

Exploring the Mechanism of Grignard Methathesis

Polymerization of Poly-3-alkylthiophenes

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58		H	4.564054	0.654972	-1.031014
		C	2.747173	3.886665	0.135563
NiCl2 SCF Done: -2817.54367747 A.U.		H	1.028742	2.629638	0.486458
Ni	-0.010775	-0.129906	1.001384		
		C	4.082860	3.942193	-0.272611
P	1.720799	-0.062929	-0.407424		
		H	5.777653	2.808897	-0.999247
P	-1.674300	-0.082605	-0.486805		
		H	2.240109	4.790799	0.481574
C	1.329182	-0.129211	-2.235655		
		H	4.623527	4.891915	-0.253176
H	1.184997	-1.187819	-2.506551		
		C	2.902796	-1.481460	-0.240245
H	2.220256	0.227722	-2.773535		
		C	3.042222	-2.157514	0.985014
C	0.103935	0.686117	-2.661649		
		C	3.658480	-1.925474	-1.344046
H	0.135584	0.804455	-3.758257		
		C	3.915053	-3.243428	1.098755
H	0.166707	1.708894	-2.252918		
		H	2.478541	-1.815182	1.854177
C	-1.227570	0.013904	-2.302533		
		C	4.532864	-3.008743	-1.222793
H	-1.209422	-1.030643	-2.653250		
		H	3.577996	-1.433852	-2.314399
H	-2.066507	0.500483	-2.823890		
		C	4.662530	-3.672822	-0.000223
C	2.697774	1.498244	-0.309396		
		H	4.007600	-3.755034	2.060062
C	4.040772	1.559580	-0.713333		
		H	5.111832	-3.334317	-2.090887
C	2.058772	2.670834	0.125873		
		H	5.343283	-4.522888	0.093647
C	4.729071	2.775949	-0.692390		

C	-2.703709	1.429149	-0.225869	H	-3.418118	-2.099604	1.464233
C	-3.690016	1.447718	0.777041	H	-3.837910	-1.755523	3.136404
C	-2.489450	2.592136	-0.986317	C	-1.750128	-1.498550	2.723515
C	-4.448606	2.598652	0.998541	H	-1.553382	-2.474245	3.194330
H	-3.846090	0.564505	1.396450	H	-1.535687	-0.732856	3.486331
C	-3.245683	3.745303	-0.754298	Cl	-0.759642	2.207356	-1.349456
H	-1.729212	2.617905	-1.768178	C	1.083926	-1.554799	2.275956
C	-4.229141	3.750817	0.237136	C	1.301288	-0.898790	3.499721
H	-5.212592	2.594914	1.779940	C	2.109760	-2.350834	1.741275
H	-3.062821	4.640243	-1.354478	C	2.510103	-1.052431	4.183323
H	-4.821594	4.651262	0.418210	H	0.535138	-0.248510	3.928048
C	-2.851858	-1.495913	-0.515098	C	3.318070	-2.500457	2.425938
C	-4.085678	-1.384509	-1.178178	H	1.975562	-2.842179	0.776477
C	-2.484414	-2.725522	0.053439	C	3.520901	-1.856604	3.649680
C	-4.936875	-2.488792	-1.273253	H	2.662448	-0.536354	5.134703
H	-4.394207	-0.430477	-1.613107	H	4.108343	-3.117907	1.992144
C	-3.335658	-3.828848	-0.050543	H	4.467685	-1.974512	4.182719
H	-1.545416	-2.810384	0.602689	C	-3.601797	2.472438	0.519628
C	-4.561843	-3.713116	-0.711857	C	-4.891683	2.813540	0.084943
H	-5.897749	-2.389747	-1.784761	C	-2.804611	3.450123	1.137254
H	-3.043007	-4.780041	0.400882	C	-5.379425	4.110646	0.272599
H	-5.229488	-4.575600	-0.783754	H	-5.518761	2.070305	-0.412856
Cl	-1.608475	-0.542615	2.486562	C	-3.298184	4.742052	1.330914
Cl	1.486330	0.292516	2.586116	H	-1.785064	3.207605	1.444225

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NiCl-3BTanti-I SCF Done: -5640.02303209 A.U.

Ni	-0.676188	0.510151	0.078329	H	-6.382954	4.367047	-0.076733
P	-2.953978	0.752321	0.382296	H	-2.666385	5.496270	1.806721
P	-0.491695	-1.288930	1.355667	H	-4.966081	6.090275	1.040631
C	-3.677605	0.019006	1.936547	C	-0.743669	-2.825921	0.367598
H	-4.775916	0.079478	1.881010	C	-0.663343	-4.100089	0.959248
H	-3.380084	0.718973	2.735486	C	-1.065206	-2.727404	-0.995010
C	-3.218990	-1.401021	2.294210	C	-0.904327	-5.247872	0.202224
				H	-0.397786	-4.203073	2.014485

C	-1.308389	-3.878580	-1.751432
H	-1.124523	-1.745602	-1.470069
C	-1.228795	-5.138485	-1.155046
H	-0.835112	-6.232114	0.672484
H	-1.557992	-3.784319	-2.810830
H	-1.415921	-6.038278	-1.746696
C	-3.913749	-0.022699	-0.995441
C	-5.004697	-0.883130	-0.782295
C	-3.516868	0.253910	-2.318532
C	-5.683515	-1.454616	-1.863913
H	-5.343213	-1.119070	0.227634
C	-4.203147	-0.313414	-3.394658
H	-2.667216	0.918706	-2.495667
C	-5.285946	-1.170465	-3.172324
H	-6.528400	-2.122940	-1.678527
H	-3.884928	-0.083757	-4.414811
H	-5.818280	-1.616000	-4.016703
C	2.240256	1.010026	0.380069
C	3.551072	0.759374	-0.161401
C	1.200218	0.370678	-0.253386
C	3.473226	-0.101972	-1.230652
S	1.832210	-0.584160	-1.572805
Br	4.906059	-0.745895	-2.288490
H	2.095698	1.670199	1.239537
C	4.808360	1.400751	0.365329
C	5.084993	2.793823	-0.227838
H	5.670868	0.744760	0.160781
H	4.731827	1.484976	1.463805
C	6.348722	3.453205	0.332182
H	5.168538	2.704589	-1.325267
H	4.212943	3.446732	-0.044192
C	6.628181	4.835953	-0.258658
H	6.261292	3.532330	1.431768

H	7.215314	2.791654	0.148852
H	7.542588	5.282251	0.164899
H	6.758670	4.784425	-1.352637
H	5.795274	5.531598	-0.061069

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Ni-3BTanti-3BTanti-O SCF Done: -8462.49452658 A.U.

Ni	-0.109041	-0.985387	-0.150182
P	-1.710628	-2.573743	0.139586
P	1.660621	-2.428995	-0.287863
C	-1.274009	-4.370956	-0.141025
H	-1.299545	-4.560945	-1.225767
H	-2.073163	-4.982441	0.306141
C	0.094877	-4.781491	0.417589
H	0.143258	-5.883948	0.420705
H	0.177156	-4.478681	1.475533
C	1.284758	-4.261972	-0.404101
H	1.096798	-4.451731	-1.473519
H	2.205524	-4.811785	-0.153868
C	-2.171718	-2.600552	1.928159
C	-1.408382	-1.857567	2.843291
C	-3.232950	-3.388042	2.410154
C	-1.695130	-1.903456	4.211912
H	-0.585566	-1.234793	2.483138
C	-3.521725	-3.428825	3.775699
H	-3.848930	-3.965733	1.716129
C	-2.752256	-2.687312	4.679598
H	-1.090952	-1.318643	4.909775
H	-4.352652	-4.040809	4.136041
H	-2.980361	-2.719936	5.748062
C	-3.303518	-2.417946	-0.774118
C	-3.431396	-2.952685	-2.068025
C	-4.372753	-1.678801	-0.240930
C	-4.606825	-2.771903	-2.801029

H	-2.609294	-3.506916	-2.526406	C	-3.178858	1.910752	-1.289147
C	-5.545787	-1.497055	-0.977304	Br	-4.251468	2.914721	-2.483958
H	-4.285170	-1.228094	0.748328	H	-2.094557	0.945772	1.715435
C	-5.668619	-2.044994	-2.256713	C	-4.077171	2.847455	0.924562
H	-4.687882	-3.195544	-3.805281	C	-3.393081	4.164578	1.333425
H	-6.364591	-0.913670	-0.549314	H	-4.378717	2.301893	1.836550
H	-6.585959	-1.897916	-2.832158	H	-5.005200	3.079143	0.375883
C	2.930970	-2.326158	1.045365	C	-4.273817	5.060873	2.208652
C	3.790011	-1.212692	1.096601	H	-2.451976	3.935587	1.864652
C	3.025427	-3.298397	2.056528	H	-3.098444	4.711224	0.420407
C	4.728946	-1.089434	2.122643	C	-3.597313	6.371210	2.614548
H	3.724959	-0.436819	0.331928	H	-5.214161	5.282180	1.670980
C	3.961373	-3.166608	3.087322	H	-4.572722	4.503391	3.115708
H	2.371074	-4.171582	2.056211	H	-4.257531	6.992484	3.241278
C	4.817310	-2.063419	3.121614	H	-2.673105	6.184375	3.186813
H	5.386250	-0.216979	2.144960	H	-3.319127	6.968165	1.729850
H	4.019502	-3.933214	3.864287	C	2.626597	2.302213	-0.368030
H	5.549373	-1.960913	3.926700	C	2.447355	2.375370	0.993545
C	2.604855	-2.205427	-1.858341	C	1.846364	1.223897	-0.922795
C	3.939365	-2.619794	-1.998489	S	1.331356	1.168857	1.575245
C	1.933369	-1.676002	-2.973096	C	1.094791	0.496142	-0.025033
C	4.588493	-2.503828	-3.231112	H	1.848421	1.021258	-1.996052
H	4.480308	-3.026028	-1.140718	Br	3.256221	3.599523	2.191291
C	2.582406	-1.566369	-4.206134	C	3.529716	3.186001	-1.189158
H	0.899143	-1.335124	-2.871989	C	4.935832	2.600983	-1.412891
C	3.912046	-1.978154	-4.336382	H	3.624561	4.170318	-0.701780
H	5.628960	-2.824832	-3.327096	H	3.054864	3.366223	-2.169384
H	2.049311	-1.147704	-5.063400	C	5.837785	3.491897	-2.272164
H	4.422925	-1.885821	-5.298216	H	5.412409	2.432855	-0.430455
C	-2.232623	1.040595	0.635417	H	4.845738	1.604738	-1.883097
C	-1.490694	0.326664	-0.279606	C	7.237595	2.915069	-2.488712
C	-3.204755	1.951501	0.084355	H	5.353100	3.662937	-3.250922
S	-1.985249	0.789816	-1.892815	H	5.917864	4.488364	-1.800746

H	7.859735	3.579632	-3.109752	C	3.518689	-0.640549	3.772661
H	7.762829	2.768241	-1.529834	H	1.475904	-1.321638	3.680891
H	7.193520	1.934238	-2.991859	C	4.418872	0.389206	3.482653
				H	4.655069	2.355644	2.609651
Ni-3BTanti-3BTanti-O-Pr SCF Done: -8462.51589736 A.U.				H	3.868475	-1.553177	4.262602
Ni	-0.725385	0.259386	0.251491	H	5.474966	0.288285	3.745649
P	-0.079183	0.792996	2.308136	C	-3.928888	1.400864	-0.783852
P	-2.343719	1.775829	0.098456	C	-4.086196	1.737393	-2.140620
C	-0.466785	2.585157	2.672743	C	-4.959527	0.685798	-0.147149
H	0.018866	3.137263	1.852612	C	-5.244794	1.380168	-2.835326
H	0.025941	2.909814	3.602660	H	-3.299144	2.288900	-2.660400
C	-1.965868	2.958239	2.730252	C	-6.117959	0.329516	-0.843851
H	-2.038679	4.039515	2.528574	H	-4.865496	0.393786	0.901085
H	-2.323441	2.818430	3.763476	C	-6.266314	0.676087	-2.189582
C	-2.960054	2.214519	1.811196	H	-5.350120	1.656702	-3.887729
H	-3.894606	2.793863	1.746064	H	-6.908070	-0.223948	-0.329660
H	-3.222764	1.245607	2.263989	H	-7.172515	0.397759	-2.733279
C	-0.966084	-0.123609	3.649934	C	-1.879522	3.424991	-0.605550
C	-1.749238	-1.237998	3.307354	C	-2.752861	4.527014	-0.557632
C	-0.892754	0.266752	4.999172	C	-0.612693	3.589977	-1.187196
C	-2.449538	-1.944741	4.291665	C	-2.363836	5.764471	-1.074633
H	-1.800298	-1.559434	2.263994	H	-3.750143	4.417398	-0.123546
C	-1.596419	-0.435478	5.980384	C	-0.224080	4.829811	-1.708549
H	-0.273820	1.119701	5.290320	H	0.074738	2.741563	-1.234175
C	-2.377179	-1.542626	5.627545	C	-1.097375	5.918185	-1.651596
H	-3.047089	-2.814779	4.008165	H	-3.052470	6.612416	-1.030670
H	-1.532426	-0.120692	7.025366	H	0.765038	4.939380	-2.160586
H	-2.924463	-2.093510	6.397001	H	-0.795155	6.886937	-2.057954
C	1.690513	0.659322	2.823851	C	-0.684510	-0.960150	-1.313521
C	2.607946	1.680496	2.518974	C	0.480518	-1.148170	-0.474188
C	2.166380	-0.509090	3.444880	C	-1.644613	-2.065639	-1.200945
C	3.958845	1.548163	2.850412	S	0.379262	-2.749929	0.369286
H	2.276399	2.589630	2.012486	C	-1.209845	-3.028007	-0.341137

Br	-2.149168	-4.593312	0.178042
H	-0.613218	-0.429235	-2.270777
C	-2.904560	-2.126776	-2.022436
C	-2.664177	-2.617821	-3.462661
H	-3.363859	-1.125749	-2.051648
H	-3.631744	-2.794655	-1.533362
C	-3.939484	-2.657590	-4.309903
H	-1.918571	-1.966707	-3.953945
H	-2.210785	-3.624155	-3.427763
C	-3.704678	-3.148317	-5.739355
H	-4.683505	-3.307204	-3.813595
H	-4.391329	-1.649454	-4.332420
H	-4.640374	-3.168486	-6.321227
H	-2.993516	-2.497036	-6.275069
H	-3.285000	-4.168314	-5.748681
C	1.815845	-0.636409	-0.768471
C	3.043488	-1.039225	-0.291484
S	2.025268	0.716830	-1.875575
C	4.166820	-0.289268	-0.778821
H	3.155597	-1.869345	0.407916
C	3.753909	0.694525	-1.644842
Br	4.829030	1.947873	-2.563702
C	5.593246	-0.593603	-0.405179
C	6.206808	-1.757131	-1.204470
H	5.631975	-0.831783	0.671833
H	6.209004	0.309018	-0.549058
C	7.649896	-2.073118	-0.800571
H	5.580900	-2.658454	-1.075902
H	6.167616	-1.513475	-2.280931
C	8.265336	-3.228077	-1.591904
H	8.268970	-1.166262	-0.928338
H	7.681803	-2.306848	0.279587
H	9.301798	-3.428786	-1.276288

H	7.689439	-4.158829	-1.455728
H	8.283050	-3.008458	-2.672587

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Ni-3BTanti-3BTanti-O-TS-2 SCF Done: -8462.47491704 A.U.

Ni	-0.022749	0.805934	-0.330358
P	1.150463	2.740752	-0.212069
P	-1.915874	1.661448	-1.254706
C	0.781546	3.935913	-1.603595
H	1.175964	3.482383	-2.527805
H	1.353753	4.862643	-1.439091
C	-0.710608	4.261667	-1.775933
H	-0.784566	5.121550	-2.464203
H	-1.127802	4.615000	-0.817643
C	-1.578481	3.132842	-2.359003
H	-1.084940	2.704253	-3.247461
H	-2.541628	3.532179	-2.715444
C	0.759743	3.759030	1.281781
C	-0.123324	3.243723	2.244373
C	1.300427	5.043558	1.476692
C	-0.460599	3.994438	3.376328
H	-0.552502	2.247783	2.106826
C	0.963420	5.792448	2.605829
H	2.000968	5.460936	0.748702
C	0.080928	5.268660	3.558118
H	-1.150225	3.578119	4.114683
H	1.392544	6.788194	2.745212
H	-0.181819	5.855925	4.441890
C	2.993265	2.663279	-0.238203
C	3.653240	2.357372	-1.442478
C	3.757901	2.781673	0.935064
C	5.040700	2.202129	-1.476699
H	3.084517	2.218051	-2.364466
C	5.146567	2.624036	0.898874

H	3.270492	3.000693	1.887104
C	5.792899	2.337891	-0.306307
H	5.533635	1.960548	-2.421571
H	5.724723	2.724395	1.821248
H	6.878340	2.213088	-0.332964
C	-3.264903	2.215681	-0.120669
C	-3.686312	1.308844	0.870831
C	-3.871167	3.482001	-0.175493
C	-4.695533	1.656289	1.771111
H	-3.218028	0.325055	0.943949
C	-4.874724	3.831789	0.734696
H	-3.573134	4.211347	-0.930497
C	-5.291390	2.920361	1.707947
H	-5.010113	0.935351	2.529917
H	-5.333566	4.822389	0.677852
H	-6.076836	3.194603	2.416884
C	-2.793487	0.564839	-2.461621
C	-4.188852	0.552159	-2.617158
C	-2.011826	-0.269651	-3.279958
C	-4.787540	-0.272558	-3.574933
H	-4.815999	1.185644	-1.986447
C	-2.610495	-1.085301	-4.243547
H	-0.925007	-0.287150	-3.159047
C	-4.001194	-1.090429	-4.391664
H	-5.875384	-0.273818	-3.682954
H	-1.988044	-1.726799	-4.872682
H	-4.471343	-1.733974	-5.139698
C	2.304190	-0.895993	0.738359
C	1.301323	-0.544223	-0.157443
C	3.484118	-1.469188	0.164943
S	1.840156	-0.971410	-1.796446
C	3.369387	-1.575496	-1.203212
Br	4.653276	-2.256068	-2.413091

H	2.185470	-0.776632	1.817276
C	4.661456	-1.930563	0.984490
C	4.507639	-3.359342	1.535565
H	4.801656	-1.230567	1.826290
H	5.577722	-1.873803	0.374236
C	5.686581	-3.804073	2.406209
H	3.571446	-3.425769	2.118362
H	4.387067	-4.058623	0.689424
C	5.541597	-5.227019	2.947711
H	6.620746	-3.724919	1.820416
H	5.801934	-3.098113	3.249293
H	6.403868	-5.514078	3.571012
H	4.634385	-5.329603	3.566597
H	5.464078	-5.961140	2.128244
C	-1.829638	-2.880536	0.614411
C	-1.806260	-2.343995	1.884038
C	-1.062912	-2.085984	-0.295409
S	-0.849027	-0.884295	1.978761
C	-0.467362	-0.948393	0.240024
H	-0.920458	-2.379216	-1.336798
Br	-2.665521	-3.014595	3.429670
C	-2.577413	-4.122864	0.203784
C	-3.969575	-3.838906	-0.388247
H	-2.684451	-4.790739	1.074035
H	-1.973165	-4.670425	-0.540312
C	-4.716501	-5.105708	-0.815826
H	-4.570740	-3.289913	0.358344
H	-3.866381	-3.159923	-1.253353
C	-6.102279	-4.827222	-1.400079
H	-4.106721	-5.654416	-1.557028
H	-4.810637	-5.782635	0.052854
H	-6.610133	-5.757101	-1.702991
H	-6.750452	-4.317573	-0.667365

H	-6.037906	-4.176925	-2.288687	C	-3.036428	-4.642660	-2.778761
96				H	-1.351716	-5.120464	-4.049531
Ni-3BTanti-3BTanti-S SCF Done: -8462.49109961 A.U.				H	-4.501078	-4.038393	-1.304707
Ni	0.565476	-0.791357	0.079504	H	-3.782038	-4.997054	-3.494859
P	0.113573	-3.023280	0.241265	C	3.620501	0.183923	1.537501
P	2.781460	-1.129700	0.553557	C	4.264587	1.251316	0.889476
C	1.611951	-4.090104	-0.072550	C	3.553152	0.184839	2.941612
H	1.984362	-3.756618	-1.054050	C	4.836402	2.287928	1.630391
H	1.300614	-5.139023	-0.193513	H	4.306475	1.286090	-0.200393
C	2.748976	-4.004649	0.964585	C	4.128707	1.222914	3.679806
H	3.668128	-4.355654	0.468088	H	3.047390	-0.621124	3.477166
H	2.548893	-4.723586	1.775650	C	4.772727	2.276709	3.026564
C	3.028476	-2.639372	1.623961	H	5.326803	3.113433	1.108808
H	4.046414	-2.632547	2.042975	H	4.069806	1.206511	4.771181
H	2.341071	-2.491414	2.471359	H	5.219662	3.089919	3.603992
C	-0.478790	-3.574872	1.900001	C	3.904093	-1.419867	-0.881741
C	-0.545051	-2.644491	2.949756	C	5.272732	-1.691280	-0.704665
C	-0.831832	-4.912532	2.151273	C	3.377544	-1.395725	-2.183359
C	-0.949845	-3.043293	4.228153	C	6.092921	-1.940628	-1.806997
H	-0.283173	-1.600024	2.760582	H	5.706246	-1.696609	0.298840
C	-1.235138	-5.309718	3.428091	C	4.200854	-1.643434	-3.286948
H	-0.803329	-5.648057	1.342972	H	2.318777	-1.171544	-2.336628
C	-1.293931	-4.375796	4.468804	C	5.557763	-1.917462	-3.100139
H	-1.001726	-2.307979	5.035043	H	7.155338	-2.149218	-1.657080
H	-1.508554	-6.352012	3.611288	H	3.778910	-1.613403	-4.294490
H	-1.613092	-4.687833	5.466497	H	6.202125	-2.108098	-3.962158
C	-1.118109	-3.721997	-0.936739	C	-2.327009	-0.283415	0.716580
C	-0.722238	-4.252114	-2.176702	C	-1.289964	-0.420904	-0.184042
C	-2.489281	-3.649938	-0.636670	C	-3.622438	-0.006278	0.148312
C	-1.676505	-4.711123	-3.089537	S	-1.912270	-0.186587	-1.798491
H	0.333093	-4.307291	-2.450314	C	-3.539260	0.062603	-1.222307
C	-3.438938	-4.109438	-1.550833	Br	-4.956660	0.391803	-2.434733
H	-2.819502	-3.216293	0.308611	H	-2.195422	-0.370395	1.798389

C	-4.866475	0.217746	0.968614
C	-5.053278	1.677847	1.419221
H	-4.830839	-0.432294	1.861036
H	-5.751295	-0.093847	0.388620
C	-6.306207	1.898784	2.271425
H	-4.159505	2.001030	1.982878
H	-5.095051	2.323421	0.524436
C	-6.496459	3.351355	2.710938
H	-7.194386	1.566221	1.703479
H	-6.260966	1.246286	3.163263
H	-7.405218	3.475840	3.321856
H	-5.640835	3.703911	3.311402
H	-6.585193	4.023762	1.841237
C	0.841833	1.090590	-0.097150
C	0.582884	2.127614	0.770260
S	1.569168	1.746708	-1.550930
C	0.966005	3.441855	0.319896
H	0.104420	1.976138	1.741496
C	1.519355	3.379506	-0.936604
Br	2.161985	4.823697	-1.980142
C	0.726077	4.699099	1.114491
C	-0.674545	5.301362	0.901678
H	1.485699	5.453671	0.850381
H	0.864906	4.475910	2.186983
C	-0.926040	6.566249	1.727621
H	-0.805746	5.527189	-0.171188
H	-1.438270	4.541132	1.145093
C	-2.315188	7.168771	1.511645
H	-0.786383	6.335352	2.800081
H	-0.155005	7.319428	1.481777
H	-2.462832	8.077828	2.116982
H	-2.471861	7.442780	0.454876
H	-3.109219	6.453646	1.785053

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Ni-3BTanti-3BTanti-S-Pr SCF Done: -8462.51277387 A.U.

Ni	-0.660237	-0.188068	0.333239
P	-0.456689	-2.272142	1.085221
P	-1.707513	0.613208	2.108018
C	-0.484137	-2.307120	2.954916
H	0.332095	-1.628134	3.247934
H	-0.208290	-3.306373	3.326824
C	-1.797695	-1.858607	3.635004
H	-1.538024	-1.544752	4.659241
H	-2.453792	-2.737314	3.745413
C	-2.648728	-0.746506	2.980620
H	-3.327926	-0.323410	3.737569
H	-3.283392	-1.184217	2.193723
C	-1.881223	-3.359143	0.615185
C	-2.794709	-2.910614	-0.352251
C	-2.080090	-4.620993	1.203977
C	-3.886139	-3.704797	-0.722627
H	-2.645434	-1.936286	-0.824421
C	-3.173483	-5.409928	0.839800
H	-1.370243	-4.997961	1.945148
C	-4.079061	-4.952471	-0.124936
H	-4.579814	-3.344137	-1.486172
H	-3.317080	-6.388313	1.306023
H	-4.931527	-5.573349	-0.412857
C	1.003080	-3.335648	0.694247
C	2.163724	-3.305266	1.487216
C	1.007269	-4.116867	-0.475350
C	3.291543	-4.048725	1.128985
H	2.203440	-2.691948	2.390125
C	2.136161	-4.858955	-0.830781
H	0.122682	-4.146743	-1.115228
C	3.281257	-4.830017	-0.029563

H	4.184846	-4.011484	1.757801
H	2.119684	-5.461982	-1.742424
H	4.164296	-5.409771	-0.309862
C	-2.982265	1.948934	1.967787
C	-2.566048	3.290723	1.880289
C	-4.354052	1.664807	1.846254
C	-3.494076	4.316537	1.690390
H	-1.504917	3.537857	1.969471
C	-5.282174	2.693363	1.652823
H	-4.714657	0.635481	1.896646
C	-4.857481	4.021989	1.576236
H	-3.150560	5.352729	1.632635
H	-6.344435	2.451195	1.563349
H	-5.583870	4.824959	1.428352
C	-0.599598	1.279063	3.437400
C	-1.100230	1.691105	4.685392
C	0.782538	1.358223	3.202018
C	-0.237126	2.165333	5.675641
H	-2.174736	1.651618	4.883651
C	1.647315	1.836061	4.193868
H	1.182415	1.043457	2.233537
C	1.139374	2.238493	5.431431
H	-0.639702	2.482242	6.641378
H	2.720537	1.893231	3.994745
H	1.813692	2.611660	6.206646
C	-0.665362	1.136113	-1.145499
C	0.322380	0.105737	-1.375312
C	-1.839835	0.985921	-2.012034
S	-0.176140	-0.928568	-2.778188
C	-1.705791	-0.064765	-2.870730
Br	-2.997301	-0.677178	-4.120091
H	-0.389416	2.142295	-0.811186
C	-2.998509	1.947350	-1.980363

C	-2.732699	3.244172	-2.768111
H	-3.227798	2.199938	-0.932651
H	-3.894999	1.456661	-2.392740
C	-3.908263	4.225196	-2.733977
H	-1.830424	3.739635	-2.366035
H	-2.495313	2.985820	-3.815190
C	-3.645314	5.516777	-3.509934
H	-4.807080	3.726539	-3.140628
H	-4.148880	4.465380	-1.682587
H	-4.509799	6.199094	-3.468628
H	-2.774446	6.058330	-3.103375
H	-3.435304	5.310372	-4.572851
C	1.744710	0.284350	-1.098408
C	2.379418	1.377405	-0.536075
S	2.918748	-0.973754	-1.435115
C	3.794380	1.234406	-0.357783
H	1.845880	2.287895	-0.258657
C	4.215558	0.004892	-0.810888
Br	5.980873	-0.666981	-0.820157
C	4.681525	2.320446	0.193539
C	5.160234	3.326433	-0.869141
H	5.560269	1.864594	0.678762
H	4.133230	2.863786	0.983096
C	6.045134	4.437507	-0.297508
H	5.711222	2.780005	-1.654717
H	4.282244	3.772322	-1.370233
C	6.528423	5.434969	-1.351425
H	5.489272	4.975881	0.492396
H	6.916730	3.982707	0.207885
H	7.161157	6.219754	-0.906583
H	7.120997	4.933985	-2.135083
H	5.680514	5.934059	-1.849947

Ni-3BTanti-3BTanti-S-TS-2 SCF Done: -8462.46981047 A.U.

Ni	-0.432459	-0.832751	0.124686
P	-2.488881	-1.781435	-0.154475
P	0.396119	-2.486712	1.445360
C	-2.375295	-3.627397	0.128965
H	-1.600250	-3.930046	-0.594530
H	-3.301521	-4.123727	-0.201780
C	-1.994067	-4.118823	1.542226
H	-1.565000	-5.128417	1.430514
H	-2.910206	-4.248491	2.141581
C	-1.028792	-3.256516	2.378265
H	-0.664300	-3.838840	3.239066
H	-1.569763	-2.393019	2.798507
C	-3.927943	-1.220472	0.852925
C	-4.033635	0.153626	1.138346
C	-4.911784	-2.092970	1.351829
C	-5.100977	0.639735	1.898240
H	-3.274719	0.845629	0.767561
C	-5.973152	-1.604659	2.120407
H	-4.863677	-3.162468	1.136678
C	-6.070468	-0.237254	2.394293
H	-5.170615	1.710513	2.105466
H	-6.728849	-2.296207	2.502271
H	-6.901467	0.143902	2.993475
C	-3.115765	-1.759718	-1.895647
C	-2.171965	-1.875042	-2.931590
C	-4.475346	-1.644147	-2.226176
C	-2.580256	-1.894555	-4.267114
H	-1.106276	-1.937368	-2.693106
C	-4.880997	-1.653432	-3.564465
H	-5.224346	-1.538419	-1.438767
C	-3.936927	-1.782477	-4.586809
H	-1.833406	-1.982745	-5.060186

H	-5.942339	-1.556035	-3.807692
H	-4.256719	-1.786515	-5.632009
C	1.438189	-1.838595	2.827871
C	2.794173	-2.170877	2.976311
C	0.871771	-0.905659	3.717371
C	3.559329	-1.597245	3.998057
H	3.261849	-2.881828	2.292691
C	1.634124	-0.343147	4.743085
H	-0.173659	-0.604646	3.605773
C	2.982697	-0.687450	4.887128
H	4.613779	-1.867930	4.097631
H	1.174066	0.372931	5.429131
H	3.581375	-0.243267	5.686352
C	1.348668	-3.932794	0.805183
C	1.511976	-5.120212	1.542706
C	1.925203	-3.842670	-0.473140
C	2.231075	-6.192942	1.010505
H	1.085668	-5.209801	2.545103
C	2.650918	-4.916152	-1.001505
H	1.808349	-2.926050	-1.056931
C	2.802418	-6.092294	-0.263273
H	2.349291	-7.110183	1.593410
H	3.097953	-4.828187	-1.994887
H	3.366493	-6.931960	-0.677612
C	-0.716815	1.891131	0.869462
C	-0.568640	1.028756	-0.219504
C	-1.445699	3.096239	0.619715
S	-1.349845	1.765298	-1.624113
C	-1.841095	3.161267	-0.700000
Br	-2.759939	4.584811	-1.541195
H	-0.271736	1.678624	1.844445
C	-1.671637	4.166071	1.657544
C	-0.513437	5.173628	1.771434

H	-1.827519	3.683944	2.638640	Ni	0.539862	0.580315	-0.345281
H	-2.600864	4.712394	1.425772	P	2.502019	1.750265	-0.291980
C	-0.741127	6.239149	2.847324	P	-0.702059	2.253572	-1.310020
H	0.423792	4.627626	1.982280	C	2.661487	3.262583	-1.377105
H	-0.365873	5.660582	0.791531	H	2.797952	2.918426	-2.414937
C	0.405700	7.244465	2.962950	H	3.586391	3.785570	-1.087999
H	-1.682573	6.776693	2.631436	C	1.461074	4.216322	-1.310425
H	-0.897606	5.743288	3.823228	H	1.762587	5.171025	-1.774494
H	0.208833	7.996879	3.743587	H	1.230496	4.458994	-0.259227
H	1.354934	6.742751	3.215987	C	0.216228	3.711280	-2.054183
H	0.562718	7.783045	2.013439	H	0.511185	3.376095	-3.061821
C	1.079890	0.173524	-0.414918	H	-0.509536	4.526445	-2.201913
C	2.225629	0.675097	0.193490	C	2.672843	2.503142	1.389057
S	1.498608	-0.307102	-2.075643	C	1.578376	2.480079	2.268469
C	3.420756	0.638811	-0.590982	C	3.858034	3.143231	1.794745
H	2.214598	1.076958	1.208877	C	1.663383	3.086730	3.526501
C	3.175282	0.123139	-1.845891	H	0.653914	1.979111	1.970769
Br	4.418363	-0.117998	-3.249865	C	3.942421	3.746377	3.051138
C	4.750614	1.150057	-0.098757	H	4.727269	3.160265	1.132288
C	4.933217	2.667353	-0.281741	C	2.844669	3.719600	3.919343
H	5.564698	0.622947	-0.623031	H	0.803244	3.056002	4.199664
H	4.852425	0.899864	0.971641	H	4.870794	4.236147	3.356166
C	6.272801	3.185691	0.249628	H	2.914013	4.189146	4.903940
H	4.839729	2.912688	-1.354358	C	4.109897	0.893788	-0.570151
H	4.104852	3.196677	0.222618	C	4.740000	0.907697	-1.826036
C	6.457249	4.693182	0.069469	C	4.688399	0.141183	0.466829
H	6.363467	2.927836	1.320994	C	5.927254	0.200433	-2.035336
H	7.096077	2.649627	-0.257132	H	4.309385	1.462741	-2.661382
H	7.429825	5.033065	0.460520	C	5.874746	-0.564022	0.254967
H	6.408297	4.977930	-0.994957	H	4.210659	0.103327	1.446973
H	5.670297	5.258839	0.596187	C	6.498475	-0.536469	-0.995569
				H	6.402355	0.222845	-3.019317
				H	6.308749	-1.145677	1.071896

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Ni-3BTanti-3BTsyn-O-2 SCF Done: -8462.49051367 A.U.

H	7.423929	-1.093739	-1.160586
C	-2.043810	3.037697	-0.319154
C	-3.231862	2.326236	-0.070144
C	-1.881334	4.306065	0.264939
C	-4.235670	2.880844	0.726458
H	-3.375105	1.333031	-0.499558
C	-2.885620	4.854650	1.068663
H	-0.969639	4.883648	0.102230
C	-4.066423	4.144766	1.299307
H	-5.151002	2.312559	0.908282
H	-2.741529	5.842843	1.513025
H	-4.851990	4.573918	1.926380
C	-1.542094	1.620413	-2.827501
C	-2.646804	2.274146	-3.398249
C	-0.999576	0.500859	-3.479454
C	-3.198221	1.812922	-4.596972
H	-3.087381	3.142131	-2.902281
C	-1.548237	0.045820	-4.681974
H	-0.149883	-0.027700	-3.039314
C	-2.649713	0.699577	-5.241594
H	-4.061477	2.326421	-5.028203
H	-1.117653	-0.829208	-5.175124
H	-3.083814	0.339688	-6.177932
C	1.886878	-1.849435	1.035570
C	1.452822	-1.069156	-0.020318
C	2.550005	-3.061846	0.619025
S	1.854416	-1.855990	-1.541048
C	2.609735	-3.206403	-0.738079
Br	3.387346	-4.630962	-1.705446
C	-3.008882	-1.752156	0.211130
C	-3.009743	-1.207384	1.473755
C	-1.892470	-1.255462	-0.554063
S	-1.666342	-0.122221	1.720996

C	-1.063581	-0.363605	0.090438
H	-1.710375	-1.596715	-1.575473
Br	-4.255366	-1.529673	2.864134
C	-4.028987	-2.716174	-0.336464
C	-5.130760	-2.044411	-1.175520
H	-4.495908	-3.269106	0.494947
H	-3.509798	-3.465619	-0.959217
C	-6.149585	-3.034311	-1.748035
H	-5.652684	-1.298834	-0.549004
H	-4.664996	-1.476093	-2.001003
C	-7.245703	-2.368325	-2.581058
H	-5.620648	-3.783323	-2.365487
H	-6.609272	-3.601998	-0.918623
H	-7.960134	-3.107468	-2.978028
H	-7.818778	-1.640929	-1.981533
H	-6.820019	-1.822285	-3.439989
C	1.694861	-1.526035	2.499983
H	1.274617	-0.513054	2.594722
H	2.679216	-1.497413	3.007526
C	0.787175	-2.516591	3.248235
H	-0.188074	-2.558151	2.734734
H	1.212900	-3.534295	3.178990
C	0.574691	-2.156551	4.721378
H	0.165023	-1.132006	4.784811
H	1.553374	-2.122219	5.235792
C	-0.358700	-3.120963	5.455181
H	-1.360827	-3.129278	4.995257
H	-0.480253	-2.842585	6.514783
H	0.027176	-4.154143	5.424879
H	2.967475	-3.794165	1.312661

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Ni-3BTanti-3BTsyn-O-Pr SCF Done: -8462.51167740 A.U.

