.905964	-3.793902	N	1.909698	-0.719682	2.542280
H	-0.202373	0.343777	-4.726289	C	2.845681	-1.809190	2.857692
H	-0.086047	2.304923	-3.223534	C	3.149779	-1.587874	4.348849
H	-0.781914	2.122857	-0.866882	C	2.992169	-0.066171	4.525937
N	3.694478	0.374349	-0.281474	C	1.802343	0.275383	3.614881
N	2.821447	2.293735	0.269843	C	0.642207	-0.286474	-1.847394
C	2.505616	1.012006	-0.081187	C	1.072185	0.990861	-2.390646
C	1.874843	3.282100	0.691366	C	0.358801	1.635908	-3.367629
C	1.511058	4.304963	-0.204313	C	-0.840602	1.067778	-3.906311
C	1.354538	3.247342	2.000654	C	-1.340169	-0.089165	-3.368904
C	0.613570	5.289633	0.228978	C	-0.705860	-0.734058	-2.245399
C	0.459824	4.251976	2.388885	H	5.804066	-2.630704	-2.520083
C	0.078715	5.283838	1.521841	H	3.358221	-2.878755	-2.372546
H	0.322649	6.076433	-0.465134	H	3.077144	0.808890	-0.172457
H	0.050825	4.226840	3.397913	H	5.120448	2.097723	0.340957
C	3.838085	-0.983597	-0.715216	H	7.577733	2.353046	2.210235
C	3.754776	-1.296771	-2.086244	H	8.958355	0.639256	-0.964602
C	4.103540	-1.979634	0.241811	H	7.877840	-1.328553	-2.006279
C	3.944540	-2.626665	-2.477524	H	1.290992	-2.272007	-1.457314
C	4.288759	-3.297667	-0.197162	H	3.750893	-1.726723	2.241329
C	4.216396	-3.641458	-1.551151	H	2.391229	-2.782105	2.649369
H	3.874252	-2.875869	-3.535210	H	4.142343	-1.954699	4.629610
H	4.493220	-4.073165	0.539573	H	2.410845	-2.115588	4.965777
C	3.435484	-0.233678	-3.109756	H	3.894268	0.448735	4.171694
H	3.490185	-0.643459	-4.123656	H	2.821814	0.232881	5.565432
H	2.426263	0.164119	-2.954488	H	0.844855	0.171895	4.146928
H	4.131405	0.612346	-3.051315	H	1.842635	1.288681	3.204427
C	4.443245	-5.064670	-2.010560	H	2.017570	1.414307	-2.071524
H	5.418368	-5.172817	-2.504572	H	0.737016	2.572390	-3.771474
H	4.421068	-5.765529	-1.168855	H	-1.339331	1.552962	-4.742223
H	3.679693	-5.379494	-2.732199	H	-2.234805	-0.544945	-3.789693
C	4.155340	-1.648312	1.715293	H	-0.952413	-1.786719	-2.087695
H	4.937879	-0.914234	1.945734	N	-3.166909	1.443005	0.536730
H	3.203186	-1.223979	2.053036	N	-3.506450	-0.707248	0.397492
H	4.364261	-2.546316	2.307000	C	-2.583427	0.269121	0.181713
C	2.057991	4.334776	-1.612338	C	-3.295334	-2.111470	0.201538
H	1.935009	3.363975	-2.103458	C	-3.793223	-2.727842	-0.961393
H	1.546078	5.094713	-2.211918	C	-2.643712	-2.863599	1.198923
H	3.130176	4.572541	-1.629050	C	-3.605157	-4.107305	-1.120013
C	-0.859792	6.376934	1.982374	C	-2.478292	-4.238016	0.996098
H	-1.625199	5.988899	2.664422	C	-2.946072	-4.879287	-0.157673
H	-0.315793	7.165798	2.520080	H	-3.981103	-4.587308	-2.022130
H	-1.369545	6.850657	1.136113	H	-1.969173	-4.822447	1.760695
C	1.727993	2.145327	2.964752	C	-2.572323	2.746964	0.444715
H	1.358511	1.174392	2.615612	C	-2.738419	3.501124	-0.732009
H	2.815340	2.053605	3.077356	C	-1.894855	3.275369	1.559260
H	1.305253	2.340996	3.956054	C	-2.201391	4.793076	-0.776130
C	4.876276	1.253635	-0.171838	C	-1.376386	4.573111	1.468315
H	5.325130	1.419433	-1.161079	C	-1.514379	5.346506	0.310408
H	5.641010	0.807076	0.472917	H	-2.322282	5.379759	-1.685241
C	4.271056	2.537188	0.417996	H	-0.850088	4.988226	2.326377
H	4.530441	2.673667	1.477384	C	-3.461570	2.933023	-1.929862
H	4.578470	3.439429	-0.121656	H	-3.478720	3.658507	-2.749688
H				H	-2.966646	2.025766	-2.291309
H				H	-4.502456	2.672884	-1.697408
H				C	-0.915658	6.732698	0.225934
H				H	-0.868212	7.210007	1.211292
H				H	0.108801	6.696757	-0.169590
H				H	-1.497813	7.381895	-0.437886
C				C	-1.701357	2.461188	2.816209
C				H	-2.649598	2.067636	3.203118
H				H	-1.043504	1.607651	2.618837
H				H	-1.248786	3.072468	3.604530
C				C	-4.521037	-1.934221	-2.021665
C				H	-4.027082	-0.977455	-2.214034
H				H	-4.567964	-2.494107	-2.961570
H				H	-5.556231	-1.714962	-1.724520
H				C	-2.723464	-6.360679	-0.364440
C				H	-3.445108	-6.779998	-1.074129
H				H	-1.718743	-6.557621	-0.762810
H				H	-2.812758	-6.914815	0.577147
N_{TS}_{3a}							
SCF done: -2150.951504							
C	5.072359	0.229384	-0.758833	H			
C	5.868112	-0.755315	-1.433310	H			
C	5.209558	-1.873899	-2.012608	H			
C	3.841872	-2.011267	-1.929581	C			
C	3.038601	-1.031334	-1.277984	H			
C	3.664510	0.062711	-0.701774	H			
C	5.724652	1.349611	-0.168065	H			
C	7.093846	1.491270	-0.242607	C			
C	7.879565	0.516613	-0.911354	H			
C	7.278109	-0.580195	-1.492236	H			
C	1.563882	-1.240585	-1.253556	H			
Ni	-0.798138	0.040176	-0.430415	C			
O	0.414179	0.336170	1.195542	H			
C	1.199767	-0.638898	1.382071	H			
O	1.379159	-1.614901	0.538323	H			

C	-2.130557	-2.209591	2.460112	C	0.130152	2.627918	-1.269439
H	-1.376678	-1.449507	2.232614	C	-0.163662	3.456830	-0.172975
H	-2.935335	-1.708831	3.013610	C	-0.790799	2.448830	-2.320128
H	-1.681455	-2.954107	3.125339	C	-1.421479	4.074650	-0.125741
C	-4.564860	1.305518	0.997917	C	-2.028630	3.092723	-2.231121
H	-5.245637	1.837977	0.322593	C	-2.367914	3.903864	-1.140496
H	-4.683422	1.734771	1.999372	H	-1.658545	4.714082	0.722706
C	-4.777620	-0.218054	0.972215	H	-2.750346	2.950397	-3.033770
H	-4.931437	-0.640543	1.973461	C	0.842485	3.697941	0.928081
H	-5.627146	-0.516529	0.348177	H	0.457670	4.427354	1.648024
N4a				H	1.076997	2.779519	1.474498
SCF done: -2151.003332				H	1.788996	4.089465	0.533883
C	-4.079505	-0.373093	1.601848	C	-3.720811	4.576166	-1.072587
C	-4.689270	-1.666167	1.718388	H	-3.909113	5.186585	-1.964791
C	-3.840439	-2.803280	1.817412	H	-4.529496	3.836252	-1.012616
C	-2.471226	-2.667311	1.816899	H	-3.799673	5.229316	-0.196970
C	-1.845383	-1.385123	1.729745	C	-0.463759	1.577624	-3.508328
C	-2.663993	-0.269849	1.605703	H	0.369509	1.982061	-4.098192
C	-4.920599	0.770312	1.482057	H	-0.188646	0.572262	-3.176061
C	-6.293906	0.644417	1.487202	H	-1.326370	1.499596	-4.177546
C	-6.895037	-0.635208	1.609406	C	5.282886	1.517188	0.864196
C	-6.107520	-1.762804	1.720716	H	4.330329	2.036417	1.002366
C	-0.371736	-1.316478	1.759625	H	5.821423	1.529160	1.817835
Ni	0.697271	-0.195798	0.420278	H	5.881335	2.107852	0.156250
O	-0.496212	-0.598047	-1.026484	C	6.802043	-3.297436	0.845203
C	-0.648285	-1.861912	-1.332004	H	6.365480	-3.815340	1.710094
O	0.100654	-2.793664	-0.966637	H	6.997222	-4.055056	0.078099
N	-1.728128	-2.133532	-2.147127	H	7.763909	-2.881203	1.164966
C	-2.066842	-3.517121	-2.496953	C	2.973506	-1.916768	-2.134138
C	-3.365391	-3.371981	-3.306039	H	2.715616	-1.069630	-2.777988
C	-4.026904	-2.127455	-2.685708	H	3.365724	-2.720075	-2.767916
C	-2.832125	-1.200846	-2.404225	H	2.039583	-2.275177	-1.679514
C	0.384669	-0.400638	2.566284	C	2.490935	2.723211	-2.132564
C	-0.152153	0.588566	3.453980	H	2.727846	3.677694	-1.643784
C	0.675535	1.476488	4.104648	H	2.165342	2.936347	-3.154070
C	2.078253	1.466627	3.887494	C	3.647089	1.721856	1.721856
C	2.625180	0.547036	3.016666	H	3.784176	1.168325	-3.002628
C	1.798074	-0.378322	2.327246	H	4.601087	2.183284	-1.797053
H	-4.290817	-3.791202	1.892652	NTS_{3c}			
H	-1.838978	-3.549259	1.883418	SCF done: -2150.946982			
H	-2.220521	0.713424	1.471491	C	-4.323618	0.683420	1.334609
H	-4.457415	1.750431	1.387793	C	-5.025634	0.755993	0.087682
H	-6.922665	1.527085	1.398090	C	-4.351115	1.303359	-1.040395
H	-7.978608	-0.723377	1.613934	C	-3.058909	1.763522	-0.940124
H	-6.565196	-2.745895	1.813130	C	-2.353717	1.699473	0.295263
H	0.118462	-2.266548	1.547629	C	-2.985392	1.162352	1.398707
H	-2.220184	-4.117135	-1.588219	C	-4.991292	0.141241	2.467394
H	-1.255291	-3.987511	-3.062377	C	-6.293140	-0.307407	2.375366
H	-3.992693	-4.268513	-3.252720	C	-6.988371	-0.233128	1.141588
H	-3.134329	-3.187934	-4.363967	C	-6.366286	0.287411	0.024804
H	-4.519930	-2.394276	-1.742567	C	-0.943910	2.254881	0.417670
H	-4.775960	-1.663376	-3.337090	Ni	0.452946	-0.259103	-0.223556
H	-2.615030	-0.566525	-3.276897	O	1.688442	1.799583	1.188679
H	-2.986027	-0.542465	-1.545630	C	1.446729	1.492653	0.018528
H	-1.218390	0.586607	3.655706	O	-0.068818	1.568264	-0.501016
H	0.249545	2.185709	4.810959	N	2.265532	1.821947	-1.038564
H	2.714613	2.164190	4.426038	C	2.029577	1.466942	-2.438797
H	3.699877	0.492791	2.876835	C	3.430327	1.545894	-3.070858
H	2.269442	-1.229890	1.835485	C	4.153726	2.593251	-2.203853
N	1.429475	2.021616	-1.374764	C	3.630087	2.302383	-0.789264
N	3.191559	0.792244	-1.004113	C	-0.896695	3.759148	0.160072
C	1.882752	0.947034	-0.691179	C	-0.587824	4.286931	-1.099623
C	4.079082	-0.241396	-0.548473	C	-0.587551	5.669205	-1.310746
C	5.093649	0.099159	0.371510	C	-0.894952	6.542726	-0.264061
C	3.989301	-1.541359	-1.084765	C	-1.198410	6.023361	0.998691
C	5.968533	-0.903834	0.803597	C	-1.196176	4.642543	1.206335
C	4.889438	-2.509514	-0.616162	H	-4.878760	1.358675	-1.990462
C	5.873118	-2.219751	0.333889	H	-2.564463	2.186187	-1.809715
H	6.746339	-0.648254	1.521528	H	-2.456287	1.102335	2.348471
H	4.818362	-3.518590	-1.018260	H	-4.458748	0.091252	3.415089

