

**Supporting Information for the Paper Entitled “Understanding
Intermolecular C–F Bond Activation by a Transient Titanium
Neopentylidyne: Experimental and Theoretical Studies on the
Competition Between 1,2-CF Bond Addition and
[2+2]-Cycloaddition/ β -Fluoride Elimination.”**

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S1 Optimized Structures

=====				H	-0.015498075	-3.892270288	-0.582841641
(PNP)Ti(=CtBu)(CH2tBu)				H	-1.334797655	-4.526727427	-1.584553275
=====				H	-1.657025333	-3.267669255	-0.374470794
Ti	0.309196307	-0.062948847	-0.169481247	H	0.578667707	-2.304897717	-3.971394791
P	2.710724866	-0.885470565	0.736913018	H	0.012394801	-3.962154539	-3.691656828
C	2.508391034	-0.058247482	2.371101202	H	1.331518761	-3.294652171	-2.713010592
C	3.504068643	0.485078086	3.185931182	C	4.492329137	-0.604078906	-1.427000439
C	3.215336802	1.044016022	4.441312424	H	4.442785015	0.675669008	0.297150138
C	1.882392701	1.027753962	4.863045710	C	3.443683736	-3.141954545	2.458493355
C	0.865595282	0.516092089	4.058585493	H	1.610530338	-2.863791207	1.384956609
C	1.150074064	-0.013797726	2.787339702	C	4.313244086	1.627454580	5.302282047
N	0.159488058	-0.434581494	1.883942976	C	-4.635337980	-3.168261488	3.533631092
C	-1.005230603	-1.047326955	2.374462644	C	-3.110766998	2.165193044	2.918336537
C	-0.989900991	-2.027666974	3.388159168	H	-1.127517764	2.116810577	2.119043146
C	-2.153764839	-2.688853039	3.758582997	C	-3.597816649	1.249009400	-1.780039045
C	-3.383377000	-2.420124539	3.135575115	H	-3.878386317	-0.493881878	-0.563992292
C	-3.404558801	-1.431270565	2.147982236	H	0.211456493	-0.484146614	-2.202417387
C	-2.250157676	-0.726479691	1.779014523	H	0.505228072	2.395437218	-0.050071484
P	-2.156119919	0.663152348	0.577706567	H	2.122561196	1.820109386	-0.369866314
C	4.420894643	-0.404692243	0.098348633	C	1.125725106	2.609966081	-2.121521887
C	2.681622185	-2.726902080	1.190381006	C	1.595547621	4.061102715	-1.859510406
C	-2.148298711	2.183846569	1.719920948	C	2.105497156	1.956290623	-3.113912207
C	-3.768392070	0.586554747	-0.402161808	C	-0.272308051	2.659531511	-2.767518889
C	-0.132587084	-1.282349781	-1.484086656	H	2.126321304	2.501951628	-4.065536221
C	-0.653059564	-2.527915651	-2.170546182	H	3.126028438	1.952457749	-2.713837962
C	-1.968760254	-2.219140446	-2.926535220	H	1.821578776	0.919559668	-3.326263571
C	-0.932075320	-3.619866599	-1.116014032	H	-0.259444184	3.250601027	-3.692258498
C	0.379697502	-3.053957665	-3.196235977	H	-0.628573519	1.654323188	-3.014487199
C	1.101409281	1.822301182	-0.790511387	H	-1.006005863	3.117250372	-2.094419845
H	4.537858919	0.476128253	2.852971703	H	1.643312944	4.645272606	-2.788202696
H	1.626381802	1.441377481	5.836673873	H	0.912363271	4.577775099	-1.174956671
H	-0.162630266	0.541537240	4.406768701	H	2.592428684	4.073605340	-1.403498764
H	-0.048102699	-2.275011615	3.869425965	H	-5.506752553	-2.816000668	2.973561516
H	-2.106104215	-3.446333520	4.538959460	H	-4.855676046	-3.045504966	4.601217298
H	-4.352048416	-1.204308089	1.668745076	H	-4.537095778	-4.245231361	3.349785941
C	5.647070545	-1.044239198	0.774785578	H	3.920632845	1.978035763	6.261598811
C	3.053209306	-3.610358077	-0.010292559	H	4.801235667	2.480257756	4.814402909
C	-2.255289520	3.497681257	0.930391583	H	5.096531339	0.889793545	5.516277764
C	-5.040925521	1.103857575	0.290084181	H	5.425537779	-0.179116125	-1.816150097
H	-2.745387228	-1.879949665	-2.233944645	H	3.658590935	-0.121342423	-1.939643429
H	-2.342431902	-3.112483941	-3.444037595	H	4.479948654	-1.666353907	-1.691820435
H	-1.818201020	-1.434181178	-3.676325349	H	6.560100814	-0.552182494	0.417545522

H	5.732413541	-2.104282669	0.518306767	C	3.362901897	-3.068929479	1.968525361
H	5.633212130	-0.966714791	1.863704966	C	1.763079883	-4.117133960	-0.481312448
H	2.810116830	-4.657073041	0.207370678	C	0.801562746	-0.060143126	-1.200582415
H	4.125117875	-3.566239383	-0.230519624	C	0.115047230	-0.062041614	-2.546635153
H	2.506088538	-3.319528589	-0.910539880	C	-0.399511981	-1.476160741	-2.906032330
H	3.189466963	-4.178640049	2.712026084	C	1.148739877	0.366083252	-3.617504418
H	3.186431562	-2.515118074	3.315736823	C	-1.077575262	0.922243135	-2.577937785
H	4.527419083	-3.098517304	2.320164604	H	4.197708675	3.573802284	3.175444965
H	-2.843549888	2.972657463	3.611457239	H	7.299305271	0.634360836	3.345444890
H	-3.060371860	1.222297252	3.468716636	H	6.213735386	-0.642464102	1.550684724
H	-4.149105066	2.327307427	2.616966095	H	6.109405934	0.478606289	-1.035735636
H	-2.059525084	4.347544589	1.594956602	H	7.134905906	-1.020384984	-2.697634486
H	-3.256663825	3.639051696	0.510344863	H	4.144348112	-3.979176938	-1.917581820
H	-1.533756538	3.546739440	0.110218747	C	2.392249377	5.208711765	1.890929671
H	-4.496953211	1.085440208	-2.386348581	C	2.028084275	3.833566084	-1.572582671
H	-2.743283175	0.835471116	-2.319140147	C	2.328036412	-3.574431310	2.986557902
H	-3.452734677	2.331017487	-1.692988307	C	2.464752760	-5.471177892	-0.278249869
H	-5.916428733	0.852058205	-0.320741767	H	0.426227371	-2.194648481	-2.921232508
H	-5.023634169	2.192988651	0.392687808	H	-0.872806092	-1.480145836	-3.896971108
H	-5.195437670	0.678215158	1.283872910	H	-1.140197995	-1.826177562	-2.179485854
=====				H	1.519167556	1.376705584	-3.420411534
A-TS				H	0.700015497	0.355097207	-4.619925428
=====				H	2.007844524	-0.312016776	-3.615792112
H	-0.039830249	-0.094608343	0.189382150	H	-1.859925350	0.615292869	-1.876003245
C	-0.113658969	-0.182111679	1.644708237	H	-1.525347225	0.963460822	-3.579602346
Ti	1.706502382	-0.090094005	0.312173073	H	-0.760366456	1.934391189	-2.306726499
P	2.488707363	2.455034155	0.866318923	C	0.215029102	3.967612239	1.612900539
C	4.015037388	1.956074817	1.766396321	H	1.811947307	3.417382614	2.933133452
C	4.633828286	2.648528438	2.810071425	C	4.393871819	4.075309776	-0.658246438
C	5.819264565	2.194788315	3.409004874	H	3.441805166	2.255499283	-1.272494399
C	6.374585660	1.011390165	2.912069829	C	6.466625625	2.966971792	4.536994604
C	5.765215594	0.285760362	1.890961170	C	6.320782389	-3.512366595	-3.483013659
C	4.557934153	0.721363609	1.307516004	C	4.597571929	-3.981918899	1.912504459
N	3.839117459	-0.018860704	0.366094299	H	3.706121099	-2.080692459	2.302868949
C	4.525420946	-0.883254049	-0.500317517	C	0.278510698	-4.217799835	-0.093656256
C	5.680361131	-0.503350308	-1.214132791	H	1.806709493	-3.859122680	-1.547601735
C	6.251330963	-1.351084346	-2.154511344	H	0.326733371	-1.095213356	2.085667017
C	5.702147223	-2.611939755	-2.438117815	H	0.235278025	0.663531796	2.259538307
C	4.572930428	-3.002530159	-1.714229316	C	-1.656370825	-0.285352012	1.799789727
C	3.996801232	-2.176447355	-0.739420797	C	-1.994777875	-0.498038955	3.292142140
P	2.552444622	-2.598252386	0.314889406	C	-2.340656037	1.008849153	1.319736673
C	1.716335084	3.825706059	1.917337298	C	-2.201993992	-1.479132844	0.995016811
C	3.151399407	3.178132413	-0.755480547	H	-3.431775337	0.907472637	1.358622471
				H	-2.069308939	1.858238023	1.956155840