Ni	-0.439358	0.540151	-0.148213
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P	-2.285245	1.602549	-0.796914	C	2.597229	2.364297	-0.401002
P	0.820569	2.373491	0.125057	C	3.645995	2.901251	0.362487
C	-2.291014	3.361687	-0.160212	C	2.895700	1.789935	-1.649754
H	-2.156953	3.231121	0.926008	C	4.958773	2.880720	-0.121606
H	-3.286242	3.814778	-0.291087	H	3.445073	3.337514	1.342594
C	-1.208427	4.305461	-0.717654	C	4.204360	1.779344	-2.136020
H	-1.100758	5.135317	0.000305	H	2.101336	1.326926	-2.241422
H	-1.576528	4.762836	-1.651212	C	5.240823	2.327067	-1.373076
C	0.184465	3.717929	-1.018615	H	5.764138	3.301958	0.486171
H	0.921051	4.533767	-1.087430	H	4.417313	1.322987	-3.105735
H	0.183264	3.226625	-2.005485	H	6.266852	2.312620	-1.749653
C	-2.595360	1.779582	-2.610704	C	0.828796	3.181815	1.788445
C	-1.969643	0.873063	-3.484181	C	1.106228	4.548768	1.973929
C	-3.401730	2.794209	-3.157894	C	0.518612	2.396611	2.912777
C	-2.152602	0.970413	-4.867187	C	1.075695	5.115012	3.251204
H	-1.326602	0.090946	-3.072858	H	1.357909	5.180380	1.118641
C	-3.580231	2.895158	-4.540501	C	0.493953	2.963878	4.191546
H	-3.903317	3.511823	-2.504296	H	0.292962	1.333989	2.786152
C	-2.957095	1.982410	-5.397943	C	0.770069	4.322847	4.363130
H	-1.658937	0.256095	-5.530965	H	1.292883	6.178810	3.378967
H	-4.209201	3.690105	-4.949797	H	0.253840	2.338264	5.055053
H	-3.096539	2.063064	-6.479037	H	0.746502	4.766643	5.361818
C	-3.890652	1.014270	-0.089369	C	-0.754047	-1.414885	-0.295921
C	-3.909418	0.715508	1.285540	C	0.509643	-1.127408	0.359736
C	-5.067363	0.839457	-0.835709	C	-1.765288	-2.028814	0.571192
C	-5.082275	0.275433	1.902973	S	0.294859	-1.501079	2.138346
H	-2.994342	0.809253	1.876906	C	-1.340214	-2.099040	1.859561
C	-6.238491	0.388915	-0.216865	Br	-2.340095	-2.687711	3.360609
H	-5.076006	1.049953	-1.906935	H	-0.763972	-1.700317	-1.355595
C	-6.251031	0.110586	1.152540	C	-3.063458	-2.565829	0.032495
H	-5.074782	0.041541	2.970274	C	-2.931198	-3.976988	-0.570767
H	-7.145772	0.254763	-0.811919	H	-3.444129	-1.876474	-0.739818
H	-7.167020	-0.242674	1.633026	H	-3.819158	-2.584273	0.833625

C	-4.242020	-4.510248	-1.156468	P	2.894306	-0.686024	-0.128169
H	-2.154028	-3.970816	-1.356351	C	1.921256	-3.638208	0.773763
H	-2.565524	-4.667421	0.209542	H	2.088797	-3.702285	-0.312977
C	-4.116846	-5.914025	-1.750549	H	1.727752	-4.662956	1.128231
H	-5.017387	-4.509697	-0.368733	C	3.198265	-3.112855	1.461539
H	-4.604762	-3.811072	-1.932298	H	4.036897	-3.693102	1.043311
H	-5.075590	-6.267344	-2.163305	H	3.158523	-3.373598	2.531913
H	-3.373837	-5.939754	-2.565441	C	3.546199	-1.607510	1.363903
H	-3.793002	-6.643408	-0.989248	H	4.635657	-1.473640	1.451632
C	1.814489	-1.397241	-0.237062	H	3.099653	-1.067596	2.214271
C	3.101993	-1.243305	0.255779	C	0.034230	-2.714453	2.772379
S	1.860458	-2.051331	-1.878495	C	0.151735	-1.561287	3.564970
C	4.109325	-1.637397	-0.687735	C	-0.316968	-3.929089	3.388244
C	3.597218	-2.076653	-1.875574	C	-0.064582	-1.621787	4.946253
Br	4.559217	-2.627769	-3.402091	H	0.406800	-0.606807	3.097195
C	3.471469	-0.731900	1.627020	C	-0.534208	-3.988294	4.766484
C	3.928083	-1.827167	2.607616	H	-0.433373	-4.834160	2.786158
H	2.626252	-0.177114	2.064195	C	-0.406725	-2.834560	5.548803
H	4.283404	0.008418	1.515097	H	0.028413	-0.714779	5.549026
C	4.319607	-1.283177	3.984674	H	-0.808562	-4.938453	5.232321
H	3.119674	-2.570232	2.718601	H	-0.580497	-2.882014	6.626964
H	4.784542	-2.371493	2.169794	C	-0.924945	-3.675241	0.215590
C	4.793311	-2.366451	4.954827	C	-0.652669	-4.819727	-0.552789
H	5.112802	-0.521990	3.864913	C	-2.263600	-3.271313	0.374550
H	3.455858	-0.749191	4.420873	C	-1.695416	-5.549097	-1.135455
H	5.063993	-1.943165	5.935644	H	0.372790	-5.157635	-0.709828
H	4.008931	-3.123137	5.123530	C	-3.301139	-4.002934	-0.204024
H	5.679659	-2.894294	4.564180	H	-2.495194	-2.369196	0.945752
H	5.179370	-1.571707	-0.485809	C	-3.020713	-5.145994	-0.960337
				H	-1.465526	-6.437926	-1.729054
96				H	-4.333288	-3.668550	-0.075233
Ni-3BTanti-3BTsyn-O-TS-3 SCF Done: -8462.46582316 A.U.				H	-3.833612	-5.715897	-1.417528
Ni	0.651726	-0.490593	0.149171	C	3.940594	0.834026	-0.151268
P	0.381265	-2.603420	0.957025				

C	4.399530	1.374444	-1.365196
C	4.200617	1.535780	1.039376
C	5.112429	2.576121	-1.385299
H	4.203827	0.853513	-2.304993
C	4.913605	2.737214	1.016336
H	3.836105	1.158080	1.996453
C	5.373089	3.260764	-0.195039
H	5.465158	2.978404	-2.338656
H	5.101092	3.270856	1.951293
H	5.928715	4.201748	-0.211597
C	3.529695	-1.646323	-1.575097
C	4.858613	-2.100343	-1.652790
C	2.652028	-1.935267	-2.633041
C	5.294776	-2.832100	-2.759742
H	5.563733	-1.873779	-0.848618
C	3.090611	-2.663139	-3.744955
H	1.615573	-1.589753	-2.581691
C	4.411260	-3.114368	-3.808241
H	6.329823	-3.180608	-2.807096
H	2.396081	-2.877424	-4.561148
H	4.755133	-3.685100	-4.674733
C	-2.189759	0.495730	0.812862
C	-1.101535	0.253964	-0.031461
C	-3.486616	0.317301	0.242060
S	-1.746670	-0.219643	-1.623195
C	-3.398394	-0.068375	-1.078670
Br	-4.825684	-0.396823	-2.275070
H	-2.059184	0.851836	1.836250
C	-4.764750	0.592524	0.992965
C	-5.170523	2.077445	0.989919
H	-4.644584	0.254497	2.037217
H	-5.583363	-0.006478	0.561199
C	-6.449336	2.360225	1.783592

H	-4.340086	2.680900	1.398017
H	-5.301353	2.410435	-0.054830
C	-6.852909	3.835481	1.780814
H	-7.274605	1.750359	1.372442
H	-6.314242	2.016613	2.825767
H	-7.774518	4.005510	2.360482
H	-6.062232	4.467532	2.218890
H	-7.032524	4.199453	0.755239
C	0.316760	1.380799	0.042870
C	0.568024	2.391855	-0.897447
S	0.541834	2.048071	1.686230
C	0.908961	3.648251	-0.304562
C	0.934813	3.628270	1.064336
Br	1.377997	5.051691	2.219798
C	0.506484	2.220642	-2.395736
C	-0.655089	2.966221	-3.075465
H	0.448736	1.149254	-2.643915
H	1.459883	2.574858	-2.831078
C	-0.702718	2.764494	-4.592587
H	-1.605880	2.628628	-2.629315
H	-0.577295	4.045478	-2.850271
C	-1.860573	3.500093	-5.268835
H	0.255460	3.093595	-5.036258
H	-0.778660	1.683189	-4.808843
H	-1.866049	3.335116	-6.358490
H	-2.832610	3.159037	-4.875178
H	-1.799736	4.588169	-5.097359
H	1.144460	4.541396	-0.886444

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Ni-3BTanti-3BTsyn-S SCF Done: -8462.48809838 A.U.

Ni	0.382947	-0.603031	-0.058122
P	-0.495247	-2.705444	0.127182
P	2.517419	-1.387916	0.254593

C	0.723839	-4.040510	-0.336861	C	3.968186	-0.501143	2.544256
H	1.070981	-3.757828	-1.342754	C	5.205636	1.596965	1.179847
H	0.196837	-5.000865	-0.445792	H	4.112826	0.931088	-0.551746
C	1.936782	-4.216838	0.596990	C	4.849889	0.350595	3.218544
H	2.724341	-4.722994	0.015619	H	3.492397	-1.308153	3.103786
H	1.664753	-4.911425	1.408215	C	5.474267	1.398251	2.537836
C	2.536971	-2.960001	1.259785	H	5.677326	2.421704	0.640242
H	3.567075	-3.177665	1.580863	H	5.048105	0.189753	4.281367
H	1.967862	-2.713675	2.170290	H	6.164001	2.062145	3.065055
C	-1.046138	-3.188624	1.820428	C	3.446053	-1.844205	-1.275578
C	-0.859612	-2.291777	2.884556	C	4.771492	-2.310398	-1.216617
C	-1.613236	-4.448613	2.082033	C	2.811900	-1.749562	-2.524481
C	-1.227770	-2.647386	4.186623	C	5.442041	-2.683979	-2.383016
H	-0.426821	-1.307491	2.688651	H	5.289425	-2.369775	-0.255757
C	-1.979282	-4.803187	3.382336	C	3.485263	-2.122734	-3.692579
H	-1.780958	-5.154396	1.264322	H	1.789109	-1.369079	-2.585566
C	-1.786770	-3.903109	4.436752	C	4.799099	-2.591897	-3.622905
H	-1.081339	-1.937821	5.004790	H	6.472774	-3.043140	-2.325459
H	-2.419978	-5.784962	3.573660	H	2.982296	-2.035968	-4.658812
H	-2.077153	-4.181145	5.453120	H	5.327205	-2.879775	-4.535517
C	-1.928594	-3.103931	-0.958630	C	-2.351860	0.395458	0.716858
C	-1.725299	-3.538335	-2.280002	C	-1.386786	0.104987	-0.226979
C	-3.242720	-2.894414	-0.508748	C	-3.609357	0.880726	0.205188
C	-2.812624	-3.771379	-3.126048	S	-2.032869	0.449904	-1.813357
H	-0.716437	-3.690162	-2.669006	C	-3.573898	0.947641	-1.167146
C	-4.326880	-3.126701	-1.357889	Br	-4.966573	1.515423	-2.318437
H	-3.422572	-2.534001	0.505208	H	-2.193509	0.275007	1.791605
C	-4.116233	-3.567309	-2.667215	C	-4.764697	1.294379	1.079291
H	-2.636897	-4.108245	-4.150831	C	-4.669044	2.746727	1.580508
H	-5.342327	-2.951448	-0.994567	H	-4.818780	0.616846	1.950260
H	-4.966174	-3.743615	-3.331102	H	-5.709253	1.168047	0.524417
C	3.702587	-0.316399	1.176680	C	-5.837703	3.160260	2.479641
C	4.324136	0.751350	0.504249	H	-3.716967	2.880874	2.125168

H	-4.615085	3.421815	0.708420	H	-1.060984	-3.739670	0.197506
C	-5.744099	4.603787	2.976391	H	-1.119554	-4.304678	1.868353
H	-6.785769	3.020545	1.928598	C	0.869919	-4.344403	1.010832
H	-5.892142	2.474564	3.345596	H	0.753240	-5.213469	0.343130
H	-6.598961	4.868843	3.619459	H	1.174659	-4.752518	1.988266
H	-4.823644	4.767185	3.562010	C	2.048342	-3.486651	0.500955
H	-5.727166	5.316141	2.134614	H	2.850582	-4.151898	0.145000
C	0.998486	1.196275	-0.311140	H	2.468392	-2.906099	1.337389
C	1.021223	2.296481	0.527596	C	0.397471	-1.845554	3.220713
S	1.586041	1.655228	-1.900532	C	1.406144	-0.881684	3.378043
C	1.518736	3.492864	-0.102705	C	0.148848	-2.746588	4.271482
C	1.864584	3.304613	-1.412369	C	2.155116	-0.822374	4.559002
Br	2.563836	4.591924	-2.606837	H	1.599379	-0.165414	2.575446
C	0.528311	2.278910	1.957057	C	0.901893	-2.692451	5.446331
C	1.509676	2.838141	2.997639	H	-0.647433	-3.490210	4.179252
H	0.273044	1.239565	2.221621	C	1.907504	-1.729326	5.591987
H	-0.422236	2.842355	2.022696	H	2.927646	-0.057165	4.668296
C	0.972653	2.780738	4.431356	H	0.699095	-3.399849	6.254819
H	2.461722	2.282910	2.937586	H	2.492214	-1.683883	6.514540
H	1.757313	3.886528	2.751121	C	-2.304093	-1.686226	2.265864
C	1.940680	3.346130	5.471880	C	-3.362828	-2.526857	1.884015
H	0.013435	3.327699	4.483493	C	-2.585213	-0.578796	3.087650
H	0.730630	1.731877	4.686121	C	-4.667555	-2.270967	2.318401
H	1.526039	3.285221	6.491261	H	-3.185855	-3.386297	1.234599
H	2.897693	2.797580	5.466735	C	-3.887840	-0.326977	3.520982
H	2.170563	4.405898	5.269864	H	-1.779380	0.095751	3.386941
H	1.607022	4.458365	0.398199	C	-4.934681	-1.172364	3.138201
				H	-5.478791	-2.935762	2.010033
96				H	-4.086284	0.537596	4.159758
Ni-3BTanti-3BTsyn-S-Pr SCF Done: -8462.51055967 A.U.				H	-5.954874	-0.972891	3.475709
Ni	0.323138	-0.615987	0.048905	C	3.316844	-1.825068	-1.490599
P	-0.575423	-1.897652	1.642734	C	3.452571	-1.471869	-2.845776
P	1.642959	-2.200138	-0.793495	C	4.459205	-1.784494	-0.670817
C	-0.528432	-3.702034	1.161508				

C	4.694433	-1.100447	-3.366761
H	2.580791	-1.494548	-3.504219
C	5.701403	-1.412720	-1.193934
H	4.390234	-2.036628	0.389481
C	5.824907	-1.070583	-2.543248
H	4.779127	-0.835316	-4.423934
H	6.577215	-1.390457	-0.540113
H	6.796585	-0.781770	-2.951540
C	0.865666	-3.189888	-2.152519
C	1.464167	-4.354883	-2.665794
C	-0.367049	-2.772168	-2.679350
C	0.839654	-5.086250	-3.678380
H	2.430963	-4.690200	-2.280727
C	-0.991241	-3.503799	-3.696523
H	-0.842576	-1.869195	-2.287116
C	-0.390096	-4.661464	-4.195897
H	1.315311	-5.990014	-4.068379
H	-1.949963	-3.163725	-4.096271
H	-0.876484	-5.233923	-4.990053
C	0.763547	1.142759	-0.750566
C	-0.506138	1.178041	-0.049786
C	1.846822	1.816640	-0.024760
S	-0.311941	2.179526	1.470609
C	1.406681	2.359719	1.146895
Br	2.469373	3.275541	2.429319
H	0.796121	1.114860	-1.845855
C	3.237697	1.958597	-0.585542
C	3.371038	3.123422	-1.584918
H	3.524664	1.020141	-1.085007
H	3.953598	2.111093	0.238338
C	4.782557	3.268716	-2.161492
H	2.650883	2.981714	-2.411122
H	3.077564	4.062837	-1.083886

C	4.916132	4.418169	-3.161562
H	5.498169	3.415336	-1.331877
H	5.075674	2.319349	-2.644944
H	5.942420	4.496873	-3.555280
H	4.239375	4.281371	-4.021894
H	4.663387	5.385918	-2.696614
C	-1.782327	1.308246	-0.746915
C	-2.306792	2.402167	-1.419114
S	-2.873713	-0.065482	-0.856302
C	-3.579279	2.125655	-2.020609
C	-4.002024	0.840026	-1.808709
Br	-5.597867	0.055889	-2.440949
C	-1.643976	3.754629	-1.515269
C	-2.290408	4.832184	-0.626537
H	-1.677394	4.092465	-2.567253
H	-0.579327	3.661484	-1.252383
C	-1.619367	6.202805	-0.754914
H	-3.363354	4.922736	-0.876773
H	-2.245540	4.496747	0.423765
C	-2.258199	7.277852	0.125498
H	-0.548995	6.104463	-0.498799
H	-1.647200	6.526066	-1.812045
H	-1.751243	8.249594	0.011350
H	-3.321541	7.425554	-0.128622
H	-2.210762	7.001024	1.191977
H	-4.149042	2.855892	-2.597443

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Ni-3BTanti-3BTsyn-S-TS-3 SCF Done: -8462.46591066 A.U.

Ni	-0.428274	-0.618492	-0.178359
P	0.164188	-2.809715	-0.450616
P	-2.345509	-0.786914	-1.405071
C	-1.364502	-3.839580	-0.764927
H	-2.012287	-3.587905	0.090639

H	-1.134183	-4.911490	-0.661566
C	-2.117596	-3.587602	-2.088739
H	-3.160914	-3.912362	-1.942236
H	-1.704316	-4.245463	-2.870982
C	-2.113998	-2.155942	-2.657965
H	-2.864168	-2.076903	-3.460632
H	-1.136344	-1.946805	-3.121918
C	1.357027	-3.324648	-1.760512
C	2.375720	-2.424256	-2.121104
C	1.292847	-4.571148	-2.409323
C	3.308251	-2.765872	-3.105495
H	2.437385	-1.451169	-1.628239
C	2.221256	-4.906327	-3.399005
H	0.521961	-5.296205	-2.139074
C	3.231405	-4.004457	-3.748735
H	4.097165	-2.057287	-3.369987
H	2.157652	-5.878240	-3.895438
H	3.958276	-4.268760	-4.521169
C	0.804095	-3.613889	1.087219
C	0.098368	-3.397700	2.284983
C	1.967519	-4.397929	1.119444
C	0.534567	-3.970598	3.480984
H	-0.791326	-2.761909	2.290852
C	2.408613	-4.961594	2.321252
H	2.539647	-4.568775	0.205857
C	1.692976	-4.754109	3.502699
H	-0.025221	-3.791048	4.402377
H	3.320123	-5.564963	2.330980
H	2.041038	-5.193742	4.440858
C	-2.735268	0.661782	-2.484776
C	-3.677499	1.623267	-2.079555
C	-2.031558	0.872136	-3.685085
C	-3.918768	2.756331	-2.861599

H	-4.231131	1.486705	-1.148267
C	-2.278037	2.003550	-4.467047
H	-1.278998	0.154135	-4.018891
C	-3.223613	2.949675	-4.059023
H	-4.658333	3.490836	-2.532391
H	-1.726477	2.145787	-5.400056
H	-3.416720	3.833953	-4.671410
C	-3.983952	-1.180891	-0.643128
C	-5.093797	-1.558416	-1.421799
C	-4.125579	-1.108675	0.751962
C	-6.313356	-1.866579	-0.816229
H	-5.011760	-1.602816	-2.510909
C	-5.351332	-1.411984	1.356795
H	-3.276318	-0.803119	1.367976
C	-6.443933	-1.794383	0.575931
H	-7.167263	-2.160067	-1.432486
H	-5.447790	-1.344688	2.443358
H	-7.400167	-2.033145	1.048697
C	1.881198	0.951838	-0.631101
C	1.143942	0.297795	0.361524
C	3.289573	1.068128	-0.390914
S	2.248826	-0.160415	1.664224
C	3.621819	0.512800	0.824666
Br	5.333952	0.486291	1.628820
H	1.424245	1.330964	-1.546238
C	4.241958	1.771795	-1.324330
C	4.360289	3.284296	-1.064178
H	3.908456	1.610326	-2.364583
H	5.242030	1.314819	-1.240890
C	5.314315	3.994616	-2.028756
H	3.357497	3.743812	-1.129656
H	4.698688	3.441982	-0.025116
C	5.440342	5.496012	-1.766276

H	6.312239	3.523589	-1.963524	C	1.278783	3.674737	-2.332898
H	4.972960	3.828488	-3.067340	H	2.013918	3.938666	-1.553898
H	6.133472	5.975598	-2.476089	H	1.394467	4.438559	-3.120711
H	4.464965	6.002699	-1.859639	C	1.623908	2.310743	-2.948648
H	5.816180	5.693864	-0.748478	H	2.512984	2.397679	-3.592541
C	-0.563938	0.955352	0.874358	H	0.792877	1.978256	-3.592009
C	-0.875088	2.316819	0.747659	C	2.458891	-0.456451	-2.777973
S	-1.047744	0.393120	2.496709	C	2.004157	-0.593852	-4.099848
C	-1.520803	2.859034	1.905468	C	3.281576	-1.461047	-2.237305
C	-1.688854	1.955036	2.921318	C	2.376820	-1.701113	-4.869441
Br	-2.517773	2.257860	4.589030	H	1.351680	0.156931	-4.548417
C	-0.491493	3.142080	-0.455224	C	3.654733	-2.562655	-3.008793
C	-1.106007	4.542976	-0.540986	H	3.631490	-1.385651	-1.205833
H	-0.740614	2.582688	-1.373015	C	3.204803	-2.686330	-4.327502
H	0.613061	3.236566	-0.466321	H	2.014801	-1.790239	-5.896847
C	-0.665884	5.314501	-1.789314	H	4.294596	-3.332856	-2.571302
H	-2.208404	4.466672	-0.530003	H	3.496366	-3.550933	-4.929203
H	-0.829892	5.128866	0.353982	C	-2.317157	3.214319	-0.013739
C	-1.270637	6.716000	-1.885165	C	-2.757592	3.686752	1.233249
H	0.437030	5.387707	-1.799796	C	-3.252565	3.089456	-1.056198
H	-0.937730	4.732349	-2.687952	C	-4.097541	4.034425	1.428540
H	-0.932624	7.243592	-2.791703	H	-2.056675	3.788066	2.062945
H	-2.372699	6.675338	-1.915260	C	-4.588950	3.443612	-0.860342
H	-0.989863	7.335416	-1.016628	H	-2.950618	2.696052	-2.028482
H	-1.854157	3.893324	1.986162	C	-5.016069	3.917371	0.383110
				H	-4.421572	4.399010	2.406669
96				H	-5.301459	3.334654	-1.681614
Ni-3BTsyn-3BTsyn-O SCF Done: -8462.48524409 A.U.				H	-6.063489	4.188343	0.537505
Ni	0.099481	0.499536	-0.391623	C	3.556213	1.510014	-0.973897
P	-0.556462	2.727146	-0.308483	C	4.709083	1.629095	-1.772761
P	1.949663	0.954626	-1.703077	C	3.634497	1.851277	0.383934
C	-0.151131	3.789959	-1.787146	C	5.907306	2.088377	-1.224092
H	-0.393803	4.836782	-1.547201	H	4.677239	1.348146	-2.828626
H	-0.867911	3.488712	-2.568297				

C	4.836483	2.311888	0.932996
H	2.755277	1.756048	1.021180
C	5.972968	2.431773	0.131454
H	6.795579	2.173342	-1.855388
H	4.879534	2.571903	1.993336
H	6.913118	2.787208	0.561102
C	0.338233	3.537222	1.094035
C	0.777952	4.871463	1.061306
C	0.569230	2.781692	2.257685
C	1.436245	5.431766	2.159921
H	0.608439	5.492909	0.180416
C	1.217639	3.345693	3.360267
H	0.234749	1.743677	2.303963
C	1.656886	4.671823	3.312357
H	1.774981	6.469955	2.114405
H	1.381578	2.742149	4.256411
H	2.168964	5.113067	4.171208
C	0.643910	-2.534619	-0.426226
C	1.397053	-3.502886	0.331824
C	0.770681	-1.240389	0.045087
C	2.087972	-2.955189	1.376214
S	1.836903	-1.231955	1.450112
Br	3.187002	-3.855750	2.623138
H	1.418823	-4.569131	0.098262
C	-0.195255	-2.954554	-1.610577
C	-1.421070	-3.806550	-1.240787
H	0.435738	-3.523019	-2.319422
H	-0.531797	-2.057178	-2.151364
C	-2.257790	-4.224933	-2.453399
H	-1.091448	-4.710680	-0.695960
H	-2.050585	-3.238643	-0.534536
C	-3.486953	-5.059076	-2.089093
H	-2.579623	-3.318045	-2.996368

H	-1.620594	-4.790222	-3.159221
H	-4.056984	-5.354931	-2.985017
H	-3.202648	-5.982423	-1.555961
H	-4.169125	-4.493776	-1.433062
C	-1.619739	-0.112225	0.178980
C	-2.283393	-0.449947	1.344178
S	-2.711590	-0.295060	-1.190922
C	-3.662062	-0.824174	1.136769
C	-4.039597	-0.787837	-0.175379
H	-4.340440	-1.109733	1.942954
C	-1.664664	-0.489018	2.722796
C	-1.562702	-1.900566	3.325226
H	-2.243881	0.154706	3.412221
H	-0.650856	-0.064665	2.674171
C	-0.923627	-1.922637	4.716903
H	-2.569096	-2.354635	3.377728
H	-0.977642	-2.536661	2.639207
C	-0.787290	-3.328471	5.303871
H	0.075153	-1.452902	4.660230
H	-1.518110	-1.289691	5.402254
H	-0.338706	-3.306450	6.310443
H	-1.768484	-3.825882	5.387766
H	-0.147167	-3.962552	4.668484
Br	-5.737384	-1.206790	-0.893072

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Ni-3BTsyn-3BTsyn-O-Pr-3 SCF Done: -8462.50373808 A.U.

Ni	-1.320272	-0.440661	-0.264495
P	-0.822191	-2.501030	0.187923
P	-3.443139	-0.398366	-0.723819
C	-2.132590	-3.675980	-0.456439
H	-1.946860	-4.687546	-0.060587
H	-1.947650	-3.741462	-1.541960
C	-3.588877	-3.252197	-0.194514

H	-3.730888	-2.998581	0.870591	H	-3.278815	-0.724813	2.138776
H	-4.228079	-4.135357	-0.369888	C	-6.198091	0.895927	2.829207
C	-4.122246	-2.119270	-1.086155	H	-7.470772	1.836343	1.354105
H	-5.221223	-2.089836	-1.016152	H	-4.721589	-0.108164	4.053940
H	-3.870774	-2.329013	-2.139900	H	-6.825338	1.186987	3.675885
C	-4.038858	0.506482	-2.234956	C	-0.837460	-2.814809	2.021055
C	-5.260194	0.225122	-2.876354	C	-1.379725	-3.961774	2.626632
C	-3.200912	1.483578	-2.797010	C	-0.287546	-1.820919	2.851951
C	-5.635722	0.911185	-4.034788	C	-1.362778	-4.115032	4.017328
H	-5.933545	-0.535775	-2.475797	H	-1.822741	-4.752772	2.018557
C	-3.576477	2.172496	-3.954464	C	-0.261686	-1.976716	4.240439
H	-2.239840	1.695883	-2.324485	H	0.115738	-0.912392	2.398171
C	-4.795197	1.889248	-4.575816	C	-0.800804	-3.125349	4.828199
H	-6.588832	0.678760	-4.517495	H	-1.792065	-5.014176	4.467447
H	-2.908809	2.929643	-4.373774	H	0.173862	-1.192561	4.865247
H	-5.088431	2.424241	-5.482960	H	-0.788594	-3.246108	5.914545
C	0.690757	-3.409461	-0.396609	C	1.683803	3.194537	-0.198581
C	1.308929	-4.447012	0.321366	C	0.434646	3.851255	0.053637
C	1.214387	-3.050905	-1.650734	C	1.556517	1.821451	-0.301785
C	2.418736	-5.113983	-0.207728	C	-0.627347	2.990630	0.095382
H	0.928308	-4.737691	1.303038	S	-0.147012	1.320034	-0.136436
C	2.313601	-3.727597	-2.185454	Br	-2.414346	3.453200	0.455638
H	0.764256	-2.222247	-2.205432	H	0.339091	4.928399	0.197430
C	2.920100	-4.760421	-1.463772	C	2.983341	3.954119	-0.307150
H	2.892312	-5.915559	0.365906	C	3.523355	4.459000	1.042770
H	2.711998	-3.433498	-3.159367	H	2.834664	4.820714	-0.976267
H	3.788244	-5.281140	-1.876124	H	3.742692	3.318226	-0.788115
C	-4.579063	0.151187	0.641532	C	4.822768	5.259554	0.914284
C	-5.759234	0.886680	0.442829	H	2.755739	5.081051	1.537805
C	-4.214563	-0.189043	1.957852	H	3.685467	3.594185	1.710319
C	-6.559388	1.257865	1.528632	C	5.364447	5.761663	2.253456
H	-6.057085	1.185546	-0.563668	H	5.586141	4.633967	0.416970
C	-5.022135	0.169744	3.040253	H	4.654178	6.118097	0.238701

H	6.296287	6.335000	2.123869	H	2.691297	2.429297	-4.113678
H	4.637128	6.418629	2.759467	C	2.037210	0.520917	-3.386638
H	5.582007	4.924382	2.937744	H	2.761484	0.061602	-4.077724
C	2.595827	0.844656	-0.613724	H	1.051370	0.468657	-3.877243
C	3.298929	-0.004115	0.222630	C	1.695487	-2.228688	-2.518831
S	3.115195	0.655339	-2.286528	C	1.074638	-2.475591	-3.755513
C	4.264632	-0.795850	-0.484497	C	2.087878	-3.327176	-1.731918
C	4.280752	-0.541785	-1.829580	C	0.865335	-3.785334	-4.199539
H	4.916573	-1.529226	-0.009095	H	0.745189	-1.649372	-4.388493
C	3.105556	-0.084950	1.715969	C	1.880043	-4.633664	-2.178332
C	4.340331	0.325150	2.536245	H	2.563075	-3.161751	-0.762249
H	2.824825	-1.119195	1.983768	C	1.268803	-4.868323	-3.414418
H	2.252375	0.551018	1.999913	H	0.384711	-3.956858	-5.166265
C	4.119723	0.226481	4.048928	H	2.196566	-5.473520	-1.554347
H	5.202156	-0.305248	2.251925	H	1.106509	-5.891317	-3.763180
H	4.624996	1.359222	2.271289	C	-0.490753	3.818648	-0.543157
C	5.345917	0.625874	4.870904	C	-0.266622	4.999255	0.184775
H	3.261861	0.863576	4.331747	C	-1.753742	3.611600	-1.125757
H	3.821889	-0.806764	4.304807	C	-1.279599	5.954817	0.314845
H	5.152463	0.545831	5.952575	H	0.701183	5.179808	0.656163
H	6.211164	-0.017746	4.639143	C	-2.760449	4.572053	-1.002360
H	5.645959	1.666684	4.662913	H	-1.961457	2.686314	-1.668405
Br	5.398324	-1.347381	-3.117410	C	-2.526330	5.746975	-0.281477
				H	-1.089640	6.867674	0.885704
96				H	-3.735977	4.389808	-1.460016
Ni-3BTsyn-3BTsyn-O-TS-3 SCF Done: -8462.46417319 A.U.				H	-3.316291	6.495515	-0.178763
Ni	0.311913	0.300768	-0.462651	C	3.688847	-0.591252	-1.274340
P	0.797045	2.509524	-0.784997	C	4.736236	-0.937307	-2.148075
P	1.925626	-0.523505	-1.841077	C	3.991343	-0.305782	0.065767
C	1.296794	2.874464	-2.550117	C	6.055263	-0.979574	-1.693852
H	1.566261	3.939307	-2.633114	H	4.522832	-1.190863	-3.189818
H	0.369602	2.753213	-3.135288	C	5.314045	-0.353226	0.521919
C	2.408970	1.992631	-3.140117	H	3.187259	-0.056896	0.760707
H	3.316600	2.050492	-2.515783				

C	6.347011	-0.685412	-0.356281
H	6.859192	-1.249392	-2.383790
H	5.532091	-0.129101	1.568999
H	7.380120	-0.721676	-0.000801
C	2.218899	3.128226	0.225600
C	3.192883	4.019101	-0.256520
C	2.313639	2.689731	1.558583
C	4.232891	4.455961	0.570243
H	3.148476	4.388639	-1.282629
C	3.344537	3.136364	2.389197
H	1.574205	1.986469	1.948701
C	4.310598	4.018127	1.895101
H	4.984156	5.145035	0.175598
H	3.395515	2.787117	3.423604
H	5.122779	4.362442	2.540449
C	-0.621975	-2.526157	0.484061
C	-0.158703	-3.305874	1.592615
C	-0.303174	-1.163994	0.590963
C	0.502525	-2.584006	2.549343
S	0.563990	-0.895569	2.133276
Br	1.274485	-3.231299	4.145076
H	-0.310746	-4.384781	1.663308
C	-1.391229	-3.190490	-0.633452
C	-2.857049	-3.505995	-0.285056
H	-0.879367	-4.133448	-0.894346
H	-1.352301	-2.574295	-1.542196
C	-3.620675	-4.174324	-1.432111
H	-2.887699	-4.157396	0.607531
H	-3.370194	-2.573026	0.002887
C	-5.082728	-4.473513	-1.097659
H	-3.574274	-3.521025	-2.322199
H	-3.104989	-5.109653	-1.718609
H	-5.601544	-4.959247	-1.940074

H	-5.166629	-5.142827	-0.224641
H	-5.631946	-3.547954	-0.857278
C	-1.495313	0.218736	0.135941
C	-2.332385	0.859537	1.061582
S	-2.429800	-0.114385	-1.350966
C	-3.666120	1.056782	0.582200
C	-3.874877	0.597159	-0.690670
H	-4.443217	1.549396	1.169796
C	-1.938191	1.341486	2.437239
C	-2.461824	0.469208	3.591819
H	-2.321242	2.370129	2.567719
H	-0.843622	1.423539	2.508326
C	-2.025235	0.966108	4.972840
H	-3.565396	0.428892	3.545563
H	-2.112994	-0.567207	3.447092
C	-2.536804	0.097299	6.122807
H	-0.921141	1.005670	5.006075
H	-2.368342	2.008064	5.112919
H	-2.207648	0.483142	7.101269
H	-3.639157	0.056183	6.135196
H	-2.169496	-0.938516	6.032126
Br	-5.469525	0.700561	-1.696160

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Ni-3BTsyn-3BTsyn-S SCF Done: -8462.48422430 A.U.