H	-6.792484	-0.715045	3.250874	C	-4.264303	-1.369878	1.184289
H	-8.015567	-0.584013	1.080360	C	-3.671533	-0.214596	0.727159
H	-6.899897	0.351318	-0.921540	C	-2.536117	0.339354	1.384935
H	-0.579933	2.072277	1.433455	C	-2.027375	-0.308179	2.493129
H	1.336717	2.180894	-2.908457	C	-2.095621	-2.182069	4.133962
H	1.577486	0.469807	-2.515217	C	-2.685172	-3.339361	4.600419
H	3.395064	1.811536	-4.132942	C	-3.822386	-3.875873	3.944496
H	3.935793	0.575800	-2.983259	C	-4.345226	-3.244006	2.834132
H	3.862324	3.605272	-2.513045	C	-1.857942	1.601259	0.839899
H	5.245138	2.523652	-2.266045	Ni	0.308201	0.279505	-0.531819
H	4.233147	1.534266	-0.286132	O	1.429950	0.693531	1.896592
H	3.606345	3.185684	-0.142791	C	1.338565	1.158187	0.760225
H	-0.332316	3.611932	-1.910323	O	-1.155050	1.333616	-0.342210
H	-0.342438	6.063374	-2.294421	N	1.878778	2.352378	0.411247
H	-0.891828	7.617520	-0.427973	C	1.684814	3.033846	-0.878834
H	-1.428514	6.693242	1.823737	C	2.615310	4.252702	-0.776191
H	-1.423639	4.245724	2.193726	C	2.598398	4.584158	0.727139
N	2.320536	-2.414775	0.536656	C	2.576515	3.201907	1.397558
N	0.290055	-3.051736	0.044756	C	-2.868679	2.734737	0.620967
C	1.107571	-1.962011	0.119296	C	-3.087817	3.269880	-0.653400
C	-1.050436	-3.047219	-0.467719	C	-4.005123	4.310735	-0.841730
C	-2.128834	-3.010106	0.438134	C	-4.711354	4.834725	0.244172
C	-1.269495	-3.145980	-1.854817	C	-4.494578	4.307812	1.523076
C	-3.430062	-3.077585	-0.069981	C	-3.582052	3.266708	1.706367
C	-2.590252	-3.210039	-2.316862	H	-5.138991	-1.774944	0.677788
C	-3.682500	-3.185278	-1.443384	H	-4.071368	0.295030	-0.145602
H	-4.267788	-3.032745	0.623232	H	-1.144175	0.089993	2.989324
H	-2.767091	-3.278245	-3.388871	H	-1.224461	-1.766231	4.636010
C	3.491649	-1.639735	0.829660	H	-2.280809	-3.843114	5.475101
C	3.611482	-0.973599	2.065328	H	-4.282656	-4.786058	4.321356
C	4.550474	-1.647162	-0.097779	H	-5.220061	-3.652135	2.331052
C	4.817183	-0.323403	2.352175	H	-1.166242	1.944405	1.627439
C	5.737816	-0.982108	0.234967	H	0.635202	3.327806	-0.997949
C	5.893067	-0.318301	1.456740	H	1.942238	2.370582	-1.711568
H	4.912587	0.200521	3.301681	H	2.279408	5.083221	-1.405667
H	6.559213	-0.984364	-0.479689	H	3.631891	3.981738	-1.090321
C	2.468920	-0.913413	3.049057	H	1.684636	5.137369	0.977702
H	2.831598	-0.642199	4.046252	H	3.454311	5.189194	1.044820
H	1.749933	-0.150355	2.728599	H	3.589364	2.814105	1.574012
H	1.935127	-1.866814	3.126435	H	2.042341	3.183347	2.352020
C	7.183986	0.387462	1.807182	H	-2.524691	2.860879	-1.486149
H	7.899613	0.348111	0.978882	H	-4.165049	4.714535	-1.839531
H	7.007966	1.443058	2.049387	H	-5.421836	5.645172	0.098649
H	7.662608	-0.068639	2.683589	H	-5.036666	4.708233	2.376967
C	4.421008	-2.348402	-1.430901	H	-3.424037	2.858082	2.703012
H	4.389590	-3.440883	-1.321458	N	2.756319	-1.508143	-0.905361
H	3.503063	-2.053029	-1.950594	N	1.020166	-1.817475	-2.191633
H	5.273598	-2.112211	-2.076109	C	1.516269	-1.055827	-1.185860
C	-1.891934	-2.876520	1.924256	C	-0.286493	-1.650654	-2.766694
H	-1.282007	-1.993932	2.148161	C	-1.382079	-2.328886	-2.197526
H	-2.842159	-2.782519	2.458991	C	-0.436036	-0.850645	-3.917217
H	-1.362219	-3.746149	2.334983	C	-2.635055	-2.184767	-2.804631
C	-5.099886	-3.285099	-1.959932	C	-1.708623	-0.738763	-4.486070
H	-5.146720	-3.102159	-3.038969	C	-2.820933	-1.394330	-3.943764
H	-5.518727	-4.283927	-1.776021	H	-3.488266	-2.699370	-2.367578
H	-5.755478	-2.561421	-1.462067	H	-1.835119	-0.118650	-5.371680
C	-0.117819	-3.160413	-2.832545	C	3.670368	-1.044821	0.102819
H	0.480574	-2.245697	-2.745565	C	3.583479	-1.565343	1.407868
H	0.559710	-4.006012	-2.659396	C	4.691603	-0.150958	-0.263094
H	-0.484278	-3.234713	-3.861505	C	4.548735	-1.172130	2.339723
C	2.321506	-3.852421	0.887038	C	5.630013	0.220595	0.708685
H	2.408786	-3.971367	1.975524	C	5.577671	-0.280659	2.013571
H	3.169428	-4.366554	0.423922	H	4.484307	-1.562382	3.353851
C	0.964143	-4.328259	0.351751	H	6.422129	0.915400	0.435030
H	1.059708	-4.939686	-0.555822	C	2.454587	-2.477931	1.818857
H	0.393632	-4.905067	1.087475	H	2.659255	-2.931569	2.793874
				H	1.525639	-1.902045	1.900367
				H	2.285096	-3.287582	1.099540
				C	6.591555	0.138352	3.054124
				H	7.410193	0.713321	2.608195
				H	6.127769	0.764126	3.827998
¹⁴C							
SCF done:	-2150.978144						
C	-2.611293	-1.506682	2.993005				
C	-3.758469	-2.051736	2.328166				

H	7.027240	-0.731204	3.561304	H	-0.582714	6.120211	-3.189863
C	4.787037	0.407983	-1.664522	H	-0.818401	7.357220	-1.037631
H	5.040180	-0.365999	-2.401409	N	-1.650957	-2.625966	0.654568
H	3.840926	0.857894	-1.983859	N	0.311325	-3.120174	-0.167604
H	5.565063	1.175941	-1.721325	C	-0.585824	-2.104687	-0.009232
C	-1.232744	-3.166287	-0.948996	C	1.526419	-3.024502	-0.926028
H	-1.076790	-2.533630	-0.066917	C	1.489335	-3.159666	-2.327307
H	-2.134282	-3.759842	-0.771950	C	2.747202	-2.853471	-0.243046
H	-0.380646	-3.853172	-1.009884	C	2.698563	-3.108564	-3.032782
C	-4.192740	-1.227040	-4.556002	C	3.928543	-2.811121	-0.990879
H	-4.132421	-1.055905	-5.636588	C	3.926576	-2.933581	-2.386087
H	-4.818648	-2.109729	-4.384909	H	2.676969	-3.207676	-4.116657
H	-4.714290	-0.365841	-4.116869	H	4.873500	-2.670205	-0.469090
C	0.738463	-0.116861	-4.522820	C	-2.828607	-1.934482	1.093178
H	1.225978	0.531751	-3.786293	C	-4.016108	-2.093873	0.354373
H	1.503663	-0.805514	-4.904052	C	-2.812089	-1.194612	2.291949
H	0.412554	0.507890	-5.360239	C	-5.192212	-1.509306	0.841697
C	3.145540	-2.686177	-1.718273	C	-4.012851	-0.630766	2.739100
H	3.314523	-3.549416	-1.064259	C	-5.213910	-0.780260	2.035526
H	4.077411	-2.484609	-2.256600	H	-6.113280	-1.631198	0.274209
C	1.940422	-2.874411	-2.656155	H	-4.005039	-0.055117	3.663296
H	2.194893	-2.725956	-3.712118	C	-4.034310	-2.870482	-0.942566
H	1.472023	-3.860170	-2.557770	H	-5.004551	-2.769663	-1.439905