H	-2.060099146	1.255075736	0.291171573	C	3.662454445	0.595619173	2.394250929
H	-3.287929606	-1.567096961	1.117402416	C	3.655292649	1.498321672	3.464359929
H	-1.992162497	-1.368998127	-0.073584677	C	2.411499262	1.854920523	4.000324099
H	-1.751509411	-2.419617424	1.330371214	C	1.222624174	1.336192785	3.494568658
H	-3.079234244	-0.560684573	3.446531859	C	1.222430484	0.419597401	2.427319389
H	-1.549297681	-1.425343141	3.671539903	N	0.052897306	-0.069154090	1.818330440
H	-1.616257387	0.328607390	3.904979504	C	-1.052778466	-0.468875612	2.565639355
H	5.104188017	-3.972589520	2.885821109	C	-0.962548563	-0.830322645	3.933569108
H	5.315479608	-3.646728183	1.159346285	C	-2.059701801	-1.300539421	4.639094277
H	4.333987927	-5.019905519	1.692732755	C	-3.320735717	-1.445055955	4.040346448
H	2.787705444	-3.658836119	3.978558906	C	-3.419958119	-1.098432661	2.691790012
H	1.946776709	-4.566462039	2.721213956	C	-2.331463637	-0.618323749	1.945391519
H	1.470946940	-2.898794114	3.077147313	P	-2.428409193	-0.252297579	0.145399087
H	-0.201034500	-5.032369382	-0.650186142	C	4.025248217	-0.901863075	-0.525417840
H	-0.253921919	-3.292575062	-0.319505898	C	2.347716495	-2.825343313	1.263892736
H	0.153807463	-4.433231404	0.973605296	C	-3.420775231	1.339687208	-0.037211826
H	1.997684224	-6.225611209	-0.923398643	C	-3.322146917	-1.738675262	-0.625521856
H	2.360906508	-5.821944754	0.753384683	H	4.619191539	0.318586728	1.959817658
H	3.530499615	-5.444602231	-0.515195285	H	2.369962674	2.566200981	4.822842028
H	5.789213845	-4.466290029	-3.553302325	H	0.273059827	1.659079185	3.909831823
H	7.370724961	-3.733795036	-3.254721775	H	-0.002059897	-0.760008082	4.432269521
H	6.301285844	-3.049132552	-4.477344891	H	-1.930639995	-1.576036511	5.684793481
H	7.398904166	2.491939854	4.857824350	H	-4.384500864	-1.209128455	2.205277897
H	5.811781051	3.031552682	5.415289413	C	5.287708968	-1.616912457	-0.017278989
H	6.706563249	3.996102444	4.241421198	C	2.273785565	-3.948012974	0.216065127
H	4.799568945	4.244479107	-1.663505720	C	-3.612359365	1.682796700	-1.522906171
H	5.180517234	3.617887534	-0.052461181	C	-4.859060721	-1.757904341	-0.617259261
H	4.163701715	5.055522124	-0.231566659	C	3.761905424	-1.246456444	-2.002658578
H	2.383031555	4.049719766	-2.587319654	H	4.182590737	0.181617155	-0.464750849
H	1.704760893	4.784018782	-1.134249521	C	3.382573462	-3.131432064	2.357254540
H	1.158123067	3.176147049	-1.654526815	H	1.366045712	-2.756962193	1.752060189
H	1.952760252	5.845845091	2.668617254	C	4.948161322	2.052621144	4.018297151
H	2.227376938	5.710358954	0.932653574	C	-4.506284559	-1.957062662	4.825629850
H	3.469521667	5.167906858	2.063200905	C	-4.722770723	1.462393038	0.765438471
H	-0.249405555	4.661140516	2.324904843	H	-2.699778482	2.057605766	0.375546483
H	-0.305351517	3.011330510	1.681896589	C	-2.791710764	-1.976456251	-2.052331454
H	0.044108961	4.365273918	0.607508249	H	-2.968993648	-2.563265635	0.007626786
=====				C	0.614717764	1.402720096	-0.993869559
A				C	1.064771854	2.806312989	-1.325577008
=====				C	2.610008380	2.864474070	-1.403247615
Ti	0.150856298	-0.110633947	-0.250096434	C	0.484277298	3.231164100	-2.695631089
P	2.425291942	-1.117238973	0.447352933	C	0.583104643	3.798475275	-0.241086756
C	2.484593452	0.041637257	1.881048154	H	0.895557559	4.826488857	-0.473177913
				H	-0.509410683	3.785414380	-0.164251166

H	0.990950826	3.528175748	0.737557115	C	3.452340526	0.913155898	2.446399399
H	2.955293726	3.874018881	-1.666132924	C	3.292593946	1.813810398	3.507127640
H	3.054463405	2.592807475	-0.438263958	C	1.995868005	2.015088237	3.996165719
H	2.986926363	2.167680295	-2.161245926	C	0.898424221	1.361423210	3.442388090
H	0.808795279	4.245193651	-2.967601708	C	1.050841102	0.469370274	2.365273772
H	0.809926046	2.543765675	-3.483989104	N	-0.030450861	-0.127794654	1.699385299
H	-0.611193863	3.219484817	-2.671135772	C	-1.071071230	-0.707266881	2.421052378
H	-5.384303366	-2.086484927	4.185443314	C	-0.910079723	-1.237049452	3.724279305
H	-4.786658205	-1.269301845	5.633379427	C	-1.937571853	-1.919468742	4.361367870
H	-4.292734886	-2.926096723	5.293426963	C	-3.182944989	-2.120276948	3.748504020
H	4.759864236	2.842825278	4.751237245	C	-3.358112059	-1.578420859	2.471431361
H	5.577141747	2.476102370	3.226441252	C	-2.349249021	-0.866298721	1.809080822
H	5.540838626	1.275097509	4.517700166	P	-2.491511621	-0.118357158	0.132726810
H	-4.010376218	2.699197730	-1.622350526	C	4.105570359	-0.672760909	-0.385529224
H	-4.324296077	1.006802635	-2.008585122	C	2.544585358	-2.647992609	1.422126222
H	-2.662856264	1.636087546	-2.063448612	C	-2.969241189	1.678931133	0.473941993
H	-5.102002837	2.488695927	0.686773110	C	-3.918135159	-1.036186027	-0.710315547
H	-4.567570265	1.246572712	1.825224517	H	4.453250407	0.746472074	2.057885563
H	-5.505350663	0.797107595	0.389942023	H	1.838103176	2.712205998	4.816972129
H	-3.224183430	-2.893285333	-2.471274552	H	-0.099804861	1.560472369	3.821519454
H	-1.701603221	-2.090967230	-2.069581598	H	0.049740664	-1.128776956	4.219442461
H	-3.047969437	-1.150712537	-2.723815972	H	-1.760993831	-2.324756780	5.356687680
H	-5.215510658	-2.716786165	-1.013815003	H	-4.319129578	-1.719521648	1.986211632
H	-5.276417901	-0.970127442	-1.251032398	C	5.399097422	-1.200481137	0.256503755
H	-5.278269097	-1.643197846	0.384571954	C	2.757603991	-3.827018581	0.458946695
H	6.153298853	-1.294451904	-0.607936614	C	-3.279328797	2.424121447	-0.832728435
H	5.207059427	-2.702264400	-0.132393648	C	-5.355295013	-0.621422477	-0.348082915
H	5.507065149	-1.408312292	1.032385916	C	3.989756544	-1.152336065	-1.844553716
H	4.646004314	-1.011640663	-2.607355308	H	4.145988829	0.422796018	-0.405197912
H	2.916029998	-0.673964693	-2.393100433	C	3.479916387	-2.741930017	2.636959032
H	3.548780466	-2.313010507	-2.135793697	H	1.513479572	-2.705622999	1.796281240
H	3.077230879	-4.027492330	2.911797643	C	4.485502730	2.518147645	4.112359355
H	3.468617584	-2.309995909	3.073448521	C	-4.286506251	-2.880680591	4.448290409
H	4.374319046	-3.328742844	1.942044152	C	-4.030681725	1.926707878	1.555027161
H	2.048943878	-4.904463797	0.702222286	H	-2.008692592	2.055614512	0.847557335
H	3.223045075	-4.070316912	-0.316583579	C	-3.738159816	-1.017824836	-2.239862212
H	1.492865077	-3.762896199	-0.529512967	H	-3.761960474	-2.068090944	-0.366989114
=====				C	0.627969754	1.194862487	-1.206955323
A-Pyf				C	1.067208779	2.566620431	-1.673615276
=====				C	2.611792089	2.638796301	-1.747150082
Ti	0.123062148	-0.283653955	-0.403937993	C	0.495845224	2.862522574	-3.082685235
P	2.470572669	-0.983481564	0.503756027	C	0.577457391	3.659688679	-0.692316604
C	2.369306948	0.228534151	1.886175450	H	0.904781460	4.660646773	-1.009178805
				H	-0.515738344	3.666741586	-0.631952051