Ni	-0.166973	0.441162	0.266702
P	1.006316	2.440645	0.167940
P	-1.975437	1.359083	1.367162
C	0.623948	3.726661	1.460081
H	1.120041	4.669718	1.185031
H	1.116153	3.378301	2.382685
C	-0.862799	3.968626	1.751380
H	-1.403539	4.233791	0.826955
H	-0.932921	4.858323	2.399720

C	-1.558421	2.805468	2.472538	H	-6.600914	3.179394	0.822874
H	-2.493267	3.146661	2.943673	H	-4.140505	3.207698	-2.724808
H	-0.905409	2.437727	3.280322	H	-6.304787	3.729397	-1.593794
C	-2.796538	0.189438	2.535290	C	0.550657	3.260431	-1.432925
C	-2.464083	0.140256	3.899457	C	0.636512	4.650593	-1.622685
C	-3.738573	-0.728777	2.036075	C	0.145444	2.456240	-2.512316
C	-3.069389	-0.792923	4.747869	C	0.314353	5.221287	-2.856310
H	-1.727264	0.825562	4.321596	H	0.965219	5.304222	-0.812125
C	-4.343660	-1.656181	2.886013	C	-0.166045	3.027832	-3.750480
H	-4.001802	-0.722095	0.976765	H	0.080215	1.373275	-2.390160
C	-4.012124	-1.691636	4.244389	C	-0.086810	4.411586	-3.923937
H	-2.799287	-0.814040	5.806740	H	0.383396	6.304496	-2.985396
H	-5.073131	-2.360554	2.478859	H	-0.471993	2.383653	-4.578510
H	-4.485819	-2.420179	4.907273	H	-0.333098	4.859878	-4.889836
C	2.857608	2.512686	0.099892	C	-1.357310	-2.384032	0.413227
C	3.511678	1.941581	-1.006473	C	-2.251697	-3.231895	-0.333459
C	3.635439	3.113128	1.104301	C	-1.202758	-1.122796	-0.132943
C	4.902896	1.982133	-1.109945	C	-2.764281	-2.627797	-1.447675
H	2.935202	1.452985	-1.793679	S	-2.168866	-0.997937	-1.599763
C	5.030399	3.150906	0.998790	Br	-3.972117	-3.367151	-2.698859
H	3.172000	3.561174	1.983890	H	-2.500944	-4.254836	-0.044776
C	5.667984	2.588679	-0.108839	C	-0.665796	-2.882115	1.660770
H	5.389316	1.527846	-1.976368	C	0.364903	-3.995080	1.405637
H	5.617018	3.625928	1.789415	H	-1.425097	-3.256431	2.373149
H	6.757416	2.619411	-0.190741	H	-0.171727	-2.033768	2.159675
C	-3.391433	2.066993	0.409455	C	1.003636	-4.542482	2.685982
C	-4.614780	2.364006	1.038673	H	-0.119347	-4.826116	0.861172
C	-3.237251	2.376315	-0.949861	H	1.149081	-3.609554	0.732061
C	-5.654709	2.958830	0.322052	C	2.042627	-5.635427	2.429945
H	-4.764094	2.118889	2.093147	H	1.474546	-3.711262	3.242752
C	-4.278856	2.975829	-1.666043	H	0.211049	-4.933050	3.351167
H	-2.301340	2.147295	-1.459457	H	2.484246	-6.006941	3.369084
C	-5.488508	3.266933	-1.032946	H	1.595382	-6.498364	1.908333

H	2.865061	-5.262363	1.797195	H	4.754778	-1.364218	1.197550
C	1.366533	-0.556166	-0.300965	H	3.742434	-0.002829	1.674916
C	2.451968	-0.938647	0.475720	C	1.416924	0.844462	3.369278
S	1.554985	-1.178171	-1.925649	C	1.812226	2.045473	2.759361
C	3.433142	-1.705601	-0.246579	C	1.630313	0.682181	4.749869
C	3.093700	-1.900833	-1.558605	C	2.415177	3.061161	3.510382
H	4.356621	-2.090911	0.186315	H	1.635351	2.190905	1.691111
C	2.571815	-0.616838	1.951520	C	2.238776	1.692488	5.497863
C	3.996806	-0.491908	2.503717	H	1.309049	-0.235526	5.250006
H	2.035881	-1.385181	2.540233	C	2.633186	2.884577	4.878665
H	2.022619	0.322403	2.148295	H	2.705773	3.993223	3.019365
C	4.038190	-0.071671	3.976677	H	2.400544	1.552360	6.569960
H	4.522879	-1.457522	2.397812	H	3.104345	3.676722	5.466499
H	4.565934	0.234392	1.898012	C	-0.960410	-0.755112	3.235589
C	5.454443	0.027478	4.545448	C	-1.410418	-2.021593	3.642919
H	3.527653	0.902894	4.090046	C	-1.799155	0.356622	3.438951
H	3.448520	-0.788561	4.577216	C	-2.661691	-2.170378	4.250966
H	5.448293	0.333306	5.604197	H	-0.794946	-2.909211	3.484409
H	5.979082	-0.940643	4.482135	C	-3.045705	0.205862	4.048044
H	6.057989	0.763581	3.988232	H	-1.474216	1.348448	3.114328
Br	4.102873	-2.813627	-2.870439	C	-3.481486	-1.059038	4.457726
				H	-2.995736	-3.163862	4.561629
96				H	-3.682156	1.081397	4.200476
Ni-3BTsyn-3BTsyn-S-Pr SCF Done: -8462.50664153 A.U.				H	-4.458892	-1.177354	4.932294
Ni	0.727340	-0.127069	0.134165	C	3.891856	-0.320669	-1.374215
P	0.633415	-0.484117	2.339428	C	4.228978	-0.911434	-2.604049
P	2.708926	-1.098659	-0.181613	C	4.394972	0.962446	-1.085647
C	1.630637	-2.003495	2.771839	C	5.058374	-0.244305	-3.511907
H	1.223266	-2.789889	2.115786	H	3.845393	-1.901458	-2.858441
H	1.429868	-2.321015	3.806910	C	5.230071	1.622954	-1.989623
C	3.160438	-1.897781	2.576064	H	4.124617	1.461149	-0.151582
H	3.545104	-2.927672	2.494702	C	5.565611	1.021349	-3.207178
H	3.603183	-1.481249	3.495610	H	5.310053	-0.721242	-4.462902
C	3.713101	-1.067974	1.397330				

H	5.614330	2.616302	-1.743670
H	6.215695	1.539819	-3.916407
C	2.718816	-2.889097	-0.647377
C	3.886430	-3.673435	-0.607340
C	1.509550	-3.496074	-1.024346
C	3.843445	-5.029944	-0.937089
H	4.841811	-3.222942	-0.325973
C	1.467119	-4.854821	-1.357061
H	0.593918	-2.899959	-1.050087
C	2.632689	-5.623382	-1.313114
H	4.758596	-5.626926	-0.901598
H	0.517648	-5.310870	-1.648724
H	2.600411	-6.685095	-1.571261
C	0.192690	0.747835	-1.560028
C	-0.893863	0.784920	-0.579346
C	0.908646	2.025568	-1.572757
S	-1.069438	2.479428	0.093680
C	0.372941	2.982015	-0.772607
Br	1.074713	4.720551	-0.493324
C	-2.122656	0.004638	-0.692606
C	-3.360713	0.303399	-1.245793
S	-2.099967	-1.651388	-0.097741
C	-4.272950	-0.803934	-1.191401
C	-3.730655	-1.922732	-0.618970
Br	-4.566409	-3.598695	-0.388833
C	-3.762402	1.622629	-1.862025
C	-4.713453	2.458766	-0.988258
H	-4.255577	1.419884	-2.830088
H	-2.865156	2.217564	-2.086138
C	-5.123283	3.783465	-1.638128
H	-5.616989	1.866386	-0.754428
H	-4.222712	2.660524	-0.020257
C	-6.074623	4.615853	-0.777393

H	-4.213882	4.371223	-1.858206
H	-5.593750	3.579048	-2.617600
H	-6.348206	5.560946	-1.273505
H	-7.008794	4.068233	-0.566426
H	-5.616697	4.870288	0.193183
H	-5.290265	-0.766148	-1.584344
H	1.792525	2.198783	-2.189238
C	0.162746	-0.097814	-2.825413
C	-0.512366	0.580304	-4.030190
C	-0.523772	-0.292844	-5.288804
C	-1.184166	0.378488	-6.494097
H	1.199135	-0.361717	-3.101184
H	-0.351150	-1.049457	-2.616645
H	0.001921	1.533438	-4.250099
H	-1.548325	0.850533	-3.762043
H	0.514496	-0.572990	-5.545967
H	-1.043115	-1.242837	-5.065744
H	-1.175054	-0.276522	-7.380346
H	-0.665733	1.313530	-6.765616
H	-2.235377	0.636675	-6.282095

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Ni-3BTsyn-3BTsyn-S-TS-3 SCF Done: -8462.45935939 A.U.

Ni	-0.172659	0.433449	0.255377
P	0.710034	2.547429	0.274820
P	-2.078799	0.920229	1.409986
C	0.181728	3.586912	1.730675
H	0.527402	4.621586	1.585380
H	0.749243	3.191950	2.590142
C	-1.316761	3.588897	2.072099
H	-1.914082	3.879072	1.191042
H	-1.481571	4.387814	2.815152
C	-1.852495	2.279178	2.672121
H	-2.816399	2.456740	3.174918

H	-1.148137	1.914254	3.437852	H	-6.592084	3.023153	-1.486084
C	-2.805156	-0.455013	2.402526	C	0.149479	3.520086	-1.205665
C	-2.577092	-0.601715	3.782040	C	-0.147086	4.892620	-1.172397
C	-3.547801	-1.446936	1.734333	C	0.042389	2.838696	-2.431505
C	-3.088980	-1.702126	4.477339	C	-0.543225	5.564658	-2.332570
H	-1.999256	0.142231	4.333428	H	-0.069364	5.457489	-0.241261
C	-4.061564	-2.541942	2.431932	C	-0.342441	3.513409	-3.593563
H	-3.730856	-1.362460	0.661103	H	0.260882	1.769165	-2.480001
C	-3.834283	-2.674493	3.805655	C	-0.640231	4.878268	-3.546412
H	-2.905539	-1.795014	5.550994	H	-0.774168	6.632176	-2.286465
H	-4.640365	-3.298123	1.895382	H	-0.414454	2.965772	-4.536648
H	-4.236354	-3.532649	4.350114	H	-0.947375	5.406160	-4.452847
C	2.542065	2.859463	0.242615	C	-0.925576	-2.612984	-0.033475
C	3.303682	2.171979	-0.718155	C	-1.776124	-3.245017	-0.997855
C	3.205568	3.730455	1.124784	C	-0.524931	-1.319318	-0.401690
C	4.685213	2.356200	-0.802694	C	-2.033312	-2.484180	-2.105482
H	2.818945	1.472613	-1.401397	S	-1.245025	-0.932084	-2.005346
C	4.590321	3.911060	1.041539	Br	-3.109446	-2.944546	-3.584481
H	2.657521	4.282594	1.888969	H	-2.179294	-4.250946	-0.864330
C	5.334274	3.226879	0.077505	C	-0.473710	-3.372762	1.189037
H	5.255018	1.803248	-1.553487	C	0.620814	-4.420640	0.908844
H	5.087094	4.593438	1.736443	H	-1.349650	-3.888985	1.621051
H	6.416349	3.368183	0.015389	H	-0.132157	-2.675986	1.965690
C	-3.550353	1.556771	0.480438	C	1.025930	-5.221779	2.150100
C	-4.807047	1.690611	1.099810	H	0.263480	-5.115606	0.127708
C	-3.409882	1.954909	-0.857783	H	1.507493	-3.920244	0.484422
C	-5.892810	2.216207	0.397566	C	2.108399	-6.266777	1.875046
H	-4.943650	1.371531	2.136342	H	1.376673	-4.526272	2.934744
C	-4.498942	2.483634	-1.560546	H	0.131711	-5.717165	2.571896
H	-2.447533	1.845760	-1.359316	H	2.375253	-6.826302	2.786338
C	-5.740366	2.614992	-0.935699	H	1.774978	-6.998938	1.120428
H	-6.863528	2.311633	0.891226	H	3.028771	-5.797054	1.489713
H	-4.371481	2.787131	-2.602535	C	1.224134	-0.805169	-0.269778

C	2.142711	-1.147231	0.739612	Br	2.047761	-0.903329	-2.311743
S	1.996593	-1.050068	-1.857198	C	0.337173	-0.386374	3.095230
C	3.415037	-1.571481	0.238025	C	0.718422	-1.523204	3.828283
C	3.492106	-1.563346	-1.128388	C	-1.000440	0.039749	3.152360
H	4.248409	-1.870657	0.876523	C	-0.213025	-2.208369	4.613061
C	1.882522	-1.026096	2.224695	H	1.744048	-1.895937	3.787439
C	2.789872	-0.021741	2.956840	C	-1.930118	-0.650804	3.933035
H	2.005038	-2.014383	2.707630	H	-1.325639	0.903102	2.570321
H	0.830255	-0.734069	2.380821	C	-1.539499	-1.773003	4.668946
C	2.471113	0.105908	4.449710	H	0.101197	-3.089598	5.178100
H	3.845866	-0.322607	2.836508	H	-2.968779	-0.312312	3.956437
H	2.709627	0.966280	2.472853	H	-2.269137	-2.311479	5.278917
C	3.386425	1.083020	5.189328	C	5.316640	-0.628679	-1.029936
H	1.417989	0.422702	4.570102	C	6.389211	-0.110933	-1.770722
H	2.535267	-0.890591	4.923833	C	5.177449	-2.021078	-0.905348
H	3.124671	1.157746	6.257174	C	7.311947	-0.973567	-2.371683
H	4.441264	0.767439	5.126738	H	6.504528	0.968456	-1.890534
H	3.324463	2.096343	4.757747	C	6.106101	-2.879045	-1.497327
Br	4.976954	-2.047955	-2.187711	H	4.325211	-2.437800	-0.363357
				C	7.174694	-2.356897	-2.233617
96				H	8.139683	-0.559370	-2.953161
NiBr-TTBTBr SCF Done: -8462.56786435 A.U.				H	5.984023	-3.960474	-1.397677
Ni	1.912815	-0.247064	-0.044391	H	7.894877	-3.029420	-2.706633
P	4.123474	0.457490	-0.136463	C	1.013117	2.243790	2.007270
P	1.565354	0.483046	2.027802	C	0.720283	2.933522	3.198275
C	5.011254	0.590518	1.498669	C	0.918000	2.926461	0.784826
H	6.000864	1.040736	1.324662	C	0.346897	4.278112	3.163194
H	5.207584	-0.453668	1.794679	H	0.768162	2.417733	4.160657
C	4.262320	1.317179	2.622643	C	0.545650	4.274304	0.751725
H	3.961803	2.329314	2.303693	H	1.132264	2.402081	-0.149090
H	4.965665	1.464704	3.460169	C	0.260582	4.951453	1.938986
C	3.048414	0.553060	3.163737	H	0.118019	4.801842	4.094847
H	2.707538	0.996414	4.112197	H	0.477341	4.790911	-0.208469
H	3.335999	-0.486788	3.388354				

H	-0.033565	6.003849	1.913457
C	4.314153	2.130394	-0.904226
C	5.114457	3.142163	-0.345355
C	3.612895	2.403898	-2.094481
C	5.212227	4.395382	-0.959008
H	5.675657	2.969254	0.573906
C	3.720084	3.654260	-2.708024
H	2.986381	1.626893	-2.540034
C	4.516961	4.654658	-2.142344
H	5.837914	5.169677	-0.507605
H	3.173570	3.845598	-3.635063
H	4.595858	5.633545	-2.622322
C	-0.400645	-2.104505	0.252872
C	-1.820772	-2.194753	0.095910
C	0.097133	-0.846695	-0.043810
C	-2.427656	-1.027086	-0.318932
S	-1.202454	0.215892	-0.517133
H	-2.382381	-3.116880	0.267848
C	0.452371	-3.290507	0.638054
C	0.626834	-4.323403	-0.488692
H	0.017743	-3.791219	1.523033
H	1.449571	-2.930888	0.947120
C	1.496400	-5.519528	-0.090218
H	-0.368109	-4.684656	-0.806649
H	1.062366	-3.818024	-1.367448
C	1.663505	-6.551983	-1.206355
H	2.492257	-5.154505	0.224608
H	1.062715	-6.007749	0.802541
H	2.297311	-7.396429	-0.889691
H	0.689219	-6.965611	-1.516636
H	2.126651	-6.101719	-2.100098
C	-3.828568	-0.756933	-0.575852
C	-4.402913	0.211277	-1.374822

S	-5.079920	-1.723545	0.187776
C	-5.835211	0.194767	-1.413768
H	-3.805078	0.913369	-1.959486
C	-6.328279	-0.810883	-0.612892
Br	-8.140665	-1.266519	-0.336063
C	-6.659762	1.168752	-2.214158
C	-6.926239	2.498233	-1.485681
H	-7.622778	0.702695	-2.478985
H	-6.139644	1.375593	-3.165534
C	-7.739825	3.493193	-2.318403
H	-7.454174	2.288110	-0.538647
H	-5.962247	2.956573	-1.199729
C	-8.011320	4.813449	-1.595820
H	-7.208368	3.693546	-3.266863
H	-8.699107	3.025874	-2.606579
H	-8.595986	5.505938	-2.222550
H	-8.576925	4.650600	-0.663028
H	-7.071140	5.322897	-1.324927

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NiCl-3BTsyn SCF Done: -5640.01644833 A.U.

Ni	0.369279	0.063358	-0.384621
P	-0.141607	-1.074626	1.457960
P	2.615547	-0.516627	-0.224049
C	0.981219	-2.553422	1.659154
H	0.984154	-3.048028	0.673825
H	0.516326	-3.255668	2.367645
C	2.423851	-2.266761	2.112435
H	2.999215	-3.189475	1.934280
H	2.430085	-2.115500	3.203765
C	3.161619	-1.072865	1.469843
H	4.248422	-1.248508	1.471782
H	3.010859	-0.165052	2.075038
Cl	0.880443	1.185647	-2.232947

C	0.074227	-0.152153	3.043748
C	0.640495	1.131775	3.038651
C	-0.283459	-0.733744	4.273781
C	0.849157	1.822555	4.237187
H	0.916349	1.596225	2.089246
C	-0.073554	-0.043982	5.469686
H	-0.739912	-1.726475	4.299221
C	0.493409	1.235541	5.453562
H	1.285454	2.824172	4.216040
H	-0.357842	-0.505691	6.418672
H	0.652740	1.775565	6.390301
C	-1.820032	-1.814750	1.608935
C	-2.072732	-3.140207	1.219980
C	-2.890320	-1.019005	2.052052
C	-3.368125	-3.661978	1.282856
H	-1.268709	-3.777720	0.848258
C	-4.182110	-1.543457	2.112832
H	-2.718852	0.020035	2.338406
C	-4.424982	-2.865888	1.728945
H	-3.549643	-4.694068	0.972737
H	-5.005429	-0.910450	2.452294
H	-5.438647	-3.272016	1.770587
C	3.852158	0.820536	-0.518025
C	5.163634	0.529995	-0.925621
C	3.493790	2.154429	-0.264422
C	6.104067	1.554884	-1.064444
H	5.455142	-0.498902	-1.148686
C	4.438521	3.175408	-0.394690
H	2.463838	2.399176	0.001017
C	5.744776	2.878399	-0.794574
H	7.120066	1.316759	-1.389785
H	4.145959	4.210265	-0.200019
H	6.479677	3.679763	-0.906480

C	3.078616	-1.894182	-1.362028
C	3.968887	-2.917033	-0.986588
C	2.507013	-1.929086	-2.648321
C	4.277904	-3.952973	-1.873892
H	4.436396	-2.914838	-0.000014
C	2.822845	-2.964303	-3.531893
H	1.821009	-1.134607	-2.952684
C	3.704746	-3.979162	-3.148035
H	4.970834	-4.740399	-1.566121
H	2.372011	-2.976091	-4.527372
H	3.945722	-4.789538	-3.840861
C	-2.231794	1.613834	-0.334887
C	-1.472490	0.502586	-0.653541
C	-3.578936	1.545852	-0.842033
S	-2.417237	-0.620487	-1.604284
C	-3.828198	0.397292	-1.542186
H	-4.325949	2.327578	-0.689684
Br	-5.451363	-0.104016	-2.370516
C	-1.714995	2.840698	0.380731
C	-1.361876	4.001428	-0.565996
H	-0.818268	2.572082	0.961897
H	-2.463659	3.190148	1.116695
C	-0.829276	5.241637	0.157509
H	-0.617278	3.640947	-1.295823
H	-2.256686	4.276120	-1.153639
C	-0.476234	6.393384	-0.785205
H	-1.575738	5.586321	0.897551
H	0.064894	4.962064	0.746306
H	-0.092208	7.268386	-0.235587
H	0.293721	6.090134	-1.514065
H	-1.357909	6.722754	-1.360353

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Ni-TTBTBr-BTanti-O SCF Done: -9171.23479601 A.U.

Ni	-1.677119	-0.849023	0.380140	H	-8.332928	1.412032	-1.301184
P	-3.572967	-1.745841	-0.599914	C	-0.050063	-3.975111	0.379202
P	-1.087030	-2.828227	1.392212	C	0.532879	-5.123191	0.946276
C	-4.356685	-3.241858	0.197972	C	0.124844	-3.731075	-0.991168
H	-5.110927	-3.645797	-0.495101	C	1.267590	-6.008484	0.155717
H	-4.925773	-2.842267	1.053061	H	0.425192	-5.322607	2.015450
C	-3.412829	-4.348951	0.685871	C	0.859219	-4.620543	-1.782962
H	-2.801867	-4.738740	-0.145523	H	-0.311203	-2.840377	-1.446124
H	-4.038201	-5.195830	1.016662	C	1.431158	-5.759029	-1.211887
C	-2.510896	-3.944058	1.859764	H	1.718752	-6.894578	0.609639
H	-2.091746	-4.838565	2.346299	H	0.986195	-4.414589	-2.848438
H	-3.112195	-3.416905	2.618376	H	2.009581	-6.451439	-1.828976
C	-0.155545	-2.700523	2.980170	C	-3.108843	-2.321969	-2.295508
C	-0.796211	-2.787334	4.227657	C	-3.521589	-3.552240	-2.834360
C	1.228455	-2.452063	2.946377	C	-2.291587	-1.483890	-3.077684
C	-0.068265	-2.642965	5.413397	C	-3.123018	-3.937840	-4.118085
H	-1.870812	-2.965406	4.294206	H	-4.160617	-4.227025	-2.263311
C	1.952645	-2.311437	4.131447	C	-1.902976	-1.867241	-4.364201
H	1.745054	-2.360963	1.988854	H	-1.970946	-0.520377	-2.678257
C	1.307573	-2.406908	5.368712	C	-2.313395	-3.097557	-4.886721
H	-0.583400	-2.715198	6.374674	H	-3.450626	-4.900889	-4.517941
H	3.026601	-2.115704	4.083461	H	-1.273940	-1.199501	-4.958263
H	1.876013	-2.294043	6.295374	H	-2.004777	-3.399954	-5.890669
C	-5.091852	-0.726997	-0.871430	C	0.459956	0.641086	1.941420
C	-5.533300	-0.351787	-2.148813	C	1.844316	0.998556	1.849455
C	-5.828667	-0.308142	0.250546	C	0.015606	-0.102215	0.859306
C	-6.693143	0.415406	-2.299819	C	2.484037	0.553970	0.711340
H	-4.974336	-0.655170	-3.035301	S	1.334662	-0.347249	-0.268279
C	-6.991854	0.447173	0.097175	H	2.357290	1.590721	2.611849
H	-5.488869	-0.557458	1.259454	C	-0.404337	1.059578	3.108441
C	-7.427408	0.812242	-1.180465	C	-0.548219	2.581126	3.275193
H	-7.021840	0.702640	-3.301817	H	0.006741	0.632958	4.043012
H	-7.551028	0.765311	0.980553	H	-1.406123	0.616472	2.986432

C	-1.473988	2.982096	4.427149
H	0.447976	3.032692	3.434806
H	-0.930160	3.007391	2.332310
C	-1.637014	4.495437	4.578625
H	-2.465904	2.521935	4.265390
H	-1.092164	2.552081	5.372077
H	-2.303695	4.751252	5.418353
H	-0.666698	4.987290	4.762527
H	-2.064480	4.941139	3.665102
C	3.865673	0.717963	0.306858
C	4.435880	0.593977	-0.944615
S	5.100616	1.119730	1.489246
C	5.848789	0.828112	-0.994804
H	3.845963	0.361277	-1.833460
C	6.332834	1.127967	0.258742
Br	8.114995	1.539161	0.730440
C	6.666913	0.727913	-2.255718
C	7.081674	-0.711285	-2.610489
H	7.570730	1.350790	-2.156843
H	6.084326	1.152180	-3.092058
C	7.889501	-0.807092	-3.908015
H	7.669842	-1.131147	-1.775325
H	6.177705	-1.341922	-2.690500
C	8.301122	-2.236064	-4.265027
H	7.299184	-0.374448	-4.736658
H	8.791109	-0.173695	-3.821489
H	8.880752	-2.269320	-5.201543
H	8.923750	-2.683347	-3.472104
H	7.419607	-2.886274	-4.395900
C	-2.061341	0.918463	-0.253542
C	-1.573188	1.688511	-1.289184
S	-3.194021	1.887143	0.666309
C	-2.087836	3.030625	-1.383716

H	-0.801450	1.331196	-1.976580
C	-2.981091	3.274874	-0.368144
C	-1.637267	4.025361	-2.421953
C	-0.366750	4.796372	-2.020511
H	-2.448133	4.745495	-2.622179
H	-1.450706	3.491702	-3.370618
C	0.111878	5.782711	-3.089873
H	-0.562450	5.337979	-1.078373
H	0.439072	4.075911	-1.792682
C	1.370883	6.552442	-2.687789
H	0.299008	5.235478	-4.032459
H	-0.701404	6.496692	-3.315831
H	1.688551	7.252629	-3.477332
H	1.204046	7.139656	-1.769232
H	2.212860	5.868013	-2.490125
Br	-3.912792	4.886143	-0.020226

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Ni-TTBTBr-BTanti-O-Pr SCF Done: -9171.23697497 A.U.

P	1.024580	-1.708312	1.900245
P	0.542665	1.646231	2.107815
C	1.637982	-1.066019	3.550317
H	2.522835	-0.464058	3.291673
H	1.998086	-1.894962	4.180221
C	0.633458	-0.211233	4.346168
H	1.210297	0.350110	5.099842
H	-0.034432	-0.881536	4.912753
C	-0.260909	0.776453	3.569029
H	-0.677416	1.518266	4.268675
H	-1.121450	0.244746	3.133508
C	-0.356728	-2.829351	2.422357
C	-1.605697	-2.706373	1.792588
C	-0.218348	-3.761619	3.467777
C	-2.688980	-3.496835	2.192977

H	-1.730959	-1.979973	0.986780
C	-1.298803	-4.551364	3.867237
H	0.743721	-3.880412	3.972501
C	-2.537909	-4.420280	3.229695
H	-3.653625	-3.384021	1.692422
H	-1.174221	-5.271112	4.680677
H	-3.384055	-5.036621	3.544336
C	2.406768	-2.863090	1.462332
C	3.699892	-2.324087	1.316584
C	2.222603	-4.235218	1.221769
C	4.781827	-3.140150	0.981877
H	3.866693	-1.252867	1.456607
C	3.306569	-5.049876	0.877003
H	1.229043	-4.678579	1.310013
C	4.590204	-4.509451	0.766318
H	5.777687	-2.701193	0.880277
H	3.143672	-6.116253	0.699186
H	5.436885	-5.149688	0.505822
C	-0.639749	3.053552	1.853914
C	-0.217974	4.390297	1.752471
C	-2.006068	2.768364	1.675626
C	-1.139923	5.413356	1.505771
H	0.837583	4.642262	1.873788
C	-2.927489	3.791088	1.439570
H	-2.361384	1.735391	1.706050
C	-2.498095	5.119582	1.356306
H	-0.791458	6.447388	1.436459
H	-3.983340	3.543318	1.305696
H	-3.218037	5.920432	1.169325
C	1.981763	2.484633	2.934839
C	1.839362	3.197857	4.140244
C	3.259629	2.378207	2.365322
C	2.946355	3.785779	4.756015

H	0.853320	3.306184	4.599365
C	4.369857	2.970153	2.979630
H	3.385759	1.828272	1.430400
C	4.215704	3.672867	4.176343
H	2.818598	4.336580	5.691745
H	5.356594	2.879400	2.518070
H	5.081383	4.134155	4.658809
C	-0.010059	2.030241	-1.670242
C	0.619378	0.782640	-1.365907
C	-1.403639	1.931701	-1.664467
S	-0.632876	-0.525340	-1.286104
C	-1.926232	0.642572	-1.491872
C	1.962527	0.351123	-1.741862
C	2.333367	-0.742856	-2.501161
S	3.402369	1.255603	-1.281952
C	3.738879	-0.884371	-2.736728
C	4.432808	0.133511	-2.121116
Br	6.298063	0.434192	-2.130405
H	-2.057915	2.791993	-1.810032
C	0.774112	3.284378	-1.968585
H	1.372280	3.563047	-1.079952
C	-3.307124	0.232943	-1.485888
C	-3.866107	-1.036636	-1.502747
S	-4.588156	1.442195	-1.505949
C	-5.295531	-1.070751	-1.562588
H	-3.259105	-1.944517	-1.508821
C	-5.814118	0.205204	-1.567271
C	-6.106738	-2.340200	-1.605647
C	-6.522040	-2.867577	-0.220864
H	-5.524297	-3.116880	-2.130276
H	-7.014211	-2.170255	-2.208562
C	-7.348630	-4.155147	-0.287089
H	-5.617219	-3.039610	0.389906

H	-7.097077	-2.084852	0.304083
C	-7.771229	-4.680277	1.085682
H	-8.246470	-3.975431	-0.905817
H	-6.770122	-4.932734	-0.818853
H	-8.364946	-5.604502	1.000826
H	-6.894790	-4.905552	1.716631
H	-8.383488	-3.939564	1.626799
Br	-7.633568	0.700872	-1.652572
H	1.592436	-1.425979	-2.919113
Ni	0.649320	0.026528	0.558986
C	4.333930	-1.974430	-3.590526
H	3.951142	-1.857240	-4.621473
C	4.032206	-3.401507	-3.107138
H	4.404255	-3.522839	-2.075636
H	2.939186	-3.550993	-3.049627
C	4.642030	-4.479415	-4.008640
H	4.274113	-4.341164	-5.041957
H	5.736519	-4.333216	-4.060308
C	4.338144	-5.904632	-3.544768
H	4.722262	-6.084266	-2.526800
H	4.794615	-6.653842	-4.211332
H	3.252093	-6.095749	-3.522815
H	5.423908	-1.829845	-3.652648
H	1.521237	3.060990	-2.752859
C	-0.053384	4.499901	-2.396147
H	-0.768667	4.758491	-1.595980
H	-0.660079	4.240342	-3.282233
C	0.806317	5.727700	-2.713450
H	1.420984	5.978367	-1.829528
H	1.524723	5.473247	-3.513905
C	-0.011425	6.951188	-3.129785
H	-0.608041	6.745831	-4.034477
H	-0.714701	7.251310	-2.334830

H	0.634789	7.816756	-3.347298
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Ni-TTBTBr-BTanti-S-Pr SCF Done: -9171.25378081 A.U.