¹⁵N

SCF done: -2150.936851

C	1.166615	2.301363	-1.146828
Ni	-0.175814	-0.402763	-0.635225
O	-1.073506	1.698533	0.923275
C	-1.194746	1.277285	-0.232601
O	0.072481	1.357973	-1.271099
N	-2.336020	1.470825	-0.973745
C	-2.546435	1.082081	-2.366814
C	-3.848661	1.810938	-2.735843
C	-4.627663	1.838880	-1.408322
C	-3.534329	2.048602	-0.347372
C	2.248573	1.967337	-0.127512
C	3.601700	2.142190	-0.537229
C	4.650928	1.898266	0.321061
C	4.413539	1.461010	1.652502
C	3.055758	1.282237	2.075383
C	1.995513	1.540687	1.162690
H	-2.656811	-0.010491	-2.462469
H	-1.695419	1.384470	-2.982419
H	-4.391789	1.312055	-3.546096
H	-3.622061	2.833969	-3.062079
H	-5.125537	0.875301	-1.243800
H	-5.393240	2.621632	-1.375814
H	-3.367856	3.114002	-0.132021
H	-3.759635	1.549481	0.600015
H	3.807577	2.474492	-1.553007
H	5.676839	2.034538	-0.015374
H	0.967535	1.411742	1.488473
C	2.805928	0.855804	3.410703
H	1.774450	0.728217	3.731934
C	5.464768	1.198583	2.574260
H	6.494266	1.334752	2.248524
C	3.845675	0.614222	4.284136
H	3.639254	0.292366	5.301988
C	5.189575	0.784831	3.861061
H	6.001905	0.591579	4.557433
H	1.643588	2.213091	-2.130987
C	0.623805	3.728374	-1.063824
C	0.491458	4.434957	0.138458
C	0.231593	4.355351	-2.256889
C	-0.028300	5.732320	0.146774
H	0.788636	3.969623	1.071624
C	-0.288258	5.651561	-2.253694
H	0.334368	3.818269	-3.198167
C	-0.419904	6.345507	-1.046775
H	-0.126156	6.264469	1.089928

¹⁴d

SCF done: -2150.976724

C	1.430923	1.897435	-1.590850
Ni	-0.488806	-0.196464	-0.448009
O	-0.443512	-0.424064	2.285744
C	-0.914123	0.221958	1.338884
O	0.271231	1.160491	-1.360675
N	-1.692324	1.311465	1.545040
C	-2.278524	2.184533	0.511578
C	-2.568294	3.482294	1.279175
C	-2.921409	2.984106	2.692440
C	-1.958507	1.805922	2.912105
C	2.662849	1.536001	-0.755585
C	3.945253	1.885827	-1.270317
C	5.098176	1.629217	-0.563716
C	5.045348	1.006552	0.715372
C	3.761754	0.649766	1.242503
C	2.592254	0.924961	0.477934
H	-3.208040	1.742301	0.127729

H	-1.581150	2.312748	-0.318269	H	0.643424	-4.248000	2.006667
H	-3.368782	4.068431	0.815590	H	2.084954	-3.399170	2.569583
H	-1.667302	4.106715	1.306751	C	-2.725301	-3.770214	-0.267225
H	-3.960195	2.630201	2.716652	H	-3.316441	-4.002993	-1.161706
H	-2.813692	3.755072	3.462967	H	-3.261252	-4.158794	0.603581
H	-1.016254	2.121958	3.378840	C	-1.278734	-4.287343	-0.357843
H	-2.377434	1.007135	3.532873	H	-0.980019	-4.861335	0.526176
H	4.007155	2.368524	-2.244261	H	-1.099106	-4.907075	-1.242773
H	6.067370	1.902216	-0.977359				
H	1.630788	0.634801	0.889160				
C	3.692354	0.034466	2.523904	*le			
H	2.714722	-0.230434	2.920711	SCF done: -2150.958284			
C	6.208649	0.730870	1.485135	C	-1.754192	3.149984	-1.243799
H	7.181917	1.005423	1.082355	C	-2.000489	3.207723	-2.656200
C	4.839333	-0.217276	3.249219	C	-1.974390	1.993615	-3.401110
H	4.772124	-0.683182	4.229592	C	-1.697303	0.796669	-2.790701
C	6.110336	0.132815	2.725176	C	-1.410806	0.738625	-1.392461
H	7.007160	-0.068393	3.306263	C	-1.469308	1.896083	-0.638222
H	1.721485	1.717308	-2.642599	C	-1.803485	4.357094	-0.491437
C	1.111317	3.401178	-1.498674	C	-2.077498	5.560144	-1.102283
C	1.241053	4.128601	-0.307417	C	-2.317658	5.615176	-2.498527
C	0.614132	4.061441	-2.631728	C	-2.281036	4.464779	-3.255619
C	0.877420	5.477657	-0.249178	C	-1.118807	-0.570068	-0.766301
H	1.639825	3.640086	0.577803	Ni	1.289001	-0.395607	-0.347271
C	0.250541	5.410006	-2.580765	O	-2.246875	-2.257207	0.934031
H	0.507307	3.507422	-3.562680	C	-2.883134	-1.866813	-0.096131
C	0.380725	6.124326	-1.385395	O	-2.381684	-1.208971	-1.140785
H	0.992472	6.027268	0.682668	N	-4.224463	-2.132423	-0.212220
H	-0.128692	5.903457	-3.472967	C	-5.051239	-1.716608	-1.362665
H	0.105246	7.175425	-1.341780	C	-6.486072	-2.045109	-0.879115
N	-2.539181	-2.304448	-0.157360	C	-6.275504	-3.271250	0.052984
N	-0.497637	-3.034528	-0.442896	C	-4.953131	-2.936145	0.787589
C	-1.251312	-1.925102	-0.308378	C	-0.124336	-1.482508	-1.326425
C	0.925415	-3.067605	-0.654971	C	0.868541	-1.016123	-2.258953
C	1.419849	-2.965375	-1.967992	C	1.876845	-1.914163	-2.703939
C	1.786022	-3.258464	0.443764	C	1.910879	-3.220793	-2.253791
C	2.803796	-3.049920	-2.163693	C	0.926055	-3.684918	-1.345980
C	3.160303	-3.336110	0.194647	C	-0.059415	-2.840358	-0.879261
C	3.690252	-3.230586	-1.097274	H	-2.200280	2.029337	-4.461934
H	3.196254	-2.965500	-3.175352	H	-1.726743	-0.132428	-3.344365
H	3.836843	-3.465659	1.037105	H	-1.283519	1.858914	0.428650
C	-3.687104	-1.444935	-0.091125	H	-1.623289	4.307916	0.576817
C	-4.182536	-0.854355	-1.268379	H	-2.112661	6.473047	-0.518695
C	-4.340399	-1.271332	1.146113	H	-2.532596	6.569092	-2.966300
C	-5.349096	-0.081350	-1.183764	H	-2.468403	4.501901	-4.323792
C	-5.501624	-0.491956	1.177232	H	-1.340123	-0.685693	0.287716
C	-6.025416	0.109165	0.024810	H	-4.793573	-2.294036	-2.260016
H	-5.737457	0.379529	-2.089971	H	-4.897722	-0.657188	-1.579889
H	-6.009610	-0.348724	2.129707	H	-7.167138	-2.254171	-1.708037
C	-3.480478	-1.018997	-2.596308	H	-6.880256	-1.205207	-0.296508
H	-4.113784	-0.661107	-3.414199	H	-6.141251	-4.173512	-0.553720
H	-2.543903	-0.448237	-2.621772	H	-7.108155	-3.427223	0.743735
H	-3.224564	-2.065146	-2.800655	H	-5.143711	-2.350860	1.697778
C	-7.287495	0.939274	0.094807	H	-4.371354	-3.818959	1.064497
H	-7.161084	1.801600	0.761881	H	0.751463	-0.055271	-2.752948
H	-7.571353	1.319615	-0.891912	H	2.613592	-1.563697	-3.419100
H	-8.129521	0.352395	0.483163	H	2.682919	-3.897368	-2.603250
C	-3.805946	-1.892339	2.416453	H	0.946665	-4.719412	-1.019798
H	-3.957503	-2.980217	2.433902	H	-0.835698	-3.171929	-0.197530
H	-2.733661	-1.707343	2.537383	N	3.389518	0.125307	1.514632
H	-4.324751	-1.483694	3.289636	N	1.465040	0.553369	2.480810
C	0.500004	-2.739438	-3.146137	C	2.039767	0.180541	1.299177
H	0.084171	-1.723956	-3.135510	C	0.052248	0.700207	2.703581
H	1.043432	-2.864319	-4.088122	C	-0.475308	1.998876	2.847949
H	-0.347025	-3.436004	-3.152546	C	-0.789319	-0.424128	-2.759594
C	5.183895	-3.279037	-1.322901	C	-1.850747	2.154789	3.040779
H	5.424817	-3.468118	-2.374609	C	-2.171492	-0.225788	2.895168
H	5.650505	-2.326281	-1.040388	C	-2.713934	1.051767	3.049939
H	5.655631	-4.063149	-0.718988	H	-2.259058	3.154965	3.150063
C	1.256537	-3.348880	1.855912	H	-2.818729	-1.089751	2.802026
H	0.640643	-2.477192	2.104629	C	4.364619	-0.146882	0.493722