H	0.966994517	3.471683995	0.313293575
H	2.946864449	3.620848946	-2.110386379
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H	3.007455461	1.874117726	-2.424979376
H	0.785732801	3.863354262	-3.433427783
H	0.864101454	2.130394556	-3.811323544
H	-0.598256584	2.808145137	-3.078807588
H	-5.158489280	-3.006880000	3.798745584
H	-4.625519638	-2.364528911	5.355861710
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H	4.174163251	3.357291767	4.741851716
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H	-5.539595755	-0.599218968	0.727655256
H	6.265258914	-0.830162988	-0.306124685
H	5.443404812	-2.294189707	0.231710278
H	5.521753170	-0.886930647	1.295814061
H	4.884905912	-0.864189719	-2.409772393
H	3.117296627	-0.708613765	-2.331489601
H	3.901232095	-2.243611446	-1.904688583
H	3.261471530	-3.657831603	3.201071164
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H	4.532643077	-2.784021728	2.343700384
H	2.592153654	-4.776250105	0.983136158
H	3.778863671	-3.849284400	0.063448023
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N	-0.062825283	-1.847522789	-2.028091427
C	0.121714716	-1.564811510	-3.338739865
C	-0.011393539	-2.534827079	-4.326587965
C	-0.333786863	-3.842128935	-3.951030923
C	-0.525806456	-4.141867242	-2.603132661
C	-0.376101681	-3.093917955	-1.707079166
H	0.379523522	-0.531144402	-3.538314044

H	0.142117180	-2.270918579	-5.366866350
H	-0.435455353	-4.623619913	-4.698059174
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B			
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C	3.260588849	1.779824093	3.592145711
C	1.959802126	1.926498133	4.089842272
C	0.876489649	1.286581260	3.494690986
C	1.047110587	0.464428148	2.366126738
N	-0.028195571	-0.092741209	1.657944672
C	-1.065790025	-0.735990676	2.323202365
C	-0.922003256	-1.351120210	3.592297134
C	-1.949911805	-2.093100621	4.159758683
C	-3.180129201	-2.273046389	3.507418865
C	-3.343313156	-1.641530977	2.269836097
C	-2.335212308	-0.867086042	1.679022774
P	-2.456325852	0.017718843	0.066737683
C	4.125147416	-0.457483392	-0.451660462
C	2.631978287	-2.566894194	1.255760519
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H	4.443214669	0.823811108	2.085497775
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H	0.025522626	-1.259173202	4.113780097
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H	-4.295332545	-1.756583331	1.759118666
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C	-5.318637315	-0.441794874	-0.470057182
C	4.021771127	-0.879975495	-1.929529502
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C	3.593152494	-2.711697779	2.445264496
H	1.610411296	-2.666715749	1.648995830
C	4.438196339	2.471401818	4.241002888
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C	-3.686595102	-0.628432452	-2.388278178
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C	0.640741343	1.330710975	-1.199560403
C	1.055110469	2.703744499	-1.684593393
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H	0.880570125	4.802029283	-1.040861113
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H	2.990969796	2.030905809	-2.463544021
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H	-0.640082724	2.925422051	-3.054579184
H	-5.137427586	-3.198289727	3.450136296
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H	-5.505396012	-0.540437275	0.601388533
H	6.288937858	-0.535729992	-0.384503227
H	5.526736242	-2.056319853	0.076453843
H	5.557642770	-0.706693942	1.214656487
H	4.891141371	-0.510133506	-2.487437433
H	3.118141901	-0.478803435	-2.394677359
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H	3.402830430	-3.661009492	2.962558455
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N	-0.143471989	-1.996614582	-1.835858014
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C	-0.572254298	-4.408456238	-3.175329621
C	-1.003534120	-4.245810680	-1.852416762
C	-0.771128312	-3.031729953	-1.226954167
F	0.882170997	-1.163290655	-3.671803148
H	0.432291829	-3.419224981	-4.833675953
H	-0.736744427	-5.344716797	-3.700237291
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D