P	0.912494	0.430598	2.448891
P	0.232590	3.149959	0.664089
C	1.515614	1.915486	3.407326
H	2.404580	2.259188	2.853484
H	1.862672	1.617581	4.409032
C	0.512129	3.080135	3.562316
H	1.101512	3.977878	3.811078
H	-0.121136	2.881482	4.442408
C	-0.436574	3.418165	2.391578
H	-0.807213	4.448898	2.506267
H	-1.323327	2.766436	2.433076
C	-0.588893	-0.092592	3.404775
C	-1.818158	-0.230542	2.741004
C	-0.530843	-0.346048	4.786965
C	-2.969079	-0.602959	3.445602
H	-1.871925	-0.062038	1.662912
C	-1.679774	-0.713917	5.490232
H	0.421074	-0.267371	5.319307
C	-2.902393	-0.841364	4.820217
H	-3.916505	-0.712523	2.911999
H	-1.620693	-0.907499	6.564588
H	-3.800485	-1.133010	5.371034
C	2.126771	-0.886323	2.908375
C	3.372357	-0.624262	3.502125
C	1.798674	-2.217740	2.589454
C	4.259116	-1.669630	3.787238
H	3.667865	0.396394	3.752043
C	2.682788	-3.257793	2.876985
H	0.841610	-2.441521	2.111237
C	3.916575	-2.987954	3.479908

H	5.221622	-1.447959	4.256012	C	4.350977	-1.545260	-1.265194
H	2.408823	-4.285122	2.623863	C	3.879856	-2.642902	-1.948485
H	4.609382	-3.802893	3.703961	Br	4.915226	-4.013612	-2.740003
C	-1.029966	4.046405	-0.350504	H	-1.821547	1.316677	-2.156597
C	-0.684261	5.020124	-1.303042	C	0.994662	1.318846	-2.637029
C	-2.382243	3.672311	-0.233043	C	0.886353	0.719619	-4.050672
C	-1.665861	5.613404	-2.104067	C	1.693716	1.489651	-5.099975
H	0.357598	5.323916	-1.422780	C	1.581243	0.904283	-6.508666
C	-3.361537	4.271062	-1.028802	H	0.646889	2.367034	-2.662681
H	-2.680589	2.896797	0.476653	H	2.056507	1.353234	-2.346660
C	-3.006678	5.245370	-1.967555	H	-0.176057	0.690410	-4.353446
H	-1.377169	6.370417	-2.838078	H	1.222736	-0.331540	-4.024462
H	-4.405079	3.965182	-0.920234	H	1.363210	2.544980	-5.111331
H	-3.772298	5.711223	-2.592995	H	2.756152	1.511893	-4.794815
C	1.709914	4.263213	0.603439	H	2.174718	1.480210	-7.237188
C	1.700246	5.562876	1.141384	H	0.535197	0.901955	-6.858782
C	2.893153	3.784163	0.017915	H	1.938649	-0.138603	-6.537301
C	2.847054	6.359346	1.098078	C	-3.273733	-0.936997	-1.170729
H	0.787771	5.963558	1.590070	C	-3.890320	-2.121572	-0.817105
C	4.041207	4.582673	-0.029642	S	-4.484698	0.265705	-1.590521
H	2.908830	2.775641	-0.402880	C	-5.321478	-2.106167	-0.883228
C	4.020502	5.869972	0.512920	H	-3.325466	-3.008994	-0.524446
H	2.824938	7.367180	1.520946	C	-5.771038	-0.869422	-1.287708
H	4.953201	4.195896	-0.491487	C	-6.186087	-3.283887	-0.516800
H	4.917118	6.494272	0.479279	C	-6.461456	-3.399965	0.993436
C	0.197176	0.562782	-1.584682	H	-5.693648	-4.207658	-0.866523
C	0.692869	-0.614305	-0.867899	H	-7.145384	-3.217635	-1.055240
C	-1.251991	0.505177	-1.695654	C	-7.317652	-4.615333	1.361291
S	-0.672088	-1.795609	-0.611803	H	-5.500249	-3.446913	1.536689
C	-1.859115	-0.629350	-1.226070	H	-6.960657	-2.476844	1.338146
C	2.000283	-1.221952	-1.098192	C	-7.595936	-4.732686	2.860465
C	3.256035	-0.755700	-0.777871	H	-8.274345	-4.564454	0.810247
S	2.145530	-2.716278	-2.025997	H	-6.816090	-5.533838	1.005411

H	-8.213516	-5.615815	3.089707	C	1.475597	2.353387	-2.206203
H	-6.659462	-4.823375	3.436192	C	1.475566	1.851882	-3.520723
H	-8.130671	-3.845519	3.239408	C	2.709202	2.539144	-1.560239
Br	-7.561634	-0.325151	-1.531950	C	2.674736	1.574809	-4.180992
H	3.400330	0.149619	-0.185417	H	0.532609	1.663426	-4.040672
C	5.801654	-1.220588	-1.016926	C	3.908430	2.254394	-2.219744
C	6.382786	-1.873801	0.249246	H	2.738959	2.901954	-0.531732
H	5.911938	-0.124765	-0.943037	C	3.896394	1.776630	-3.532178
H	6.398935	-1.535549	-1.888908	H	2.652893	1.191575	-5.204554
C	7.851577	-1.515356	0.493926	H	4.857588	2.400158	-1.698378
H	5.776121	-1.579635	1.123325	H	4.835445	1.552069	-4.043943
H	6.278947	-2.969705	0.164405	C	-4.696671	0.457589	-1.294059
C	8.438912	-2.172898	1.743603	C	-5.951255	0.387102	-0.668675
H	8.448792	-1.804835	-0.390025	C	-4.428355	-0.410668	-2.368076
H	7.950410	-0.416860	0.573824	C	-6.917146	-0.520845	-1.116268
H	9.494362	-1.893297	1.892129	H	-6.181942	1.043461	0.172383
H	7.884952	-1.876097	2.650189	C	-5.397085	-1.308144	-2.821955
H	8.392356	-3.272768	1.676311	H	-3.450229	-0.387281	-2.856699
Ni	0.557395	0.973184	0.319474	C	-6.646479	-1.366224	-2.195281
				H	-7.888907	-0.563411	-0.617549
115				H	-5.172382	-1.969630	-3.662785
Ni-TTBTBr-Btanti-S-TS-3 SCF Done: -9171.21333939 A.U.				H	-7.404661	-2.071501	-2.545017
Ni	-1.246745	0.791152	-0.559439	C	0.249143	3.851560	-0.016548
P	-3.364369	1.643550	-0.793347	C	0.902896	5.067932	-0.286361
P	-0.135379	2.617581	-1.339536	C	-0.147234	3.575884	1.301803
C	-3.485850	2.855707	-2.213938	C	1.151196	5.983664	0.737993
H	-4.521938	3.223708	-2.272796	H	1.235639	5.300135	-1.301392
H	-3.331157	2.253692	-3.124711	C	0.100692	4.493654	2.328378
C	-2.492120	4.029099	-2.188352	H	-0.657090	2.635447	1.525012
H	-2.500553	4.522062	-1.201140	C	0.749833	5.697873	2.048322
H	-2.854804	4.790501	-2.900568	H	1.662660	6.923456	0.513910
C	-1.053157	3.672418	-2.586189	H	-0.216512	4.262892	3.348294
H	-0.469803	4.589412	-2.764279	H	0.945574	6.415334	2.849466
H	-1.059149	3.116184	-3.537303				

C	-4.120919	2.559475	0.626342
C	-4.839624	3.760319	0.489516
C	-3.969017	2.011133	1.913208
C	-5.390208	4.394038	1.607891
H	-4.984780	4.215999	-0.491204
C	-4.529553	2.640064	3.028222
H	-3.403634	1.086072	2.046436
C	-5.239249	3.835178	2.879901
H	-5.943328	5.328386	1.481111
H	-4.404021	2.192655	4.017536
H	-5.672568	4.330780	3.752476
C	0.597305	-1.237357	-1.592058
C	1.979575	-1.556537	-1.542611
C	0.151520	-0.510996	-0.469103
C	2.647210	-1.119959	-0.413064
S	1.524378	-0.257139	0.625332
H	2.483927	-2.117809	-2.333135
C	-0.277068	-1.651954	-2.752787
C	-0.332821	-3.168780	-3.005816
H	0.084246	-1.156848	-3.674477
H	-1.296566	-1.265389	-2.595223
C	-1.252631	-3.559581	-4.166705
H	0.685708	-3.543917	-3.209379
H	-0.659233	-3.680958	-2.083875
C	-1.292070	-5.064471	-4.436653
H	-2.276355	-3.196934	-3.957569
H	-0.929391	-3.028467	-5.081150
H	-1.962373	-5.309690	-5.276207
H	-0.290328	-5.452570	-4.686290
H	-1.647448	-5.620572	-3.553029
C	4.035662	-1.273686	-0.052308
C	4.660891	-1.014579	1.154653
S	5.214053	-1.849564	-1.223203

C	6.067810	-1.275859	1.178195
H	4.114785	-0.657485	2.030157
C	6.495099	-1.735432	-0.047920
Br	8.251223	-2.225941	-0.538072
C	6.941174	-1.035949	2.382123
C	7.442508	0.414859	2.498920
H	7.807495	-1.716702	2.349553
H	6.371955	-1.296415	3.291160
C	8.301396	0.663664	3.741971
H	8.020316	0.667974	1.592319
H	6.574911	1.099295	2.506069
C	8.801941	2.104235	3.857299
H	7.719496	0.401411	4.644564
H	9.164121	-0.027227	3.731558
H	9.416301	2.248832	4.760461
H	9.418594	2.384876	2.986911
H	7.962130	2.817617	3.908454
C	-1.447612	-0.879243	0.347525
C	-2.186144	-2.033617	0.070349
S	-1.414350	-0.678526	2.119563
C	-2.714930	-2.737884	1.195174
H	-2.341620	-2.397989	-0.944973
C	-2.381241	-2.107932	2.374842
C	-3.541588	-3.994198	1.085449
C	-5.058847	-3.741888	1.035897
H	-3.316041	-4.653634	1.940381
H	-3.235160	-4.543369	0.178589
C	-5.882350	-5.029183	0.933845
H	-5.357659	-3.184218	1.941001
H	-5.292015	-3.082468	0.181566
C	-7.391866	-4.785899	0.897084
H	-5.576581	-5.587236	0.029541
H	-5.635649	-5.686682	1.787411

H	-7.954214	-5.730561	0.821387	H	6.701897	0.555733	0.452932
H	-7.735397	-4.266018	1.807244	C	5.494326	-3.138031	0.310998
H	-7.674893	-4.158783	0.034963	H	3.536605	-2.367358	0.790194
Br	-2.819316	-2.654634	4.129786	C	6.833395	-2.828630	0.057958
				H	8.306334	-1.249866	-0.087756
115				H	5.149502	-4.173938	0.263888
Ni-TTBTBr-BTsyn-O SCF Done: -9171.23047347 A.U.				H	7.543577	-3.623139	-0.184703
Ni	1.601560	-0.085547	0.741736	C	-0.053586	1.384555	3.330470
P	3.787898	0.500857	1.200666	C	-0.787364	1.496508	4.524696
P	0.923220	-0.132385	2.928238	C	-0.007079	2.481720	2.456219
C	4.338295	0.689762	2.991811	C	-1.459411	2.680990	4.833807
H	5.174834	1.405169	3.010451	H	-0.847005	0.650606	5.214230
H	4.765910	-0.288110	3.264373	C	-0.676771	3.669196	2.769184
C	3.270845	1.067581	4.026384	H	0.545977	2.405364	1.517581
H	2.771100	2.016041	3.763972	C	-1.404345	3.770282	3.957055
H	3.786636	1.260885	4.982497	H	-2.032005	2.752799	5.762096
C	2.230002	-0.035672	4.261113	H	-0.634739	4.511833	2.074648
H	1.711851	0.113303	5.221108	H	-1.933650	4.695357	4.199491
H	2.739681	-1.010625	4.318218	C	4.366991	2.064431	0.413825
C	-0.128937	-1.533355	3.507095	C	4.401133	3.271255	1.134317
C	0.432174	-2.649393	4.151991	C	4.707205	2.079955	-0.951249
C	-1.508614	-1.534417	3.234864	C	4.780223	4.463953	0.510650
C	-0.368960	-3.730777	4.531919	H	4.128596	3.295990	2.191409
H	1.502200	-2.693739	4.363339	C	5.092181	3.272636	-1.568843
C	-2.306037	-2.615644	3.615531	H	4.674763	1.160143	-1.537153
H	-1.965050	-0.691507	2.712590	C	5.129765	4.466774	-0.842397
C	-1.740655	-3.715764	4.267433	H	4.803101	5.392193	1.087206
H	0.085076	-4.587721	5.036087	H	5.358366	3.264727	-2.628633
H	-3.374725	-2.598457	3.388394	H	5.429776	5.397669	-1.330187
H	-2.366759	-4.561199	4.563745	C	-0.528989	-2.055177	0.007425
C	5.004737	-0.780908	0.664407	C	-1.916012	-2.178668	-0.326482
C	6.354046	-0.479060	0.415964	C	-0.127312	-0.742612	0.218760
C	4.585321	-2.119558	0.609620	C	-2.602821	-0.984274	-0.385501
C	7.260537	-1.498169	0.110813				

S	-1.495904	0.324689	-0.008451
H	-2.398161	-3.137289	-0.533308
C	0.379642	-3.258932	0.125640
C	0.400137	-4.174219	-1.108525
H	0.087845	-3.858116	1.009518
H	1.404646	-2.906493	0.328217
C	1.367474	-5.354520	-0.977047
H	-0.616720	-4.562912	-1.297635
H	0.667175	-3.574647	-1.995388
C	1.376424	-6.275429	-2.198112
H	2.388593	-4.966532	-0.803976
H	1.111217	-5.939773	-0.074147
H	2.082891	-7.112015	-2.072298
H	0.378141	-6.707908	-2.380290
H	1.667310	-5.726801	-3.109313
C	-4.001289	-0.739799	-0.677647
C	-4.620838	0.417206	-1.105841
S	-5.190100	-2.017207	-0.479363
C	-6.036829	0.311758	-1.300062
H	-4.065040	1.334763	-1.309116
C	-6.471967	-0.959399	-0.999262
Br	-8.237606	-1.620483	-1.109879
C	-6.906631	1.457395	-1.747343
C	-7.369022	2.367573	-0.595308
H	-7.791625	1.062754	-2.272667
H	-6.348729	2.061241	-2.483873
C	-8.236348	3.541048	-1.060635
H	-7.928882	1.760558	0.137960
H	-6.484083	2.752423	-0.056981
C	-8.700949	4.445574	0.081676
H	-7.672680	4.139068	-1.800102
H	-9.116214	3.148629	-1.602284
H	-9.321068	5.278370	-0.287116

H	-9.300639	3.884575	0.817951
H	-7.843652	4.882419	0.621183
C	1.939141	0.151540	-1.137465
C	1.693051	1.256524	-1.944600
S	2.590470	-1.147613	-2.110490
C	2.036917	1.047189	-3.325458
C	2.535538	-0.204976	-3.568882
Br	3.120585	-0.897790	-5.226914
H	1.920521	1.794492	-4.109894
C	1.117066	2.557496	-1.418241
C	0.991373	3.699923	-2.431187
H	1.739067	2.906313	-0.573764
H	0.117345	2.356800	-0.994664
C	0.430632	4.987569	-1.819041
H	1.979453	3.913339	-2.877317
H	0.339863	3.385376	-3.266266
C	0.289502	6.132487	-2.823320
H	-0.553836	4.773650	-1.363597
H	1.084663	5.306364	-0.986430
H	-0.113301	7.042490	-2.349858
H	1.262746	6.393951	-3.271991
H	-0.388728	5.859649	-3.649187

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Ni-TTBTBr-BTsyn-O-Pr-2 SCF Done: -9171.23980128 A.U.

Ni	1.822864	-0.087527	0.147765
P	3.367963	-1.236778	1.302242
P	1.750653	1.668298	1.566811
C	4.447989	-0.028393	2.241992
H	4.758274	0.703773	1.479184
H	5.367294	-0.528482	2.584730
C	3.776343	0.691103	3.426576
H	4.382878	1.583640	3.652580
H	3.842301	0.048046	4.319936

C	2.301039	1.109781	3.271551	H	-1.522785	5.285110	2.858511
H	2.053511	1.880478	4.018268	H	-3.049353	1.252397	2.686761
H	1.636884	0.257303	3.487141	H	-3.411199	3.677878	3.147755
C	2.852009	-2.417763	2.633088	C	2.851930	3.120384	1.239155
C	1.496997	-2.775588	2.729191	C	3.307035	3.983317	2.253777
C	3.752285	-2.930189	3.585695	C	3.284274	3.345082	-0.079780
C	1.051420	-3.629670	3.744000	C	4.163502	5.046692	1.955384
H	0.784571	-2.373780	2.004546	H	2.990372	3.833535	3.288506
C	3.308392	-3.782275	4.600056	C	4.137929	4.412999	-0.377828
H	4.812390	-2.668942	3.534851	H	2.952451	2.677937	-0.879932
C	1.956527	-4.134731	4.680589	C	4.579325	5.265123	0.637725
H	-0.006607	-3.897439	3.802334	H	4.507366	5.707409	2.755623
H	4.020635	-4.172330	5.331930	H	4.460552	4.573227	-1.409745
H	1.610373	-4.800567	5.475294	H	5.249283	6.097021	0.405386
C	4.668764	-2.146251	0.347057	C	1.292512	-1.186710	-1.435933
C	5.389298	-1.418511	-0.618931	C	0.700632	0.159514	-1.500837
C	4.934552	-3.518205	0.489608	C	2.422309	-1.316280	-2.360942
C	6.365435	-2.039999	-1.400549	S	1.608277	1.127515	-2.778994
H	5.176138	-0.358612	-0.779804	C	2.686660	-0.212630	-3.093251
C	5.906495	-4.141100	-0.300775	Br	4.135948	0.029365	-4.288739
H	4.381916	-4.112542	1.219231	C	-0.693514	0.555613	-1.324596
C	6.628181	-3.404705	-1.243576	C	-1.264839	1.832476	-1.395720
H	6.909283	-1.456354	-2.147148	S	-1.959152	-0.632109	-0.995176
H	6.098687	-5.210011	-0.175523	C	-2.673009	1.819002	-1.187150
H	7.387175	-3.893149	-1.859927	C	-3.215220	0.573773	-0.950940
C	0.109797	2.396166	2.030330	C	-0.495501	3.107583	-1.668263
C	-0.108648	3.761830	2.273654	C	-1.248072	4.414715	-1.394337
C	-0.966203	1.502928	2.179163	H	-0.164695	3.117256	-2.722003
C	-1.369077	4.218391	2.674437	H	0.432743	3.099122	-1.071759
H	0.703281	4.479965	2.146457	C	-0.385494	5.658374	-1.632901
C	-2.222009	1.958949	2.586429	H	-2.141529	4.473890	-2.041282
H	-0.826441	0.441707	1.955837	H	-1.617956	4.419338	-0.354355
C	-2.426347	3.319213	2.837955	C	-1.129885	6.970809	-1.383159

H	0.508466	5.610812	-0.985198
H	-0.002967	5.642719	-2.669797
H	-0.482593	7.844848	-1.559875
H	-2.006725	7.067221	-2.045474
H	-1.496106	7.032073	-0.344421
H	-3.286995	2.718854	-1.214143
H	3.017435	-2.224647	-2.439982
C	0.487083	-2.452088	-1.126364
H	-0.261042	-2.601427	-1.928677
H	-0.097271	-2.311781	-0.203710
C	1.291298	-3.749893	-0.989842
H	1.792344	-3.987092	-1.944170
H	2.097446	-3.615856	-0.249291
C	0.422780	-4.945763	-0.583761
H	-0.400308	-5.061055	-1.312281
H	-0.063548	-4.730396	0.385189
C	1.201236	-6.258142	-0.480796
H	1.671157	-6.522312	-1.443087
H	0.547353	-7.095807	-0.189299
H	2.006354	-6.187953	0.269694
C	-4.589183	0.207431	-0.672094
C	-5.216092	-1.015258	-0.821003
S	-5.713143	1.387282	-0.025058
C	-6.596725	-1.036518	-0.442336
H	-4.692672	-1.884327	-1.220080
C	-6.990867	0.207901	0.001464
Br	-8.716804	0.704934	0.576932
C	-7.515119	-2.233138	-0.537526
H	-8.095478	-2.306877	0.398957
H	-8.268052	-2.040984	-1.324578
C	-6.828779	-3.573379	-0.816438
H	-6.295771	-3.525937	-1.782878
H	-6.054265	-3.758866	-0.050353

C	-7.806407	-4.752488	-0.844308
H	-8.584543	-4.561087	-1.605541
H	-8.340562	-4.803744	0.121905
C	-7.132355	-6.095432	-1.128220
H	-6.620499	-6.089079	-2.105218
H	-6.375335	-6.333996	-0.362291
H	-7.862900	-6.919931	-1.141414

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Ni-TTBTBr-BTsyn-O-TS-3 SCF Done: -9171.20910605 A.U.

Ni	1.633697	0.463070	0.637330
P	3.805636	1.171321	0.716452
P	0.810890	1.724615	2.343793
C	4.285181	2.377207	2.078424
H	5.142794	2.970334	1.723176
H	4.669299	1.745111	2.895228
C	3.183608	3.289633	2.636438
H	2.726308	3.901392	1.839726
H	3.665929	4.010697	3.318547
C	2.095466	2.544232	3.426374
H	1.577956	3.228745	4.116734
H	2.568246	1.759565	4.039488
C	-0.305697	0.917992	3.574145
C	0.087702	0.620212	4.890877
C	-1.585329	0.515865	3.148299
C	-0.778019	-0.054536	5.758513
H	1.072386	0.911369	5.260110
C	-2.449214	-0.153469	4.017212
H	-1.911832	0.725936	2.127808
C	-2.048541	-0.442156	5.325728
H	-0.454485	-0.274083	6.779418
H	-3.436047	-0.459020	3.660545
H	-2.724002	-0.968612	6.004879
C	5.117603	-0.105377	0.994418

C	6.443061	0.048696	0.554398
C	4.785138	-1.236468	1.758012
C	7.409816	-0.910765	0.868422
H	6.725699	0.918888	-0.042153
C	5.754138	-2.191185	2.078759
H	3.756827	-1.373443	2.101728
C	7.068378	-2.031919	1.631158
H	8.436066	-0.780086	0.515218
H	5.476630	-3.067058	2.670744
H	7.825572	-2.782018	1.873365
C	-0.160197	3.207337	1.800840
C	-1.026371	3.896020	2.668206
C	0.011714	3.689910	0.493479
C	-1.700955	5.040084	2.235615
H	-1.185161	3.531579	3.686123
C	-0.659934	4.838707	0.062018
H	0.671640	3.157358	-0.195205
C	-1.518690	5.514706	0.931951
H	-2.375684	5.561998	2.919247
H	-0.516479	5.197905	-0.960220
H	-2.050542	6.408124	0.594708
C	4.335725	2.027877	-0.829047
C	4.354658	3.429851	-0.936015
C	4.629138	1.261593	-1.972738
C	4.669238	4.049817	-2.149620
H	4.121744	4.056449	-0.072795
C	4.951998	1.883557	-3.180807
H	4.609541	0.171234	-1.923112
C	4.971066	3.278954	-3.275354
H	4.680408	5.141137	-2.211551
H	5.184850	1.270025	-4.054881
H	5.220896	3.763249	-4.222755
C	-0.268645	-1.749714	0.858396

C	-1.655308	-2.027836	0.775939
C	0.131892	-0.616709	0.107576
C	-2.393988	-1.151791	0.001630
S	-1.329586	0.097202	-0.627333
H	-2.116653	-2.874326	1.289761
C	0.655698	-2.574357	1.725483
C	0.566808	-4.095734	1.528396
H	0.443267	-2.339044	2.786536
H	1.696425	-2.247800	1.569758
C	1.562467	-4.874259	2.393733
H	-0.456576	-4.440796	1.759445
H	0.736719	-4.333532	0.464424
C	1.463341	-6.390991	2.224430
H	2.588628	-4.543650	2.148590
H	1.406713	-4.609712	3.456155
H	2.194695	-6.919415	2.857146
H	0.460121	-6.759772	2.496967
H	1.649674	-6.689458	1.179272
C	-3.809969	-1.140821	-0.267767
C	-4.525905	-0.388650	-1.182678
S	-4.906334	-2.172215	0.644461
C	-5.938372	-0.621264	-1.187290
H	-4.043812	0.315512	-1.863677
C	-6.277711	-1.566254	-0.244752
Br	-8.000098	-2.237609	0.137232
C	-6.901484	0.106861	-2.088123
C	-7.326213	1.484869	-1.549697
H	-7.798918	-0.513850	-2.242373
H	-6.434166	0.234250	-3.080075
C	-8.291206	2.227937	-2.478176
H	-7.793407	1.353288	-0.557673
H	-6.426009	2.102973	-1.380426
C	-8.712464	3.598837	-1.947079

H	-7.821941	2.344878	-3.472321	C	3.517973	-0.865430	3.906750
H	-9.188473	1.603963	-2.643026	H	3.079372	0.112491	4.168774
H	-9.406741	4.104901	-2.636971	H	4.115783	-1.165673	4.784384
H	-9.217756	3.512069	-0.970542	C	2.410171	-1.909172	3.710760
H	-7.840517	4.259991	-1.807990	H	1.958348	-2.181211	4.677307
C	1.586454	-0.664183	-0.934046	H	2.850389	-2.827843	3.291069
C	1.567651	-0.149319	-2.251236	C	-0.103388	-2.816706	2.610251
S	2.487373	-2.208428	-0.955475	C	0.374053	-4.125934	2.794980
C	2.211768	-0.988047	-3.209926	C	-1.478925	-2.625662	2.387259
C	2.746092	-2.129058	-2.671770	C	-0.503146	-5.215047	2.769374
Br	3.642221	-3.510524	-3.592166	H	1.435875	-4.317663	2.957816
H	2.279392	-0.750082	-4.272346	C	-2.352151	-3.714789	2.361771
C	0.974643	1.181961	-2.651774	H	-1.873660	-1.621133	2.223594
C	0.024277	1.143602	-3.858807	C	-1.868387	-5.012698	2.553716
H	1.801927	1.884383	-2.870833	H	-0.113242	-6.225169	2.919061
H	0.447960	1.623154	-1.791910	H	-3.415734	-3.543527	2.179152
C	-0.582887	2.510856	-4.188309	H	-2.553681	-5.863902	2.532764
H	0.563444	0.766749	-4.746259	C	4.932511	-0.802972	-0.071242
H	-0.783088	0.418184	-3.660213	C	6.240347	-0.352863	-0.316958
C	-1.515089	2.488682	-5.400595	C	4.503818	-2.001057	-0.666339
H	-1.135192	2.882554	-3.305812	C	7.095473	-1.084343	-1.146728
H	0.231486	3.238723	-4.361592	H	6.596568	0.573784	0.137331
H	-1.937922	3.485135	-5.607343	C	5.363512	-2.736905	-1.486422
H	-0.983934	2.157830	-6.309020	H	3.487516	-2.360934	-0.488967
H	-2.358035	1.794917	-5.243996	C	6.661175	-2.277899	-1.731228

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Ni-TTBTBr-BTsyn-S SCF Done: -9171.22812415 A.U.

Ni	1.567405	-0.306702	0.604585	H	8.108671	-0.719428	-1.333867
P	3.798892	0.021730	1.135003	H	5.013618	-3.667046	-1.941029
P	1.028228	-1.358120	2.579415	H	7.332409	-2.848661	-2.377784
C	4.472393	-0.750384	2.711110	C	0.181106	-0.123171	3.665265
H	5.385178	-0.199586	2.986273	C	-0.463532	-0.513715	4.852912
H	4.802015	-1.760148	2.418491	C	0.224070	1.239851	3.332903
				C	-1.046331	0.440506	5.688971
				H	-0.524888	-1.571203	5.122309

C	-0.357209	2.195319	4.173324	H	1.806774	-6.239466	-4.205456
H	0.703270	1.561076	2.405513	H	0.101554	-5.745504	-4.313153
C	-0.992798	1.797753	5.351410	H	1.382763	-4.625093	-4.822072
H	-1.549303	0.122674	6.605912	C	-4.053894	-0.400884	-0.865217
H	-0.318658	3.251440	3.895727	C	-4.666187	0.835928	-0.884117
H	-1.453123	2.543128	6.005043	S	-5.254510	-1.667127	-1.065167
C	4.393977	1.763728	1.232585	C	-6.086676	0.807108	-1.073395
C	4.574400	2.402730	2.471257	H	-4.102614	1.766476	-0.790943
C	4.596365	2.506034	0.054754	C	-6.532034	-0.490477	-1.189885
C	4.962376	3.744880	2.531856	Br	-8.307018	-1.070825	-1.473284
H	4.410076	1.865075	3.406837	C	-6.948897	2.041695	-1.110692
C	4.995048	3.842394	0.118699	C	-7.368612	2.543467	0.282809
H	4.431597	2.042601	-0.919521	H	-7.852534	1.840839	-1.709027
C	5.179096	4.466600	1.355947	H	-6.398526	2.843222	-1.633221
H	5.096244	4.224408	3.504866	C	-8.227390	3.810751	0.236990
H	5.145245	4.402343	-0.807397	H	-7.921004	1.739711	0.801063
H	5.483881	5.515097	1.402748	H	-6.465095	2.730663	0.890619
C	-0.592195	-1.894590	-0.716058	C	-8.650829	4.309318	1.619460
C	-1.983547	-1.887415	-1.054110	H	-7.670934	4.608208	-0.288763
C	-0.174180	-0.728909	-0.084393	H	-9.125524	3.617946	-0.377644
C	-2.653699	-0.736371	-0.694889	H	-9.265476	5.221262	1.550924
S	-1.526191	0.368406	0.069592	H	-9.242514	3.548465	2.155756
H	-2.482024	-2.714878	-1.564611	H	-7.774160	4.545066	2.246014
C	0.298429	-3.088053	-0.987088	C	1.695486	0.967766	-0.827634
C	0.241916	-3.638658	-2.420078	C	1.925702	0.975108	-2.193826
H	0.040517	-3.905721	-0.287368	S	1.264131	2.589929	-0.300645
H	1.339385	-2.810718	-0.749627	C	1.779084	2.277530	-2.796620
C	1.185259	-4.822868	-2.654097	C	1.423064	3.248232	-1.901738
H	-0.790361	-3.953698	-2.654984	Br	1.135060	5.081398	-2.259465
H	0.478082	-2.829874	-3.132888	H	1.919702	2.476485	-3.860451
C	1.117559	-5.389754	-4.072934	C	2.225413	-0.245220	-3.034190
H	2.222976	-4.509121	-2.433567	C	3.508986	-0.162866	-3.875416
H	0.954450	-5.621316	-1.924940	H	1.370885	-0.424729	-3.714240

H	2.275373	-1.126742	-2.378231	H	-1.109359	-1.843292	6.437272
C	3.715803	-1.374876	-4.789300	H	-3.382442	-1.738905	5.411248
H	3.491035	0.751874	-4.495025	C	2.549569	-0.902839	2.978074
H	4.379315	-0.054743	-3.203571	C	3.722626	-0.467127	3.617879
C	4.995410	-1.302827	-5.623625	C	2.441951	-2.260894	2.623171
H	3.727059	-2.293911	-4.175525	C	4.757189	-1.367005	3.900063
H	2.842791	-1.474935	-5.459945	H	3.846316	0.578619	3.904089
H	5.108074	-2.185792	-6.273542	C	3.471402	-3.157714	2.911398
H	5.000659	-0.410603	-6.272355	H	1.545581	-2.620853	2.112556
H	5.889282	-1.245344	-4.979891	C	4.634708	-2.713417	3.550158
				H	5.661295	-1.009633	4.400286
115				H	3.367768	-4.207321	2.625756
Ni-TTBTBr-BTsyn-S-Pr SCF Done: -9171.24550859 A.U.				H	5.442557	-3.415361	3.772081
Ni	0.915896	0.721398	0.309637	C	-0.416318	3.839546	-0.646685
P	1.173613	0.229597	2.484584	C	0.188031	4.475744	-1.746887
P	0.628416	2.928553	0.579833	C	-1.819964	3.819317	-0.573032
C	1.534938	1.772512	3.472315	C	-0.588364	5.084857	-2.735460
H	2.453737	2.188543	3.030452	H	1.277329	4.502024	-1.830711
H	1.770556	1.508465	4.515533	C	-2.596059	4.429456	-1.564003
C	0.427786	2.848592	3.472908	H	-2.326293	3.316451	0.253203
H	0.897639	3.787078	3.809814	C	-1.984339	5.065196	-2.647203
H	-0.317144	2.590310	4.243232	H	-0.098987	5.577955	-3.579525
C	-0.346371	3.129494	2.164543	H	-3.685777	4.399503	-1.487648
H	-0.789772	4.136425	2.214089	H	-2.591820	5.541014	-3.421078
H	-1.183729	2.421218	2.066333	C	2.028370	4.120150	0.838959
C	-0.271140	-0.463869	3.419204	C	1.803905	5.482110	1.111217
C	-1.552732	-0.418471	2.848092	C	3.349701	3.652128	0.791619
C	-0.125909	-0.985212	4.717549	C	2.876125	6.348727	1.334295
C	-2.667521	-0.870565	3.563213	H	0.783691	5.873898	1.138123
H	-1.678871	-0.044805	1.830355	C	4.425728	4.519671	1.012858
C	-1.238173	-1.439864	5.429377	H	3.536246	2.597339	0.579578
H	0.864775	-1.043835	5.175670	C	4.190415	5.868957	1.285789
C	-2.512643	-1.381164	4.854031	H	2.686062	7.404554	1.544515
H	-3.656941	-0.831053	3.100598				

H	5.448417	4.136919	0.967453
H	5.028632	6.549011	1.458065
C	0.472564	0.240648	-1.577120
C	0.761190	-0.950476	-0.777003
C	-0.963603	0.437276	-1.704509
S	-0.810630	-1.798635	-0.383387
C	-1.767349	-0.516588	-1.141095
C	1.882789	-1.867069	-0.959960
C	3.256769	-1.708699	-0.833235
S	1.505879	-3.527114	-1.467450
C	3.985960	-2.911587	-1.124521
C	3.182450	-3.961750	-1.468445
Br	3.728273	-5.720847	-1.877653
C	3.985524	-0.451118	-0.419894
C	5.083604	-0.023763	-1.410858
H	4.446925	-0.615953	0.570717
H	3.252755	0.364184	-0.277040
C	5.833906	1.250172	-1.011726
H	5.814845	-0.844441	-1.516702
H	4.643482	0.109016	-2.415103
C	7.001204	1.581438	-1.943655
H	5.129287	2.099477	-0.996528
H	6.206375	1.143827	0.023994
H	7.514276	2.507939	-1.639417
H	7.750701	0.772381	-1.950066
H	6.657101	1.718157	-2.982495
H	5.071330	-2.991656	-1.058324
H	-1.373577	1.288094	-2.254666
C	1.371039	0.757988	-2.690687
C	1.178027	0.022664	-4.029296
C	2.085020	0.544095	-5.147899
C	1.886429	-0.177196	-6.482044
H	1.164908	1.833090	-2.837437

H	2.427319	0.689657	-2.394674
H	0.121976	0.109571	-4.342548
H	1.360048	-1.055950	-3.878917
H	1.909534	1.627487	-5.284079
H	3.140753	0.449622	-4.833098
H	2.554713	0.220245	-7.263102
H	0.850037	-0.070267	-6.844187
H	2.090209	-1.256800	-6.386391
C	-3.214015	-0.576532	-1.092836
C	-4.020487	-1.611829	-0.660148
S	-4.206624	0.765752	-1.641369
C	-5.428628	-1.371686	-0.767217
H	-3.611395	-2.551932	-0.284580
C	-5.664917	-0.117060	-1.282298
C	-6.480363	-2.361261	-0.339165
C	-6.817146	-2.297442	1.161536
H	-6.132781	-3.378476	-0.589007
H	-7.399509	-2.192376	-0.923247
C	-7.871597	-3.322246	1.589735
H	-5.893494	-2.450682	1.748944
H	-7.168531	-1.279403	1.406548
C	-8.214267	-3.258574	3.078749
H	-8.788852	-3.168447	0.992660
H	-7.515965	-4.337471	1.335474
H	-8.975755	-4.006744	3.351154
H	-7.325030	-3.447245	3.703621
H	-8.607796	-2.266599	3.357439
Br	-7.340815	0.685123	-1.615781

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Ni-TTBTBr-BTsyn-S-TS-3 SCF Done: -9171.20623808 A.U.

Ni	1.524618	0.407621	0.484580
P	3.206612	1.923767	0.167731
P	0.926042	1.081662	2.575745

C	4.013944	2.531384	1.733916
H	4.710567	3.349980	1.495694
H	4.635880	1.692963	2.088946
C	3.063144	2.960102	2.862879
H	2.338046	3.708153	2.498851
H	3.669040	3.482976	3.622170
C	2.336215	1.801907	3.564666
H	1.945126	2.132320	4.540014
H	3.053929	0.987946	3.759491
C	0.250550	-0.215863	3.700005
C	0.987122	-0.778383	4.757291
C	-1.043884	-0.706865	3.444204
C	0.439795	-1.796141	5.545746
H	1.995478	-0.428144	4.984041
C	-1.589863	-1.717966	4.237466
H	-1.633884	-0.293143	2.623681
C	-0.850555	-2.267159	5.290307
H	1.026085	-2.217016	6.366809
H	-2.599023	-2.080205	4.026114
H	-1.279326	-3.059177	5.909478
C	4.675159	1.498566	-0.884099
C	4.436833	1.125397	-2.218851
C	6.000629	1.502377	-0.415476
C	5.492536	0.775656	-3.062629
H	3.416050	1.095426	-2.605507
C	7.057002	1.149147	-1.262145
H	6.233523	1.780950	0.612935
C	6.807464	0.786561	-2.587527
H	5.280322	0.480883	-4.093167
H	8.080811	1.160336	-0.878875
H	7.633814	0.509555	-3.247115
C	-0.331964	2.432817	2.726983
C	-0.951108	2.725574	3.956077

C	-0.649218	3.214369	1.605813
C	-1.860875	3.779475	4.058691
H	-0.730524	2.119442	4.838492
C	-1.557725	4.273395	1.710661
H	-0.188366	2.992834	0.642536
C	-2.165511	4.556911	2.935280
H	-2.337120	3.993401	5.019100
H	-1.792255	4.872280	0.827130
H	-2.879942	5.380246	3.016395
C	2.597496	3.468008	-0.662656
C	3.194823	4.727302	-0.485818
C	1.507337	3.357690	-1.543788
C	2.709292	5.847780	-1.165080
H	4.052888	4.846940	0.178922
C	1.028625	4.477202	-2.231693
H	1.032394	2.386144	-1.700242
C	1.625565	5.725927	-2.040493
H	3.184377	6.820471	-1.013033
H	0.184372	4.369179	-2.917331
H	1.249714	6.602820	-2.573801
C	-0.367214	-2.095390	0.464159
C	-1.761228	-2.214357	0.215515
C	0.165289	-0.851442	0.061689
C	-2.368286	-1.113764	-0.361209
S	-1.164150	0.148282	-0.594227
H	-2.325948	-3.118051	0.449081
C	0.477102	-3.217822	1.006509
C	-0.262449	-4.504202	1.388013
H	1.039173	-2.857986	1.887118
H	1.247815	-3.458330	0.248343
C	0.667824	-5.587202	1.944783
H	-1.040900	-4.279564	2.138959
H	-0.792594	-4.905659	0.505855

C	-0.058184	-6.877928	2.326791
H	1.451200	-5.812070	1.198331
H	1.200294	-5.188515	2.827534
H	0.638176	-7.633731	2.724437
H	-0.824635	-6.693086	3.098416
H	-0.570171	-7.322490	1.456836
C	-3.754146	-0.909364	-0.704108
C	-4.339098	0.122978	-1.416249
S	-4.987410	-2.053812	-0.191850
C	-5.757771	0.023376	-1.575358
H	-3.756583	0.943478	-1.840068
C	-6.235666	-1.112738	-0.960844
Br	-8.026081	-1.706699	-0.889007
C	-6.594160	1.056337	-2.284505
C	-7.033143	2.218582	-1.375510
H	-7.488257	0.574297	-2.712450
H	-6.017621	1.458924	-3.135195
C	-7.864137	3.279688	-2.102870
H	-7.612419	1.811065	-0.528296
H	-6.138069	2.689968	-0.930764
C	-8.300519	4.433974	-1.199410
H	-7.282564	3.676157	-2.955358
H	-8.755956	2.800792	-2.546686
H	-8.898083	5.177533	-1.750894
H	-8.913749	4.072473	-0.356974
H	-7.430123	4.958343	-0.770071
C	1.684220	-0.851545	-0.972375
C	2.768975	-1.750454	-0.889345
S	1.198676	-0.687859	-2.677133
C	3.170964	-2.277946	-2.157715
C	2.431972	-1.796026	-3.204835
Br	2.627559	-2.239382	-5.028992
H	3.992124	-2.982064	-2.294207

C	3.563919	-1.972336	0.380167
H	2.902583	-1.817319	1.250263
H	4.322441	-1.170412	0.450063
C	4.265921	-3.331699	0.509293
H	3.527427	-4.135088	0.346488
H	5.015930	-3.441433	-0.294405
C	4.956085	-3.560830	1.862120
H	4.207074	-3.472197	2.670414
H	5.312202	-4.605208	1.899038
C	6.134508	-2.627490	2.154113
H	6.901198	-2.693662	1.363619
H	6.619625	-2.884351	3.109764
H	5.822108	-1.572546	2.218753

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Pd-3BTanti-3BTanti-O SCF Done: -8419.48899869 A.U.