C	4.809413	0.893933	-0.342814	H	-3.184012	5.705752	-4.159738
C	4.873057	-1.447781	0.353549	H	-2.608563	3.519975	-5.168125
C	5.783280	0.616292	-1.304848	H	-1.299921	-0.647897	0.325131
C	5.851789	-1.689603	-0.616751	H	-4.905444	-3.514791	-1.774960
C	6.320469	-0.669400	-1.449248	H	-5.416615	-1.824980	-1.694104
H	6.125545	1.415866	-1.954668	H	-7.289670	-3.834023	-1.392117
H	6.245438	-2.694622	-0.729257	H	-7.396244	-2.360045	-0.414545
C	4.204752	2.280140	-0.227103	H	-6.088349	-5.011611	0.400008
H	4.661942	2.960616	-0.950843	H	-7.305452	-4.107108	1.316695
H	3.126526	2.233033	-0.420520	H	-5.690479	-2.404150	1.949476
H	4.347702	2.697043	0.776644	H	-4.600549	-3.792107	1.858498
C	7.390393	-0.940015	-2.493007	H	0.957842	-0.684437	-2.687877
H	7.045920	-0.642651	-3.490331	H	2.727114	-2.381289	-3.004790
H	8.302817	-0.373566	-2.269547	H	2.663434	-4.511275	-1.736668
H	7.647750	-2.002976	-2.522424	H	0.882660	-4.893353	-0.030593
C	4.318790	-2.580326	1.195139	H	-0.824861	-3.137139	0.414439
H	4.374703	-2.354017	2.265311	N	3.398711	0.502397	1.380378
H	3.265127	-2.744469	0.939973	N	1.529210	1.202252	2.260420
H	4.871691	-3.505063	1.007235	C	2.052373	0.547640	1.199215
C	0.428231	3.214527	2.750256	C	0.139779	1.455584	2.524585
H	1.071085	3.146216	1.866758	C	-0.338097	2.769443	2.332128
H	-0.167544	4.129336	2.680415	C	-0.695922	0.441812	3.028752
H	1.074968	3.306068	3.632103	C	-1.669987	3.047960	2.653736
C	-4.211068	1.237748	3.221553	C	-2.032944	0.765293	3.304370
H	-4.486375	1.188115	4.283247	C	-2.537661	2.056085	3.132344
H	-4.535111	2.208326	2.832336	H	-2.043903	4.061003	2.513851
H	-4.759757	0.451658	2.693193	H	-2.693675	-0.028802	3.644459
C	-0.264067	-1.844892	2.675877	C	4.338275	-0.010994	0.423661
H	0.631257	-1.904576	2.054008	C	4.745666	0.795993	-0.658978
H	-0.024287	-2.218331	3.680869	C	4.871734	-1.298699	0.614465
H	-1.036978	-2.472700	2.227910	C	5.696461	0.282426	-1.547218
C	3.803594	0.544498	2.897063	C	5.824928	-1.766555	-0.299345
H	4.305059	1.517148	2.858730	C	6.253128	-0.992949	-1.383099
H	4.477049	-0.195198	3.334197	H	6.012382	0.896793	-2.388788
C	2.438909	0.615514	3.626201	H	6.236556	-2.764565	-0.161477
H	2.277936	-0.242506	4.286741	C	4.166999	2.175715	-0.873079
H	2.309907	1.539982	4.190538	H	4.585532	2.634849	-1.774203

Ni^{TS_{5e}}

SCF done: -2150.940625

C	-2.091822	2.738293	-1.856562	H	4.381680	2.844939	-0.030324
C	-2.158298	2.562576	-3.278220	C	7.301618	-1.505830	-2.344552
C	-1.841982	1.282957	-3.816893	H	7.003206	-1.344182	-3.387378
C	-1.454224	0.245399	-3.004102	H	8.259299	-0.988428	-2.198924
C	-1.347158	0.418409	-1.588810	H	7.481073	-2.577299	-2.207131
C	-1.692623	1.646836	-1.043039	C	4.408987	-2.176701	1.753550
C	-2.435540	4.005817	-1.306248	H	4.594491	-1.716249	2.732009
C	-2.819540	5.050741	-2.120372	H	3.332432	-2.372014	1.687763
C	-2.879119	4.876205	-3.526708	H	4.930149	-3.139061	1.736684
C	-2.557137	3.657770	-4.090002	C	0.550654	3.854861	1.767718
C	-0.966106	-0.690998	-0.704603	H	0.987402	3.554657	0.808426
Ni	1.274168	-0.440132	-0.262586	H	-0.019525	4.774996	1.605693
O	-2.745103	-2.071358	1.286066	H	1.384082	4.102205	2.438191
C	-3.333605	-2.115861	0.171052	C	-3.989948	2.362516	3.419788
O	-2.834004	-1.756040	-0.966901	H	-4.156924	3.438021	3.545481
N	-4.632505	-2.591523	0.118178	H	-4.631633	2.019913	2.597243
C	-5.381438	-2.761541	-1.127753	H	-4.333013	1.855799	4.328980
C	-6.764981	-3.228875	-0.644334	C	-0.229512	-0.972357	3.285166
C	-6.443372	-4.002509	0.648323	H	0.791132	-1.146596	2.937933
C	-5.301408	-3.184790	1.276581	H	-0.270224	-1.199507	4.359193
C	-0.047514	-1.758264	-1.055545	H	-0.895885	-1.675181	2.772121
C	0.990439	-1.540314	-2.018467	C	3.856288	1.241254	2.576929
C	1.960424	-2.550086	-2.252946	H	4.355441	2.173560	2.280205
C	1.922115	-3.738936	-1.546824	H	4.565798	0.644776	3.158050
C	0.911269	-3.954140	-0.577782	C	2.533291	1.489541	3.311724
C	-0.038780	-2.986359	-0.319978	H	2.385459	0.801345	4.154847
H	-1.933781	1.128820	-4.890133	H	2.430350	2.512423	3.683590
H	-1.273713	-0.736484	-3.428769				
H	-1.653842	1.783669	0.034074	N_{2e}			
H	-2.393343	4.133186	-0.227293	SCF done: -2150.959332			
H	-3.081239	6.012686	-1.686524	C	1.236083	1.142768	1.963342
				C	0.882475	0.377389	3.118796
				C	0.563858	-1.015420	2.956239

H	-0.188646	0.572262	-3.176061	H	-7.138908	-1.428088	0.713841
H	-1.326370	1.499596	-4.177546	H	-4.242041	0.422341	3.053304
C	5.282886	1.517188	0.864196	H	-4.520176	-1.315049	3.342076
H	4.330329	2.036417	1.002366	H	-5.881900	-0.254840	2.907977
H	5.821423	1.529160	1.817835	H	-4.431659	1.168452	-2.229443
H	5.881335	2.107852	0.156250	H	-5.912778	0.183368	-2.297752
C	6.802043	-3.297436	0.845203	H	-4.387471	-0.464089	-2.952064
H	6.365480	-3.815340	1.710094	H	-6.331906	2.723276	-0.029149
H	6.997222	-4.055056	0.078099	C	-8.857629	-0.151726	0.547046
H	7.763909	-2.881203	1.164966	H	-9.580808	-0.946313	0.718103
C	2.973506	-1.916768	-2.134138	H	-2.068610	-0.498700	0.333097
H	2.715616	-1.069630	-2.777988	O	-4.047433	1.439955	0.465680
H	3.365724	-2.720075	-2.767916	H	-4.407654	2.088457	1.085575
H	2.039583	-2.275177	-1.679514	N	1.805226	-3.062823	-0.977114
C	2.490935	2.723211	-2.132564	N	3.836836	-2.261422	-0.891129
H	2.727846	3.677694	-1.643784	C	2.532922	-1.958570	-0.690849
H	2.165342	2.936347	-3.154070	C	4.957205	-1.361940	-0.898112
C	3.647089	1.721856	-2.064363	C	5.120105	-0.458710	-1.968042
H	3.784176	1.168325	-3.002628	C	5.937102	-1.486988	0.107216
H	4.601087	2.183284	-1.797053	C	6.272044	0.338322	-1.988681

#5

SCF done: -2856.475454

C	-0.372032	-1.007538	4.005646	H	7.820698	-0.746429	0.823422
C	0.238637	-1.926006	4.867339	C	0.374039	-3.211273	-0.927051
C	1.581116	-2.256252	4.665151	C	-0.374544	-2.973093	-2.100747
C	2.297538	-1.678640	3.612960	C	-0.238473	-3.714833	0.236566
C	1.703627	-0.758135	2.727489	C	-1.757030	-3.189463	-2.059918
C	0.349058	-0.436302	2.954510	C	-1.628059	-3.912001	0.225325
Ni	1.682378	-0.318581	-0.178973	C	-2.410433	-3.652948	-0.907298
O	0.872561	0.327980	-1.963696	H	-2.342815	-2.998934	-2.956864
N	-0.527408	2.148673	-1.872863	H	-2.108532	-4.292085	1.124919
C	0.213700	1.196414	-1.278996	C	0.286061	-2.513250	-3.378992
O	0.267981	1.113648	0.012162	H	-0.445251	-2.471808	-4.192540
C	-1.234424	3.212602	-1.129798	H	0.722883	-1.517578	-3.257799
C	-1.543575	4.245291	-2.225468	H	1.086348	-3.197166	-3.690115
C	-1.700021	3.387940	-3.495262	C	-3.908641	-3.835944	-0.887014
C	-0.621906	2.303807	-3.332223	H	-4.218238	-4.496699	-0.070486
C	2.517541	-0.161641	1.616877	H	-4.406788	-2.866663	-0.748099
C	2.806468	1.317023	1.665172	H	-4.266617	-4.263711	-1.831017
C	3.872736	1.827474	0.930020	C	0.561823	-4.091906	1.459961
C	4.197118	3.208594	0.912543	H	0.958636	-5.113065	1.367481
C	3.413676	4.121396	1.691555	H	1.403809	-3.417713	1.625187
C	2.340502	3.590017	2.455980	H	-0.061831	-4.067760	2.358136
C	2.045943	2.245974	2.441261	C	4.101864	-0.342738	-3.078226
C	-9.315242	1.153764	0.344606	H	3.168068	0.115489	-2.733679
C	-8.398476	2.186726	0.142443	H	4.498382	0.268301	-3.895310
C	-7.026870	1.902088	0.143905	H	3.839264	-1.323920	-3.492612
C	-6.524560	0.604135	0.348719	C	8.478871	1.142616	-1.031082
C	-7.483817	-0.409155	0.546628	H	8.390712	1.964834	-0.308419
B	-4.934910	0.230983	0.330078	H	9.386345	0.583426	-0.775155
O	-4.569978	-0.779388	1.371446	H	8.622736	1.587131	-2.021564
C	-4.817305	-0.460963	2.718145	C	5.816444	-2.496998	1.226105
O	-4.490860	-0.450360	-0.912463	H	4.773874	-2.713418	1.473899
C	-4.823768	0.141519	-2.145509	H	6.295870	-3.448635	0.955938
H	2.076297	-2.958529	5.332137	H	6.315071	-2.133779	2.130726
H	3.347067	-1.934355	3.480963	C	2.635055	-4.236383	-1.330334
H	-0.128054	0.292202	2.306008	H	2.285896	-4.683518	-2.265944
H	-0.594761	3.600614	-0.332429	H	2.563657	-4.994386	-0.541317
H	-2.151578	2.814054	-0.677695	C	4.037343	-3.625314	-1.437530
H	-0.700894	4.939222	-2.339421	H	4.786667	-4.167511	-0.854139
H	-2.436594	4.834499	-1.995338	H	4.394275	-3.556713	-2.472750
H	-1.574438	3.959321	-4.420564	C	5.280792	3.725216	0.145176
H	-2.694669	2.925972	-3.515741	H	5.872088	3.034229	-0.451006
H	-0.886325	1.353304	-3.805227	C	3.741737	5.504166	1.677779
H	0.345309	2.625169	-3.742815	H	3.144002	6.190408	2.274636
H	3.468405	-0.693018	1.548824	C	5.573424	5.072973	0.148322
H	4.486870	1.151884	0.340875	H	6.402151	5.451968	-0.445188
H	1.745515	4.266507	3.066892	C	4.797353	5.973663	0.923293
H	1.225151	1.888418	3.050823	H	5.038239	7.033771	0.919958
H	-8.762151	3.201972	-0.001683	H	-0.321664	-2.367469	5.687458