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C	1.191817456	1.456927791	3.746075915
C	1.123288690	0.481175358	2.729377813
N	-0.088378337	-0.003644973	2.205121009
C	-1.176611395	-0.251380510	3.041877296
C	-1.029226085	-0.543065711	4.422144338
C	-2.117800570	-0.823031576	5.233181268
C	-3.430498890	-0.829788013	4.736199399
C	-3.587380059	-0.566222161	3.375373521
C	-2.505454915	-0.293708777	2.520586568
P	-2.673706762	-0.081704419	0.707209059
C	3.749002234	-0.914726911	-0.317565782
C	2.213018655	-2.837220689	1.591645934
C	-3.516359416	1.577877852	0.406915532
C	-3.782731077	-1.478792393	0.064040409
H	4.498326838	0.265160518	2.155415698
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H	-0.032092616	-0.564993338	4.848417047
H	-1.943336915	-1.051608526	6.283551587
H	-4.592033876	-0.571019649	2.964513051
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C	-3.206914754	-2.834548726	0.513144573	H	4.965237816	-2.706548195	0.003858396
C	3.397108842	-1.261620449	-1.776583526	H	5.336430987	-1.404732234	1.139039910
H	3.903987984	0.170054860	-0.267425008	H	4.241081760	-1.020519466	-2.434966497
C	3.326717532	-3.126108159	2.609294318	H	2.524602024	-0.693799806	-2.111517196
H	1.267624511	-2.774210494	2.148281682	H	3.181944592	-2.330005432	-1.897043412
C	4.947064625	2.070299764	4.140662930	H	3.076278354	-4.026167063	3.184953345
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C	0.286332885	1.217048253	-0.774416881	C	-0.628097291	-2.201545676	-2.620528251
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C	2.251356020	2.692668819	-1.279596184	C	-0.989921020	-3.699428783	-4.247564763
C	0.127789722	2.943797866	-2.598341311	C	-0.934496969	-2.701005799	-5.216781526
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H	0.494207137	2.237459609	-3.352923335	B-TS			
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H	-4.758416957	-0.322105495	6.379454802	P	2.718774507	-0.534234833	0.465204803
H	-4.470914780	-2.051248276	6.196496331	C	2.365264382	0.688094647	1.797369908
H	4.878547889	3.131691861	4.402863710	C	3.287938278	1.542368611	2.410125235
H	5.736230607	1.962320313	3.389640505	C	2.915056030	2.427072368	3.430820373
H	5.280264496	1.537639387	5.041652508	C	1.572023959	2.431854946	3.827706190
H	-4.162592101	2.761169154	-1.296896780	C	0.629261082	1.611869528	3.214316482
H	-4.671079804	1.072834676	-1.391281979	C	0.996202141	0.744102970	2.169938905
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H	-5.573829694	1.337498682	1.150015712	C	-1.707378251	-2.138013501	3.937795230
H	-5.750990775	-0.495158407	-0.026335511	C	-2.904224417	-2.431053811	3.267861208
H	-5.527121322	-1.527782411	1.395303998	C	-3.111022238	-1.819893450	2.024337950
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C	-2.609641825	1.738882214	0.422603368	H	3.850528321	-0.348050628	-2.265929694
C	-3.855507503	-0.707652025	-0.997476491	H	4.713397061	-1.740145044	-1.603187875
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H	-0.412357687	1.658659475	3.519464998	H	4.636966686	-2.258048264	2.552549174
H	0.189045119	-1.129602673	3.910526059	H	2.950178596	-4.304725461	0.965745743
H	-1.519400952	-2.582119418	4.913863559	H	4.189521727	-3.320956595	0.185353634
H	-4.042189733	-2.021756655	1.502604442	H	2.536537677	-3.325837084	-0.453443933
C	5.640671646	-0.468781819	0.719869903	N	0.399813343	-2.023256203	-1.931622289
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C	-3.002609893	2.650110563	-0.748961320	C	-0.660903627	-2.881150364	-1.877818439
C	-5.215601151	-0.343265040	-0.374769303	C	-1.464586390	-3.144306147	-2.962729984
C	4.656431180	-0.646197297	-1.596627246	C	-1.226375567	-2.431975902	-4.166235283
H	4.382882174	0.992498337	-0.245604533	C	-0.175123143	-1.548101138	-4.242758654
C	3.557126912	-2.236940553	2.721191799	H	-0.830240254	-3.349602778	-0.911823910
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C	3.938361474	3.317884974	4.098341203	H	-1.866477310	-2.590794340	-5.029415124
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C	-3.844202551	-0.347763238	-2.495329808	C	0.030280134	2.475711490	-3.741697770
H	-3.719293532	-1.795251654	-0.916586386	C	2.446683562	2.251523610	-3.096823284
H	-4.789636094	-3.494572108	3.203185280	C	0.890832203	3.606690447	-1.654998548
H	-4.324893830	-2.963798379	4.823161294	H	0.274221613	3.356675366	-4.350760531
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H	4.625733268	3.760515440	3.368771032	H	1.132558400	4.511465498	-2.229768124
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H	-6.008690875	-0.936486658	-0.846622056	P	2.588164030	0.130976392	1.597624154
H	-5.456693484	0.710325870	-0.543050703	C	2.800020958	1.622385637	2.656608439
H	-5.259721483	-0.525102658	0.700721425	C	4.005783229	2.306360586	2.861945832
H	6.548875625	0.004844521	0.326424790	C	4.079327590	3.460204353	3.648381650
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C	-0.596526422	1.311835955	3.860358427	H	-0.983970268	4.038794318	-1.619136155
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C	-1.964130489	1.156448451	3.495758468	H	6.136982150	3.897704529	3.132833261
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C	2.271576828	-2.641063835	2.109189417	H	-2.018727248	-1.628790490	1.187082555
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C	3.883298948	-0.859147875	-0.703547492	H	5.639644382	-0.013712961	2.208420213
H	4.313983981	1.013734464	0.246939133	H	4.748272682	-0.795704445	-1.375749246
C	3.514510551	-1.378052910	3.942704569	H	2.995276253	-0.520909472	-1.242428948
H	1.498686520	-1.044830420	3.316793544	H	3.741017220	-1.917535592	-0.458079898
C	5.396894703	4.158241707	3.895805395	H	3.185844065	-2.083979105	4.715869881
C	-3.667326979	0.541513654	6.889185105	H	3.674052263	-0.408323568	4.422638516
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C	3.494940367	1.278381879	2.078827453	H	-4.287185317	1.481557899	-1.701822094
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C	-1.630629271	-1.635337221	4.339419629	H	-5.804275188	-2.047318285	-0.767076819
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P	2.432439649	-1.423631068	0.314877291	H	5.445942563	1.978749476	4.081339662
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C	1.369680779	1.668982559	2.754010394	H	-4.577969807	1.165084202	1.344323944
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H	1.860811853	2.978044112	-3.219771050	C	-3.092298433	-1.195589270	-2.433990166
H	2.430761785	2.882852179	-1.564172802	H	-3.123870224	-2.159472754	-0.519782214
F	2.303901231	0.373218446	-2.329284006	C	0.656789356	1.546679863	-1.536194010
=====				C	1.067817553	3.010446338	-1.240455486
2				C	2.608548379	3.154440093	-1.331628337
=====				C	0.429634126	3.980571465	-2.265972228
Ti	0.256812338	0.004155549	-0.477901181	C	0.615215485	3.444120232	0.167052863
P	2.599548211	-0.777731545	0.360223757	H	0.917868604	4.480349077	0.365410848
C	2.553173495	0.302283698	1.843438065	H	-0.474701135	3.390287522	0.264080932
C	3.651850548	0.901583283	2.468951587	H	1.056835206	2.818808144	0.946530424
C	3.502847644	1.746623672	3.575507688	H	2.900694196	4.207267180	-1.219384862
C	2.202902398	1.984855650	4.039201932	H	3.094032694	2.581782942	-0.534527724
C	1.092630167	1.418933441	3.418296969	H	2.983125102	2.786811526	-2.290167768
C	1.239326468	0.574864131	2.304096007	H	0.689113816	5.016535373	-2.016178994
N	0.136304973	0.058359565	1.583938364	H	0.778516787	3.784031554	-3.284119494
C	-0.899008316	-0.566823027	2.297358618	H	-0.663475488	3.901274300	-2.264377472
C	-0.708894665	-1.135108839	3.577266674	H	-4.991363298	-2.810583796	3.735208981
C	-1.733572302	-1.808481714	4.229422922	H	-4.420985716	-2.170026547	5.280190837
C	-3.001121281	-1.960802775	3.651300135	H	-3.790274965	-3.701783661	4.677621902
C	-3.192855201	-1.400183811	2.385502384	H	4.416789653	3.181728590	4.913048993
C	-2.181495974	-0.709476253	1.703667388	H	5.417090078	2.762309691	3.515962010
P	-2.340397325	0.010572828	0.021924160	H	5.251265085	1.626199779	4.854938993
C	4.304844120	-0.583304363	-0.411336527	H	-3.797248385	3.418535703	-0.841356823
C	2.369555076	-2.517648106	1.068740929	H	-4.224413391	1.894704214	-1.623177201
C	-3.195038492	1.672341227	0.300884032	H	-2.540257272	2.455011085	-1.632199704
C	-3.446027578	-1.196161388	-0.935720199	H	-4.691575834	2.722908151	1.456271085
H	4.653372383	0.711999150	2.093412880	H	-4.254035739	1.156002680	2.149732924

H	-5.304951184	1.239485595	0.725246821	C	-1.622291600	-1.991673316	4.072967519
H	-2.027125122	-1.367029221	-2.594447581	C	-2.806204096	-2.384233644	3.433570208
H	-3.369008692	-0.248034528	-2.909873335	C	-3.049712334	-1.864174866	2.155867361
H	-3.651619795	-1.990715325	-2.942763957	C	-2.156840725	-0.994222537	1.521668126
H	-5.461647454	-1.903420176	-1.270658252	P	-2.362989090	-0.205637303	-0.127966905
H	-5.348719836	-0.146042114	-1.193523657	C	4.362083696	-0.311943004	-0.210794238
H	-5.286319309	-1.101011821	0.291624748	C	2.611457406	-2.226806588	1.495063149
H	6.419510879	-0.965433337	-0.155544610	C	-2.761622979	1.595610322	0.315358302
H	5.415922800	-2.383510679	0.141060364	C	-3.873435553	-1.011071120	-0.924337124
H	5.522780475	-1.110420878	1.362045524	H	4.360185574	1.423749506	2.035234534
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H	3.501103407	-0.352138058	-2.433147657	H	-0.380578330	1.875716012	3.397907450
H	4.027006627	-2.008587320	-2.053760685	H	0.222799075	-0.899092844	3.962973283
H	2.851632783	-3.820682355	2.728197440	H	-1.405162203	-2.364880125	5.072288412
H	3.272523923	-2.129168233	3.030187017	H	-3.967865352	-2.152293538	1.653274778
H	4.280929907	-3.122718599	1.965637623	C	5.561818708	-0.714608939	0.664464467
H	2.073481613	-4.544356211	0.354357872	C	2.865735473	-3.449412342	0.597332293
H	3.401272274	-3.710436272	-0.455323303	C	-3.188721856	2.404511739	-0.917628382
H	1.719832818	-3.308820163	-0.866405007	C	-5.247641424	-0.699822838	-0.302778816
C	0.675517961	1.161153913	-2.980429415	C	4.499811193	-0.932735649	-1.612370049
F	0.012487338	-1.455168626	-1.507396352	H	4.368854851	0.780055847	-0.328684632
N	1.867857559	0.893680020	-3.566272255	C	3.444132501	-2.272481471	2.785461842
C	1.887648217	0.527131127	-4.852043566	H	1.554519160	-2.250416768	1.790748941
C	0.750262694	0.401465736	-5.647553197	C	4.050474560	3.324238775	3.949082965
C	-0.481651675	0.689607275	-5.061794852	C	-3.784746015	-3.323893506	4.101425406
C	-0.519164309	1.076137267	-3.726423064	C	-3.712790723	1.815946203	1.500861559
H	2.872734840	0.314230148	-5.268136726	H	-1.766313537	1.944376395	0.613449527
H	0.831099486	0.089489700	-6.684460610	C	-3.908478831	-0.729404083	-2.438327316
H	-1.401184235	0.611726971	-5.637271049	H	-3.661516461	-2.080881966	-0.788908768
H	-1.459653470	1.311998466	-3.243992347	H	-4.646707649	-3.524830452	3.457508349
=====				H	-4.166315483	-2.911063039	5.043770466
Ea-TS				H	-3.320931527	-4.289026187	4.340504605
=====				H	3.617642183	4.220434101	4.404259008
Ti	0.291190816	-0.286033440	-0.643651176	H	4.799710348	3.648622774	3.218719547
P	2.635953294	-0.619963106	0.487748180	H	4.585539339	2.783404745	4.741116301
C	2.354722624	0.682862978	1.754201823	H	-3.172191641	3.475613102	-0.682951343
C	3.319621694	1.512343569	2.334729247	H	-4.208489702	2.159353223	-1.233469898
C	2.985655336	2.462875569	3.308390768	H	-2.515318396	2.235896680	-1.762112970
C	1.640586005	2.560953277	3.687459549	H	-3.700500913	2.876097445	1.783667224
C	0.659597543	1.762036515	3.105740665	H	-3.416052957	1.232231204	2.375916583
C	0.989195618	0.823367809	2.113663909	H	-4.746631159	1.556678950	1.255421249
N	0.025005726	0.067666330	1.418932906	H	-2.956464844	-0.955757738	-2.920062201
C	-0.923060604	-0.662529532	2.146903937	H	-4.151240212	0.317506673	-2.643661620
C	-0.698369652	-1.157932753	3.450287234	H	-4.684196254	-1.344090989	-2.911673498