Pd	-0.078553	-0.934105	-0.146432
P	-1.736926	-2.653038	0.000713
P	1.801506	-2.416358	0.037030
C	-1.138401	-4.412862	-0.171906
H	-0.946594	-4.604691	-1.239170
H	-1.965457	-5.075127	0.128015
C	0.129163	-4.733728	0.636244
H	0.194818	-5.830577	0.734797
H	0.032693	-4.350876	1.666753
C	1.433386	-4.250044	-0.018790
H	1.416058	-4.504749	-1.090897
H	2.303507	-4.778272	0.401850
C	-2.517164	-2.701823	1.673085
C	-1.916853	-2.001306	2.731798
C	-3.667393	-3.469613	1.929456
C	-2.451429	-2.071439	4.022911
H	-1.029995	-1.391792	2.540211
C	-4.202592	-3.534133	3.217556

H	-4.158338	-4.011359	1.116903	H	1.456125	-1.795396	-2.766888
C	-3.594385	-2.836277	4.267237	C	4.739281	-2.264983	-3.568703
H	-1.974334	-1.519016	4.836233	H	6.306025	-2.742482	-2.154942
H	-5.100055	-4.130039	3.402503	H	2.977420	-1.780016	-4.730287
H	-4.015848	-2.886442	5.274479	H	5.412083	-2.244927	-4.429791
C	-3.147461	-2.569987	-1.181989	C	-2.406712	1.032344	0.613732
C	-3.110802	-3.249943	-2.411732	C	-1.591652	0.438394	-0.324049
C	-4.239788	-1.727253	-0.909511	C	-3.369161	1.973090	0.096537
C	-4.148776	-3.105599	-3.337007	S	-1.993963	1.050799	-1.905954
H	-2.268836	-3.895139	-2.669524	C	-3.258589	2.070240	-1.270669
C	-5.274260	-1.584644	-1.836204	Br	-4.294118	3.159989	-2.422992
H	-4.274433	-1.162115	0.023047	H	-2.337701	0.823178	1.684063
C	-5.234493	-2.274774	-3.050994	C	-4.308569	2.767718	0.966254
H	-4.103258	-3.644030	-4.287079	C	-3.687128	4.069050	1.505118
H	-6.109685	-0.917867	-1.610010	H	-4.627119	2.141022	1.818182
H	-6.043343	-2.157973	-3.776574	H	-5.221137	3.012846	0.397752
C	2.794209	-2.193616	1.573073	C	-4.628776	4.864642	2.413674
C	3.521780	-1.000468	1.745620	H	-2.758104	3.827974	2.052107
C	2.795558	-3.141640	2.611300	H	-3.378629	4.696322	0.650389
C	4.239911	-0.773074	2.921167	C	-4.011629	6.158685	2.946390
H	3.526568	-0.245201	0.958141	H	-5.556279	5.098765	1.859436
C	3.509201	-2.905364	3.790917	H	-4.941027	4.227948	3.262321
H	2.240288	-4.076249	2.517459	H	-4.713559	6.706362	3.595981
C	4.234081	-1.721901	3.948349	H	-3.101391	5.955646	3.535317
H	4.797625	0.159495	3.035315	H	-3.724226	6.833493	2.122738
H	3.497330	-3.653742	4.587468	C	2.855226	2.321932	-0.644422
H	4.791911	-1.537939	4.870051	C	2.470758	2.722043	0.614519
C	3.013442	-2.305260	-1.350005	C	2.112997	1.153834	-1.049189
C	4.383070	-2.566611	-1.188765	S	1.206375	1.717005	1.269138
C	2.518306	-2.021303	-2.634524	C	1.191905	0.683182	-0.138748
C	5.240403	-2.542502	-2.293523	H	2.279614	0.689087	-2.023194
H	4.788221	-2.783041	-0.197874	Br	3.150975	4.188542	1.602052
C	3.375181	-2.006738	-3.737897	C	3.923038	2.966674	-1.489818

C	5.310853	2.318061	-1.337939	C	1.848536	-2.547108	5.576395
H	3.996403	4.036813	-1.235434	H	1.647011	-0.391535	5.558464
H	3.616545	2.916656	-2.549301	H	1.926632	-4.692365	5.299294
C	6.386011	2.962646	-2.217743	H	2.268455	-2.582089	6.585073
H	5.617886	2.376544	-0.278359	C	-1.688315	-2.797149	1.437993
H	5.237436	1.241176	-1.575202	C	-2.524991	-2.600686	0.324669
C	7.764372	2.316973	-2.067021	C	-2.239822	-3.343429	2.609026
H	6.068473	2.912387	-3.275517	C	-3.871458	-2.969864	0.369612
H	6.454267	4.039255	-1.977419	H	-2.125803	-2.135050	-0.580237
H	8.514237	2.802959	-2.711959	C	-3.591899	-3.698571	2.657153
H	8.126432	2.384308	-1.027220	H	-1.616259	-3.491848	3.492699
H	7.736827	1.247373	-2.335958	C	-4.409208	-3.520226	1.537482
				H	-4.503502	-2.809093	-0.507298
96				H	-4.006813	-4.118673	3.577408
Pd-3BTanti-3BTanti-O-Pr SCF Done: -8419.51292616 A.U.				H	-5.464991	-3.800731	1.577577
Pd	0.697972	-0.328809	0.052238	C	4.132141	-0.384627	-1.278024
P	0.090247	-2.308326	1.263976	C	4.431583	0.158741	-2.540574
P	2.575047	-1.341835	-0.992543	C	4.988128	-0.086569	-0.201099
C	0.752331	-3.811433	0.362857	C	5.559822	0.963451	-2.722475
H	0.296146	-3.713551	-0.635432	H	3.781799	-0.051358	-3.393170
H	0.328661	-4.731181	0.797005	C	6.116937	0.716038	-0.385949
C	2.284176	-3.970724	0.232714	H	4.774061	-0.473272	0.797949
H	2.467676	-4.611753	-0.645530	C	6.408732	1.243816	-1.647201
H	2.655432	-4.541441	1.099976	H	5.777596	1.370740	-3.713403
C	3.178162	-2.718619	0.123865	H	6.770170	0.931964	0.463578
H	4.191308	-3.032759	-0.174495	H	7.291244	1.872130	-1.790839
H	3.275192	-2.245773	1.114529	C	2.311270	-2.197344	-2.612247
C	0.773689	-2.458080	2.974196	C	3.292064	-3.019203	-3.197318
C	0.972162	-1.275014	3.708583	C	1.080862	-2.038175	-3.269393
C	1.121379	-3.686668	3.564855	C	3.044135	-3.667972	-4.408933
C	1.501326	-1.320817	5.001906	H	4.262262	-3.146283	-2.709513
H	0.711439	-0.312041	3.260870	C	0.833422	-2.685989	-4.485428
C	1.658046	-3.730107	4.855257	H	0.314013	-1.401518	-2.819215
H	0.969417	-4.622646	3.022052				

C	1.813212	-3.502320	-5.055181
H	3.814612	-4.303967	-4.852804
H	-0.128610	-2.550183	-4.986129
H	1.620944	-4.009747	-6.004120
C	0.500981	1.818892	-0.361824
C	-0.650468	1.403292	0.389546
C	1.435853	2.632557	0.414496
S	-0.569146	2.093460	2.050875
C	0.986416	2.829260	1.686409
Br	1.890635	3.727461	3.087869
H	0.451130	1.950683	-1.447280
C	2.696127	3.202436	-0.178204
C	2.453615	4.446073	-1.053364
H	3.190029	2.421765	-0.780156
H	3.395385	3.464177	0.631816
C	3.736616	5.010639	-1.670401
H	1.739384	4.197062	-1.859271
H	1.961656	5.224241	-0.443258
C	3.501988	6.247741	-2.538359
H	4.448999	5.256753	-0.861794
H	4.227115	4.222620	-2.270087
H	4.443989	6.629276	-2.964387
H	2.822863	6.025811	-3.378888
H	3.045409	7.065425	-1.955653
C	-1.972260	1.130394	-0.167222
C	-3.208255	1.172637	0.437794
S	-2.149711	0.661028	-1.855211
C	-4.316866	0.832047	-0.409468
H	-3.338726	1.449348	1.485659
C	-3.881771	0.537634	-1.678932
Br	-4.928830	0.032758	-3.169036
C	-5.749174	0.847539	0.054614
C	-6.360723	2.258401	0.121051

H	-5.802074	0.381547	1.054171
H	-6.358294	0.220100	-0.615922
C	-7.810557	2.267350	0.615023
H	-5.742405	2.894451	0.779740
H	-6.307301	2.720018	-0.880778
C	-8.421770	3.667612	0.680855
H	-8.422951	1.627276	-0.046178
H	-7.856800	1.795917	1.613863
H	-9.464169	3.638413	1.036593
H	-7.854573	4.320774	1.365071
H	-8.421384	4.151373	-0.310285

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Pd-3BTanti-3BTanti-O-TS-2 SCF Done: -8419.46451921 A.U.

Pd	-0.078448	-0.859585	-0.267079
P	-1.659059	-2.708705	-0.454607
P	1.872634	-2.285938	-0.638241
C	-1.086534	-4.142122	-1.504605
H	-1.116359	-3.801633	-2.553418
H	-1.821191	-4.957341	-1.406676
C	0.316365	-4.677499	-1.176912
H	0.414676	-5.659915	-1.669773
H	0.399181	-4.882433	-0.095965
C	1.487407	-3.802776	-1.657040
H	1.278801	-3.419344	-2.669767
H	2.406993	-4.402381	-1.749722
C	-1.971001	-3.538410	1.172453
C	-1.125174	-3.256414	2.257657
C	-3.020135	-4.457889	1.350146
C	-1.315179	-3.888849	3.491294
H	-0.314977	-2.532655	2.135237
C	-3.210833	-5.086282	2.582585
H	-3.702318	-4.675502	0.524070
C	-2.357514	-4.804009	3.655610

H	-0.647208	-3.658917	4.325189	H	6.589017	-1.498531	-2.202904
H	-4.033112	-5.795608	2.708398	H	3.460906	0.473676	-4.429821
H	-2.510516	-5.294347	4.620538	H	5.882277	-0.036646	-4.096539
C	-3.363750	-2.395037	-1.088477	C	-1.999799	1.395546	0.905325
C	-3.940845	-3.085431	-2.168151	C	-1.213477	0.874660	-0.116970
C	-4.105198	-1.373117	-0.467150	C	-3.124329	2.180491	0.491316
C	-5.231472	-2.768632	-2.606715	S	-1.920529	1.349096	-1.665552
H	-3.395396	-3.878395	-2.681959	C	-3.194329	2.251515	-0.882445
C	-5.394496	-1.064062	-0.902407	Br	-4.481256	3.175115	-1.913629
H	-3.664336	-0.803969	0.354511	H	-1.736735	1.280135	1.958688
C	-5.962348	-1.760966	-1.973935	C	-4.039141	2.890986	1.456252
H	-5.664529	-3.315657	-3.448374	C	-3.525266	4.280547	1.874313
H	-5.951062	-0.261901	-0.412141	H	-4.162932	2.265342	2.357359
H	-6.969154	-1.512882	-2.319445	H	-5.040436	2.997085	1.006641
C	2.773298	-2.946209	0.833942	C	-4.438507	4.991315	2.877338
C	3.089120	-2.035720	1.860457	H	-2.511841	4.178732	2.302168
C	3.141225	-4.293403	0.994248	H	-3.410449	4.904622	0.970622
C	3.765287	-2.459944	3.006546	C	-3.933677	6.376724	3.283402
H	2.799700	-0.986356	1.764340	H	-5.452574	5.079392	2.446013
C	3.808524	-4.718009	2.148380	H	-4.550730	4.360345	3.778322
H	2.915938	-5.029835	0.221124	H	-4.611411	6.860137	4.005396
C	4.124588	-3.803443	3.155999	H	-2.935978	6.318683	3.749996
H	4.006378	-1.735320	3.788494	H	-3.848180	7.043327	2.408874
H	4.084316	-5.770334	2.255957	C	2.255771	2.826769	-0.112392
H	4.647971	-4.136777	4.055816	C	2.315807	2.582243	1.240642
C	3.210112	-1.550282	-1.681645	C	1.316823	1.951009	-0.749031
C	4.574952	-1.824870	-1.496549	S	1.249244	1.289009	1.735831
C	2.823292	-0.708085	-2.738904	C	0.661400	1.050146	0.081577
C	5.529737	-1.278994	-2.360061	H	1.077791	2.042955	-1.810215
H	4.898322	-2.467016	-0.674523	Br	3.381684	3.474951	2.520495
C	3.777674	-0.175216	-3.609253	C	3.063656	3.863180	-0.850898
H	1.766718	-0.461604	-2.874106	C	4.430753	3.351607	-1.338870
C	5.134055	-0.459155	-3.420979	H	3.219503	4.739145	-0.199273

H	2.478112	4.217393	-1.716684	H	-1.161990	-6.652041	3.403765
C	5.228467	4.403226	-2.115707	H	-1.438317	-5.071103	5.313295
H	5.017166	3.011849	-0.467063	C	-0.843013	-3.862557	-1.022929
H	4.281835	2.457732	-1.969894	C	-0.375761	-4.489272	-2.190735
C	6.592258	3.902019	-2.593373	C	-2.230553	-3.750376	-0.821613
H	4.634451	4.742139	-2.984493	C	-1.276932	-5.005050	-3.127945
H	5.365882	5.297983	-1.481412	H	0.693391	-4.579484	-2.389589
H	7.137775	4.678534	-3.153560	C	-3.125874	-4.268762	-1.758146
H	7.226095	3.596396	-1.744056	H	-2.614674	-3.238237	0.062715
H	6.486794	3.025300	-3.254474	C	-2.652686	-4.899131	-2.913165
				H	-0.896932	-5.490075	-4.030738
96				H	-4.200291	-4.165036	-1.589325
Pd-3BTanti-3BTanti-S SCF Done: -8419.48601392 A.U.				H	-3.355692	-5.299313	-3.648023
Pd	0.587104	-0.711808	0.057424	C	3.672365	0.412952	1.578247
P	0.294684	-3.092170	0.202400	C	4.117505	1.579723	0.932322
P	2.923039	-0.937291	0.575030	C	3.736037	0.347616	2.980572
C	1.901177	-3.985924	-0.097418	C	4.627500	2.647747	1.672354
H	2.255039	-3.595532	-1.064905	H	4.052779	1.663686	-0.154365
H	1.704764	-5.059724	-0.242076	C	4.247347	1.420126	3.718373
C	3.005375	-3.817546	0.965369	H	3.384661	-0.536287	3.516093
H	3.956040	-4.101463	0.485323	C	4.696419	2.571164	3.066912
H	2.840310	-4.553333	1.769347	H	4.963754	3.548498	1.153286
C	3.184065	-2.443684	1.642072	H	4.292662	1.352060	4.808402
H	4.181154	-2.399748	2.107112	H	5.094367	3.409319	3.644501
H	2.451733	-2.332568	2.457536	C	4.101901	-1.160392	-0.825681
C	-0.289202	-3.745293	1.826119	C	5.476357	-1.362133	-0.604708
C	-0.453460	-2.861772	2.904892	C	3.617732	-1.140078	-2.143239
C	-0.551486	-5.113541	2.017601	C	6.344449	-1.551415	-1.681711
C	-0.863381	-3.337243	4.155325	H	5.875493	-1.357949	0.413121
H	-0.266931	-1.794570	2.757599	C	4.489743	-1.326532	-3.221545
C	-0.959303	-5.586781	3.266494	H	2.554109	-0.965632	-2.324481
H	-0.449725	-5.813135	1.183640	C	5.851740	-1.534620	-2.992022
C	-1.114815	-4.699314	4.337715	H	7.410930	-1.706377	-1.499159
H	-0.992617	-2.638598	4.985780				

H	4.101325	-1.300670	-4.242612
H	6.533647	-1.677500	-3.834186
C	-2.444452	-0.386122	0.713855
C	-1.423223	-0.430194	-0.210922
C	-3.767667	-0.195315	0.173969
S	-2.086410	-0.211872	-1.807203
C	-3.715477	-0.093850	-1.196678
Br	-5.175601	0.155804	-2.377065
H	-2.281502	-0.487762	1.789955
C	-5.007596	-0.081654	1.022692
C	-5.282426	1.347035	1.525648
H	-4.909904	-0.755716	1.892350
H	-5.881263	-0.434082	0.449412
C	-6.522774	1.450276	2.418122
H	-4.397788	1.714518	2.076377
H	-5.395158	2.016275	0.654800
C	-6.801900	2.870817	2.911543
H	-7.401310	1.073138	1.863174
H	-6.404748	0.774143	3.285162
H	-7.700788	2.911501	3.547856
H	-5.957254	3.262924	3.502915
H	-6.959561	3.562931	2.067455
C	0.749655	1.319041	-0.138637
C	0.467608	2.333378	0.745243
S	1.372108	2.009421	-1.619965
C	0.753327	3.668145	0.279937
H	0.051987	2.153057	1.739769
C	1.255165	3.636982	-0.999160
Br	1.776252	5.115258	-2.062444
C	0.479741	4.907829	1.091068
C	-0.964118	5.424781	0.957226
H	1.176967	5.707830	0.791070
H	0.688640	4.691405	2.153624

C	-1.246936	6.665138	1.809864
H	-1.164687	5.651062	-0.104808
H	-1.666559	4.617417	1.231482
C	-2.677787	7.187395	1.670941
H	-1.040426	6.432644	2.871088
H	-0.533995	7.464255	1.535467
H	-2.847750	8.078765	2.296383
H	-2.902597	7.464608	0.627386
H	-3.414197	6.423473	1.972237

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Pd-3BTanti-3BTanti-S-Pr SCF Done: -8419.50970116 A.U.

Pd	-0.704984	-0.362637	0.123977
P	-0.207613	-2.696361	-0.139923
P	-2.606977	-0.782382	1.500990
C	-0.981689	-3.657505	1.270347
H	-0.571242	-3.169252	2.168581
H	-0.594903	-4.688755	1.282250
C	-2.521012	-3.694804	1.353945
H	-2.777601	-3.988481	2.385463
H	-2.892573	-4.508746	0.709484
C	-3.327476	-2.433070	0.984003
H	-4.354499	-2.536950	1.368791
H	-3.411761	-2.355342	-0.111800
C	-0.866655	-3.523783	-1.655184
C	-1.135171	-2.729580	-2.783425
C	-1.123796	-4.905568	-1.722211
C	-1.647165	-3.304153	-3.951950
H	-0.937616	-1.654731	-2.745845
C	-1.642157	-5.476715	-2.887290
H	-0.911645	-5.547793	-0.863842
C	-1.904918	-4.676435	-4.004773
H	-1.846274	-2.672584	-4.821432
H	-1.839417	-6.551418	-2.924114

H	-2.309718	-5.124784	-4.915903
C	1.536608	-3.302757	-0.021578
C	2.265513	-3.005689	1.145257
C	2.185874	-3.981437	-1.065074
C	3.598431	-3.398118	1.273677
H	1.794599	-2.445589	1.957841
C	3.525959	-4.363145	-0.939070
H	1.648289	-4.212211	-1.986692
C	4.235016	-4.077747	0.229653
H	4.148766	-3.156762	2.186616
H	4.016789	-4.886239	-1.764129
H	5.283061	-4.372156	0.324390
C	-4.100827	0.305175	1.404816
C	-4.400099	1.244331	2.407818
C	-4.909839	0.274906	0.253102
C	-5.484051	2.116494	2.268735
H	-3.786281	1.294908	3.309785
C	-5.995467	1.143696	0.118627
H	-4.689380	-0.424404	-0.556949
C	-6.288120	2.068062	1.126163
H	-5.702580	2.835852	3.062508
H	-6.612717	1.100258	-0.782531
H	-7.136497	2.748661	1.019773
C	-2.350025	-0.976313	3.323808
C	-3.331506	-1.516422	4.174790
C	-1.117478	-0.588208	3.874016
C	-3.082277	-1.668014	5.540759
H	-4.303619	-1.812618	3.771666
C	-0.869017	-0.735589	5.243505
H	-0.349499	-0.171505	3.215662
C	-1.849865	-1.277500	6.077731
H	-3.853391	-2.090411	6.190438
H	0.094348	-0.426666	5.657386

H	-1.656880	-1.395541	7.147162
C	-0.411566	1.768539	-0.322241
C	0.639569	1.022078	-0.955187
C	-1.393141	2.313353	-1.257112
S	0.382257	1.048876	-2.746462
C	-1.092544	1.980435	-2.545126
Br	-2.128894	2.356866	-4.086580
H	-0.260104	2.259356	0.643387
C	-2.546704	3.171049	-0.811561
C	-2.149068	4.631986	-0.530175
H	-2.989457	2.731495	0.097359
H	-3.334098	3.155475	-1.581801
C	-3.322680	5.499478	-0.065324
H	-1.350927	4.656442	0.234185
H	-1.705764	5.066530	-1.443654
C	-2.933236	6.951347	0.216273
H	-4.117966	5.472171	-0.832341
H	-3.768263	5.051417	0.841389
H	-3.798913	7.546981	0.548281
H	-2.164092	7.014661	1.004552
H	-2.520573	7.437515	-0.683642
C	2.016058	0.974822	-0.470784
C	2.604155	1.737286	0.517261
S	3.193977	-0.132165	-1.150240
C	3.990548	1.460012	0.756185
H	2.059669	2.509600	1.063148
C	4.436696	0.474112	-0.093923
Br	6.187967	-0.223819	-0.212147
C	4.831914	2.212714	1.753815
C	5.390005	3.540730	1.210793
H	5.669904	1.576117	2.081466
H	4.223360	2.416837	2.652195
C	6.228818	4.311605	2.234278

H	5.999250	3.331963	0.313806	C	-3.647439	1.655853	-1.232791
H	4.552738	4.174108	0.866233	C	-3.152466	1.330617	-2.507641
C	6.784355	5.630488	1.695004	C	-4.512357	2.754424	-1.101298
H	5.616019	4.508593	3.133278	C	-3.532816	2.070645	-3.629491
H	7.062700	3.671350	2.575714	H	-2.449623	0.500444	-2.619483
H	7.384075	6.158454	2.453726	C	-4.881518	3.502340	-2.223593
H	7.430471	5.463167	0.817004	H	-4.897457	3.035453	-0.118928
H	5.973171	6.308554	1.380657	C	-4.397974	3.159873	-3.489504
				H	-3.137047	1.805634	-4.613157
96				H	-5.550135	4.359131	-2.105704
Pd-3BTanti-3BTanti-S-TS-2 SCF Done: -8419.45884899 A.U.				H	-4.686444	3.747604	-4.364739
Pd	-0.868284	-0.327208	0.070957	C	-0.519179	-3.448782	1.883244
P	-3.130862	0.591140	0.188315	C	0.606248	-4.047485	1.286465
P	-1.671377	-2.504884	0.796808	C	-0.660951	-3.523127	3.279591
C	-4.402355	-0.772271	0.040590	C	1.545244	-4.728372	2.063008
H	-4.132989	-1.241143	-0.919829	H	0.751627	-3.981524	0.205410
H	-5.401888	-0.334938	-0.112730	C	0.286632	-4.199101	4.056146
C	-4.474131	-1.847278	1.145786	H	-1.510600	-3.055691	3.780349
H	-4.934277	-2.742389	0.695515	C	1.388228	-4.808386	3.451072
H	-5.175211	-1.513506	1.928098	H	2.408453	-5.192580	1.579564
C	-3.179677	-2.269686	1.867809	H	0.157486	-4.250329	5.140519
H	-3.385201	-3.185263	2.444916	H	2.125402	-5.339548	4.058538
H	-2.886223	-1.494794	2.595660	C	-2.203800	-3.775356	-0.437175
C	-3.613112	1.563007	1.677753	C	-2.730131	-5.020387	-0.047504
C	-2.642592	2.414965	2.237166	C	-2.086152	-3.485596	-1.805802
C	-4.882250	1.494838	2.279188	C	-3.140888	-5.947350	-1.007359
C	-2.939077	3.183919	3.365432	H	-2.809829	-5.274386	1.013012
H	-1.650010	2.471979	1.782316	C	-2.494706	-4.416906	-2.767467
C	-5.172535	2.257156	3.415354	H	-1.657742	-2.529528	-2.117378
H	-5.659851	0.852517	1.860366	C	-3.024599	-5.646297	-2.369764
C	-4.202627	3.104071	3.959576	H	-3.548077	-6.911763	-0.692481
H	-2.176357	3.845020	3.784698	H	-2.391772	-4.180378	-3.829510
H	-6.163021	2.191806	3.873362	H	-3.342351	-6.375072	-3.119912
H	-4.431558	3.701064	4.846126				

C	0.926141	2.048178	0.803782
C	0.470843	1.229731	-0.228005
C	1.219319	3.401205	0.443998
S	0.406307	2.180491	-1.709130
C	0.985819	3.610551	-0.898799
Br	1.260307	5.210300	-1.867117
H	1.089071	1.673958	1.817232
C	1.775600	4.420562	1.405688
C	3.313429	4.433139	1.469585
H	1.373991	4.216766	2.413757
H	1.419445	5.425604	1.124262
C	3.872863	5.452817	2.465801
H	3.674263	3.422147	1.731387
H	3.709989	4.644146	0.461026
C	5.401050	5.473488	2.522938
H	3.499819	6.459398	2.202189
H	3.468581	5.238556	3.472487
H	5.770274	6.216320	3.248314
H	5.804668	4.490360	2.818413
H	5.834582	5.723555	1.540163
C	1.148242	-0.553036	-0.331194
C	2.182831	-0.929047	0.516594
S	1.477046	-1.207540	-1.940065
C	3.224518	-1.711516	-0.075034
H	2.220613	-0.619243	1.562947
C	2.972165	-1.937746	-1.410780
Br	4.055978	-2.881926	-2.638953
C	4.451802	-2.158112	0.676931
C	5.532710	-1.068137	0.788314
H	4.882394	-3.045488	0.184750
H	4.150941	-2.475434	1.690754
C	6.765007	-1.509754	1.582883
H	5.836699	-0.760583	-0.227747

H	5.093632	-0.168617	1.256355
C	7.837029	-0.424843	1.696631
H	6.451207	-1.826551	2.594736
H	7.199449	-2.409441	1.109706
H	8.708939	-0.774687	2.272547
H	8.198069	-0.112954	0.702309
H	7.444771	0.474947	2.199783

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Pd-3BTanti-3BTsyn-O SCF Done: -8419.48339080 A.U.

Pd	-0.541037	-0.511777	-0.105144
P	-0.027749	-2.820814	-0.538138
P	-2.897699	-0.983288	-0.302782
C	-1.466906	-3.939085	-0.154220
H	-1.724432	-3.709938	0.891678
H	-1.133091	-4.988294	-0.174403
C	-2.720248	-3.794819	-1.040564
H	-3.553961	-4.259485	-0.489490
H	-2.583151	-4.402485	-1.949752
C	-3.156593	-2.388015	-1.501498
H	-4.214767	-2.425247	-1.803529
H	-2.584099	-2.092643	-2.395218
C	0.377240	-3.201785	-2.297005
C	0.296144	-2.182705	-3.259483
C	0.740673	-4.498236	-2.703142
C	0.564275	-2.455413	-4.605443
H	0.030297	-1.169329	-2.947253
C	1.007420	-4.768726	-4.046848
H	0.828400	-5.300103	-1.965210
C	0.918608	-3.747700	-5.000275
H	0.502407	-1.652154	-5.343881
H	1.290501	-5.779598	-4.351367
H	1.131895	-3.960735	-6.050886
C	1.351120	-3.579818	0.415514

C	1.123330	-4.335430	1.578299
C	2.676357	-3.324403	0.020459
C	2.197843	-4.836148	2.320246
H	0.108196	-4.538947	1.923664
C	3.745651	-3.827859	0.762685
H	2.875692	-2.714741	-0.863094
C	3.510398	-4.586200	1.913549
H	2.003938	-5.423504	3.221445
H	4.768861	-3.612692	0.445893
H	4.349180	-4.975220	2.496171
C	-3.970098	0.349797	-0.979369
C	-4.387492	1.382831	-0.121852
C	-4.308828	0.419004	-2.340671
C	-5.136277	2.452354	-0.614077
H	-4.114545	1.360846	0.935033
C	-5.060218	1.492116	-2.829983
H	-3.985076	-0.355357	-3.038284
C	-5.475758	2.510110	-1.969367
H	-5.444761	3.251633	0.063858
H	-5.315785	1.531862	-3.891940
H	-6.056436	3.351940	-2.354449
C	-3.788249	-1.522281	1.221756
C	-5.153270	-1.860683	1.192360
C	-3.089863	-1.613060	2.435768
C	-5.800126	-2.289454	2.353036
H	-5.719619	-1.777387	0.260946
C	-3.740023	-2.040007	3.599217
H	-2.033144	-1.336895	2.468910
C	-5.094059	-2.380353	3.558519
H	-6.861373	-2.548951	2.318942
H	-3.185691	-2.098944	4.539170
H	-5.603653	-2.711522	4.466972
C	2.326295	0.302569	-1.042829

C	1.450587	-0.041917	-0.037624
C	3.688992	0.537998	-0.632481
S	2.307010	-0.068280	1.481856
C	3.817993	0.365686	0.725439
Br	5.392832	0.556906	1.760166
H	2.023495	0.403673	-2.088093
C	4.782515	0.958116	-1.580097
C	4.805089	2.470984	-1.863601
H	4.656599	0.416555	-2.534695
H	5.761304	0.653343	-1.173881
C	5.901305	2.887584	-2.848572
H	3.819134	2.783164	-2.251983
H	4.937682	3.010821	-0.909548
C	5.924517	4.389629	-3.135818
H	6.884147	2.571879	-2.452891
H	5.769130	2.332697	-3.796002
H	6.723956	4.655105	-3.846459
H	4.968119	4.729597	-3.567445
H	6.091966	4.970767	-2.213556
C	-0.873016	1.491809	0.207399
C	-1.050705	2.248093	1.351737
S	-0.998965	2.504875	-1.211356
C	-1.317313	3.638320	1.076003
C	-1.323212	3.927008	-0.261133
Br	-1.622225	5.614549	-1.059898
C	-0.957867	1.712285	2.763021
C	0.104432	2.398866	3.636827
H	-0.731883	0.634392	2.710931
H	-1.940606	1.797158	3.267597
C	0.201742	1.812974	5.048486
H	1.083422	2.317275	3.134340
H	-0.114587	3.479692	3.707895
C	1.258118	2.493827	5.920319

H	-0.785558	1.881908	5.542658	C	5.036939	0.686100	1.126943
H	0.427081	0.732968	4.975813	C	5.460411	0.150409	-1.582731
H	1.302630	2.049707	6.928105	H	3.466313	0.896688	-1.897159
H	2.261705	2.405547	5.472098	C	6.244012	0.119800	0.702048
H	1.045770	3.569756	6.040000	H	4.886244	0.887878	2.189156
H	-1.492953	4.391496	1.846125	C	6.462720	-0.144764	-0.652238
				H	5.615082	-0.063771	-2.643380
96				H	7.018521	-0.112638	1.437860
Pd-3BTanti-3BTsyn-O-Pr SCF Done: -8419.50928540 A.U.				H	7.407080	-0.585237	-0.981813
Pd	0.423307	0.452288	0.054652	C	-2.585669	2.586003	-0.173365
P	2.372181	1.669403	0.679399	C	-3.547356	3.115528	-1.049856
P	-0.787855	2.413815	-0.586682	C	-2.997943	2.153731	1.100168
C	2.402165	3.296284	-0.248510	C	-4.884925	3.222946	-0.654521
H	2.292932	2.996733	-1.303416	H	-3.257285	3.446037	-2.048877
H	3.397607	3.761216	-0.165295	C	-4.330965	2.275743	1.498978
C	1.327576	4.339470	0.112123	H	-2.272513	1.700718	1.781578
H	1.319613	5.077286	-0.707363	C	-5.279706	2.810804	0.621508
H	1.657040	4.893718	1.006903	H	-5.621447	3.634633	-1.349882
C	-0.120300	3.876400	0.380157	H	-4.630563	1.932877	2.492420
H	-0.799358	4.737484	0.275139	H	-6.324980	2.898896	0.928923
H	-0.221517	3.541151	1.425298	C	-0.672440	2.936680	-2.354960
C	2.578063	2.166535	2.447707	C	-0.750666	4.277887	-2.771966
C	1.819328	1.494020	3.420431	C	-0.477854	1.937016	-3.325075
C	3.439676	3.200438	2.858324	C	-0.636016	4.610611	-4.124887
C	1.922210	1.840427	4.772093	H	-0.909747	5.073577	-2.040208
H	1.138683	0.697004	3.107795	C	-0.371990	2.270616	-4.679186
C	3.538165	3.550461	4.207350	H	-0.403958	0.890775	-3.014269
H	4.048312	3.734292	2.123901	C	-0.447704	3.607262	-5.081096
C	2.779948	2.870251	5.167026	H	-0.696145	5.657638	-4.433667
H	1.326205	1.305681	5.515994	H	-0.223947	1.481170	-5.420459
H	4.210851	4.356739	4.511584	H	-0.358400	3.868787	-6.138705
H	2.858218	3.145432	6.222006	C	0.681648	-1.709002	0.331231
C	4.026683	0.992922	0.200082	C	-0.634067	-1.479433	-0.203659
C	4.250762	0.704359	-1.160053				

C	1.609929	-2.339444	-0.603264
S	-0.660883	-2.067395	-1.917348
C	1.024189	-2.553245	-1.814478
Br	1.856936	-3.220422	-3.380623
H	0.836328	-1.856025	1.404781
C	3.008707	-2.726647	-0.208282
C	3.071270	-4.006798	0.645515
H	3.463018	-1.892275	0.351584
H	3.620902	-2.866112	-1.112926
C	4.495891	-4.386189	1.060693
H	2.449066	-3.878781	1.549966
H	2.615209	-4.839067	0.080633
C	4.564188	-5.651954	1.916364
H	5.113831	-4.519100	0.153950
H	4.950629	-3.541554	1.609749
H	5.601665	-5.898541	2.194233
H	3.988227	-5.536633	2.850026
H	4.147824	-6.521075	1.379877
C	-1.866383	-1.540004	0.576937
C	-3.187608	-1.309072	0.221368
S	-1.754494	-1.986067	2.282578
C	-4.093156	-1.477568	1.321478
C	-3.471208	-1.824280	2.488280
Br	-4.272298	-2.092228	4.174324
C	-3.680771	-0.922462	-1.151116
C	-4.335084	-2.076545	-1.932553
H	-2.853932	-0.499854	-1.743706
H	-4.414226	-0.104535	-1.040106
C	-4.848798	-1.657921	-3.313233
H	-3.606077	-2.898264	-2.041617
H	-5.170409	-2.489814	-1.338443
C	-5.510879	-2.798720	-4.087385
H	-5.565180	-0.823695	-3.197941

H	-4.007711	-1.250523	-3.903148
H	-5.866689	-2.465821	-5.075777
H	-4.807542	-3.632461	-4.249913
H	-6.378976	-3.203620	-3.540281
H	-5.170066	-1.324340	1.240675

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Pd-3BTanti-3BTsyn-O-TS-2 SCF Done: -8419.45531977 A.U.