H	-1.412414	-0.728501	4.159739	C	-3.342557	4.376184	-1.383378
O	-10.677419	1.425567	0.391423	C	-2.390388	5.354000	-1.075399
C	-11.327556	1.400857	-0.875673	H	-0.280669	5.766314	-0.975261
H	-12.380440	1.631006	-0.691023	H	-4.400752	4.615446	-1.292728
H	-10.903375	2.152604	-1.556468	C	0.854451	3.445195	-1.742988
H	-11.246482	0.409654	-1.344534	H	1.441907	4.366312	-1.681227

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SCF done: -2086.005749

C	-4.169752	-2.464835	0.653020
C	-3.457214	-3.469060	1.385849
C	-2.190974	-3.128508	1.939021
C	-1.651552	-1.871380	1.785634
C	-2.352463	-0.855618	1.061675
C	-3.585478	-1.177676	0.509826
C	-5.437433	-2.792194	0.095013
C	-5.974635	-4.053330	0.250523
C	-5.266853	-5.047737	0.973248
C	-4.036351	-4.759314	1.527728
Ni	-0.020301	0.392930	0.074111
O	1.003058	0.356167	1.661132
C	-1.821945	0.536643	0.899164
C	6.049213	0.481974	0.268796
C	5.862026	-0.763848	0.883093
C	4.639580	-1.067942	1.481851
C	3.550776	-0.169343	1.496375
C	3.783881	1.070888	0.881092
B	2.169377	-0.491427	2.311528
O	2.147279	0.067692	3.655323
C	3.009262	-0.461790	4.631850
O	1.801968	-1.897287	2.363393
C	1.746385	-2.676639	1.198401
H	-1.636757	-3.886247	2.489077
H	-0.670056	-1.657978	2.200724
H	-4.143799	-0.418307	-0.035467
H	-5.981413	-2.027462	-0.456229
H	-6.945388	-4.288962	-0.178550
H	-5.700182	-6.037636	1.091877
H	-3.492631	-5.518890	2.085646
H	6.687026	-1.472114	0.888537
H	2.992076	1.817954	0.891135
H	2.822652	0.066001	5.575696
H	4.069138	-0.319897	4.362113
H	2.833451	-1.536741	4.789424
H	1.472007	-3.702153	1.480525
H	2.705390	-2.710184	0.662166
H	0.984041	-2.312236	0.488969
H	4.531015	-2.037072	1.965673
C	5.002668	1.410644	0.271854
H	5.121513	2.391663	-0.178360
O	7.285352	0.696225	-0.299140
C	7.551121	1.966897	-0.865488
H	8.580640	1.924778	-1.228292
H	6.878719	2.183504	-1.708036
H	7.460782	2.767900	-0.118499
H	0.654950	0.884030	2.398696
N	-1.218140	1.499154	-2.420995
N	-0.189820	-0.410856	-2.689517
C	-0.556349	0.508550	-1.772971
C	0.561600	-1.621773	-2.475460
C	1.967506	-1.576269	-2.533734
C	-0.130443	-2.841711	-2.337702
C	2.670967	-2.782956	-2.428722
C	0.619665	-4.016826	-2.231872
C	2.019882	-4.009940	-2.271885
H	3.758228	-2.756120	-2.461941
H	0.094299	-4.962487	-2.112798
C	-1.607045	2.781198	-1.903395
C	-0.620263	3.746963	-1.616052
C	-2.978068	3.091630	-1.804181
C	-1.037395	5.017657	-1.201124

C	-3.342557	4.376184	-1.383378
C	-2.390388	5.354000	-1.075399
H	-0.280669	5.766314	-0.975261
H	-4.400752	4.615446	-1.292728
C	0.854451	3.445195	-1.742988
H	1.441907	4.366312	-1.681227
H	1.196878	2.776819	-0.943550
H	1.094035	2.955511	-2.694018
C	-2.813916	6.725779	-0.602416
H	-3.095668	6.706631	0.458845
H	-2.005299	7.455526	-0.715293
H	-3.682778	7.091666	-1.161398
C	-4.055550	2.090510	-2.156215
H	-4.359921	2.185867	-3.208052
H	-3.724254	1.059770	-2.001901
H	-4.951132	2.256788	-1.548554
C	2.731429	-0.280755	-2.684467
H	2.919596	0.186067	-1.709010
H	3.709490	-0.464574	-3.140267
H	2.200149	0.449211	-3.304120
C	2.805937	-5.291411	-2.118808
H	3.771140	-5.234284	-2.633724
H	3.012664	-5.496877	-1.059800
H	2.255584	-6.150885	-2.517511
C	-1.638974	-2.896158	-2.299094
H	-2.046697	-2.231802	-1.531514
H	-2.085245	-2.602730	-3.258956
H	-1.982564	-3.910860	-2.078273
C	-1.278342	1.296058	-3.889296
H	-0.743080	2.108769	-4.394246
C	-2.316206	1.306636	-4.235741
H	-0.602229	-0.070216	-4.069813
H	-1.283903	-0.834688	-4.456695
H	0.274911	-0.035448	-4.724846
H	-2.390667	1.064160	0.132757
C	-1.733563	1.412359	2.116157
C	-1.675283	2.811573	1.942355
C	-1.736826	0.921181	3.436852
C	-1.613838	3.678443	3.032255
H	-1.678143	3.219107	0.936458
C	-1.673295	1.789355	4.529206
H	-1.788945	-0.146161	3.618960
C	-1.609005	3.171383	4.336221
H	-1.567668	4.751857	2.863361
H	-1.668244	1.378298	5.535388
H	-1.554441	3.843852	5.188430

N7S,

SCF done: -2427.608433

C	-4.904308	1.483494	-0.011901
C	-5.371796	0.567437	0.985753
C	-4.406710	-0.044372	1.833296
C	-3.063573	0.229194	1.706481
C	-2.573150	1.151027	0.727351
C	-3.510995	1.750797	-0.103812
C	-5.857319	2.103218	-0.868680
C	-7.204455	1.830517	-0.746794
C	-7.664599	0.921811	0.240328
C	-6.764969	0.305828	1.086783
Ni	0.196372	-0.094890	0.485382
O	-0.041463	-0.395669	2.410795
C	-1.116304	1.492626	0.588009
C	4.840831	-1.536817	0.397355
C	3.917755	-2.570594	0.179674
C	2.567383	-2.363272	0.453401
C	2.054463	-1.140547	0.947765
C	3.024763	-0.127198	1.137241
B	1.013803	-1.367285	2.671289
O	1.872733	-0.906053	3.680362
C	2.836837	-1.773708	4.246929
O	0.639420	-2.715385	2.745503