H	-6.003769591	-1.369632567	-0.731250993	P	2.549192995	-0.891199105	0.404283980
H	-5.558181744	0.324240737	-0.531637500	C	2.435290180	0.442371827	1.659545273
H	-5.272670600	-0.818806466	0.781974985	C	3.494875033	1.201981711	2.166628984
H	6.486043068	-0.321243183	0.223135291	C	3.287781026	2.233291960	3.090866642
H	5.666361876	-1.802964664	0.714076715	C	1.969994839	2.490216229	3.490806302
H	5.495148445	-0.339683591	1.688037532	C	0.898303135	1.759298670	2.985532118
H	5.478561341	-0.681419114	-2.038744840	C	1.101664539	0.726080485	2.054750416
H	3.732881976	-0.559912244	-2.293670304	N	0.038559583	0.019139731	1.446997842
H	4.423999904	-2.024438125	-1.581372216	C	-0.957937040	-0.533436521	2.264429393
H	3.135570296	-3.135990609	3.388100818	C	-0.749596566	-0.851123250	3.625327731
H	3.303038018	-1.374557727	3.393720223	C	-1.733497658	-1.477098345	4.380561395
H	4.512980027	-2.383045108	2.584113382	C	-2.973293451	-1.828260282	3.830323697
H	2.659879979	-4.370258147	1.156132502	C	-3.185442101	-1.509689261	2.485301114
H	3.908853343	-3.499703473	0.265005944	C	-2.219375785	-0.865894149	1.700555796
H	2.221942791	-3.442060220	-0.287040744	P	-2.399982675	-0.437373096	-0.079135288
N	0.488448769	-1.883455087	-1.967497540	C	4.236060067	-0.743179434	-0.418649750
C	0.784183090	-0.982886535	-2.993077655	C	2.433110954	-2.485514675	1.421739541
C	-0.483011105	-2.789259823	-2.175648383	C	-3.148801523	1.299317468	-0.075735136
C	-1.193685017	-2.951445200	-3.330622634	C	-3.637637101	-1.694565140	-0.767233279
C	-0.938720721	-2.001445364	-4.367366289	H	4.510368044	0.995090346	1.840784835
C	0.009392218	-1.028039022	-4.203910632	H	1.775529621	3.291586505	4.200712536
F	-0.729720817	-3.573391193	-1.106156251	H	-0.115274877	1.997047552	3.295039342
H	-1.914234188	-3.752869769	-3.432899252	H	0.204890084	-0.615725312	4.084144883
H	-1.493103816	-2.074799170	-5.299079602	H	-1.524879415	-1.713007497	5.422821350
H	0.241906421	-0.332806204	-5.003447310	H	-4.138988740	-1.779056054	2.042920104
C	0.690747547	1.103877902	-1.689679651	C	5.459582274	-1.220645193	0.382479079
C	1.101805398	2.339401769	-2.449113556	C	2.571012780	-3.735219428	0.535652059
C	0.066965730	2.708098490	-3.539686064	C	-3.536117095	1.728596430	-1.499834033
C	2.488128417	2.166163394	-3.115639437	C	-5.131992632	-1.453083505	-0.486277753
C	1.188516388	3.503768992	-1.430021536	C	4.211679494	-1.410626046	-1.806750877
H	0.380066046	3.609713407	-4.082788613	H	4.319712328	0.341460509	-0.570837298
H	-0.913578964	2.904597241	-3.096869038	C	3.311407689	-2.571558197	2.679508636
H	-0.050742228	1.898897684	-4.266482363	H	1.389218678	-2.426836738	1.757545851
H	1.487294685	4.434190001	-1.931560583	C	4.451132863	3.020963611	3.648476717
H	1.919790598	3.282723189	-0.646399269	C	-4.031284807	-2.519883314	4.659868903
H	0.220402454	3.670196370	-0.947717533	C	-4.268051927	1.574166734	0.938649823
H	2.796722372	3.092937119	-3.616081055	H	-2.273050754	1.890029682	0.223889335
H	2.476046919	1.373564646	-3.872032370	C	-3.417629937	-1.915428446	-2.273657874
H	3.249707927	1.913917500	-2.371180367	H	-3.334717884	-2.612421785	-0.245332779
H	1.817108657	-0.674738392	-3.058255244	H	-4.914060029	-2.762366931	4.060291684
=====				H	-4.363547700	-1.892784992	5.496849945
F				H	-3.658123265	-3.456512534	5.092208623
=====				H	4.118317382	3.967226457	4.085478955
Ti	0.219140645	-0.350658493	-0.601128803	H	5.189015584	3.252165509	2.872545289

H	4.975423252	2.463855134	4.436016671
H	-3.756288698	2.802590982	-1.520446706
H	-4.433432437	1.206874765	-1.849141736
H	-2.729195219	1.534478797	-2.211920211
H	-4.470617703	2.651827343	0.976047828
H	-3.992212676	1.250305088	1.945655300
H	-5.202834937	1.076907872	0.665272980
H	-2.387516956	-2.185818641	-2.506984905
H	-3.662487572	-1.018751887	-2.851815633
H	-4.070857877	-2.723898876	-2.625300494
H	-5.705381552	-2.331125570	-0.807898250
H	-5.509715535	-0.597167163	-1.053657133
H	-5.359351819	-1.278874583	0.567090398
H	6.377336207	-0.925506622	-0.140729154
H	5.474220215	-2.311521759	0.468393348
H	5.503953101	-0.806522555	1.392474414
H	5.157173038	-1.218840182	-2.328356879
H	3.397806943	-1.029761610	-2.427055490
H	4.092663042	-2.496178057	-1.729675868
H	2.980118789	-3.415068109	3.297890919
H	3.243219945	-1.665569800	3.288123127
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H	2.307841658	-4.628307376	1.115141917
H	3.600853968	-3.870536343	0.186722415
H	1.916377172	-3.700243010	-0.339474446
N	0.354812016	-1.469447085	-2.164703861
C	0.621694406	-0.187815810	-2.931934123
C	0.188943653	-2.569443352	-2.919671069
C	-0.195780814	-2.567669769	-4.223658035
C	-0.605491221	-1.283901263	-4.762462070
C	-0.325731065	-0.130395344	-4.117445065
F	0.323639711	-3.734301808	-2.236909306
H	-0.330204200	-3.497080024	-4.762434499
H	-1.200180295	-1.276492869	-5.673774198
H	-0.697086693	0.822095769	-4.475291736
C	0.605805978	0.949487653	-1.862347480
C	1.058986170	2.363114384	-2.203187451
C	-0.016194626	3.147266436	-2.999098691
C	2.366817281	2.353804894	-3.030576565
C	1.312277193	3.130726292	-0.886934237
H	0.305024588	4.186719863	-3.142971747
H	-0.968445350	3.159414404	-2.461068413
H	-0.189841492	2.720725164	-3.990821303
H	1.616341482	4.165293790	-1.090767890

H	2.098311061	2.654040245	-0.293896231
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H	2.712223505	3.378621933	-3.212975907
H	2.227235425	1.873820654	-4.005193267
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H	1.655191399	-0.268069702	-3.321087580

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Ti	0.157105645	0.076423829	-0.677715025
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C	4.166818344	1.366394864	2.122617719
C	3.091117081	2.129312425	2.603616150
C	1.776388017	1.740609907	2.381333267
C	1.484022291	0.548839370	1.690948170
N	0.169986975	0.154091330	1.340776725
C	-0.827778106	-0.059140708	2.289019911
C	-0.645503821	0.121028971	3.677776238
C	-1.682130326	-0.108905132	4.575349432
C	-2.946655994	-0.533926204	4.147622294
C	-3.118538440	-0.749319498	2.775553422
C	-2.096395962	-0.529473710	1.842269372
P	-2.177979180	-0.911179502	0.043915844
C	3.634165164	-2.358630026	-0.580761884
C	1.536570341	-2.971267258	1.627300759
C	-3.584236925	0.091146710	-0.717024147
C	-2.535897053	-2.771550278	-0.028899391
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H	3.289423851	3.054320622	3.140887441
H	0.956780863	2.364994283	2.722970009
H	0.320856571	0.438058098	4.053909666
H	-1.500564778	0.045326392	5.637414571
H	-4.085361048	-1.100907068	2.430287783
C	4.704773022	-3.046564572	0.284096220
C	1.207579708	-4.353348301	1.039075766
C	-3.751065179	-0.289641961	-2.198670098
C	-3.947777190	-3.245125897	0.348262567
C	3.273322434	-3.243173847	-1.790130795
H	4.049200295	-1.420685650	-0.974447464
C	2.443120922	-3.076138785	2.863553065
H	0.593623511	-2.514205777	1.951900128
C	5.592666332	1.796955313	2.377558837