Pd	0.129241	0.434901	-0.417917
P	-0.491037	2.779222	-0.800331
P	2.290760	0.725667	-1.514501
C	0.183371	3.458433	-2.406807
H	-0.091145	4.523558	-2.477378
H	-0.401574	2.947884	-3.190792
C	1.688410	3.285175	-2.677057
H	2.280220	3.701247	-1.844721
H	1.932106	3.912202	-3.552072
C	2.169152	1.859238	-2.993822
H	3.155748	1.904967	-3.482509
H	1.475914	1.383911	-3.707661
C	3.084990	-0.786821	-2.211465
C	3.145663	-1.069449	-3.586828
C	3.596155	-1.734964	-1.305487
C	3.713314	-2.263768	-4.044097
H	2.751558	-0.364034	-4.320186
C	4.167886	-2.922555	-1.764279
H	3.545065	-1.546653	-0.230321
C	4.227784	-3.192326	-3.135978
H	3.753493	-2.465402	-5.117780
H	4.559757	-3.644328	-1.043310
H	4.672581	-4.123992	-3.494827
C	-2.256750	3.324605	-0.950160
C	-2.662690	4.648312	-0.703302
C	-3.215570	2.385499	-1.361466

C	-3.998065	5.022065	-0.872874
H	-1.936721	5.393039	-0.369313
C	-4.551763	2.762308	-1.532625
H	-2.921533	1.348752	-1.535190
C	-4.945429	4.080307	-1.289176
H	-4.300861	6.053725	-0.674544
H	-5.285290	2.014183	-1.843351
H	-5.990792	4.373972	-1.415746
C	3.681655	1.481950	-0.554920
C	4.979555	1.586286	-1.088132
C	3.438079	1.970167	0.737777
C	6.005156	2.175347	-0.346789
H	5.196377	1.192482	-2.084740
C	4.466830	2.560571	1.480781
H	2.437351	1.884197	1.165910
C	5.749930	2.664679	0.940040
H	7.009824	2.247993	-0.771597
H	4.260334	2.935456	2.486203
H	6.555127	3.121811	1.521130
C	0.171322	3.932292	0.490097
C	0.816068	5.148565	0.208160
C	0.011900	3.556762	1.836860
C	1.288569	5.964238	1.242419
H	0.955993	5.478585	-0.822613
C	0.473369	4.375864	2.869586
H	-0.479392	2.611604	2.077415
C	1.117634	5.582116	2.575025
H	1.791161	6.904659	1.001594
H	0.333319	4.066779	3.908594
H	1.486138	6.220920	3.381702
C	0.444583	-2.721000	-0.244474
C	1.168421	-3.630490	0.592965
C	0.179568	-1.490328	0.372644

C	1.487579	-3.118473	1.820792
S	0.904225	-1.488733	1.996943
Br	2.431622	-3.978805	3.209810
H	1.453854	-4.635739	0.278372
C	0.084240	-3.103558	-1.660820
C	-0.853527	-4.316163	-1.786500
H	1.020123	-3.323241	-2.207407
H	-0.354932	-2.238620	-2.180896
C	-1.207687	-4.655713	-3.237270
H	-0.382968	-5.196200	-1.311828
H	-1.778295	-4.121340	-1.217295
C	-2.130610	-5.867723	-3.372658
H	-1.684792	-3.775906	-3.706332
H	-0.277531	-4.832403	-3.808647
H	-2.367087	-6.082859	-4.427357
H	-1.669135	-6.773427	-2.943874
H	-3.084597	-5.704016	-2.844166
C	-1.529368	-0.632633	0.277292
C	-2.342017	-0.386349	1.392058
S	-2.542794	-1.245911	-1.048801
C	-3.723586	-0.695165	1.171636
C	-3.988680	-1.164272	-0.085629
H	-4.497933	-0.558468	1.928515
C	-1.883347	0.182010	2.713802
C	-2.117567	-0.736298	3.925181
H	-2.411331	1.139477	2.888547
H	-0.815025	0.438799	2.655327
C	-1.629395	-0.134179	5.245847
H	-3.194184	-0.970301	4.007499
H	-1.608376	-1.698904	3.747948
C	-1.872067	-1.039413	6.454482
H	-0.549591	0.087319	5.163692
H	-2.125514	0.840876	5.408841

H	-1.510599	-0.577234	7.387291	H	-0.561130	-4.252765	-2.528469
H	-2.946066	-1.255181	6.584474	C	-4.178957	-3.136874	-1.665061
H	-1.354410	-2.006267	6.339322	H	-3.357305	-2.302219	0.141780
Br	-5.663867	-1.670602	-0.790910	C	-3.918929	-3.818674	-2.857751
				H	-2.398648	-4.743374	-4.088366
96				H	-5.193901	-2.807920	-1.429885
Pd-3BTanti-3BTsyn-S SCF Done: -8419.48374469 A.U.				H	-4.731394	-4.033461	-3.556388
Pd	0.372598	-0.557949	-0.051504	C	3.778860	-0.251305	1.223968
P	-0.477064	-2.801007	0.107029	C	4.349263	0.840611	0.544423
P	2.617488	-1.350580	0.307431	C	4.072349	-0.428964	2.586612
C	0.844261	-4.054902	-0.279484	C	5.207895	1.718138	1.208228
H	1.228341	-3.755955	-1.267395	H	4.113820	1.014981	-0.507538
H	0.383844	-5.047075	-0.407136	C	4.932083	0.454421	3.248810
C	2.014130	-4.171553	0.716745	H	3.635793	-1.253959	3.151694
H	2.828791	-4.693551	0.188984	C	5.504683	1.526911	2.561545
H	1.712764	-4.837417	1.541786	H	5.638597	2.561788	0.663679
C	2.584425	-2.889415	1.358276	H	5.153163	0.299119	4.307947
H	3.598309	-3.102206	1.730706	H	6.175761	2.216116	3.080220
H	1.979676	-2.607673	2.235275	C	3.579367	-1.841016	-1.189404
C	-1.116130	-3.317557	1.758412	C	4.896106	-2.325301	-1.091026
C	-1.019455	-2.429515	2.841459	C	2.981994	-1.739291	-2.455734
C	-1.676646	-4.590373	1.966236	C	5.593927	-2.711148	-2.237154
C	-1.464990	-2.809279	4.112367	H	5.386455	-2.388477	-0.115928
H	-0.601438	-1.432164	2.680908	C	3.683420	-2.124383	-3.603442
C	-2.119361	-4.968626	3.235383	H	1.966312	-1.344465	-2.542387
H	-1.780327	-5.287078	1.130207	C	4.987737	-2.612464	-3.495138
C	-2.013264	-4.078773	4.310710	H	6.617546	-3.084388	-2.149918
H	-1.388978	-2.106962	4.946272	H	3.209569	-2.032741	-4.583856
H	-2.554034	-5.960185	3.385652	H	5.537660	-2.909708	-4.391734
H	-2.364597	-4.375096	5.302369	C	-2.503726	0.421058	0.705716
C	-1.825848	-3.258988	-1.060427	C	-1.531214	0.179692	-0.241340
C	-1.571822	-3.936650	-2.265205	C	-3.763112	0.906831	0.198844
C	-3.142279	-2.855514	-0.774121	S	-2.161182	0.570893	-1.818863
C	-2.613493	-4.214845	-3.156064				

C	-3.714648	1.024605	-1.170441
Br	-5.105420	1.613309	-2.313498
H	-2.350741	0.260870	1.775942
C	-4.932897	1.271610	1.075796
C	-4.869832	2.710466	1.619352
H	-4.979186	0.567795	1.925978
H	-5.870898	1.142707	0.510549
C	-6.053672	3.075248	2.519613
H	-3.925010	2.847341	2.175747
H	-4.822248	3.410939	0.767122
C	-5.992512	4.505676	3.057628
H	-6.994369	2.932729	1.956821
H	-6.101611	2.364591	3.365622
H	-6.857375	4.735367	3.700900
H	-5.080022	4.670436	3.655189
H	-5.983398	5.241884	2.236514
C	0.989675	1.384056	-0.314405
C	0.959574	2.488250	0.515175
S	1.626072	1.830246	-1.885030
C	1.466026	3.684949	-0.110182
C	1.865957	3.487951	-1.402849
Br	2.583920	4.775174	-2.586100
C	0.433744	2.484724	1.931779
C	1.466088	2.862979	3.005439
H	0.029270	1.483345	2.149113
H	-0.425516	3.178062	2.003775
C	0.897696	2.846177	4.427903
H	2.326100	2.173739	2.941844
H	1.872459	3.868410	2.791825
C	1.915589	3.236430	5.500731
H	0.027341	3.525797	4.480685
H	0.499844	1.837643	4.647279
H	1.475236	3.208752	6.510765

H	2.783350	2.555380	5.495447
H	2.300535	4.256735	5.334415
H	1.517615	4.656384	0.384979

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Pd-3BTanti-3BTsyn-S-Pr SCF Done: -8419.50751732 A.U.

Pd	0.408682	-0.504757	-0.004117
P	-0.403575	-2.135646	1.557024
P	2.236074	-1.874920	-0.693042
C	0.194299	-3.832824	1.053278
H	-0.154002	-3.944574	0.014029
H	-0.320477	-4.608664	1.642069
C	1.714241	-4.100137	1.121316
H	1.906133	-4.983009	0.489320
H	1.969505	-4.404969	2.149671
C	2.715830	-2.991507	0.729124
H	3.695998	-3.455786	0.534693
H	2.855710	-2.303913	1.578456
C	0.275740	-1.930903	3.268862
C	0.996311	-0.768428	3.585996
C	0.096438	-2.911411	4.261366
C	1.534797	-0.592269	4.866148
H	1.125497	0.006602	2.825812
C	0.638904	-2.738241	5.536418
H	-0.480462	-3.813799	4.041172
C	1.360740	-1.577689	5.840606
H	2.085894	0.322544	5.098329
H	0.493894	-3.508812	6.298294
H	1.781091	-1.441305	6.840508
C	-2.198325	-2.427122	1.889565
C	-2.932943	-3.441906	1.252843
C	-2.881936	-1.528196	2.729705
C	-4.311366	-3.560959	1.460228
H	-2.440228	-4.147606	0.581032

C	-4.256149	-1.651836	2.938339	Br	1.723663	3.766820	2.554511
H	-2.333555	-0.722109	3.223913	H	0.600313	1.498474	-1.859877
C	-4.977154	-2.669653	2.304311	C	2.819932	2.687908	-0.471445
H	-4.865789	-4.356892	0.955962	C	2.854895	3.867438	-1.461011
H	-4.768117	-0.946118	3.597734	H	3.252971	1.795213	-0.951838
H	-6.054086	-2.763689	2.464892	H	3.463017	2.924795	0.391403
C	3.864689	-1.150072	-1.186581	C	4.263024	4.186964	-1.971995
C	4.075725	-0.756019	-2.521478	H	2.195083	3.647020	-2.319909
C	4.866216	-0.867967	-0.240160	H	2.426867	4.760199	-0.971388
C	5.256849	-0.114426	-2.899747	C	4.302984	5.359125	-2.953537
H	3.310021	-0.957247	-3.275023	H	4.919587	4.403782	-1.109655
C	6.047046	-0.221947	-0.620259	H	4.687291	3.285908	-2.450605
H	4.731753	-1.144510	0.807634	H	5.328451	5.562126	-3.302236
C	6.248894	0.155457	-1.950223	H	3.682798	5.158275	-3.843466
H	5.403669	0.175704	-3.943529	H	3.920486	6.283928	-2.489769
H	6.813543	-0.013899	0.130964	C	-2.037295	1.231015	-0.858952
H	7.172976	0.658104	-2.246288	C	-2.807022	2.217928	-1.456513
C	1.894535	-3.060312	-2.074175	S	-2.750826	-0.352865	-1.104156
C	2.828993	-4.029450	-2.482253	C	-3.968900	1.689239	-2.109984
C	0.651529	-3.000371	-2.724911	C	-4.063151	0.325944	-2.008438
C	2.522623	-4.920543	-3.513075	Br	-5.409976	-0.770250	-2.746250
H	3.808582	-4.083982	-1.999379	C	-2.488504	3.692901	-1.439852
C	0.345574	-3.892303	-3.759458	C	-3.394142	4.519171	-0.509742
H	-0.078212	-2.247165	-2.413269	H	-2.580726	4.085904	-2.468771
C	1.279357	-4.853686	-4.153439	H	-1.437953	3.839305	-1.145366
H	3.257615	-5.669054	-3.820809	C	-3.061117	6.013958	-0.514176
H	-0.624977	-3.831081	-4.258454	H	-4.450783	4.375912	-0.801164
H	1.042138	-5.550336	-4.961738	H	-3.302886	4.124541	0.516848
C	0.498861	1.552645	-0.772162	C	-3.964792	6.841401	0.401032
C	-0.774823	1.359867	-0.137037	H	-2.006912	6.147983	-0.211335
C	1.434310	2.353530	0.013169	H	-3.128337	6.400196	-1.548020
S	-0.802621	2.291493	1.417137	H	-3.695524	7.909667	0.378683
C	0.866453	2.777145	1.181384	H	-5.023364	6.758762	0.101677

H	-3.892101	6.501730	1.447754	H	2.570625	4.903904	0.207113
H	-4.696124	2.302391	-2.644672	C	2.738522	4.724241	-3.193261
				H	1.485471	3.472942	-4.438552
96				H	3.843625	5.832586	-1.699690
Pd-3BTanti-3BTsyn-S-TS-2 SCF Done: -8419.45537346 A.U.				H	3.303538	5.135633	-4.033568
Pd	-0.405734	0.597217	0.018970	C	-3.563051	-0.196427	1.669297
P	0.270403	2.929903	0.331024	C	-4.103665	-1.275525	0.944850
P	-2.670573	1.118586	0.733618	C	-3.658829	-0.210603	3.071541
C	-1.222239	4.054305	0.246992	C	-4.749172	-2.322586	1.604631
H	-1.649459	3.804309	-0.737637	H	-4.021999	-1.298199	-0.144682
H	-0.897101	5.104300	0.172609	C	-4.299896	-1.265426	3.730346
C	-2.306911	3.926980	1.337817	H	-3.235288	0.600009	3.667599
H	-3.239862	4.334299	0.914265	C	-4.852268	-2.320638	3.000117
H	-2.049186	4.587396	2.181853	H	-5.168825	-3.147621	1.023570
C	-2.603902	2.539237	1.938744	H	-4.370146	-1.256688	4.821255
H	-3.540304	2.600300	2.515689	H	-5.357755	-3.141011	3.515830
H	-1.808706	2.261238	2.650241	C	-3.937060	1.653336	-0.503966
C	1.160273	3.408020	1.872505	C	-5.223489	2.071541	-0.117614
C	2.097979	2.496688	2.392367	C	-3.604578	1.648874	-1.867766
C	0.949925	4.622632	2.548804	C	-6.149703	2.489153	-1.075193
C	2.808823	2.796519	3.557379	H	-5.509320	2.061212	0.937727
H	2.269182	1.548427	1.876468	C	-4.535550	2.062819	-2.827597
C	1.654930	4.915817	3.720523	H	-2.615186	1.304171	-2.178192
H	0.240158	5.355779	2.160268	C	-5.806247	2.486454	-2.432553
C	2.585881	4.003995	4.226724	H	-7.146094	2.812884	-0.763082
H	3.537616	2.080455	3.945631	H	-4.265539	2.047679	-3.886518
H	1.478895	5.863442	4.236359	H	-6.534140	2.809323	-3.181372
H	3.137786	4.235192	5.141444	C	2.173337	-0.894393	0.649090
C	1.292836	3.657443	-1.026899	C	1.293425	-0.527147	-0.371287
C	1.008905	3.257730	-2.344693	C	3.552696	-1.004987	0.276070
C	2.321556	4.588190	-0.808031	S	2.223663	-0.313798	-1.856050
C	1.718593	3.795345	-3.420615	C	3.720506	-0.719215	-1.060121
H	0.234456	2.508230	-2.529313	Br	5.333025	-0.773466	-2.045156
C	3.040904	5.114201	-1.885705				

H	1.845235	-1.067453	1.673816
C	4.640425	-1.438642	1.225681
C	4.802317	-2.966284	1.322923
H	4.420154	-1.035464	2.230054
H	5.600352	-0.994643	0.914358
C	5.891438	-3.401509	2.307608
H	3.836576	-3.416032	1.616128
H	5.029585	-3.365335	0.318848
C	6.056296	-4.919132	2.401694
H	6.852593	-2.943260	2.010819
H	5.661958	-2.992196	3.308899
H	6.846093	-5.198224	3.117654
H	5.121852	-5.404061	2.730903
H	6.324140	-5.353809	1.424119
C	-0.415114	-1.380035	-0.598241
C	-0.690900	-2.578681	0.073161
S	-0.962860	-1.504014	-2.279745
C	-1.311192	-3.561059	-0.764321
C	-1.517816	-3.137277	-2.050914
Br	-2.316152	-4.111395	-3.455393
C	-0.299611	-2.838178	1.506547
C	-1.029060	-3.988264	2.209871
H	-0.446353	-1.912349	2.089062
H	0.791086	-3.034927	1.539242
C	-0.633850	-4.134632	3.683028
H	-2.119562	-3.831349	2.139194
H	-0.819167	-4.940395	1.690430
C	-1.350700	-5.282296	4.395569
H	0.459589	-4.280830	3.754744
H	-0.844956	-3.185898	4.209307
H	-1.047408	-5.357677	5.452304
H	-2.444900	-5.144896	4.371669
H	-1.131261	-6.251747	3.917238

H	-1.593698	-4.557382	-0.424988
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Pd-3BTsyn-3BTsyn-O SCF Done: -8419.48239425 A.U.

Pd	-0.049711	0.527333	-0.380559
P	-1.509620	2.454532	-0.561062
P	1.798365	1.693814	-1.395688
C	-1.109251	3.614679	-1.966819
H	-1.787181	4.479113	-1.898917
H	-1.400760	3.080140	-2.885039
C	0.349342	4.080612	-2.085261
H	0.708337	4.485762	-1.123735
H	0.367527	4.931149	-2.787769
C	1.325104	3.021413	-2.619080
H	2.253570	3.500597	-2.966842
H	0.880778	2.520879	-3.494160
C	2.978101	0.669306	-2.377746
C	2.697377	0.342415	-3.715766
C	4.131694	0.134245	-1.779896
C	3.560947	-0.479904	-4.444480
H	1.795802	0.718009	-4.204401
C	4.990274	-0.691789	-2.509063
H	4.356857	0.348692	-0.734111
C	4.711734	-0.997395	-3.843973
H	3.328113	-0.719554	-5.485160
H	5.878521	-1.104004	-2.024233
H	5.385363	-1.643329	-4.412678
C	-3.317974	2.204323	-0.843567
C	-4.263803	2.412331	0.171922
C	-3.760230	1.746095	-2.097165
C	-5.621702	2.178473	-0.066271
H	-3.946124	2.755941	1.157638
C	-5.117330	1.524776	-2.336051
H	-3.043958	1.539049	-2.896475

C	-6.053015	1.739656	-1.319888
H	-6.344714	2.340528	0.737103
H	-5.442716	1.168126	-3.316486
H	-7.114678	1.556700	-1.503164
C	2.873175	2.634473	-0.226076
C	4.022334	3.314547	-0.670700
C	2.521380	2.712311	1.129772
C	4.795575	4.057744	0.222544
H	4.326542	3.255199	-1.718907
C	3.296223	3.458694	2.024324
H	1.636035	2.183560	1.487844
C	4.432720	4.132136	1.572578
H	5.687472	4.578601	-0.135165
H	3.008198	3.508576	3.077104
H	5.040467	4.713000	2.271106
C	-1.442273	3.526707	0.942410
C	-1.626264	4.919926	0.901172
C	-1.217484	2.912769	2.186789
C	-1.578156	5.678694	2.073773
H	-1.814652	5.430019	-0.045275
C	-1.180595	3.671682	3.360446
H	-1.078202	1.832008	2.235330
C	-1.356209	5.057037	3.306295
H	-1.718450	6.761480	2.022896
H	-1.011202	3.174662	4.318915
H	-1.321390	5.652259	4.222325
C	1.351846	-2.250537	-0.892194
C	2.391719	-3.112939	-0.386606
C	1.178503	-1.105010	-0.139502
C	2.997010	-2.625508	0.737658
S	2.306690	-1.094932	1.203076
Br	4.391630	-3.429644	1.729316
H	2.674155	-4.059594	-0.850783

C	0.557484	-2.605305	-2.127945
C	-0.282055	-3.886101	-1.994754
H	1.244964	-2.715011	-2.988142
H	-0.107709	-1.761293	-2.372053
C	-1.107458	-4.205019	-3.244429
H	0.379806	-4.741869	-1.767442
H	-0.954960	-3.780853	-1.127090
C	-1.965938	-5.463076	-3.103553
H	-1.759112	-3.341883	-3.472255
H	-0.431141	-4.311376	-4.113363
H	-2.539702	-5.668935	-4.021962
H	-1.346005	-6.351107	-2.892748
H	-2.687270	-5.360099	-2.275935
C	-1.532745	-0.648228	0.446227
C	-1.805888	-1.092408	1.729837
S	-2.715707	-1.302022	-0.668139
C	-2.973845	-1.934541	1.807454
C	-3.566380	-2.143421	0.593327
H	-3.350154	-2.368861	2.735313
C	-0.979980	-0.786697	2.959301
C	-0.382973	-2.025328	3.647780
H	-1.595335	-0.235385	3.697332
H	-0.155342	-0.113884	2.674759
C	0.484156	-1.685664	4.863634
H	-1.195429	-2.706404	3.959125
H	0.218567	-2.583400	2.910762
C	1.117833	-2.912983	5.520732
H	1.281375	-0.987037	4.551086
H	-0.125269	-1.138279	5.607190
H	1.720468	-2.637446	6.401542
H	0.349779	-3.631410	5.854093
H	1.780630	-3.440976	4.815329
Br	-5.096487	-3.193283	0.231608

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Pd-3BTsyn-3BTsyn-O-Pr SCF Done: -8419.50958129 A.U.

Pd	1.270965	0.267217	-0.238196
P	1.028551	2.577509	0.057508
P	3.508492	0.006433	-0.913652
C	2.419147	3.472794	-0.822217
H	2.423408	4.529151	-0.506349
H	2.118020	3.482737	-1.883262
C	3.831802	2.871435	-0.684846
H	4.057665	2.645674	0.372059
H	4.546774	3.662079	-0.970806
C	4.139416	1.646004	-1.567366
H	5.229270	1.568913	-1.714473
H	3.686780	1.786799	-2.563426
C	4.015167	-1.166120	-2.260396
C	4.719155	-0.792252	-3.418277
C	3.625059	-2.511241	-2.121753
C	5.026945	-1.737131	-4.404633
H	5.037892	0.240155	-3.568949
C	3.944147	-3.455265	-3.098602
H	3.060531	-2.818632	-1.238102
C	4.644582	-3.070683	-4.247507
H	5.571484	-1.424325	-5.299737
H	3.634146	-4.495202	-2.966200
H	4.885900	-3.807002	-5.018522
C	-0.390709	3.646798	-0.492282
C	-0.636022	4.927527	0.033573
C	-1.229000	3.160698	-1.508613
C	-1.689641	5.705464	-0.453910
H	-0.006101	5.320369	0.835397
C	-2.276907	3.943894	-2.004434
H	-1.065219	2.153617	-1.903107
C	-2.509326	5.217262	-1.477175

H	-1.871572	6.697780	-0.032064
H	-2.922136	3.549452	-2.793199
H	-3.333180	5.826710	-1.858083
C	4.761180	-0.342154	0.412833
C	6.094178	-0.686532	0.127827
C	4.361778	-0.235761	1.755079
C	7.006042	-0.911796	1.162031
H	6.421839	-0.790426	-0.909979
C	5.277136	-0.453424	2.790486
H	3.321121	0.012493	1.982634
C	6.600037	-0.793201	2.496090
H	8.038193	-1.184666	0.925840
H	4.950650	-0.364850	3.829999
H	7.314403	-0.971583	3.304235
C	1.240645	3.072851	1.834542
C	2.113680	4.076739	2.286251
C	0.483396	2.369046	2.789857
C	2.219842	4.373945	3.650042
H	2.725054	4.640479	1.579240
C	0.578605	2.673627	4.149203
H	-0.180017	1.566357	2.456826
C	1.450524	3.677504	4.584767
H	2.908906	5.155876	3.980411
H	-0.022689	2.116971	4.872855
H	1.534197	3.910805	5.649370
C	-2.218271	-3.230437	0.124379
C	-1.065055	-3.966438	0.549171
C	-1.948612	-1.886737	-0.074379
C	0.062970	-3.195070	0.636105
S	-0.240876	-1.527519	0.230194
Br	1.756329	-3.770096	1.222701
H	-1.081737	-5.031062	0.786577
C	-3.575302	-3.873476	-0.027945

C	-4.284437	-4.143552	1.311178
H	-3.458849	-4.828876	-0.570110
H	-4.217861	-3.237769	-0.656412
C	-5.647344	-4.823506	1.149528
H	-3.635574	-4.766850	1.952905
H	-4.409217	-3.186713	1.848776
C	-6.356147	-5.089683	2.478192
H	-6.290678	-4.196716	0.505622
H	-5.515478	-5.775609	0.603684
H	-7.332566	-5.576644	2.325763
H	-5.754879	-5.746263	3.129364
H	-6.534678	-4.152552	3.031873
C	-2.846919	-0.838033	-0.548579
C	-3.413734	0.222117	0.136914
S	-3.325976	-0.825797	-2.243187
C	-4.250673	1.031056	-0.702054
C	-4.302124	0.583875	-1.995228
H	-4.785718	1.915200	-0.354418
C	-3.212958	0.503078	1.605047
C	-4.481136	0.324557	2.457404
H	-2.845111	1.538448	1.719521
H	-2.417636	-0.152166	1.992956
C	-4.259865	0.633940	3.941074
H	-5.286427	0.971751	2.065277
H	-4.847583	-0.711785	2.346486
C	-5.517232	0.461226	4.794228
H	-3.456307	-0.017459	4.330487
H	-3.882898	1.667978	4.042843
H	-5.322010	0.690179	5.854075
H	-6.327583	1.127619	4.453835
H	-5.898535	-0.572483	4.742259
Br	-5.277430	1.349419	-3.416431

Pd-3BTsyn-3BTsyn-O-TS-2 SCF Done: -8419.45532151 A.U.

Pd	0.127652	0.435237	-0.418368
P	-0.497718	2.777945	-0.801066
P	2.288699	0.730604	-1.514873
C	0.175398	3.458767	-2.407404
H	-0.101457	4.523285	-2.477972
H	-0.408272	2.947006	-3.191550
C	1.680879	3.288805	-2.677424
H	2.271683	3.706048	-1.844952
H	1.923370	3.916436	-3.552338
C	2.164664	1.863915	-2.994184
H	3.151121	1.911676	-3.482955
H	1.472374	1.387067	-3.707921
C	3.086027	-0.780194	-2.211979
C	3.145694	-1.063267	-3.587299
C	3.600679	-1.726668	-1.306242
C	3.715796	-2.256333	-4.044767
H	2.748882	-0.359173	-4.320470
C	4.174813	-2.913023	-1.765238
H	3.550445	-1.538015	-0.231099
C	4.233717	-3.183219	-3.136896
H	3.755184	-2.458301	-5.118416
H	4.569396	-3.633494	-1.044446
H	4.680431	-4.113904	-3.495904
C	-2.264603	3.319506	-0.950894
C	-2.673432	4.642264	-0.703766
C	-3.221390	2.378334	-1.362246
C	-4.009643	5.013104	-0.873150
H	-1.949054	5.388523	-0.369750
C	-4.558426	2.752235	-1.533219
H	-2.925095	1.342240	-1.536081
C	-4.954966	4.069327	-1.289516
H	-4.314697	6.044061	-0.674628

H	-5.290348	2.002549	-1.843965
H	-6.000989	4.360703	-1.415926
C	3.678014	1.489669	-0.555204
C	4.975601	1.596978	-1.088589
C	3.433572	1.976942	0.737687
C	6.000038	2.188051	-0.347245
H	5.193105	1.203911	-2.085336
C	4.461164	2.569357	1.480696
H	2.433126	1.888583	1.165988
C	5.743942	2.676436	0.939771
H	7.004473	2.263038	-0.772196
H	4.254042	2.943468	2.486277
H	6.548224	3.135166	1.520869
C	0.162258	3.932311	0.489450
C	0.803946	5.150211	0.207551
C	0.004258	3.556099	1.836187
C	1.274864	5.966791	1.241812
H	0.942666	5.480813	-0.823198
C	0.464128	4.376089	2.868926
H	-0.484622	2.609690	2.076707
C	1.105355	5.583962	2.574397
H	1.775060	6.908494	1.001007
H	0.325216	4.066429	3.907916
H	1.472602	6.223484	3.381079
C	0.451199	-2.719619	-0.243678
C	1.177546	-3.626888	0.594013
C	0.182863	-1.489497	0.373081
C	1.495368	-3.113618	1.821663
S	0.907584	-1.485416	1.997341
Br	2.441705	-3.971036	3.210917
H	1.465731	-4.631443	0.279726
C	0.092031	-3.103427	-1.659975
C	-0.842147	-4.318800	-1.785491

H	1.028586	-3.320412	-2.206495
H	-0.349645	-2.239831	-2.180167
C	-1.194452	-4.660304	-3.236254
H	-0.369304	-5.197174	-1.310014
H	-1.767795	-4.126312	-1.216916
C	-2.114240	-5.874726	-3.371368
H	-1.673405	-3.782044	-3.706329
H	-0.263455	-4.835123	-3.806833
H	-2.348932	-6.091640	-4.426101
H	-1.651028	-6.778801	-2.941014
H	-3.069252	-5.712797	-2.844180
C	-1.528250	-0.636029	0.277541
C	-2.341492	-0.391410	1.392235
S	-2.540208	-1.252086	-1.048419
C	-3.722320	-0.703555	1.171860
C	-3.986293	-1.173607	-0.085284
H	-4.496994	-0.568523	1.928702
C	-1.884236	0.178412	2.713838
C	-2.115853	-0.740298	3.925417
H	-2.414779	1.134483	2.888451
H	-0.816615	0.438057	2.655197
C	-1.629221	-0.136603	5.245930
H	-3.191816	-0.977243	4.007861
H	-1.604018	-1.701525	3.748347
C	-1.869417	-1.042242	6.454759
H	-0.550014	0.087741	5.163671
H	-2.127913	0.837166	5.408759
H	-1.508790	-0.579081	7.387406
H	-2.942865	-1.260542	6.585074
H	-1.349496	-2.007878	6.339583
Br	-5.660288	-1.684147	-0.790382

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Pd-3BTsyn-3BTsyn-S SCF Done: -8419.48073668 A.U.