C	-0.509960	-3.197449	2.084803	C	-0.718137	-0.825315	-3.597598
H	-4.746302	-0.749832	2.589998	H	-1.793258	-0.684905	-3.765397
H	-2.350141	-0.276311	2.347176	H	-0.373371	-1.637070	-4.244173
H	-3.180833	2.468452	-0.852317	H	-0.972163	2.017192	-0.353991
H	-5.505577	2.803954	-1.623712	C	-0.525739	2.346610	1.677171
H	-7.919941	2.314706	-1.407060	C	0.667715	3.064878	1.428512
H	-8.728197	0.715228	0.329148	C	-1.089832	2.483578	2.964679
H	-7.113705	-0.389703	1.847829	C	1.261156	3.863733	2.403460
H	4.285066	-3.529857	-0.176965	H	1.133296	2.989276	0.450710
H	2.718325	0.829865	1.554711	C	-0.489676	3.281664	3.946820
H	3.296676	-1.251032	5.092462	C	-2.024972	1.984870	3.198870
H	3.619468	-2.022532	3.516386	C	0.690125	3.975948	3.677508
H	2.377382	-2.704589	4.601479	H	2.177908	4.400583	2.168629
H	-0.551995	-4.281707	2.234661	H	-0.958343	3.361574	4.925167
H	-0.476784	-2.990844	1.007718	H	1.155590	4.594330	4.440572
H	-1.426433	-2.748712	2.491950				
H	1.892491	-3.205578	0.324931	ng			
C	4.389882	-0.302333	0.884932	SCF done: -2427.594345			
H	5.080564	0.512002	1.081070	C	1.525959	5.160642	-1.741130
O	6.148797	-1.832622	0.119117	C	2.250954	4.765856	-2.869104
C	7.140900	-0.855231	0.398057	C	2.123771	3.448932	-3.324961
H	8.094512	-1.314757	0.130524	C	1.291992	2.543552	-2.662550
H	6.993211	0.051751	-0.203569	C	0.541529	2.918734	-1.527666
H	7.149674	-0.587086	1.462689	C	0.683964	4.253546	-1.091720
H	0.065482	0.400255	2.962512	Ni	0.331885	0.107053	-0.139249
N	0.376088	0.843751	-2.370388	O	0.228092	-0.565148	-2.206567
N	-0.478101	-1.156837	-2.175569	C	-0.375450	1.985764	-0.796389
C	0.089943	-0.142135	-1.469187	C	-0.213249	-4.616657	0.508115
C	-0.858674	-2.476466	-1.741652	C	1.094120	-4.137536	0.363210
C	0.068808	-3.527757	-1.910122	C	1.332164	-2.762503	0.277564
C	-2.181305	-2.740609	-1.339959	C	0.301090	-1.803770	0.333088
C	-0.316847	-4.821896	-1.545066	C	-0.998502	-2.326382	0.479359
C	-2.518580	-4.054341	-0.985473	B	0.646425	-1.773111	-2.778504
C	-1.599586	-5.104568	-1.059289	O	-0.322021	-2.599748	-3.258997
H	0.401858	-5.632156	-1.654801	C	0.003047	-3.849802	-3.864764
H	-3.535090	-4.257221	-0.652988	O	1.963959	-2.066432	-2.939861
C	1.203343	2.007971	-2.192153	C	3.014586	-1.173817	-2.574855
C	2.607073	1.847742	-2.141086	H	2.681647	3.121629	-4.200414
C	0.630143	3.291746	-2.247200	H	1.227017	1.520242	-3.016581
C	3.403836	2.989074	-2.020175	H	0.110930	4.588677	-0.229611
C	1.474704	4.406908	-2.135954	H	1.911467	-4.853420	0.311652
C	2.857398	4.280314	-1.997692	H	-1.853772	-1.654332	0.526111
H	4.484279	2.867558	-1.966905	H	-0.925609	-4.262488	-4.267028
H	1.029446	5.400227	-2.159140	H	0.416560	-4.538131	-3.120051
C	3.250689	0.491176	-2.297289	H	0.729101	-3.719117	-4.674953
H	4.333296	0.561215	-2.163577	H	3.947762	-1.613960	-2.935959
H	2.873195	-0.233036	-1.573875	H	3.067795	-1.052240	-1.489957
H	3.070511	0.086694	-3.302634	H	2.875641	-0.190730	-3.036263
C	3.744450	5.493631	-1.837178	H	2.364888	-2.445681	0.156620
H	4.025664	5.639807	-0.785544	C	-1.269987	-3.701618	0.564683
H	4.673933	5.389312	-2.409078	H	-2.298706	-4.034440	0.664314
H	3.240150	6.406479	-2.171626	O	-0.353860	-5.984236	0.580048
C	-0.848912	3.530576	-2.455558	C	-1.659402	-6.516168	0.728335
H	-1.016709	4.096899	-3.381050	H	-1.538342	-7.601014	0.767049
H	-1.416118	2.600238	-2.519171	H	-2.132167	-6.169840	1.658146
H	-1.269758	4.123035	-1.634585	H	-2.302179	-6.251929	-0.122841
C	1.419833	-3.303483	-2.549204	H	-0.708575	-0.394481	-2.419019
H	1.908862	-2.398229	-2.186894	N	0.130005	1.294193	2.567713
H	2.087400	-4.147600	-2.351238	N	2.186783	0.923932	1.917610
H	1.323552	-3.218214	-3.641459	C	0.882318	0.768347	1.555135
C	-1.975052	-6.503421	-0.627754	C	3.372086	0.397018	1.293813
H	-1.486198	-7.261157	-1.250700	C	3.862588	-0.850973	1.738833
H	-1.668047	-6.688805	0.410520	C	4.117764	1.186898	0.400251
H	-3.057358	-6.663328	-0.682646	C	5.053460	-1.334252	1.186889
C	-3.252857	-1.680147	-1.362253	C	5.303805	0.655519	-0.128618
H	-2.861541	-0.686541	-1.146191	C	5.781845	-0.605068	0.237374
H	-3.734081	-1.644795	-2.350470	H	5.426845	-2.302441	1.516217
H	-4.036693	-1.895117	-0.631042	H	5.872951	1.258186	-0.834312
C	0.077642	0.465637	-3.770865	C	-1.288035	1.185975	2.790798
H	1.013125	0.316828	-4.324525	C	-1.814089	-0.017961	3.319476
H	-0.488580	1.258287	-4.268536	C	-2.107178	2.320819	2.646562

C	-3.184357	-0.086197	3.583654	C	-0.368097	1.924286	-1.431981
C	-3.475717	2.202516	2.937289	O	0.881065	5.249741	-2.272357
C	-4.038560	1.009027	3.388338	C	1.853933	6.183013	-1.839705
H	-3.592992	-1.015895	3.976141	C	-2.991050	2.026970	1.629192
H	-4.111817	3.076197	2.805506	C	-4.338741	2.254332	1.246797
C	-0.927469	-1.188222	3.675024	C	-5.039986	1.234461	0.524338
H	-1.532529	-2.057989	3.948096	C	-4.335438	0.042649	0.203382
H	-0.279775	-1.482360	2.847753	C	-3.024610	-0.139967	0.584021
H	-0.290794	-0.949414	4.538209	C	-5.025941	3.460959	1.562448
C	-5.516797	0.897396	3.684850	C	-6.339465	3.648225	1.186042
H	-6.021749	1.862223	3.571613	C	-7.031994	2.636208	0.472003
H	-6.006185	0.185007	3.008162	C	-6.392603	1.456948	0.148705
H	-5.692679	0.541797	4.707885	H	-0.505670	1.675594	2.093519
C	-1.582070	3.676006	2.227659	H	0.915964	0.954527	3.726828
H	-1.803357	4.423762	3.000310	H	1.872040	-0.798164	5.172044
H	-0.504110	3.671556	2.056742	H	1.128189	-3.173214	4.933913
H	-2.064396	4.014785	1.303128	H	-0.572374	-3.748951	3.213974
C	3.168761	-1.631201	2.830913	H	-1.574839	-2.004894	1.808360
H	2.096839	-1.726482	2.647926	H	2.146877	2.112909	0.832991
H	3.586721	-2.639411	2.910042	H	2.433558	4.296498	-0.205321
H	3.301176	-1.145567	3.808188	H	-1.194674	1.300323	-1.762154
C	7.048693	-1.169298	-0.364762	H	1.729877	7.063058	-2.474869
H	6.820931	-1.921199	-1.132409	H	2.873888	5.790210	-1.960133
H	7.650443	-0.386462	-0.838697	H	1.700687	6.468290	-0.789291
H	7.668442	-1.661250	0.394196	H	-2.474981	2.811679	2.179586
C	3.726132	2.604457	0.068093	H	-4.843463	-0.730034	-0.370723
H	2.646900	2.751656	0.078920	H	-2.514981	-1.043769	0.267332
H	4.168519	3.301969	0.794286	H	-4.494520	4.237659	2.108581
H	4.089919	2.895734	-0.921118	H	-6.850010	4.575365	1.435084
C	0.940584	1.758582	3.715997	H	-8.067252	2.794602	0.180164
H	0.798565	1.086077	4.571268	H	-6.919154	0.678551	-0.400608
H	0.630857	2.763250	4.019013	C	-0.209140	3.171511	-2.041515
C	2.361188	1.711038	3.156364	H	-0.876246	3.495729	-2.836718
H	2.749800	2.707675	2.910863	N	0.828921	-2.293720	-1.577591
H	3.074153	1.221982	3.826387	N	2.671016	-1.261043	-1.044292
H	-0.669504	2.456173	0.140077	C	1.348432	-1.338985	-0.763762
C	-1.629460	1.564528	-1.500917	C	3.658738	-0.482505	-0.350740
C	-2.696290	1.026014	-0.776009	C	4.218159	0.636886	-0.992019
C	-1.809042	1.658123	-2.922344	C	4.118195	-0.908674	0.912094
C	-3.896394	0.580871	-1.383860	C	5.232424	1.341792	-0.329489
H	-2.612350	0.942506	0.304133	C	5.126738	-0.166619	1.535491
C	-2.964399	1.233031	-3.544419	C	5.696876	0.962925	0.933256
H	-1.023003	2.099406	-3.525700	H	5.661665	2.216191	-0.814923
C	-4.043387	0.677503	-2.807265	H	5.482948	-0.486106	-2.513578
H	-3.061550	1.331212	-4.624352	C	-0.538679	-2.726740	-1.629861
H	2.899253	5.469968	-3.384920	C	-1.429334	-2.146316	-2.550389
H	1.603954	6.181547	-1.372480	C	-0.936000	-3.809117	-0.815792
C	-5.246285	0.227741	-3.415560	C	-2.745947	-2.628777	-2.595222
H	-5.347860	0.305874	-4.496409	C	-2.258629	-4.254297	-0.896787
C	-4.972151	0.029978	-0.627022	C	-3.183922	-3.671073	-1.774223
H	-4.863150	-0.044963	0.452771	H	-3.444088	-2.172104	-3.294325
C	-6.127054	-0.399420	-1.245651	C	-2.573249	-5.083406	-0.265053
H	-6.937723	-0.818107	-0.653700	H	-0.994475	-1.063872	-3.510584
C	-6.268935	-0.300537	-2.654957	H	-1.843550	-0.435933	-3.799037
H	-7.184828	-0.642219	-3.130522	H	-0.226480	-0.416215	-3.082822
				H	-0.590088	-1.501621	-4.434361
				C	-4.613605	-4.160460	-1.822893
ng				H	-4.660071	-5.253705	-1.898121
SCF done:	-2096.557955			H	-5.160614	-3.876078	-0.914246
C	-2.313071	0.850610	1.331780	H	-5.151641	-3.740079	-2.678964
Ni	0.301640	-0.202675	0.471938	C	0.049356	-4.503200	0.095843
C	-0.892171	0.712296	1.761084	H	0.839863	-5.004421	-0.478508
C	-0.402510	-0.368713	2.630743	H	0.539139	-3.802107	0.777357
C	0.597500	-0.078392	3.606879	H	-0.453046	-5.268812	0.695884
C	1.133109	-1.064151	4.419412	C	3.747431	1.088405	-2.354657
C	0.717248	-2.402968	4.286401	H	2.655504	1.133411	-2.403467
C	-0.230775	-2.722140	3.321408	H	4.135128	2.085529	-2.582803
C	-0.779639	-1.728507	2.490829	H	4.094552	0.414419	-3.150240
C	0.480298	1.484711	-0.397545	C	6.783808	1.745013	1.636147
C	1.473365	2.381615	0.021403	H	6.411131	2.199765	2.563208
C	1.646518	3.644347	-0.571999	H	7.627746	1.099471	1.910358
C	0.803767	4.040233	-1.615542				