C	-4.079845218	-0.737490170	5.126595387
C	-4.931049381	0.151572981	0.017142850
H	-3.138022931	1.092595507	-0.690633553
C	-2.105909951	-3.368949910	-1.379852746
H	-1.839095055	-3.140962823	0.736193279
H	-4.882066058	-1.340528976	4.689985130
H	-4.522696085	0.217898948	5.437496211
H	-3.739838785	-1.243514807	6.037214840
H	5.717942106	2.874583196	2.226958039
H	6.292590105	1.280731160	1.714229126
H	5.895334363	1.579694455	3.410043728
H	-4.394091491	0.445544210	-2.696820747
H	-4.230067955	-1.268401660	-2.311748292
H	-2.789150071	-0.307146910	-2.719506647
H	-5.600689527	0.837687511	-0.516926690
H	-4.823297595	0.527573426	1.037329041
H	-5.430122729	-0.821176641	0.058332841
H	-1.100733155	-3.060331692	-1.671095880
H	-2.783628648	-3.072689105	-2.186160636
H	-2.127759615	-4.464498279	-1.321162323
H	-3.972782106	-4.342141211	0.365119721
H	-4.690242903	-2.917335753	-0.385903742
H	-4.260310723	-2.896699780	1.335052583
H	5.619848744	-3.188075881	-0.304468515
H	4.374327186	-4.038809525	0.607204102
H	4.969860785	-2.478786540	1.179186856
H	4.176333563	-3.463241569	-2.372351313
H	2.552752018	-2.760662992	-2.453879952
H	2.848590167	-4.201400074	-1.472335486
H	1.925928400	-3.639248367	3.650901244
H	2.691523865	-2.091749877	3.269783745
H	3.377897402	-3.600459710	2.647725185
H	0.708984736	-4.972512444	1.794425770
H	2.111778805	-4.887852587	0.728732247
H	0.543246542	-4.283904436	0.171570413
N	-0.034108474	-0.283937449	-2.761745701
C	0.608447611	1.003926330	-2.578188093
C	0.573042931	-1.097055356	-3.625919330
C	1.451891601	-0.719849081	-4.612918319
C	1.687130135	0.683267868	-4.731320330
C	1.249575721	1.557801465	-3.782035931
F	0.181887323	-2.392944883	-3.564267758
H	1.813022417	-1.440424291	-5.335065329
H	2.215080380	1.056838925	-5.605892589

H	1.430235052	2.620509172	-3.862418907
C	-0.159482747	1.739481774	-1.485695324
C	-0.227136166	3.249108778	-1.347011015
C	-0.964160634	3.878433460	-2.555290132
C	1.182586381	3.881321276	-1.201680329
C	-1.028466351	3.587057545	-0.070223277
H	-1.055363784	4.964154111	-2.423750500
H	-1.972253280	3.461501064	-2.648341764
H	-0.442853405	3.696160276	-3.498334922
H	-1.085657655	4.673111514	0.076830915
H	-0.559508157	3.144433068	0.813576501
H	-2.050719540	3.200224837	-0.136161487
H	1.101364167	4.971075307	-1.098600574
H	1.824054122	3.678335893	-2.063620276
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H	1.643460457	0.612345725	-1.796748892

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Ga

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Ti	0.186676938	0.084572793	-0.483787624
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C	2.398870395	1.918518350	3.823172881
C	1.229020243	1.394294972	3.283786792
C	1.268277807	0.524747937	2.179612381
N	0.098499248	0.048264165	1.537740650
C	-0.922600421	-0.542036274	2.299228855
C	-0.722013200	-1.025343290	3.609769918
C	-1.746400586	-1.645753572	4.314461889
C	-3.018118015	-1.828293948	3.757426595
C	-3.214129372	-1.363856843	2.452873157
C	-2.206633130	-0.724127651	1.719337080
P	-2.381971214	-0.135017324	-0.015975154
C	4.127084401	-0.810161841	-0.694411628
C	2.190702108	-2.638547313	0.924891583
C	-3.287464276	1.518871682	0.131044003
C	-3.453830304	-1.439582955	-0.879004101
H	4.662980762	0.520435872	1.742306047
H	2.333863200	2.595848207	4.672001611
H	0.266002226	1.671443854	3.701885940
H	0.254119167	-0.923363806	4.071137781
H	-1.546054885	-2.007312358	5.321568447

H	-4.189915390	-1.509496112	2.000454908	H	-5.455256202	-2.204364999	-1.166920275
C	5.312187147	-1.540021509	-0.038322096	H	-5.369327982	-0.445203874	-1.242250253
C	2.135983803	-3.724804204	-0.160530639	H	-5.306661772	-1.266447096	0.320364164
C	-3.510718637	2.138532246	-1.257998197	H	6.240776094	-1.257271628	-0.548644683
C	-4.978912835	-1.323709467	-0.719287725	H	5.209392853	-2.625537417	-0.132857136
C	3.980132310	-1.229190630	-2.168494073	H	5.432335697	-1.308788137	1.022751833
H	4.320167688	0.270457746	-0.676539879	H	4.921932466	-1.047717136	-2.699229935
C	3.105361413	-3.031050250	2.095906532	H	3.196171352	-0.659726636	-2.669612075
H	1.175123436	-2.518329901	1.322456953	H	3.746733186	-2.294594909	-2.263018588
C	4.925341696	2.181891512	3.873072636	H	2.704784442	-3.927644161	2.585085865
C	-4.128493749	-2.491238648	4.539594846	H	3.167395018	-2.241286866	2.849980983
C	-4.550875832	1.574739464	1.002729534	H	4.120747245	-3.266678418	1.765712617
H	-2.513076359	2.112078993	0.634074591	H	1.785443597	-4.667000025	0.277325167
C	-3.086720102	-1.556265778	-2.368285546	H	3.123816896	-3.916527684	-0.593495399
H	-3.119906366	-2.359384211	-0.382361185	H	1.448949528	-3.449579789	-0.966183472
C	0.567421391	1.751560526	-1.373746839	C	0.813172944	1.328936015	-2.750127874
C	0.925159554	3.191284329	-0.947164785	H	-0.146979606	-1.408026005	-1.306298225
C	2.440577758	3.333350917	-0.658694383	N	1.991723909	1.675414303	-3.369085261
C	0.537571636	4.196893751	-2.058754847	C	2.222611428	1.219950750	-4.569469365
C	0.142117262	3.583257375	0.323593401	C	1.402499646	0.360087961	-5.310502909
H	0.414769139	4.597419854	0.643127990	C	0.202239048	0.007354523	-4.707657658
H	-0.936762774	3.574019742	0.133801162	C	-0.114225642	0.513527890	-3.444261943
H	0.348802344	2.905851761	1.155857229	F	3.381912095	1.613352340	-5.141762265
H	2.682894168	4.371982416	-0.395374944	H	1.697157287	0.023844692	-6.297227967
H	2.737882001	2.695947647	0.180064766	H	-0.504503909	-0.632102271	-5.230453240
H	3.022873253	3.051055534	-1.537752083	H	-1.090961389	0.334260739	-3.014477581
H	0.725267068	5.224567943	-1.723297114	=====			
H	1.116300210	4.027157584	-2.969733252	H			
H	-0.527197333	4.114514114	-2.307267564	=====			
H	-4.998523403	-2.692591197	3.907251853	Ti	-0.012833581	-0.199369126	-0.211081322
H	-4.466539815	-1.862177765	5.372964689	P	2.333932113	-1.120476421	0.497396295
H	-3.803286898	-3.445172918	4.971166574	C	2.376689082	0.041874803	1.924487629
H	4.721562922	3.077161852	4.468163073	C	3.552610621	0.597143924	2.444830162
H	5.645412902	2.453608765	3.094077927	C	3.544124023	1.500930850	3.511848567
H	5.419669923	1.456809340	4.532779903	C	2.296270262	1.863887403	4.035459524
H	-3.879300589	3.165818661	-1.154505179	C	1.112033044	1.342533399	3.525893953
H	-4.257142231	1.582738264	-1.836401566	C	1.113899634	0.415238977	2.463832768
H	-2.580374331	2.172049715	-1.832640979	N	-0.058186021	-0.083922087	1.869102585
H	-4.829695466	2.623015953	1.167905209	C	-1.171035414	-0.383020296	2.655745359
H	-4.391310097	1.116680406	1.982509606	C	-1.059030039	-0.763311170	4.017193211
H	-5.404528354	1.083604629	0.528307175	C	-2.169488173	-1.084393356	4.781458612
H	-2.016497895	-1.734311526	-2.495369360	C	-3.468663205	-1.048981218	4.250319601
H	-3.361519444	-0.650902392	-2.922175621	C	-3.588745110	-0.699943643	2.905268522
H	-3.634112293	-2.393086701	-2.819319435	C	-2.482773152	-0.380612844	2.097830140