Pd	-0.092345	0.424545	0.254142	H	7.134421	1.327623	1.023884
P	1.472214	2.256829	0.530954	C	-2.973540	2.668401	0.112687
P	-1.924970	1.651672	1.244722	C	-4.127444	3.321147	0.585522
C	1.084918	3.415550	1.936096	C	-2.611250	2.820684	-1.233192
H	1.790231	4.259723	1.901102	C	-4.891811	4.115660	-0.270047
H	1.309590	2.861596	2.862348	H	-4.442073	3.198223	1.625245
C	-0.359212	3.937469	2.000142	C	-3.378050	3.617793	-2.090274
H	-0.667463	4.353920	1.025916	H	-1.727225	2.309594	-1.615555
H	-0.368034	4.790025	2.699735	C	-4.517175	4.266536	-1.610589
C	-1.390667	2.916345	2.504608	H	-5.787202	4.615241	0.108674
H	-2.292853	3.433744	2.866343	H	-3.082599	3.724866	-3.136713
H	-0.970054	2.369852	3.364097	H	-5.118921	4.886167	-2.280427
C	-3.171750	0.658471	2.175535	C	1.465050	3.356807	-0.960810
C	-3.137161	0.524572	3.573793	C	1.977466	4.665702	-0.922578
C	-4.161377	-0.033822	1.454406	C	0.985743	2.855145	-2.181452
C	-4.078345	-0.270493	4.236438	C	1.993363	5.456688	-2.073141
H	-2.377503	1.035348	4.167630	H	2.381436	5.076875	0.005363
C	-5.099995	-0.825046	2.118606	C	1.011631	3.644227	-3.336375
H	-4.197495	0.038492	0.365495	H	0.604573	1.833346	-2.231808
C	-5.062827	-0.945619	3.511604	C	1.510164	4.947580	-3.283561
H	-4.037729	-0.359867	5.325040	H	2.392256	6.473241	-2.025983
H	-5.858525	-1.356948	1.539389	H	0.642629	3.232860	-4.279229
H	-5.797840	-1.566727	4.029830	H	1.528641	5.566001	-4.184564
C	3.284546	1.955188	0.747973	C	-1.822648	-2.232172	0.399346
C	3.999015	1.394820	-0.326794	C	-2.807915	-2.971425	-0.350882
C	3.978131	2.268703	1.928873	C	-1.397275	-1.085565	-0.242564
C	5.373621	1.173966	-0.227289	C	-3.119063	-2.392327	-1.549642
H	3.481902	1.126871	-1.250158	S	-2.208885	-0.926274	-1.788663
C	5.356090	2.043976	2.025896	Br	-4.351438	-3.022384	-2.836544
H	3.460447	2.695402	2.788841	H	-3.268119	-3.898408	-0.004403
C	6.058002	1.500756	0.947803	C	-1.356529	-2.687315	1.762581
H	5.908684	0.736183	-1.073298	C	-0.721564	-4.086981	1.787161
H	5.879642	2.299217	2.950840	H	-2.214298	-2.675295	2.461859

H	-0.635009	-1.950791	2.150655	P	0.891417	-1.920948	1.573585
C	-0.319554	-4.551011	3.190735	P	2.956074	-0.338427	-0.748137
H	-1.426307	-4.820993	1.356543	C	2.268487	-3.055336	1.013325
H	0.159772	-4.094951	1.121602	H	2.008449	-3.309598	-0.026952
C	0.313013	-5.943295	3.217736	H	2.242315	-3.997654	1.583621
H	0.383062	-3.818969	3.629852	C	3.707312	-2.495928	1.067103
H	-1.210034	-4.537232	3.846103	H	4.324537	-3.158068	0.437395
H	0.586783	-6.246598	4.241364	H	4.090473	-2.615275	2.094067
H	-0.378012	-6.704934	2.818710	C	3.982103	-1.032488	0.655780
H	1.228277	-5.979097	2.603338	H	5.056401	-0.916397	0.440343
C	1.380847	-0.813541	-0.471857	H	3.761864	-0.361361	1.500829
C	2.307000	-1.577797	0.217866	C	1.411052	-1.445079	3.286878
S	1.575783	-1.043675	-2.194168	C	1.510785	-0.083304	3.613561
C	3.177448	-2.332257	-0.648060	C	1.722814	-2.403570	4.268210
C	2.912214	-2.136697	-1.976093	C	1.920638	0.314869	4.891424
H	3.969807	-2.994348	-0.296934	H	1.254172	0.667107	2.861163
C	2.386951	-1.655955	1.727924	C	2.136063	-2.006306	5.541617
C	3.801270	-1.682983	2.323778	H	1.632658	-3.469290	4.040756
H	1.847568	-2.556305	2.075871	C	2.236796	-0.645368	5.855178
H	1.828361	-0.801620	2.148125	H	1.984736	1.379452	5.130353
C	3.808516	-1.694755	3.855882	H	2.376418	-2.761066	6.295166
H	4.342211	-2.575298	1.960702	H	2.556391	-0.336492	6.853949
H	4.373070	-0.812677	1.960063	C	-0.492466	-3.101847	1.897456
C	5.211960	-1.753069	4.461012	C	-0.619932	-4.322238	1.211992
H	3.284720	-0.794203	4.227019	C	-1.520703	-2.716605	2.778258
H	3.214874	-2.554511	4.217414	C	-1.737604	-5.139606	1.411569
H	5.181400	-1.755129	5.562710	H	0.148321	-4.647249	0.507538
H	5.747707	-2.663030	4.142147	C	-2.632771	-3.535515	2.978615
H	5.819291	-0.888417	4.144621	H	-1.451178	-1.766485	3.314352
Br	3.817551	-2.909038	-3.444386	C	-2.746191	-4.751618	2.295961
				H	-1.817908	-6.085025	0.868525
96				H	-3.418163	-3.220011	3.670452
Pd-3BTsyn-3BTsyn-S-Pr SCF Done: -8419.50302748 A.U.				H	-3.619488	-5.390332	2.450007
Pd	0.709980	-0.102238	0.026834				

C	3.900799	1.192385	-1.176198
C	4.260432	1.513655	-2.496969
C	4.167764	2.132606	-0.161947
C	4.883354	2.731084	-2.790898
H	4.056918	0.808781	-3.305757
C	4.798599	3.343275	-0.456555
H	3.870135	1.927667	0.869490
C	5.159668	3.647993	-1.773363
H	5.156870	2.960410	-3.824316
H	5.002082	4.055518	0.347417
H	5.649408	4.597268	-2.004487
C	3.314647	-1.485321	-2.153350
C	4.616999	-1.906319	-2.478942
C	2.236129	-1.975422	-2.907841
C	4.832745	-2.795464	-3.534445
H	5.472671	-1.530941	-1.911437
C	2.452422	-2.863617	-3.967610
H	1.220736	-1.658690	-2.653074
C	3.750214	-3.274834	-4.281504
H	5.849752	-3.114939	-3.776975
H	1.602834	-3.234630	-4.546552
H	3.920949	-3.969595	-5.107997
C	-0.201939	1.727603	-0.789787
C	-1.208371	1.027448	-0.016728
C	0.365852	2.833829	-0.025525
S	-1.489063	1.885346	1.556322
C	-0.205321	3.018677	1.193842
Br	0.330005	4.281939	2.497845
C	-2.340075	0.295651	-0.578262
C	-3.628222	0.716934	-0.879389
S	-2.116804	-1.389373	-1.021778
C	-4.420632	-0.319683	-1.475889
C	-3.737517	-1.497320	-1.626667

Br	-4.391428	-3.091674	-2.394852
C	-4.183719	2.099451	-0.634429
C	-5.184790	2.175514	0.531654
H	-4.685771	2.444569	-1.556586
H	-3.359426	2.803221	-0.446345
C	-5.750251	3.581705	0.750775
H	-6.014564	1.467528	0.352904
H	-4.684607	1.831679	1.453806
C	-6.751647	3.662665	1.903829
H	-4.914270	4.279884	0.936953
H	-6.231062	3.930693	-0.181698
H	-7.137791	4.686392	2.034212
H	-7.616644	3.000110	1.731372
H	-6.289263	3.357522	2.857474
H	-5.455338	-0.181910	-1.793866
H	1.176976	3.456614	-0.406087
C	-0.170654	1.769639	-2.310398
C	-0.989698	2.917171	-2.927780
C	-0.908208	2.958567	-4.456965
C	-1.710739	4.100392	-5.082613
H	0.879704	1.865934	-2.635062
H	-0.532043	0.810523	-2.712673
H	-0.638696	3.880773	-2.515976
H	-2.044713	2.821103	-2.618321
H	0.151532	3.042332	-4.760832
H	-1.260648	1.993513	-4.864886
H	-1.628258	4.100274	-6.181523
H	-1.359078	5.081942	-4.722504
H	-2.781505	4.022957	-4.829622

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PdBr-TTBTBr SCF Done: -8419.56299897 A.U.

Pd	1.873817	-0.255946	-0.048739
P	4.161713	0.528464	-0.153904

P	1.513731	0.520383	2.105131	C	0.907201	2.261590	2.118763
C	5.001225	0.736545	1.496658	C	0.586091	2.909180	3.326248
H	5.968152	1.238685	1.334968	C	0.798120	2.972401	0.913758
H	5.249561	-0.290285	1.813291	C	0.169768	4.241436	3.324013
C	4.200270	1.441687	2.601305	H	0.645100	2.369329	4.274821
H	3.837884	2.425292	2.257870	C	0.381579	4.307834	0.914143
H	4.894939	1.655530	3.431432	H	1.036304	2.475677	-0.029663
C	3.035728	0.622858	3.177695	C	0.067828	4.943454	2.117124
H	2.716785	1.045493	4.143453	H	-0.081197	4.732829	4.267487
H	3.369206	-0.407834	3.378410	H	0.300204	4.847341	-0.032399
Br	2.016419	-1.040889	-2.432100	H	-0.261132	5.985794	2.117333
C	0.334964	-0.400074	3.180067	C	4.299697	2.177004	-0.974740
C	0.768965	-1.500890	3.938375	C	5.005034	3.260567	-0.423962
C	-1.027224	-0.055252	3.202126	C	3.647781	2.348759	-2.211346
C	-0.136280	-2.228071	4.716210	C	5.059183	4.488105	-1.093283
H	1.815615	-1.811923	3.924332	H	5.523173	3.165195	0.531609
C	-1.929653	-0.787365	3.976419	C	3.712718	3.573371	-2.879579
H	-1.391774	0.777510	2.598657	H	3.089554	1.515538	-2.647943
C	-1.487241	-1.872314	4.738781	C	4.415387	4.647123	-2.322591
H	0.218227	-3.079746	5.302267	H	5.610223	5.321168	-0.649230
H	-2.986916	-0.511717	3.973328	H	3.206005	3.687651	-3.841217
H	-2.195559	-2.444279	5.343354	H	4.460272	5.606030	-2.845346
C	5.403597	-0.534800	-1.005614	C	-0.575678	-2.146946	0.249204
C	6.561364	0.007352	-1.586078	C	-1.997587	-2.215311	0.086252
C	5.218528	-1.926575	-1.011785	C	-0.066611	-0.898083	-0.054744
C	7.523039	-0.832071	-2.155850	C	-2.585791	-1.041713	-0.338137
H	6.712399	1.089249	-1.604589	S	-1.343320	0.182970	-0.540231
C	6.186238	-2.762909	-1.574027	H	-2.572628	-3.128266	0.262257
H	4.301725	-2.353843	-0.601071	C	0.255571	-3.342615	0.649931
C	7.338685	-2.217772	-2.147732	C	0.444755	-4.371769	-0.477860
H	8.417677	-0.399665	-2.611319	H	-0.208111	-3.841181	1.521106
H	6.028541	-3.844244	-1.579247	H	1.246965	-2.992741	0.984708
H	8.089523	-2.872719	-2.597270	C	1.291772	-5.579122	-0.064957

H	-0.546209	-4.720483	-0.821361	C	1.339697	0.065322	-2.344085
H	0.906828	-3.866855	-1.343457	H	1.372038	-0.969239	-2.721197
C	1.473706	-6.607633	-1.182431	H	2.154889	0.616747	-2.837058
H	2.283729	-5.226200	0.274575	C	-0.008059	0.694839	-2.712468
H	0.832004	-6.067232	0.814762	H	-0.018177	0.839471	-3.806160
H	2.090088	-7.460922	-0.855197	H	-0.098986	1.706227	-2.280516
H	0.502526	-7.008439	-1.518360	C	-1.214866	-0.179314	-2.335111
H	1.963428	-6.158125	-2.062261	H	-0.993694	-1.240720	-2.534425
C	-3.983104	-0.752757	-0.597335	H	-2.094413	0.062121	-2.951325
C	-4.543747	0.221475	-1.398340	C	2.681222	1.559366	-0.251375
S	-5.247149	-1.699625	0.169396	C	4.047764	1.698623	-0.540294
C	-5.976253	0.226275	-1.435116	C	1.964579	2.669979	0.224372
H	-3.936582	0.913701	-1.985197	C	4.680483	2.933679	-0.372672
C	-6.482785	-0.770366	-0.631327	H	4.632539	0.841229	-0.877975
Br	-8.301046	-1.197948	-0.349790	C	2.598417	3.904992	0.380706
C	-6.788048	1.212146	-2.233978	H	0.913745	2.560789	0.502359
C	-7.038076	2.542927	-1.501926	C	3.957061	4.039949	0.081640
H	-7.756761	0.758762	-2.500042	H	5.747425	3.027199	-0.590723
H	-6.265095	1.414645	-3.184672	H	2.030115	4.759201	0.756837
C	-7.840760	3.549673	-2.331032	H	4.455487	5.003351	0.215887
H	-7.567522	2.336620	-0.554908	C	2.990596	-1.403273	-0.518657
H	-6.068443	2.989068	-1.215742	C	3.042517	-2.312017	0.551577
C	-8.096112	4.870811	-1.604176	C	3.859755	-1.594428	-1.612048
H	-7.308009	3.746592	-3.279465	C	3.945485	-3.379423	0.528839
H	-8.805749	3.094430	-2.619477	H	2.390439	-2.167364	1.413678
H	-8.673839	5.571676	-2.228000	C	4.763703	-2.659365	-1.626429
H	-8.662131	4.711625	-0.671002	H	3.843526	-0.916079	-2.467045
H	-7.149842	5.368836	-1.333273	C	4.807896	-3.556359	-0.555147
				H	3.971397	-4.074920	1.371321
58				H	5.433013	-2.788129	-2.480904
PdCl2 SCF Done: -2774.53356421 A.U.				H	5.512886	-4.391580	-0.568002
Pd	0.004188	-0.258951	0.964751	C	-2.640188	1.490065	-0.399046
P	1.766507	-0.017103	-0.521229	C	-3.048447	1.921034	0.877813
P	-1.730669	-0.112619	-0.554688				

C	-2.935886	2.297652	-1.512858
C	-3.740663	3.124792	1.027382
H	-2.819385	1.305952	1.751791
C	-3.624188	3.504836	-1.354919
H	-2.637123	2.001763	-2.519161
C	-4.029255	3.921302	-0.084794
H	-4.051475	3.441839	2.025985
H	-3.842747	4.119233	-2.232081
H	-4.566645	4.865189	0.037848
C	-2.999715	-1.439902	-0.498635
C	-4.314875	-1.207560	-0.930487
C	-2.626177	-2.726614	-0.079131
C	-5.241903	-2.253829	-0.950768
H	-4.624498	-0.206983	-1.241304
C	-3.553813	-3.770025	-0.108900
H	-1.615462	-2.903415	0.294421
C	-4.862297	-3.535676	-0.543194
H	-6.266099	-2.063020	-1.281243
H	-3.256514	-4.766672	0.226343
H	-5.589749	-4.351385	-0.554500
Cl	-1.658296	-0.706671	2.597661
Cl	1.673249	-0.075981	2.641133

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PdCl-3BTanti-1 SCF Done: -5597.01570183 A.U.

Pd	-0.677827	0.462451	0.063357
P	-3.063488	0.661005	0.341136
P	-0.467924	-1.444403	1.340937
C	-3.767811	-0.220169	1.821915
H	-4.866844	-0.209123	1.750873
H	-3.517785	0.428388	2.678039
C	-3.251075	-1.644767	2.075220
H	-3.357560	-2.266228	1.169914
H	-3.905903	-2.109636	2.831753

C	-1.811491	-1.721993	2.605419
H	-1.624438	-2.712302	3.049412
H	-1.672828	-0.983590	3.411066
Cl	-0.743606	2.360154	-1.370736
C	1.064339	-1.628796	2.344931
C	1.162446	-1.023421	3.609603
C	2.184606	-2.298366	1.824743
C	2.347109	-1.104853	4.346359
H	0.320241	-0.470373	4.031258
C	3.367280	-2.376786	2.563270
H	2.143552	-2.746474	0.830712
C	3.451881	-1.784458	3.826451
H	2.405509	-0.630348	5.329213
H	4.230605	-2.896362	2.140695
H	4.379385	-1.845520	4.401261
C	-3.737648	2.354543	0.604186
C	-5.068435	2.672594	0.287658
C	-2.917909	3.331640	1.191470
C	-5.573860	3.945574	0.566052
H	-5.713806	1.930408	-0.188617
C	-3.429396	4.600477	1.475321
H	-1.870208	3.106747	1.400236
C	-4.756480	4.909922	1.163160
H	-6.609124	4.185276	0.309852
H	-2.780597	5.355756	1.925730
H	-5.151402	5.906739	1.375850
C	-0.576697	-2.981847	0.328941
C	-0.404353	-4.250437	0.913256
C	-0.884497	-2.896354	-1.037565
C	-0.540849	-5.406974	0.143707
H	-0.147597	-4.340150	1.972056
C	-1.022315	-4.057060	-1.806297
H	-1.013268	-1.915978	-1.502324

C	-0.851230	-5.311731	-1.217968
H	-0.400385	-6.386675	0.607478
H	-1.260224	-3.974534	-2.869428
H	-0.955330	-6.218356	-1.819494
C	-3.986527	-0.010702	-1.108818
C	-5.059316	-0.911428	-0.995717
C	-3.571343	0.397384	-2.391639
C	-5.705366	-1.394049	-2.139165
H	-5.407928	-1.248685	-0.018056
C	-4.225641	-0.081623	-3.528675
H	-2.731820	1.092084	-2.489920
C	-5.291384	-0.979646	-3.407207
H	-6.537044	-2.095590	-2.034078
H	-3.894785	0.247855	-4.516887
H	-5.797711	-1.356708	-4.299568
C	2.348611	1.019568	0.384164
C	3.668572	0.803304	-0.152002
C	1.332932	0.368327	-0.271799
C	3.616404	-0.041656	-1.235754
S	1.988501	-0.551143	-1.601429
Br	5.069696	-0.635878	-2.294110
H	2.180231	1.663982	1.250427
C	4.907297	1.466170	0.391948
C	5.152829	2.873339	-0.181559
H	5.786324	0.833672	0.183804
H	4.821888	1.533638	1.490897
C	6.397088	3.556570	0.393301
H	5.243911	2.800247	-1.279567
H	4.263993	3.502050	0.005643
C	6.644638	4.952853	-0.179681
H	6.302169	3.620314	1.493249
H	7.280714	2.918914	0.206573
H	7.545356	5.416752	0.254098

H	6.781926	4.917669	-1.273455
H	5.793446	5.624829	0.021627

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PdCl-3BTsyn SCF Done: -5597.00771619 A.U.

Pd	0.351346	0.174684	-0.340057
P	-0.190873	-1.715184	0.873727
P	2.692583	-0.407538	-0.334732
C	0.950456	-3.101167	0.364429
H	0.916034	-3.088376	-0.736638
H	0.510966	-4.058975	0.682833
C	2.415175	-3.039120	0.848643
H	3.003802	-3.673061	0.165804
H	2.479830	-3.519083	1.838538
C	3.101242	-1.664622	0.972078
H	4.191326	-1.804219	1.040308
H	2.792001	-1.186850	1.913944
Cl	0.877652	2.022186	-1.735974
C	-0.005899	-1.607005	2.706257
C	0.434294	-0.414187	3.300350
C	-0.281151	-2.717575	3.524891
C	0.600515	-0.331580	4.687285
H	0.641866	0.455609	2.672015
C	-0.110767	-2.634494	4.908270
H	-0.643660	-3.649635	3.083458
C	0.330193	-1.441032	5.491853
H	0.935950	0.606104	5.137183
H	-0.328821	-3.503131	5.534767
H	0.457041	-1.376518	6.575499
C	-1.864834	-2.441378	0.649696
C	-2.112453	-3.439234	-0.306802
C	-2.940901	-1.925177	1.392006
C	-3.409757	-3.920074	-0.506955
H	-1.302610	-3.843555	-0.916668

C	-4.234431	-2.406605	1.187649
H	-2.772267	-1.132213	2.123141
C	-4.472520	-3.405600	0.238583
H	-3.588320	-4.695185	-1.256389
H	-5.062675	-1.989402	1.765224
H	-5.487515	-3.775935	0.074945
C	3.865536	0.962628	0.030801
C	4.294715	1.799808	-1.013870
C	4.282217	1.245182	1.343299
C	5.135428	2.882848	-0.749844
H	3.960991	1.612139	-2.034911
C	5.121688	2.332535	1.602776
H	3.956453	0.624161	2.179810
C	5.551912	3.152905	0.556986
H	5.459851	3.524698	-1.572649
H	5.439388	2.536631	2.628536
H	6.207629	4.003322	0.760333
C	3.304494	-1.143252	-1.908982
C	4.547760	-1.798195	-1.978270
C	2.512927	-1.051713	-3.065983
C	4.984401	-2.360678	-3.179315
H	5.188780	-1.863764	-1.095186
C	2.956230	-1.613384	-4.268596
H	1.561327	-0.516570	-3.027191
C	4.187582	-2.270404	-4.326572
H	5.952077	-2.867267	-3.221536
H	2.334633	-1.529561	-5.163478
H	4.531825	-2.708743	-5.266893
C	-2.282298	1.708338	0.354008
C	-1.605868	0.766244	-0.396698
C	-3.644218	1.895293	-0.078374
S	-2.632516	0.129002	-1.655391
C	-3.977945	1.109677	-1.148024

H	-4.340279	2.592445	0.392346
Br	-5.649782	1.030361	-2.026300
C	-1.671022	2.543711	1.454560
C	-1.305133	3.971413	1.012342
H	-0.759320	2.043844	1.819906
H	-2.364364	2.596624	2.315167
C	-0.677484	4.812872	2.127325
H	-0.612408	3.903808	0.156505
H	-2.211702	4.479247	0.635472
C	-0.312798	6.231796	1.687462
H	-1.370247	4.860061	2.988640
H	0.229669	4.300922	2.499395
H	0.139032	6.810685	2.509669
H	0.407749	6.216346	0.852992
H	-1.202766	6.784252	1.341523

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Pd-TTBTBr-BTanti-O SCF Done: -9128.23140288 A.U.

Pd	-1.673023	-0.811809	0.302027
P	-3.850995	-1.477747	-0.520783
P	-1.066849	-3.064208	0.909844
C	-4.514442	-3.093850	0.132927
H	-5.426937	-3.336931	-0.433415
H	-4.855303	-2.866308	1.156288
C	-3.553406	-4.291148	0.160558
H	-3.082496	-4.440737	-0.825858
H	-4.157819	-5.196790	0.338666
C	-2.483483	-4.227107	1.260174
H	-2.056070	-5.226706	1.436414
H	-2.952426	-3.906418	2.204397
C	0.027998	-3.308420	2.373631
C	-0.475537	-3.695298	3.627472
C	1.403511	-3.039349	2.251743
C	0.377629	-3.824252	4.728400

H	-1.538309	-3.900186	3.765739	H	-4.931927	-3.570234	-2.449946
C	2.252454	-3.171084	3.351995	C	-3.179976	-0.792038	-4.521467
H	1.815871	-2.716078	1.293929	H	-2.754628	0.165289	-2.632800
C	1.743434	-3.565135	4.593459	C	-3.759479	-1.889924	-5.165085
H	-0.031812	-4.128932	5.694943	H	-4.838445	-3.746781	-4.900624
H	3.316665	-2.951904	3.236521	H	-2.691902	-0.007245	-5.104890
H	2.409385	-3.665438	5.454277	H	-3.725270	-1.970670	-6.254564
C	-5.311481	-0.404862	-0.169159	C	0.654611	0.328829	2.066650
C	-6.188489	0.044845	-1.166950	C	2.055843	0.632078	2.041213
C	-5.560397	-0.050378	1.168219	C	0.192715	-0.179840	0.865764
C	-7.297568	0.828147	-0.830194	C	2.681234	0.375814	0.839063
H	-6.009420	-0.210711	-2.212880	S	1.498712	-0.268494	-0.291093
C	-6.674596	0.720173	1.503038	H	2.589354	1.049198	2.899331
H	-4.869094	-0.363582	1.956003	C	-0.204937	0.574693	3.284994
C	-7.545921	1.163217	0.502731	C	-0.336096	2.057580	3.670793
H	-7.969813	1.177706	-1.617923	H	0.204360	0.014160	4.146788
H	-6.852645	0.990737	2.546742	H	-1.209401	0.160424	3.097122
H	-8.412262	1.776722	0.762394	C	-1.246524	2.296735	4.878583
C	-0.190470	-3.954644	-0.451071	H	0.665888	2.473883	3.881609
C	0.431228	-5.197461	-0.232092	H	-0.723783	2.617606	2.803101
C	-0.179222	-3.406850	-1.743324	C	-1.384195	3.773426	5.252995
C	1.045832	-5.876505	-1.285661	H	-2.247157	1.878946	4.662218
H	0.449543	-5.633739	0.769952	H	-0.863945	1.727374	5.746212
C	0.434191	-4.090405	-2.798756	H	-2.047035	3.913607	6.122440
H	-0.647350	-2.436272	-1.923459	H	-0.405653	4.215401	5.506112
C	1.047396	-5.324337	-2.571815	H	-1.801764	4.357885	4.416321
H	1.530181	-6.838905	-1.101414	C	4.072864	0.546107	0.470122
H	0.436166	-3.649869	-3.798708	C	4.642442	0.655937	-0.782590
H	1.532284	-5.855817	-3.394721	S	5.320390	0.620928	1.703563
C	-3.846762	-1.685147	-2.355911	C	6.066343	0.817324	-0.790330
C	-4.430767	-2.781742	-3.013195	H	4.045932	0.648379	-1.697114
C	-3.215470	-0.691943	-3.128373	C	6.558517	0.819549	0.495552
C	-4.382877	-2.884400	-4.407193	Br	8.358295	1.021098	1.030843

C	6.886687	0.937665	-2.048030
C	7.268497	-0.419105	-2.667136
H	7.805088	1.508462	-1.834413
H	6.317689	1.525862	-2.788823
C	8.085297	-0.289168	-3.956110
H	7.839021	-1.003903	-1.924062
H	6.349838	-0.999405	-2.868039
C	8.468672	-1.635466	-4.572219
H	7.511814	0.304226	-4.691816
H	8.999670	0.295929	-3.748336
H	9.053870	-1.506314	-5.496858
H	9.076301	-2.236351	-3.874919
H	7.574433	-2.230034	-4.824381
C	-1.942551	1.162823	-0.218229
C	-1.363922	1.895668	-1.232910
S	-2.967536	2.220210	0.721305
C	-1.732607	3.286782	-1.297504
H	-0.643573	1.466353	-1.934040
C	-2.599784	3.600183	-0.277765
C	-1.188749	4.248609	-2.322070
C	0.146520	4.897846	-1.915629
H	-1.930552	5.041854	-2.514183
H	-1.050470	3.711257	-3.276932
C	0.706433	5.847722	-2.978570
H	0.003020	5.445592	-0.967665
H	0.885504	4.106042	-1.698507
C	2.026193	6.506281	-2.573957
H	0.845504	5.293020	-3.925135
H	-0.044182	6.629034	-3.198361
H	2.402433	7.179596	-3.361155
H	1.909566	7.102449	-1.653454
H	2.807080	5.752296	-2.378436
Br	-3.370419	5.289992	0.090873

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Pd-TTBTBr-Btanti-O-TS-2 SCF Done: -9128.20815580 A.U.

Pd	-1.547779	-0.914370	0.304638
P	-3.784348	-1.657471	-0.324321
P	-0.742947	-3.162169	0.754749
C	-4.265486	-3.353598	0.293196
H	-5.213717	-3.641803	-0.188378
H	-4.507977	-3.204792	1.358584
C	-3.224467	-4.476965	0.151313
H	-2.836534	-4.524611	-0.880589
H	-3.751380	-5.433415	0.309871
C	-2.059088	-4.424429	1.153917
H	-1.578432	-5.413730	1.220848
H	-2.449228	-4.185914	2.157437
C	0.491019	-3.396802	2.105757
C	0.248202	-4.156641	3.263130
C	1.720142	-2.720490	1.987605
C	1.213996	-4.243688	4.272231
H	-0.693406	-4.692133	3.394198
C	2.684084	-2.814863	2.992701
H	1.923814	-2.111272	1.103999
C	2.433659	-3.575871	4.139657
H	1.008900	-4.840820	5.164726
H	3.630355	-2.279950	2.879736
H	3.186855	-3.645584	4.928666
C	-5.246931	-0.694529	0.270406
C	-6.370735	-0.424699	-0.527252
C	-5.233483	-0.240202	1.600686
C	-7.459681	0.277002	-0.000626
H	-6.399383	-0.758893	-1.566429
C	-6.327273	0.449281	2.128551
H	-4.354248	-0.417735	2.225938
C	-7.442816	0.711715	1.327505

H	-8.326224	0.483975	-0.634098	H	0.050637	-0.004310	3.919744
H	-6.300415	0.797027	3.164341	H	-1.311950	0.565403	2.974813
H	-8.294458	1.261714	1.735908	C	-1.050392	2.228204	5.181855
C	0.084410	-3.942749	-0.705537	H	0.874173	2.357058	4.205271
C	0.847897	-5.117766	-0.586483	H	-0.467995	2.945318	3.222613
C	-0.072840	-3.360209	-1.973393	C	-0.965711	3.575309	5.901075
C	1.432958	-5.699409	-1.713050	H	-2.100359	2.026724	4.901021
H	0.998088	-5.575654	0.394795	H	-0.765029	1.417843	5.878055
C	0.510260	-3.946324	-3.102179	H	-1.609863	3.600430	6.794933
H	-0.650184	-2.437197	-2.073356	H	0.065398	3.791346	6.228317
C	1.263807	-5.115281	-2.973722	H	-1.279837	4.400742	5.240591
H	2.028362	-6.609980	-1.606424	C	4.002414	0.884950	0.403617
H	0.379318	-3.481033	-4.082389	C	4.606328	0.963321	-0.837573
H	1.725603	-5.570069	-3.853966	S	5.223513	0.944021	1.667450
C	-4.025411	-1.738283	-2.152861	C	6.032853	1.084554	-0.811823
C	-4.522113	-2.860818	-2.836390	H	4.033669	0.956006	-1.767214
C	-3.660497	-0.600713	-2.899415	C	6.494844	1.089142	0.485577
C	-4.653589	-2.846676	-4.229515	Br	8.285451	1.241747	1.062369
H	-4.815838	-3.760349	-2.292860	C	6.888113	1.160133	-2.049571
C	-3.804528	-0.585060	-4.288271	C	7.249119	-0.218368	-2.632340
H	-3.258353	0.277181	-2.387137	H	7.815634	1.710353	-1.821690
C	-4.298458	-1.709430	-4.958659	H	6.354599	1.749168	-2.815559
H	-5.039319	-3.730516	-4.744279	C	8.108301	-0.136405	-3.897433
H	-3.523322	0.309535	-4.849837	H	7.779653	-0.804859	-1.861565
H	-4.404494	-1.699137	-6.046464	H	6.320638	-0.776150	-2.850811
C	0.572877	0.675465	1.959490	C	8.471321	-1.505104	-4.475385
C	1.975016	0.924079	1.955955	H	7.574999	0.458117	-4.661820
C	0.077623	0.310172	0.699290	H	9.032353	0.426575	-3.672174
C	2.603723	0.750179	0.738555	H	9.088261	-1.411058	-5.383436
S	1.418503	0.228730	-0.453803	H	9.039396	-2.108939	-3.747948
H	2.519529	1.236653	2.850268	H	7.568391	-2.078909	-4.744020
C	-0.260197	0.789972	3.214369	C	-1.494687	1.146048	0.006058
C	-0.174759	2.148884	3.927866	C	-1.353304	1.810508	-1.211294

S	-2.529168	2.129925	1.047777	C	-0.509713	3.100823	3.717259
C	-2.026565	3.066858	-1.328195	C	-2.310623	2.763255	2.138450
H	-0.716436	1.427712	-2.011342	C	-1.418285	3.002833	4.774658
C	-2.700860	3.369463	-0.164952	H	0.546928	3.252627	3.947732
C	-1.925346	3.955009	-2.542048	C	-3.215486	2.659426	3.197488
C	-0.690068	4.873225	-2.528367	H	-2.669286	2.644476	1.114940
H	-2.834602	4.573029	-2.623853	C	-2.774200	2.783518	4.517826
H	-1.893897	3.322075	-3.446381	H	-1.060956	3.093255	5.803654
C	-0.573096	5.754220	-3.775675	H	-4.270077	2.467910	2.985057
H	-0.728957	5.509725	-1.626866	H	-3.483854	2.701434	5.344922
H	0.219901	4.255641	-2.423306	C	4.958059	1.126700	0.354879
C	0.653022	6.668187	-3.762670	C	5.994629	0.813099	-0.535935
H	-0.544227	5.110413	-4.674280	C	5.111719	0.808962	1.716556
H	-1.488600	6.365634	-3.875677	C	7.165341	0.203232	-0.071284
H	0.708192	7.286164	-4.673363	H	5.893172	1.040056	-1.598754
H	0.633545	7.351503	-2.897202	C	6.283749	0.208208	2.179431
H	1.586958	6.084970	-3.698492	H	4.303565	1.019595	2.423378
Br	-3.697123	4.932268	0.206256	C	7.315429	-0.096429	1.284805
				H	7.963803	-0.038085	-0.777487
115				H	6.387714	-0.031732	3.240666
Pd-TTBTBr-BTanti-S SCF Done: -9128.23154249 A.U.				H	8.231501	-0.571489	1.644590
Pd	1.297078	0.936133	0.401000	C	-0.633918	3.806422	-0.411291
P	3.399923	1.972476	-0.166900	C	-1.412358	4.965542	-0.237213
P	0.267261	3.025266	0.997377	C	-0.497527	3.266132	-1.699629
C	3.712196	3.645218	0.600943	C	-2.038456	5.567897	-1.329921
H	4.634934	4.053601	0.161046	H	-1.543651	5.396083	0.758967
H	3.958262	3.434691	1.654586	C	-1.122091	3.873449	-2.794254
C	2.573262	4.673210	0.530698	H	0.098113	2.361742	-1.844886
H	2.194988	4.770946	-0.501307	C	-1.893329	5.022974	-2.611100
H	2.999905	5.659185	0.781972	H	-2.645252	6.464731	-1.180978
C	1.414862	4.409025	1.503223	H	-1.007320	3.439810	-3.790597
H	0.802854	5.316364	1.623907	H	-2.386001	5.494951	-3.465073
H	1.819543	4.164321	2.498167	C	3.595391	2.249213	-1.982097
C	-0.946329	2.993050	2.385276				

C	4.157950	3.416024	-2.528866	H	-4.166374	-1.198626	-1.814227
C	3.154863	1.237662	-2.855905	C	-6.680072	-1.687903	0.329628
C	4.276684	3.567592	-3.913786	Br	-8.456834	-2.092626	0.827791
H	4.512414	4.221581	-1.883937	C	-6.956397	-1.773566	-2.221835
C	3.285337	1.387977	-4.239136	C	-7.463889	-0.449688	-2.821355
H	2.707957	0.326126	-2.453766	H	-7.815112	-2.439092	-2.036015
C	3.842973	2.553738	-4.772305	H	-6.318590	-2.284994	-2.963470
H	4.712557	4.483456	-4.321129	C	-8.240372	-0.634680	-4.128278
H	2.942494	0.587856	-4.899836	H	-8.104025	0.058220	-2.078388
H	3.938104	2.673331	-5.854588	H	-6.605655	0.224902	-2.992958
C	-0.866520	-0.666675	1.989963	C	-8.751534	0.677575	-4.724683
C	-2.218546	-1.139481	1.927720	H	-7.596017	-1.149294	-4.864568
C	-0.478007	0.006708	0.845299	H	-9.092586	-1.315592	-3.949969
C	-2.875858	-0.851661	0.750084	H	-9.307507	0.507908	-5.660779
S	-1.791432	0.040845	-0.304180	H	-9.427501	1.198328	-4.025823
H	-2.690834	-1.700414	2.738561	H	-7.920200	1.366145	-4.951778
C	0.025852	-0.922855	3.181951	C	1.981576	-0.937708	-0.118489
C	0.434327	-2.395691	3.351150	C	2.966933	-1.728045	0.432531
H	-0.481146	-0.582213	4.104241	S	1.240761	-1.811403	-1.443466
H	0.934480	-0.306245	3.081710	C	3.163269	-3.017355	-0.181975
C	1.352567	-2.640643	4.552025	H	3.566948	-1.417295	1.289688
H	-0.472942	-3.018673	3.453133	C	2.296019	-3.181974	-1.235656
H	0.933378	-2.732903	2.426705	C	4.207150	-4.008590	0.263922
C	1.756596	-4.105879	4.723613	C	5.582003	-3.803556	-0.396878
H	2.261352	-2.019389	4.444143	H	3.855897	-5.031964	0.051152
H	0.854810	-2.284481	5.473242	H	4.320474	-3.937903	1.360061
H	2.418600	-4.247719	5.593479	C	6.639566	-4.804825	0.077129
H	0.873130	-4.750000	4.869572	H	5.465715	-3.879891	-1.492603
H	2.289259	-4.479537	3.833109	H	5.931128	-2.774685	-0.197950
C	-4.236583	-1.158466	0.353195	C	8.006597	-4.604302	-0.579045
C	-4.773441	-1.290737	-0.911348	H	6.743216	-4.731991	1.175592
S	-5.486698	-1.395329	1.563185	H	6.282641	-5.831875	-0.121099
C	-6.172617	-1.598897	-0.947295	H	8.744039	-5.339050	-0.217310

H	7.943257	-4.708533	-1.675294	H	1.257181	-1.542657	3.648687
H	8.407602	-3.598356	-0.368275	C	4.605950	-1.374660	4.267009
Br	2.168327	-4.682655	-2.382870	H	5.852830	0.352249	3.888750
				H	3.112412	-2.920517	4.523923
Pd-TTBTBr-BTanti-S-Pr SCF Done: -9128.25048167 A.U.				H	5.425294	-1.985606	4.653962
P	1.095683	1.153994	2.514642	C	-1.214969	3.803369	-1.221951
P	0.149258	3.280317	-0.084044	C	-1.060264	4.764878	-2.234494
C	1.584517	2.924081	2.868025	C	-2.459012	3.156493	-1.091593
H	2.387635	3.138112	2.144377	C	-2.126669	5.080948	-3.083626
H	2.033252	3.003446	3.871206	H	-0.103671	5.273751	-2.366361
C	0.477640	3.990600	2.739332	C	-3.525626	3.483121	-1.931480
H	0.987197	4.968411	2.727713	H	-2.594303	2.376354	-0.337462
H	-0.130291	3.980976	3.659271	C	-3.362365	4.447265	-2.932219
C	-0.503069	3.930555	1.547939	H	-1.987083	5.829986	-3.867777
H	-0.963621	4.921333	1.407285	H	-4.481504	2.967179	-1.813000
H	-1.330805	3.240495	1.776887	H	-4.194060	4.696700	-3.596014
C	-0.289056	0.854449	3.706376	C	1.539428	4.426123	-0.500622
C	-1.511592	0.366916	3.217564	C	1.535075	5.792891	-0.167620
C	-0.162014	1.116164	5.082888	C	2.658533	3.898312	-1.166892
C	-2.589885	0.154596	4.084865	C	2.623312	6.608048	-0.490982
H	-1.610590	0.139500	2.152936	H	0.672907	6.232116	0.340277
C	-1.238716	0.906468	5.946881	C	3.744672	4.715301	-1.497472
H	0.787769	1.477606	5.486442	H	2.673549	2.835299	-1.422729
C	-2.456080	0.426806	5.448214	C	3.730102	6.070809	-1.157297
H	-3.534213	-0.228636	3.689800	H	2.606153	7.668028	-0.223984
H	-1.128017	1.114674	7.014399	H	4.605561	4.289316	-2.019125
H	-3.297575	0.261622	6.126166	H	4.580278	6.709636	-1.410122
C	2.487797	0.204444	3.274195	C	0.207276	-0.219268	-1.648734
C	3.795594	0.716621	3.342912	C	0.592688	-1.123114	-0.578845
C	2.262820	-1.117836	3.700680	C	-1.226697	-0.253898	-1.862365
C	4.844378	-0.067056	3.837061	S	-0.858050	-2.045289	-0.014945
H	4.012124	1.734257	3.011260	C	-1.931341	-1.139654	-1.089116
C	3.309877	-1.896937	4.195314	C	1.863576	-1.836562	-0.492625

C	3.120885	-1.371517	-0.182471
S	1.952462	-3.548820	-0.912977
C	4.175631	-2.340659	-0.272216
C	3.671160	-3.561876	-0.656906
Br	4.634761	-5.175494	-0.868725
H	-1.707967	0.383428	-2.608434
C	1.127629	0.181151	-2.791581
C	1.124139	-0.818381	-3.962607
C	2.049421	-0.408084	-5.112198
C	2.041333	-1.392271	-6.283015
H	0.818724	1.173734	-3.163076
H	2.157068	0.296134	-2.418590
H	0.092543	-0.929011	-4.342905
H	1.418449	-1.814948	-3.589819
H	1.759445	0.596517	-5.472307
H	3.080334	-0.302530	-4.727156
H	2.718310	-1.068935	-7.090249
H	1.031468	-1.492012	-6.715369
H	2.361261	-2.397651	-5.962046
C	-3.362844	-1.358967	-1.037161
C	-4.074081	-2.269167	-0.279508
S	-4.464161	-0.419339	-2.032495
C	-5.493483	-2.244222	-0.472294
H	-3.587683	-2.964565	0.407661
C	-5.836270	-1.282678	-1.395930
C	-6.455025	-3.129692	0.276122
C	-6.829840	-2.593432	1.669558
H	-6.006386	-4.132484	0.382629
H	-7.372488	-3.259248	-0.320426
C	-7.798805	-3.503980	2.429408
H	-5.909652	-2.454253	2.265787
H	-7.274499	-1.588505	1.559080
C	-8.171259	-2.974967	3.815098

H	-8.715451	-3.639730	1.827071
H	-7.352349	-4.510634	2.525477
H	-8.870654	-3.651260	4.332085
H	-7.279899	-2.865960	4.455740
H	-8.652658	-1.984748	3.750023
Br	-7.568239	-0.840841	-2.000480
H	3.286974	-0.342271	0.139268
Pd	0.583131	0.942421	0.186436
C	5.621056	-2.027470	0.010347
H	6.146132	-2.952749	0.297430
H	5.673191	-1.353141	0.882549
C	6.354911	-1.379324	-1.177412
H	5.825393	-0.455164	-1.472749
H	6.293123	-2.054499	-2.049251
C	7.822144	-1.055484	-0.881479
H	8.345555	-1.983686	-0.588252
H	7.877203	-0.390335	-0.000020
C	8.552373	-0.406811	-2.058401
H	9.604517	-0.189737	-1.813457
H	8.075761	0.544040	-2.350974
H	8.545656	-1.063187	-2.944689

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Pd-TTBTBr-Btanti-S-TS-2 SCF Done: -9128.20634641 A.U.