H	7.170003	2.550522	1.002686	C	-0.635746	-2.877918	-1.297941
C	3.552739	-2.137625	1.584714	C	-1.391450	-2.327293	-2.349189
H	2.518072	-1.983147	1.907519	C	-1.210569	-3.793295	-0.392127
H	3.556297	-3.006096	0.914759	C	-2.741275	-2.691052	-2.461840
H	4.141910	-2.396870	2.470080	C	-2.561524	-4.122764	-0.542005
C	1.805561	-2.854464	-2.537342	C	-3.345514	-3.583373	-1.570959
H	1.563042	-2.526396	-3.555855	H	-3.332352	-2.261336	-3.268708
H	1.782868	-3.948772	-2.516820	H	-3.012818	-4.822068	0.160228
C	3.127878	-2.267683	-2.030222	C	-0.773889	-1.374765	-3.346404
H	3.760164	-3.014400	-1.532216	H	-1.549395	-0.871505	-3.932739
H	3.718384	-1.797615	-2.821315	H	-0.169108	-0.609629	-2.851432

N_{TS10}

SCF done: -2096.530424

C	-2.307095	1.310867	0.936254
Ni	0.406898	-0.239198	0.571403
C	-0.854978	1.354671	1.325562
C	-0.375982	0.406572	2.383522
C	0.580964	0.864546	3.338976
C	1.051682	0.043067	4.350672
C	0.602001	-1.288819	4.457570
C	-0.309266	-1.771614	3.528270
C	-0.789690	-0.954863	2.482095
C	0.238623	1.598122	-0.198791
C	1.393287	2.369504	0.058847
C	1.886876	3.311989	-0.849252
C	1.214107	3.532852	-2.057911
C	-0.427613	1.863236	-1.418414
O	1.602161	4.437185	-3.019440
C	2.720990	5.264248	-2.749891
C	-3.124566	2.372300	1.288970
C	-4.510928	2.395513	0.980684
C	-5.083525	1.288987	0.272402
C	-4.228928	0.216218	-0.100937
C	-2.888560	0.227037	0.215789
C	-5.353431	3.481507	1.350799
C	-6.696680	3.473279	1.038880
C	-7.262578	2.376650	0.338400
C	-6.471539	1.310316	-0.035691
H	-0.626173	2.360507	1.670487
H	0.916135	1.898296	3.287854
H	1.759743	0.436980	5.076360
H	0.958443	-1.924968	5.263672
H	-0.679866	-2.790969	3.609715
H	-1.609192	-1.324741	1.875713
H	1.929397	2.236931	0.996318
H	2.788831	3.861097	-0.598310
H	-1.346976	1.338120	-1.658618
H	2.828170	5.916393	-3.619396
H	3.640221	4.674795	-2.624285
H	2.560464	5.877096	-1.851930
H	-2.702807	3.220609	1.825779
H	-4.645064	-0.621980	-0.655685
H	-2.253779	-0.591352	-0.112107
H	-4.918682	4.322205	1.887501
H	-7.328130	4.309439	1.328773
H	-8.322660	2.381122	0.097449
H	-6.902107	0.468106	-0.573794
C	0.052018	2.798751	-2.332672
H	-0.472848	2.982192	-3.266931
N	0.760802	-2.577199	-1.189280
N	2.651799	-1.598488	-0.727205
C	1.308193	-1.524752	-0.515582
C	3.650412	-0.737195	-0.163400
C	4.209291	0.272183	-0.969436
C	4.116995	-0.966418	1.144939
C	5.236630	1.059324	-0.435227
C	5.141404	-0.148753	1.638124
C	5.713592	0.869697	0.866830
H	5.672773	1.841881	-1.054028
H	5.505647	-0.319408	2.649890

C	-4.802135	-3.965975	-1.710154
H	-4.917258	-5.045790	-1.869924
H	-5.370167	-3.712569	-0.805882
H	-5.271479	-3.452395	-2.555862
C	-0.385709	-4.420031	0.707713
H	0.370493	-5.105526	0.301909
H	0.145728	-3.662116	1.291064
H	-1.020723	-4.998896	1.386520
C	3.710959	0.514100	-2.374534
H	2.627668	0.669116	-2.388509
H	4.184163	1.401771	-2.805492
H	3.932443	-0.331067	-3.039885
C	6.802183	1.754276	1.432478
H	7.404868	1.222304	2.177259
H	7.475312	2.114798	0.646440
H	6.377293	2.637753	1.928822
C	3.534746	-2.061923	2.006701
H	2.487874	-1.858116	2.255991
H	3.563660	-3.036098	1.502979
H	4.093892	-2.153535	2.943415
C	1.737793	-3.371395	-1.963953
H	1.579577	-3.228353	-3.040909
C	1.630730	-4.439446	-1.745615
H	3.076613	-2.793485	-1.487054
H	3.623370	-3.484801	-0.831649
H	3.740857	-2.516831	-2.311819

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SCF done: -2086.013294

C	2.316408	2.288800	1.667479
Ni	0.112892	-0.374795	0.372255
C	0.830560	2.139722	1.999516
C	0.344176	0.672491	2.072680
C	1.034885	0.333012	1.882517
C	1.603482	-0.831989	2.531134
C	0.751910	-1.731252	3.249852
C	0.653697	-1.443731	3.309542
C	1.167521	-0.295767	2.764324
C	0.032416	3.001514	1.068894
C	0.243431	3.137390	-0.293851
C	0.573204	3.908347	-1.126051
C	1.695520	4.556591	-0.603518
C	1.153652	3.673017	1.583334
O	2.575714	5.341289	-1.338220
C	2.334286	5.474586	-2.768943
C	3.060692	3.293998	2.302384
C	4.407064	3.493562	1.995850
C	5.035390	2.684137	1.046047
C	4.306703	1.677108	0.410223
C	2.957954	1.481267	0.718065
H	0.695146	2.550831	3.012412
H	1.726039	1.086600	1.516968
H	1.305502	-2.143885	3.823570
H	2.225441	-0.077941	2.868434
H	1.118470	2.653301	-0.709470
H	0.319210	4.000392	-2.173726
H	1.382535	3.592993	2.641269
H	3.141126	6.110725	-3.134502
H	1.367954	5.950536	-2.977211

H	2.371185	4.502749	-3.277885	C	2.114610	1.266221	-1.247089
H	2.576447	3.926056	3.039930	C	1.160254	0.412667	-0.621824
H	4.777359	1.029126	-0.319181	C	1.601652	-0.702023	0.059336
H	2.401339	0.683949	0.232760	C	3.459689	-2.158307	0.850630
C	1.977768	4.434753	0.763359	C	4.808958	-2.436951	0.925019
H	2.843362	4.953417	1.154410	C	5.751411	-1.581508	0.300088
N	1.037969	-1.847431	-1.985821	C	5.324988	-0.463649	-0.387021
N	1.150365	-1.710082	-1.892366	C	-0.306434	0.785601	-0.744864
C	0.003466	-1.352158	-1.238056	O	-2.596751	-0.036687	-1.964544
C	2.494069	-1.362392	-1.517649	C	-2.264273	-0.587145	-0.920737
C	3.042801	-0.135534	-1.930612	O	-1.112523	-0.307351	-0.234613
C	3.267511	-2.289420	-0.800936	N	-2.979006	-1.553806	-0.296554
C	4.379688	0.141291	-1.630839	C	-2.617398	-2.209485	0.969453
C	4.605706	-1.985611	-0.528095	C	-3.665658	-3.328504	1.091894
C	5.178420	-0.779099	-0.941714	C	-4.893016	-2.756499	0.358338
H	4.802837	1.091941	-1.939751	C	-4.278297	-1.993344	-0.824983
H	5.202640	-2.698514	0.031224	C	-0.681224	2.067731	-0.009934
C	2.424229	-1.830802	-1.613519	C	-0.211282	2.327340	1.285742
C	3.301952	-0.959368	-2.283744	C	-0.598894	3.486184	1.961179
C	2.910073	-2.730823	-0.646313	C	-1.456570	4.404764	1.345508
C	4.669294	-1.015221	-1.993968	C	-1.926251	4.155079	0.053381
C	4.281277	-2.746843	-0.369283	C	-1.541985	2.990631	-0.619309
C	5.174133	-1.902561	-1.036439	H	4.176940	1.651450	-1.666097
H	5.348508	-0.353275	-2.522838	H	1.767717	2.146798	-1.783169
H	4.658176	-3.438717	0.377157	H	0.883614	-1.364369	0.532643
C	2.765146	0.043040	-3.287915	H	2.735636	-2.814891	1.328593
H	3.552023	0.739128	-3.591735	H	5.154686	-3.315919	1.463207
H	1.940784	0.612699	-2.846629	H	6.812028	-1.810707	0.364234
H	2.384152	-0.454295	-4.188273	H	6.045624	0.194249	-0.868319
C	6.655480	-1.920482	-0.702360	H	-0.559800	0.905584	-1.801855
H	6.964651	-2.906888	-0.342284	H	-2.682511	-1.496563	1.802667
H	6.876998	-1.189120	0.085843	H	-1.592182	-2.589701	0.933596
H	7.260279	-1.666837	-1.579148	H	-3.869458	-3.592416	2.134496
C	1.964838	-3.648895	0.102036	H	-3.309540	-4.231783	0.580595
H	1.294186	-4.177272	-0.583831	H	-5.433407	-2.060945	1.012945
H	1.341549	-3.061353	0.786743	H	-5.598265	-3.528416	0.034654
H	2.526573	-4.387299	0.681516	H	-4.134226	-2.643126	-1.699472
C	2.182923	0.883693	-2.649640	H	-4.868124	-1.130536	-1.146580
H	1.382575	1.227349	-1.985226	H	0.465607	1.623471	1.763228
H	2.782471	1.749798	-2.945082	H	-0.226624	3.676400	2.964884
H	1.721077	0.456621	-3.547494	H	-1.753558	5.309909	1.869502
C	6.641692	-0.476655	-0.667068	H	-2.592759	4.863692	-0.432041
H	7.257799	-0.727699	-1.540417	H	-1.922442	2.786112	-1.616829
H	6.787805	0.586132	-0.446930				
H	7.009940	-1.058956	0.183503				
C	2.640812	-3.570205	-0.287592	arylboronic ester(OMe)			
H	1.804434	-3.328531	0.376703	SCF done: -601.405446			
H	2.259563	-4.189386	-1.108303	C	2.415339	0.202248	-0.088036
H	3.371048	-4.153999	0.278357	C	1.633459	1.307414	-0.458083
C	0.606849	-2.676000	-3.165188	C	0.245748	1.215483	-0.437027
H	1.098070	-2.329908	-4.076873	C	-0.422237	0.028340	-0.062690
H	0.864733	-3.725846	-2.991710	C	0.391606	-1.065926	0.283943
C	0.922032	-2.442822	-3.185736	B	-1.982062	-0.151159	-0.056748
H	1.490978	-3.375022	-3.197768	O	-2.452028	-1.426515	-0.239830
H	1.235594	-1.816306	-4.026656	C	-3.845864	-1.721662	-0.201224
H	6.082858	2.834107	0.809269	O	-2.926640	0.828245	0.127874
H	4.964781	4.275462	2.499273	C	-2.699950	2.174640	0.516769
C	1.319678	-2.860616	3.883437	H	2.134490	2.222872	-0.759532
H	0.666936	-3.537821	4.426082	H	-0.081039	-2.005690	0.556567
C	2.993159	-1.094107	2.499001	H	-3.951329	-2.799226	-0.353901
H	3.637779	-0.416923	1.949695	H	-4.382974	-1.186949	-0.992669
C	3.524853	-2.203532	3.135794	H	-4.281525	-1.444561	0.765682
H	4.592966	-2.387718	3.100476	H	-3.593621	2.518163	1.046781
C	2.683295	-3.096149	3.830142	H	-2.552649	2.809771	-0.365265
H	3.106503	-3.961575	4.327770	H	-1.831849	2.267120	1.178640
				H	-0.323039	2.088851	-0.743608
				C	1.787588	-0.993734	0.286175
				H	2.366122	-1.865962	0.570705
				O	3.767669	0.388885	-0.128974
				C	4.617104	-0.695307	0.223212
				H	5.636290	-0.319433	0.116979
				H	4.450961	-1.011792	1.261308