P	-2.599292076	-0.032059741	0.301320468	H	5.241828021	1.374967530	4.860974500
C	3.939864144	-0.829088088	-0.457636638	H	-3.968778506	3.022004883	-1.474396873
C	2.342308310	-2.832482830	1.315089163	H	-4.530824860	1.366029251	-1.715889647
C	-3.376766182	1.677790043	0.125195021	H	-2.821403894	1.773733885	-1.984723961
C	-3.755448605	-1.331795875	-0.447752430	H	-4.801612504	3.085185652	0.941439620
H	4.510696419	0.318821465	2.016079665	H	-4.292576891	1.854321460	2.104274343
H	2.248494915	2.582846088	4.851249533	H	-5.449666021	1.447689475	0.828081249
H	0.161957685	1.669342360	3.936502084	H	-5.671700949	-0.250838634	-0.536453869
H	-0.072462863	-0.817189657	4.464989503	H	-5.546622607	-1.377665648	0.823352984
H	-2.024685377	-1.378748446	5.819803448	H	-5.784347970	-1.990977917	-0.809279654
H	-4.583100563	-0.666748325	2.472077756	H	-3.799087125	-3.501178259	-0.609003894
C	5.205752650	-1.548229568	0.037839882	H	-3.407456206	-2.917020961	1.016985879
C	2.396016070	-3.964549664	0.275514038	H	-2.186011909	-2.863948585	-0.259068750
C	-3.691538976	1.968773346	-1.350340285	H	6.073433892	-1.189537306	-0.529459207
C	-3.252768987	-2.731827444	-0.050453377	H	5.142040134	-2.629271310	-0.120079826
C	3.719068118	-1.101838953	-1.956901109	H	5.410127223	-1.378324966	1.097349825
H	4.082161837	0.251813788	-0.340723969	H	4.644275469	-0.907244243	-2.513229843
C	3.344747203	-3.056584272	2.457328905	H	2.941278417	-0.449104619	-2.363578508
H	1.336291066	-2.832710294	1.757519505	H	3.437583853	-2.144027253	-2.146327399
C	4.832694458	2.040965750	4.089098842	H	3.085675024	-3.977961523	2.993972681
C	-4.671896750	-1.379268138	5.103264947	H	3.332656157	-2.235152409	3.178465712
C	-4.547735171	2.023982382	1.055544513	H	4.367535712	-3.173230416	2.088580516
H	-2.525479365	2.308837010	0.409431128	H	2.222390926	-4.928544676	0.769273996
C	-5.271917215	-1.217686142	-0.222673844	H	3.378865884	-4.024165095	-0.205451170
H	-3.573572727	-1.205139440	-1.523358776	H	1.640558654	-3.851167129	-0.507491575
C	0.465999631	1.328214620	-0.922126963	C	0.042453312	-1.880019121	-2.525687591
C	0.901639028	2.745239570	-1.221744538	N	0.001095443	-3.208238661	-2.299658785
C	2.442612585	2.818627004	-1.340407792	C	-0.965565351	-3.874840661	-2.883234862
C	0.279486437	3.219727226	-2.557597881	C	-1.947204490	-3.322363409	-3.713179373
C	0.450476930	3.697793821	-0.087932687	C	-1.894218926	-1.950972440	-3.928260445
H	0.772881877	4.730265922	-0.283925143	C	-0.872061221	-1.202437362	-3.326633575
H	-0.640947438	3.699535441	0.008011903	H	0.897743452	-1.345874770	-2.100514104
H	0.870787716	3.382068988	0.871989092	H	-2.705407982	-3.957929005	-4.156451022
H	2.772846104	3.841164724	-1.570154074	H	-2.630482124	-1.470344779	-4.566122194
H	2.913702941	2.511897627	-0.400936016	H	-0.772491051	-0.130879872	-3.460724613
H	2.804271241	2.159768933	-2.137532521	F	-1.003954576	-5.194637782	-2.651523002
H	0.582132684	4.249153864	-2.795164851	=====			
H	0.596417504	2.574429926	-3.385014013	Ha-TS			
H	-0.814404551	3.191562735	-2.507893036	=====			
H	-5.590215720	-1.403349302	4.508309257	H	-0.095099448	0.095178015	0.705989948
H	-4.817847461	-0.642108279	5.903365109	C	-0.153465997	-0.013491391	1.981225460
H	-4.566245770	-2.357556671	5.588494221	Ti	1.713583358	0.035615203	0.675905519
H	4.682267922	3.020208059	4.555006536	P	2.388062213	2.632967193	1.027361116
H	5.603007098	2.152090721	3.318465205	C	3.845034006	2.209866727	2.069934327

C	4.349622323	2.918509047	3.161353809	H	-1.791927853	0.944706756	-2.958225173
C	5.500646896	2.503792751	3.850557390	H	-0.737740980	1.996771502	-1.993430346
C	6.143333471	1.349836529	3.392128324	H	-0.607037382	2.043322544	2.471965976
C	5.641246641	0.602150714	2.328428627	H	-1.761271538	1.463685567	4.603017100
C	4.459483197	0.987983596	1.666395096	H	-1.952040999	-0.972053605	5.259365908
N	3.815877304	0.209290103	0.700937950	F	-0.964891454	-2.888712698	3.813642613
C	4.560426555	-0.647467642	-0.128174125	C	0.150408358	4.372728527	1.252648214
C	5.705557086	-0.230380480	-0.833250795	H	1.431692859	3.776331649	2.876593045
C	6.325691664	-1.073834708	-1.747984222	C	4.436603337	4.060831382	-0.493739745
C	5.833283234	-2.361684213	-2.008547005	H	3.493411808	2.203111211	-1.001821856
C	4.716856926	-2.789819035	-1.282885580	C	6.026355882	3.291734448	5.029426550
C	4.094706773	-1.971196621	-0.331688792	C	6.488060892	-3.249705713	-3.041408343
P	2.674590344	-2.422560983	0.749052451	C	4.861482480	-3.567576646	2.338766967
C	1.554290270	4.121270019	1.840007677	H	3.765986230	-1.782491226	2.747288127
C	3.185345362	3.176781266	-0.605787604	C	0.471423315	-4.174541373	0.479113772
C	3.531908797	-2.799970740	2.407404678	H	1.920861619	-3.768263597	-1.049768142
C	1.932746727	-3.999102821	0.024182795	H	5.347732005	-3.543708611	3.322248572
C	0.767293191	-0.013487287	-0.827136142	H	5.551108096	-3.128610970	1.613345380
C	-0.073367368	-0.094554849	-2.073492097	H	4.715210200	-4.618130442	2.073741238
C	-0.752830116	-1.480468700	-2.178075929	H	3.033753130	-3.398920786	4.431365038
C	0.834010718	0.117041608	-3.310234222	H	2.371106161	-4.478655191	3.205541846
C	-1.174017365	0.994425396	-2.052078828	H	1.616287652	-2.910351151	3.489379794
C	-0.700136736	1.009625930	2.777416460	H	0.025746813	-5.032257258	-0.040489921
C	-1.348718512	0.683393639	3.968696605	H	-0.124882722	-3.287059049	0.263383140
C	-1.459946797	-0.652507153	4.348156125	H	0.397443104	-4.360130406	1.554702043
C	-0.897056282	-1.583936699	3.476631765	H	2.264387193	-6.102823996	-0.376690851
N	-0.289870240	-1.315137783	2.347806590	H	2.681901156	-5.634021988	1.269635923
H	3.849796909	3.823214030	3.495602097	H	3.769376502	-5.229951280	-0.062352753
H	7.048438178	1.010366006	3.892410242	H	6.104112131	-4.273069977	-2.989307742
H	6.147525774	-0.308064661	2.022079963	H	7.574859323	-3.293495457	-2.904440409
H	6.088529364	0.773154949	-0.669990914	H	6.308211535	-2.882718349	-4.059987527
H	7.201611647	-0.718344410	-2.287579597	H	6.897848577	2.802517429	5.475141487
H	4.337485280	-3.791193167	-1.464150266	H	5.270109564	3.397966366	5.817051718
C	2.340867838	5.446119720	1.859176216	H	6.331192272	4.305705186	4.740231869
C	2.154217418	3.767229480	-1.577691746	H	4.921070891	4.128733263	-1.475848168
C	2.575417361	-3.427751464	3.434987797	H	5.164947811	3.651258193	0.210765201
C	2.718535956	-5.306682643	0.226309239	H	4.196626819	5.080401918	-0.178008223
H	-0.003632712	-2.277457222	-2.211370829	H	2.593490402	3.844338171	-2.579471500
H	-1.366658220	-1.549150425	-3.085978703	H	1.844607951	4.776017526	-1.283398682
H	-1.401738598	-1.663633996	-1.315105353	H	1.263962231	3.136687124	-1.651050446
H	1.315116215	1.099995800	-3.280875437	H	-0.405588678	5.064386270	1.897142445
H	0.248103088	0.049838870	-4.236496030	H	-0.438319527	3.459102901	1.144468665
H	1.622581947	-0.641253093	-3.345825159	H	0.213402468	4.831381085	0.261785602
H	-1.833517106	0.863600739	-1.186624658	H	1.842461228	6.161577886	2.525368835