Pd	1.274837	0.867032	0.407176
P	3.498196	1.814280	0.043214
P	0.358083	2.970780	1.234568
C	3.892087	3.252159	1.170017
H	4.885622	3.643496	0.899652
H	4.012165	2.804496	2.170692
C	2.861832	4.392505	1.228976
H	2.585336	4.722074	0.212839
H	3.360496	5.261169	1.692144
C	1.598575	4.100127	2.054601

H	1.091783	5.046407	2.303289	H	-0.228006	4.349283	-3.511024
H	1.886486	3.625431	3.007727	H	-1.615625	6.356419	-2.983194
C	-1.023898	2.925570	2.456990	C	3.848226	2.460743	-1.653204
C	-0.937648	3.458114	3.755260	C	4.486544	3.685722	-1.913778
C	-2.210874	2.273656	2.073415	C	3.434094	1.672628	-2.743677
C	-2.014812	3.349579	4.641959	C	4.705128	4.110667	-3.228557
H	-0.033398	3.966375	4.093316	H	4.824709	4.323860	-1.095656
C	-3.286230	2.172152	2.957825	C	3.663239	2.093675	-4.055851
H	-2.294096	1.834549	1.076408	H	2.928654	0.720376	-2.564529
C	-3.191536	2.709657	4.245901	C	4.296506	3.315869	-4.302702
H	-1.930313	3.771332	5.647070	H	5.200055	5.068063	-3.411390
H	-4.196201	1.657301	2.639927	H	3.339275	1.463406	-4.887963
H	-4.031970	2.626116	4.939736	H	4.469673	3.648896	-5.329258
C	4.956240	0.740181	0.420888	C	-0.772656	-1.000516	1.790394
C	6.116436	0.701278	-0.368852	C	-2.156920	-1.319481	1.738701
C	4.901406	-0.045860	1.585682	C	-0.276306	-0.504274	0.574840
C	7.203685	-0.093335	0.008580	C	-2.771644	-1.081562	0.523463
H	6.176513	1.294087	-1.283811	S	-1.595660	-0.413651	-0.597949
C	5.994401	-0.826270	1.969669	H	-2.700129	-1.731390	2.592817
H	3.993264	-0.048809	2.194636	C	0.048978	-1.177807	3.045546
C	7.149466	-0.851812	1.181058	C	0.077089	-2.611827	3.600822
H	8.099542	-0.115548	-0.617403	H	-0.346667	-0.503920	3.828792
H	5.939579	-1.425436	2.882262	H	1.076610	-0.827689	2.855667
H	8.002488	-1.467857	1.476717	C	0.944015	-2.760955	4.854863
C	-0.311862	4.062046	-0.103239	H	-0.952918	-2.935950	3.833217
C	-1.098137	5.192470	0.183815	H	0.435730	-3.301445	2.816634
C	-0.009464	3.767689	-1.442606	C	0.960368	-4.180669	5.423235
C	-1.561828	6.012939	-0.846496	H	1.978096	-2.445415	4.621433
H	-1.362304	5.427421	1.218337	H	0.586683	-2.056836	5.628783
C	-0.472218	4.592325	-2.473904	H	1.594962	-4.251702	6.321319
H	0.588063	2.883672	-1.679372	H	-0.053533	-4.510436	5.705578
C	-1.248260	5.715125	-2.177774	H	1.345656	-4.903751	4.684834
H	-2.175893	6.886008	-0.610372	C	-4.152485	-1.274340	0.144270

C	-4.718411	-1.344315	-1.114906
S	-5.401560	-1.437394	1.371440
C	-6.136400	-1.543949	-1.132362
H	-4.122113	-1.279896	-2.027314
C	-6.631575	-1.614276	0.150853
Br	-8.424910	-1.888818	0.671933
C	-6.952515	-1.633762	-2.395303
C	-7.392041	-0.264102	-2.943894
H	-7.845941	-2.252623	-2.211336
H	-6.360349	-2.159130	-3.164347
C	-8.209597	-0.362895	-4.235149
H	-7.982442	0.258499	-2.170675
H	-6.498896	0.362619	-3.117952
C	-8.654043	0.995640	-4.779149
H	-7.615282	-0.891994	-5.002558
H	-9.096725	-0.996920	-4.054543
H	-9.239113	0.888992	-5.706700
H	-9.282255	1.533107	-4.049095
H	-7.787720	1.640193	-5.004154
C	1.367561	-1.132093	-0.164492
C	2.074169	-2.169266	0.441127
S	1.335300	-1.440609	-1.908589
C	2.562714	-3.195734	-0.428970
H	2.219204	-2.228732	1.519798
C	2.235449	-2.923874	-1.738701
C	3.333171	-4.402908	0.043765
C	4.860665	-4.254389	-0.066862
H	3.016691	-5.286462	-0.536388
H	3.062797	-4.607412	1.093882
C	5.625053	-5.484172	0.432162
H	5.125130	-4.057969	-1.120619
H	5.181809	-3.361509	0.497445
C	7.143667	-5.348158	0.311855

H	5.354295	-5.679047	1.486474
H	5.289335	-6.374257	-0.130732
H	7.663203	-6.245394	0.685191
H	7.449960	-5.198046	-0.736978
H	7.514778	-4.483644	0.887755
Br	2.615792	-3.983376	-3.256016

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Pd-TTBTBr-BTsyn-O-Pr SCF Done: -9128.24127545 A.U.

Pd	1.776543	-0.118974	0.086595
P	3.345762	-1.483792	1.283835
P	1.759363	1.591421	1.782259
C	4.415544	-0.329863	2.300949
H	4.730870	0.436379	1.574510
H	5.333894	-0.846778	2.621747
C	3.756091	0.338704	3.522561
H	4.397794	1.189691	3.805658
H	3.793381	-0.360154	4.374920
C	2.298180	0.826596	3.406459
H	2.077963	1.514650	4.238280
H	1.602247	-0.020137	3.524841
C	2.793841	-2.747068	2.517946
C	1.468536	-3.208561	2.451428
C	3.628427	-3.240249	3.538061
C	0.988946	-4.145495	3.372978
H	0.808155	-2.819947	1.671778
C	3.148936	-4.172589	4.461934
H	4.665157	-2.902180	3.611628
C	1.828448	-4.628160	4.380257
H	-0.044713	-4.494070	3.305051
H	3.809199	-4.546056	5.249164
H	1.454937	-5.356945	5.104231
C	4.651720	-2.346927	0.293946
C	5.313856	-1.594956	-0.695869

C	4.975017	-3.707275	0.431944
C	6.289269	-2.180738	-1.505385
H	5.051906	-0.544910	-0.851487
C	5.944576	-4.294785	-0.388309
H	4.469205	-4.318878	1.181225
C	6.607918	-3.534671	-1.354830
H	6.788394	-1.578235	-2.268451
H	6.181220	-5.355353	-0.267631
H	7.364846	-3.996185	-1.994086
C	0.134041	2.306130	2.319614
C	-0.016017	3.582412	2.888613
C	-1.004482	1.494453	2.172935
C	-1.271121	4.025678	3.317223
H	0.846347	4.243227	2.995010
C	-2.257269	1.934917	2.609960
H	-0.910291	0.515141	1.695775
C	-2.393281	3.201644	3.185254
H	-1.371105	5.022140	3.756009
H	-3.132273	1.293363	2.480513
H	-3.373735	3.550639	3.519397
C	2.888225	3.046790	1.595623
C	3.435422	3.752346	2.683600
C	3.242612	3.440843	0.292613
C	4.302775	4.828521	2.473485
H	3.186645	3.466890	3.708437
C	4.105817	4.521325	0.083230
H	2.847312	2.889463	-0.564829
C	4.637606	5.217192	1.172428
H	4.719126	5.365078	3.330206
H	4.367502	4.813503	-0.936934
H	5.316271	6.058371	1.009221
C	1.227183	-1.044115	-1.850952
C	0.624537	0.280901	-1.795538

C	2.411001	-1.052813	-2.705068
S	1.549340	1.396775	-2.901933
C	2.684344	0.133306	-3.299210
Br	4.204256	0.540534	-4.349979
C	-0.768453	0.650078	-1.561258
C	-1.323416	1.926376	-1.412837
S	-2.045188	-0.565467	-1.472048
C	-2.734132	1.891358	-1.231766
C	-3.290710	0.628718	-1.228855
C	-0.527119	3.212245	-1.422699
C	-1.239750	4.442643	-0.849161
H	-0.212703	3.444571	-2.456520
H	0.409459	3.046481	-0.862987
C	-0.350610	5.690463	-0.832117
H	-2.145735	4.662331	-1.442065
H	-1.585262	4.225465	0.176445
C	-1.050241	6.926564	-0.265474
H	0.559600	5.479410	-0.243099
H	-0.000220	5.902154	-1.858923
H	-0.384590	7.804701	-0.264836
H	-1.945209	7.188592	-0.854918
H	-1.379873	6.756977	0.773283
H	-3.337619	2.788986	-1.098265
H	3.036527	-1.933569	-2.838143
C	0.457518	-2.351303	-1.665746
H	-0.252024	-2.463396	-2.508731
H	-0.163824	-2.295605	-0.759518
C	1.312804	-3.621259	-1.594911
H	1.832198	-3.779808	-2.555952
H	2.105323	-3.492628	-0.838210
C	0.491647	-4.874315	-1.272108
H	-0.322699	-4.977157	-2.012384
H	-0.007969	-4.740709	-0.295172

C	1.323831	-6.157153	-1.246288	H	2.897609	-4.251369	-0.535598
H	1.805193	-6.342138	-2.221292	H	3.819572	-4.820358	-1.915940
H	0.704990	-7.037353	-1.008691	C	2.163359	-3.575975	-2.475256
H	2.124918	-6.098215	-0.490854	H	1.687756	-4.496180	-2.850474
C	-4.671036	0.238010	-1.027645	H	2.573678	-3.044503	-3.349826
C	-5.278202	-0.983215	-1.246388	C	-0.332917	-2.230181	-3.138983
S	-5.841771	1.386893	-0.402167	C	-0.053572	-2.593428	-4.467969
C	-6.675158	-1.030166	-0.934625	C	-1.544498	-1.569010	-2.860540
H	-4.737569	-1.843013	-1.647661	C	-0.965209	-2.306566	-5.490370
C	-7.106639	0.192969	-0.471247	H	0.874595	-3.106357	-4.724891
Br	-8.856293	0.663190	0.055620	C	-2.455200	-1.291346	-3.881337
C	-7.521640	-2.269279	-1.066914	H	-1.777914	-1.266376	-1.837504
H	-8.567361	-1.980704	-1.261855	C	-2.167414	-1.656972	-5.200781
H	-7.184050	-2.839252	-1.949607	H	-0.731774	-2.597478	-6.518017
C	-7.472207	-3.178986	0.173987	H	-3.389463	-0.777999	-3.640645
H	-6.423267	-3.460825	0.377395	H	-2.878283	-1.434572	-6.000706
H	-7.805995	-2.600891	1.053804	C	5.235938	-0.177320	-0.840634
C	-8.325726	-4.443178	0.036778	C	6.540454	-0.201053	-0.319196
H	-7.991890	-5.014305	-0.849002	C	4.932924	0.728577	-1.870851
H	-9.371776	-4.153299	-0.171265	C	7.518176	0.663578	-0.819218
C	-8.280326	-5.343152	1.272350	H	6.796170	-0.893621	0.485828
H	-7.251673	-5.679239	1.485896	C	5.914103	1.585839	-2.376452
H	-8.645114	-4.812669	2.167862	H	3.917848	0.767772	-2.274067
H	-8.903469	-6.242259	1.141447	C	7.208101	1.557292	-1.849063
				H	8.527947	0.638125	-0.401199
115				H	5.661445	2.287261	-3.175611
Pd-TTBTBr-BTsyn-O-TS-2 SCF Done: -9128.20228630 A.U.				H	7.973579	2.234662	-2.236237
Pd	1.605620	-0.574057	-0.466259	C	-0.064074	-3.725345	-0.673839
P	3.912662	-1.346855	-0.289676	C	-0.882898	-4.728081	-1.222811
P	0.830500	-2.496874	-1.732881	C	0.105263	-3.675686	0.719434
C	4.370947	-2.834250	-1.329917	C	-1.509610	-5.662665	-0.395456
H	5.304878	-3.260122	-0.928638	H	-1.042693	-4.773819	-2.303187
H	4.631888	-2.416114	-2.315821	C	-0.518085	-4.615803	1.546895
C	3.307574	-3.931656	-1.509126				

H	0.722938	-2.887611	1.157952
C	-1.326688	-5.610075	0.990948
H	-2.147977	-6.433686	-0.834840
H	-0.377353	-4.562144	2.629423
H	-1.820929	-6.340581	1.636638
C	4.430948	-1.804459	1.420532
C	4.711161	-3.121831	1.820619
C	4.480443	-0.781160	2.387557
C	5.038826	-3.409124	3.150751
H	4.679016	-3.942100	1.101410
C	4.819494	-1.069115	3.710542
H	4.250587	0.248670	2.104713
C	5.097386	-2.384950	4.098211
H	5.253773	-4.440427	3.442645
H	4.861798	-0.259571	4.443664
H	5.358119	-2.609792	5.135512
C	-0.451866	1.523282	-1.395043
C	-1.853702	1.764731	-1.402523
C	-0.036890	0.697632	-0.334718
C	-2.565829	1.144760	-0.394497
S	-1.461544	0.198999	0.591064
H	-2.337905	2.399754	-2.148108
C	0.454780	2.086200	-2.465885
C	0.350187	3.605112	-2.677458
H	0.228939	1.576978	-3.422492
H	1.499094	1.815723	-2.242188
C	1.327375	4.136238	-3.730506
H	-0.680159	3.867928	-2.976801
H	0.528739	4.117860	-1.716906
C	1.211321	5.643042	-3.965548
H	2.359593	3.891385	-3.419563
H	1.164783	3.599088	-4.683346
H	1.930532	5.992890	-4.723704

H	0.201297	5.917706	-4.313717
H	1.403470	6.208043	-3.038172
C	-3.985860	1.164580	-0.128781
C	-4.671400	0.802114	1.015516
S	-5.121267	1.681264	-1.367871
C	-6.094768	0.939440	0.939367
H	-4.161269	0.460620	1.918408
C	-6.470388	1.409264	-0.299394
Br	-8.221201	1.777483	-0.900737
C	-7.029271	0.584118	2.066136
C	-7.402932	-0.908578	2.110248
H	-7.949173	1.185337	1.982157
H	-6.556277	0.867297	3.022421
C	-8.336013	-1.265581	3.270911
H	-7.878081	-1.187640	1.153175
H	-6.480458	-1.513222	2.177427
C	-8.712241	-2.747205	3.316168
H	-7.857529	-0.976274	4.224588
H	-9.253640	-0.653557	3.199604
H	-9.385737	-2.968586	4.159641
H	-9.224636	-3.058700	2.390479
H	-7.819019	-3.384774	3.427422
C	1.505147	1.148506	0.708720
C	1.458025	1.134766	2.112459
S	2.406654	2.579753	0.175543
C	2.107473	2.260088	2.714049
C	2.660365	3.123766	1.806078
Br	3.574655	4.731715	2.174315
H	2.161562	2.422601	3.791587
C	0.835844	0.047038	2.958708
C	-0.185214	0.536053	3.998433
H	1.641825	-0.500529	3.483028
H	0.363231	-0.702375	2.305261

C	-0.820282	-0.603973	4.800605	H	-2.438313	-6.451718	1.151418
H	0.302873	1.239615	4.696712	C	5.013612	-0.707875	-0.125728
H	-0.974148	1.112760	3.486176	C	6.315760	-0.193014	-0.235250
C	-1.819006	-0.125923	5.855605	C	4.625940	-1.763951	-0.967758
H	-1.324434	-1.298384	4.103795	C	7.209112	-0.723932	-1.170747
H	-0.022962	-1.195012	5.288340	H	6.637358	0.627966	0.408828
H	-2.263468	-0.970129	6.407170	C	5.524287	-2.301236	-1.893484
H	-1.336502	0.536437	6.594037	H	3.611349	-2.165157	-0.899818
H	-2.644358	0.443633	5.396239	C	6.817678	-1.780254	-1.998787
				H	8.217968	-0.310666	-1.249184
115				H	5.208432	-3.123375	-2.540385
Pd-TTBTBr-BTsyn-S SCF Done: -9128.22393439 A.U.				H	7.518630	-2.195515	-2.727216
Pd	1.517522	-0.413704	0.515765	C	0.046084	-1.031062	3.607601
P	3.830987	-0.163548	1.186433	C	-0.593729	-1.711955	4.659125
P	0.957292	-1.951457	2.287176	C	0.030906	0.372639	3.598104
C	4.434318	-1.259703	2.583354	C	-1.229437	-1.001679	5.679170
H	5.335552	-0.789517	3.006539	H	-0.608506	-2.804792	4.677128
H	4.777750	-2.184726	2.093536	C	-0.603991	1.082831	4.622692
C	3.433110	-1.620681	3.690180	H	0.508610	0.913969	2.778081
H	2.943424	-0.720070	4.098713	C	-1.234610	0.397809	5.663457
H	4.007093	-2.049962	4.528750	H	-1.727596	-1.543067	6.487576
C	2.378807	-2.656949	3.267985	H	-0.611123	2.175216	4.597227
H	1.955956	-3.157439	4.153208	H	-1.736556	0.952329	6.460504
H	2.859974	-3.434808	2.653638	C	4.395131	1.522392	1.666508
C	-0.106942	-3.421990	1.970318	C	4.617830	1.874036	3.009080
C	0.402773	-4.731668	1.945118	C	4.534048	2.512526	0.676028
C	-1.470757	-3.220917	1.687387	C	4.985470	3.178965	3.352072
C	-0.432482	-5.814998	1.653261	H	4.504207	1.137142	3.806245
H	1.455985	-4.927023	2.153006	C	4.911925	3.811432	1.021389
C	-2.301696	-4.304865	1.398155	H	4.340863	2.270844	-0.370965
H	-1.888194	-2.212197	1.688022	C	5.138219	4.149263	2.359010
C	-1.786169	-5.604873	1.379810	H	5.154118	3.433971	4.401432
H	-0.019379	-6.826893	1.641868	H	5.012956	4.566667	0.238400
H	-3.356717	-4.126315	1.176915				

H	5.426867	5.168718	2.627034
C	-0.771132	-1.679487	-1.173717
C	-2.167281	-1.592309	-1.484405
C	-0.349096	-0.685830	-0.302367
C	-2.828556	-0.550648	-0.867093
S	-1.688534	0.348427	0.118593
H	-2.673046	-2.281333	-2.165398
C	0.113627	-2.775152	-1.725471
C	0.117636	-2.900367	-3.256968
H	-0.193769	-3.746586	-1.293158
H	1.144429	-2.601268	-1.373937
C	1.042949	-4.006339	-3.774014
H	-0.908903	-3.094141	-3.616451
H	0.413206	-1.933924	-3.700012
C	1.047882	-4.138772	-5.297737
H	2.072554	-3.812267	-3.419125
H	0.748090	-4.970136	-3.319432
H	1.721473	-4.943370	-5.634700
H	0.039685	-4.366454	-5.682823
H	1.378987	-3.203277	-5.778909
C	-4.227518	-0.176491	-0.947615
C	-4.829212	1.036335	-0.680183
S	-5.438656	-1.353893	-1.427410
C	-6.250363	1.062532	-0.864283
H	-4.257785	1.916979	-0.379835
C	-6.706553	-0.170470	-1.273357
Br	-8.487180	-0.657013	-1.673738
C	-7.101792	2.279321	-0.611592
C	-7.513404	2.448246	0.862055
H	-8.008191	2.229899	-1.236817
H	-6.545313	3.175367	-0.936730
C	-8.355169	3.701820	1.116858
H	-8.075179	1.552745	1.181867

H	-6.606178	2.477465	1.492301
C	-8.767261	3.871905	2.579778
H	-7.790164	4.592646	0.786320
H	-9.258342	3.667910	0.480452
H	-9.372735	4.780659	2.727069
H	-9.364680	3.013486	2.930186
H	-7.885765	3.949164	3.238366
C	1.668043	1.212383	-0.743077
C	1.968909	1.449852	-2.072088
S	1.197599	2.710333	0.038647
C	1.845455	2.838920	-2.444025
C	1.439553	3.638923	-1.411740
Br	1.160457	5.507597	-1.458762
H	2.040849	3.220336	-3.447835
C	2.333237	0.394568	-3.090386
C	3.671919	0.618803	-3.811007
H	1.530361	0.344271	-3.850276
H	2.340015	-0.587604	-2.593875
C	3.945079	-0.400601	-4.921470
H	3.693657	1.634138	-4.246380
H	4.492735	0.590010	-3.072404
C	5.280828	-0.186997	-5.634714
H	3.913622	-1.419593	-4.494701
H	3.122203	-0.360795	-5.658562
H	5.440121	-0.930695	-6.432417
H	5.331913	0.812659	-6.098399
H	6.126127	-0.265318	-4.930562

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Pd-TTBTBr-BTsyn-S-Pr SCF Done: -9128.24764696 A.U.

P	-1.446083	-0.588205	2.504922
P	-1.391353	-3.111971	0.100665
C	-2.465081	-2.054738	3.058287
H	-3.355482	-2.031108	2.409026

H	-2.821683	-1.903608	4.089781	H	-1.928959	-4.978948	-2.222273
C	-1.795802	-3.444256	2.977651	C	1.919685	-4.721406	-1.754688
H	-2.608040	-4.186933	3.045812	H	1.502063	-3.413807	-0.099957
H	-1.181349	-3.588361	3.881814	C	1.392180	-5.494584	-2.794720
C	-0.901549	-3.803256	1.770316	H	-0.415754	-6.172560	-3.769041
H	-0.798057	-4.898662	1.714519	H	3.001791	-4.640408	-1.623647
H	0.113743	-3.406338	1.927681	H	2.059143	-6.025854	-3.478361
C	0.086085	-0.726881	3.537532	C	-3.095813	-3.779998	-0.161280
C	1.333712	-0.801968	2.897824	C	-3.454494	-5.102982	0.157072
C	0.040084	-0.769234	4.942761	C	-4.079845	-2.917956	-0.672950
C	2.511235	-0.926349	3.644328	C	-4.764483	-5.549704	-0.033018
H	1.378087	-0.753083	1.806359	H	-2.706003	-5.796265	0.549826
C	1.214652	-0.895929	5.687581	C	-5.391086	-3.366267	-0.866872
H	-0.919182	-0.690446	5.461644	H	-3.811970	-1.885078	-0.911728
C	2.452947	-0.976045	5.039006	C	-5.735334	-4.681776	-0.546088
H	3.474321	-0.978620	3.130257	H	-5.029262	-6.579943	0.219423
H	1.165113	-0.927765	6.779282	H	-6.144271	-2.682539	-1.266653
H	3.371649	-1.071715	5.623725	H	-6.759914	-5.032891	-0.693970
C	-2.319943	0.837005	3.290987	C	-0.369041	0.039599	-1.794868
C	-3.686101	0.806068	3.618408	C	-0.599836	1.161786	-0.907649
C	-1.615044	2.043371	3.463653	C	1.042770	-0.287135	-1.849380
C	-4.325821	1.946147	4.117162	S	0.979337	1.816553	-0.319812
H	-4.270360	-0.106150	3.482310	C	1.877972	0.533873	-1.134351
C	-2.253917	3.177413	3.966230	C	-1.711140	2.102689	-1.013978
H	-0.555121	2.095898	3.201342	C	-1.805083	3.317756	-1.679443
C	-3.613321	3.133659	4.295531	S	-3.237781	1.694857	-0.246083
H	-5.389451	1.902149	4.366054	C	-3.109931	3.904641	-1.571879
H	-1.687583	4.103224	4.097117	C	-3.983664	3.140293	-0.845125
H	-4.114689	4.023450	4.684488	Br	-5.797005	3.523427	-0.492088
C	-0.331570	-4.124936	-1.028268	H	1.418020	-1.118797	-2.450965
C	-0.849415	-4.899023	-2.080928	C	-1.285408	-0.338042	-2.948534
C	1.067360	-4.036156	-0.886655	C	-0.961148	0.383082	-4.269217
C	0.007067	-5.575748	-2.956373	C	-1.883358	-0.027094	-5.421439

C	-1.567086	0.679906	-6.740298
H	-1.217532	-1.427734	-3.109492
H	-2.331076	-0.130807	-2.673614
H	0.088682	0.180776	-4.548748
H	-1.029570	1.473827	-4.114605
H	-1.820024	-1.121512	-5.565104
H	-2.931621	0.176884	-5.135982
H	-2.248840	0.361614	-7.545459
H	-0.537080	0.466573	-7.072445
H	-1.659038	1.774491	-6.639924
C	3.315273	0.431488	-0.968625
C	4.217209	1.395944	-0.566058
S	4.153775	-1.077317	-1.290111
C	5.584251	0.969398	-0.524903
H	3.911166	2.415528	-0.322853
C	5.687458	-0.352777	-0.896749
C	6.723875	1.859207	-0.102404
C	6.915675	1.935321	1.423081
H	6.544688	2.874987	-0.495401
H	7.658013	1.504536	-0.567271
C	8.058148	2.864703	1.843248
H	5.973699	2.271055	1.893234
H	7.102916	0.918562	1.811662
C	8.256095	2.939845	3.357791
H	8.995032	2.526866	1.363957
H	7.867121	3.877985	1.444882
H	9.083945	3.616079	3.624635
H	7.348174	3.309994	3.862989
H	8.486901	1.948018	3.781523
Br	7.260739	-1.388364	-1.017092
Pd	-1.084689	-0.741218	0.141234
H	-3.386028	4.853137	-2.035431
C	-0.694963	3.987015	-2.453942

H	-1.093264	4.304035	-3.434909
H	0.103775	3.259673	-2.661884
C	-0.087800	5.211427	-1.747353
H	-0.883999	5.948349	-1.535905
H	0.304876	4.896717	-0.764751
C	1.029109	5.881390	-2.553051
H	0.638919	6.173540	-3.545391
H	1.823869	5.139278	-2.750136
C	1.630713	7.104619	-1.859887
H	0.867700	7.881230	-1.682196
H	2.432954	7.558974	-2.463307
H	2.061209	6.838040	-0.879986

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Pd-TTBTBr-BTsyn-S-TS-2 SCF Done: -9128.19662870 A.U.

Pd	1.507765	0.446417	0.408513
P	3.481166	1.762281	-0.121827
P	0.939578	1.723332	2.390265
C	4.247249	2.618493	1.344824
H	5.039812	3.298139	0.994859
H	4.747021	1.831119	1.933153
C	3.270197	3.389549	2.249881
H	2.624119	4.049531	1.645458
H	3.872972	4.067159	2.877422
C	2.419916	2.522489	3.197179
H	2.070585	3.129617	4.047705
H	3.043628	1.713019	3.611587
C	0.151624	0.775939	3.761324
C	0.763493	0.537211	5.003763
C	-1.118639	0.220015	3.515372
C	0.116679	-0.229309	5.979769
H	1.749083	0.947461	5.229796
C	-1.764580	-0.536724	4.494326
H	-1.606672	0.380813	2.551346

C	-1.148837	-0.765265	5.730025
H	0.606297	-0.402448	6.941766
H	-2.752637	-0.954256	4.285339
H	-1.654103	-1.360715	6.494685
C	4.931344	0.947604	-0.931329
C	4.686011	0.240754	-2.122813
C	6.240521	0.976759	-0.420401
C	5.725356	-0.406882	-2.792888
H	3.671905	0.188696	-2.526334
C	7.278927	0.320671	-1.090564
H	6.470770	1.512009	0.502250
C	7.025644	-0.369556	-2.278490
H	5.511772	-0.952369	-3.715272
H	8.291653	0.354109	-0.680113
H	7.838564	-0.880646	-2.800626
C	-0.204132	3.166994	2.201113
C	-0.754127	3.819434	3.319712
C	-0.517489	3.640569	0.918224
C	-1.588867	4.926122	3.155405
H	-0.539794	3.453572	4.327325
C	-1.352014	4.751847	0.754377
H	-0.111996	3.132331	0.042128
C	-1.888413	5.395762	1.871127
H	-2.012344	5.421805	4.032871
H	-1.585735	5.108991	-0.251677
H	-2.544877	6.260443	1.743781
C	3.135588	3.151792	-1.301476
C	4.059676	4.183905	-1.540338
C	1.927100	3.149275	-2.016322
C	3.772801	5.197171	-2.457280
H	5.021049	4.196652	-1.020719
C	1.642852	4.159469	-2.941921
H	1.209870	2.341031	-1.852184

C	2.562204	5.188011	-3.159404
H	4.500794	5.993948	-2.630899
H	0.699804	4.138312	-3.494003
H	2.340873	5.979567	-3.879946
C	-0.608288	-1.999210	0.848804
C	-2.016619	-2.107219	0.667269
C	-0.052395	-0.899101	0.172768
C	-2.596411	-1.131455	-0.121333
S	-1.353866	-0.001115	-0.635588
H	-2.605554	-2.919088	1.096046
C	0.204562	-3.020294	1.602382
C	-0.586211	-4.105784	2.340237
H	0.856032	-2.502074	2.327317
H	0.892946	-3.504935	0.883975
C	0.309958	-5.082679	3.108284
H	-1.294703	-3.635432	3.045517
H	-1.201219	-4.675039	1.620490
C	-0.467285	-6.176837	3.841591
H	1.026353	-5.547422	2.406634
H	0.924813	-4.517856	3.832753
H	0.206590	-6.858993	4.384519
H	-1.168355	-5.746960	4.576772
H	-1.061270	-6.785754	3.139495
C	-3.981267	-0.959402	-0.492637
C	-4.534868	-0.136898	-1.456857
S	-5.249302	-1.866166	0.319103
C	-5.958373	-0.219169	-1.579774
H	-3.926050	0.507755	-2.093983
C	-6.470424	-1.124030	-0.676273
Br	-8.280490	-1.606182	-0.443983
C	-6.764596	0.604636	-2.549627
C	-7.164932	1.986170	-2.001391
H	-7.675108	0.050929	-2.831178

H	-6.179575	0.737424	-3.475992
C	-7.975967	2.821345	-2.996453
H	-7.747119	1.847796	-1.073292
H	-6.254675	2.539662	-1.707932
C	-8.382441	4.191432	-2.451881
H	-7.390644	2.951154	-3.925306
H	-8.880174	2.257442	-3.289718
H	-8.965308	4.764737	-3.190575
H	-9.000430	4.093517	-1.543605
H	-7.498824	4.795010	-2.184086
C	1.508121	-1.193029	-0.897573
C	2.515915	-2.157246	-0.713780
S	1.008128	-1.181639	-2.598551
C	2.837344	-2.871890	-1.913878
C	2.124366	-2.451863	-3.004215
Br	2.241293	-3.125749	-4.763326
H	3.588356	-3.660175	-1.970581
C	3.342990	-2.288693	0.548566
H	2.753239	-1.928093	1.407058
H	4.189580	-1.582799	0.466178
C	3.890394	-3.690400	0.854708
H	3.057913	-4.414657	0.839801
H	4.580748	-4.006513	0.052209
C	4.619841	-3.800583	2.202116
H	3.929548	-3.502373	3.012526
H	4.854657	-4.863624	2.386131
C	5.911170	-2.984176	2.305660
H	6.624492	-3.263512	1.511698
H	6.410975	-3.149542	3.273952
H	5.726547	-1.901872	2.212283