Substrate(OMe)			
SCF done: -1056.244896			
C	2.988486	-1.013087	0.151128
C	3.941767	-0.149892	-0.479973
C	3.460845	0.992617	-1.179590

H 4.471703 -1.551273 -0.448739

(dimethyl boric)pyrrolidine-1-carboxylic anhydride (OMe)

SCF done: -655.847877

O 0.596242 0.471776 0.096574
N -1.593734 -0.081530 0.186174
C -0.357250 -0.334368 0.674611
O -0.103513 -1.132890 1.562757
C -2.774029 -0.760104 0.740750
C -3.946164 0.006101 0.108182
C -3.379005 0.474701 -1.244844
C -1.920170 0.834813 -0.917199
B 1.904113 0.043930 -0.139824
O 2.117765 -1.206106 -0.621892
C 3.437664 -1.698323 -0.846624
O 2.936228 0.920375 0.022658
C 2.740971 2.225110 0.567341
H -2.758654 -0.716176 1.833704
H -2.771757 -1.819754 0.451396
H -4.207143 0.873396 0.728005
H -4.842150 -0.614259 0.006828
H -3.928133 1.318389 -1.674900
H -3.406133 -0.348631 -1.969738
H -1.240990 0.684963 -1.761007
H -1.825983 1.879660 -0.589766
H 3.337602 -2.700023 -1.271645
H 3.994807 -1.757017 0.094828
H 3.984499 -1.054957 -1.544819
H 3.730901 2.668371 0.701544
H 2.228595 2.175662 1.533941
H 2.154236 2.848614 -0.116555

K[ArB(OCH₃)₂(OH)] (Ar=p-OMePh)

SCF done: -705.402969

C -3.466229 -0.034529 0.298860
C -2.726781 0.846294 1.105328
C -1.363090 1.005471 0.889439
C -0.674600 0.290227 -0.115995
C -1.440492 -0.593201 -0.896676
B 0.867566 0.441414 -0.360161
O 1.725089 -0.590595 -0.584937
C 1.544339 -1.991067 -0.273364
O 1.540262 1.658629 -0.378545
C 0.915051 2.937896 -0.429797
H -3.242532 1.390488 1.891171
H -0.958126 -1.173858 -1.679710
H 2.481806 -2.317172 0.206512
H 1.376357 -2.533735 -1.210059
H 0.685632 -2.128858 0.391233
H 0.882987 3.382673 0.571949
H -0.102798 2.876709 -0.826957
H 1.516975 3.580170 -1.080744
H -0.818930 1.692328 1.534099
C -2.817369 -0.755852 -0.712494
H -3.362685 -1.443419 -1.349600
O -4.798284 -0.118306 0.577295
C -5.604513 -1.000283 -0.195115
H -6.614380 -0.906024 0.207412
H -5.604993 -0.713988 -1.254897
H -5.266105 -2.039557 -0.094748
K 4.213872 0.251109 0.046412
O 4.477115 -1.966263 0.918086
H 4.874044 -2.741346 1.336996

potassium pyrrolidine-1-carboxylate

SCF done: -428.791561

O -1.072649 -1.132124 0.082452
N 0.899087 -0.000519 -0.022755
C -0.481451 -0.000066 -0.007792
O -1.074210 1.131979 -0.087158

C 1.703602 1.219079 -0.078761
C 3.118592 0.725390 0.272038
C 3.125898 -0.724656 -0.246789
C 1.702639 -1.218497 0.066588
H 1.320240 1.970005 0.619661
H 1.672123 1.666819 -1.084849
H 3.258596 0.732683 1.361312
H 3.904973 1.347833 -0.169667
H 3.900356 -1.346875 0.215804
H 3.294470 -0.732081 -1.331982
H 1.341873 -1.975684 -0.637210
H 1.642214 -1.658762 1.074708
K -3.393119 -0.000349 0.006181

Product (S)

SCF done: -1001.844069

C 1.156387 4.418983 -0.601664
C 0.454024 4.827270 0.536257
C -0.310212 3.898244 1.242876
C -0.376808 2.568268 0.816303
C 0.326110 2.149801 -0.318980
C 1.093164 3.091229 -1.022295
C 0.307738 0.694411 -0.809680
C 3.944910 -1.491450 0.178701
C 3.567342 -0.376385 0.938934
C 2.419620 0.340319 0.621257
C 1.609638 -0.039066 -0.460359
C 1.995851 -1.152434 -1.213039
H -0.861644 4.206366 2.124029
H -0.984196 1.853745 1.357310
H 1.647476 2.775388 -1.900185
H 4.198348 -0.090680 1.770351
H 1.382143 -1.469415 -2.050132
H 2.149643 1.210038 1.207262
C 3.149888 -1.874889 -0.905812
H 3.416257 -2.728358 -1.514618
O 5.107882 -2.132798 0.577284
C 5.538967 -3.300623 -0.182811
H 6.455029 -3.632860 0.306294
H 4.791799 -4.103174 -0.150791
H 5.750723 -3.048030 -1.229120
H 0.234310 0.727056 -1.905002
C -0.920821 -0.070284 -0.299580
C -2.104112 -0.022272 -1.007951
C -0.873782 -0.806670 0.916891
C -3.273896 -0.687707 -0.551474
H -2.157486 0.539340 -1.936144
C -1.988978 -1.457009 1.392590
H 0.064461 -0.859817 1.454796
C -3.218704 -1.421747 0.679422
H -1.940913 -2.016534 2.321125
H 0.500434 5.859240 0.864443
H 1.750179 5.134242 -1.159516
C -4.388508 -2.089081 1.136876
H -4.340906 -2.644135 2.067967
C -4.499714 -0.650545 -1.273704
H -4.539482 -0.093367 -2.203878
C -5.614482 -1.305919 -0.802649
H -6.543431 -1.270288 -1.359930
C -5.558710 -2.032840 0.414270
H -6.445268 -2.544017 0.771194

Product (R)

SCF done: -1001.843069

C -1.051794 0.285900 -0.220954
C 0.333888 0.694549 -0.731052
C 0.677486 2.146658 -0.368750
C 0.060004 3.187005 -1.082133
C 0.318892 4.524128 -0.776106
C 1.205042 4.848011 0.257272
C 1.827499 3.822626 0.972438

C	1.567937	2.483192	0.659162
C	1.434776	-0.302068	-0.353289
C	2.557573	-0.422513	-1.179883
C	3.609672	-1.294820	-0.880530
C	3.547243	-2.076921	0.280024
C	1.389915	-1.101425	0.800429
O	4.512802	-2.963209	0.673477
C	5.669315	-3.110342	-0.138103
C	-1.856474	-0.527150	-0.997192
C	-3.138619	-0.957152	-0.559622
C	-3.609924	-0.533656	0.725984
C	-2.771366	0.305350	1.509322
C	-1.535256	0.706303	1.050271
C	-3.973088	-1.791066	-1.355675
C	-5.213155	-2.189021	-0.902531
C	-5.678966	-1.769249	0.370310
C	-4.894113	-0.959790	1.164408
H	0.267276	0.667463	-1.826738
H	-0.635777	2.943677	-1.883116
H	-0.168768	5.312490	-1.344532
H	1.410208	5.888186	0.497578
H	2.522310	4.060979	1.774314
H	2.071675	1.696535	1.213687
H	2.623702	0.182028	-2.082739
H	4.456853	-1.354959	-1.554844
H	0.527848	-1.052546	1.459361
H	6.292125	-3.852920	0.364048
H	6.223009	-2.165442	-0.220528
H	5.410176	-3.471141	-1.142543
H	-1.505099	-0.859009	-1.973361
H	-3.123960	0.638046	2.483499
H	-0.923218	1.364110	1.660994
H	-3.614967	-2.112704	-2.331399
H	-5.839738	-2.827212	-1.520449
H	-6.658480	-2.088671	0.716895
H	-5.249219	-0.635858	2.140545
C	2.427860	-1.974417	1.118041
H	2.385547	-2.592173	2.010480