H	2.368260674	5.897924003	0.863042832
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Hb-TS

Ti	0.245023108	1.213917767	0.713707228
P	2.539955431	0.192526647	1.398792738
C	2.823907207	1.728633378	2.388622517
C	4.051539658	2.394891547	2.513965179
C	4.187540408	3.560789488	3.273220810
C	3.040203969	4.073738384	3.899188517
C	1.802543184	3.458254983	3.755567236
C	1.662014566	2.283579478	2.992241268
N	0.415936502	1.690033077	2.708545116
C	-0.522925207	1.452137283	3.710953528
C	-0.187397568	1.370781653	5.083229712
C	-1.142773173	1.055636349	6.040272134
C	-2.481247326	0.808196327	5.699668265
C	-2.818919997	0.894996351	4.346630204
C	-1.879605917	1.208268052	3.352764072
P	-2.246939600	1.350708229	1.559527918
C	4.108619969	-0.122662492	0.406858032
C	2.293714687	-1.146598958	2.716828193
C	-3.111787496	3.022314920	1.380945279
C	-3.407491133	-0.052935726	1.055911021
H	4.932200721	1.998191976	2.018597694
H	3.115923014	4.984518978	4.489468542
H	0.919381617	3.895464008	4.212047256
H	0.840604350	1.538944276	5.386636043
H	-0.838180935	0.991090661	7.083540626
H	-3.852250549	0.722104029	4.062733210
C	5.338296631	-0.621043640	1.186842335
C	2.076031541	-2.527150488	2.075219729
C	-3.603563202	3.242788325	-0.057605394
C	-2.769394107	-1.395522752	1.458605531
C	3.815010069	-1.045646072	-0.791321218
H	4.324163065	0.876573155	0.005541186
C	3.318650467	-1.201704954	3.860205435
H	1.338522913	-0.824939663	3.150337035
C	5.531150163	4.232252528	3.440782553
C	-3.508331381	0.467421214	6.755378063
C	-4.191690203	3.360085154	2.419251594
H	-2.264949849	3.701629406	1.546712765
C	-4.884259115	0.005336843	1.478056462

H	-3.375441218	0.009731253	-0.040126792
C	0.565682801	2.378834752	-0.589133413
C	1.095262575	3.515550502	-1.429442188
C	2.542575257	3.218588988	-1.897934909
C	0.222382064	3.841901288	-2.661849192
C	1.119402498	4.757781828	-0.502237187
H	1.553136099	5.616317831	-1.031318279
H	0.106959894	5.027326359	-0.183067591
H	1.717762160	4.568890853	0.394423525
H	2.933605615	4.054944432	-2.492672641
H	3.201100287	3.078108910	-1.034130699
H	2.581172768	2.311032822	-2.505142661
H	0.597526501	4.751328882	-3.147795970
H	0.240034651	3.034975680	-3.397747875
H	-0.819913736	4.016953245	-2.375559878
H	-4.483736844	0.251977901	6.308392069
H	-3.646802833	1.290110837	7.468115586
H	-3.211051929	-0.412785486	7.338685583
H	5.436939938	5.323384811	3.435694577
H	6.221480945	3.951424011	2.639654763
H	6.003215432	3.954543412	4.392432556
H	-3.995699570	4.260783555	-0.164093618
H	-4.413261148	2.553969600	-0.324681666
H	-2.791462980	3.121143328	-0.778751937
H	-4.500326738	4.404959701	2.292616923
H	-3.824568174	3.242701114	3.441274921
H	-5.086636319	2.741241751	2.305786421
H	-5.377292021	0.922317891	1.147528473
H	-5.009320375	-0.077949632	2.561314801
H	-5.422352409	-0.837473133	1.026511349
H	-3.352382716	-2.225541306	1.043029453
H	-2.742856913	-1.512496663	2.546695399
H	-1.744532202	-1.489122245	1.082622700
H	6.221239420	-0.575661891	0.537859194
H	5.215212373	-1.666499490	1.486900016
H	5.554061625	-0.038770628	2.085926645
H	4.711065333	-1.118112657	-1.419945663
H	2.991620880	-0.670845250	-1.404638618
H	3.569169513	-2.061428931	-0.461821023
H	2.937630925	-1.848153017	4.660791735
H	3.501885949	-0.212876855	4.289758896
H	4.276965583	-1.615250374	3.535601439
H	1.729971709	-3.240257489	2.832808603
H	3.002091304	-2.927763386	1.650046716

H	1.326587334	-2.497598453	1.277006834	C	-5.150346738	-0.372409989	-0.733740108
C	-0.061252595	0.733823806	-1.582657156	C	4.264594798	-0.642113426	-1.956841510
N	1.003339176	0.212536062	-2.283894078	H	4.282326516	0.809709170	-0.383834315
C	0.884363463	0.039166184	-3.576476285	C	3.561065739	-2.648881400	2.355232392
C	-0.245334184	0.266264410	-4.355245537	H	1.668322340	-2.627141796	1.343638196
C	-1.369637600	0.723726847	-3.647918391	C	4.351293500	2.538875061	4.301637983
C	-1.299610406	0.953344408	-2.288956207	C	-4.246053835	-3.048298701	3.901887018
H	-0.262279273	0.054613217	-0.602304385	C	-3.924753203	1.950677038	1.531459537
H	-0.245638098	0.069754396	-5.419585300	H	-1.888865400	2.190184980	0.904873334
H	-2.302264153	0.905384684	-4.177387877	C	-3.466210593	-0.412192187	-2.612670826
H	-2.166154060	1.305210278	-1.743311713	H	-3.512205516	-1.757091054	-0.938068331
F	1.994807015	-0.428475936	-4.193200053	C	0.762577076	1.590206460	-1.229764642
=====				C	1.184111238	3.040780505	-1.365197685
Gb				C	2.715520135	3.139052123	-1.577529578
=====				C	0.484215006	3.705426152	-2.573934638
Ti	0.291743349	-0.074365140	-0.572375364	C	0.818407990	3.808160080	-0.075777568
P	2.641037091	-0.742235723	0.333440857	H	1.161553633	4.849536772	-0.128897311
C	2.439725119	0.357256880	1.796573231	H	-0.265473070	3.817562404	0.078618894
C	3.466090926	1.040118214	2.459000619	H	1.278253521	3.340202078	0.800331969
C	3.220612571	1.839265131	3.582326746	H	3.023082983	4.182658929	-1.727811305
C	1.895537152	1.943935946	4.026161491	H	3.249532857	2.753238818	-0.703753349
C	0.853307607	1.296887974	3.370079716	H	3.032159728	2.564461112	-2.455294120
C	1.094624629	0.502023726	2.233822793	H	0.772184991	4.760811449	-2.663638998
N	0.068868194	-0.095289016	1.482933451	H	0.756057197	3.202132864	-3.509392920
C	-0.986477060	-0.742004486	2.139109328	H	-0.604884314	3.662034469	-2.474450005
C	-0.840637576	-1.390189848	3.383357526	H	-5.104010376	-3.114360470	3.225805016
C	-1.886386567	-2.116649143	3.939929708	H	-4.600478660	-2.605879136	4.841763597
C	-3.123394112	-2.239966443	3.292006907	H	-3.926496464	-4.071933810	4.132056552
C	-3.276258104	-1.579402687	2.068365287	H	3.972448537	3.296649544	4.994063067
C	-2.247099590	-0.823852620	1.493919802	H	5.029063747	3.037869842	3.599889034
P	-2.321570988	0.110369834	-0.088348745	H	4.956110085	1.834282640	4.887233617
C	4.289321896	-0.284218917	-0.459093188	H	-3.189891289	3.797221912	-0.430538227
C	2.723004844	-2.480678610	1.079384039	H	-4.080907717	2.496488782	-1.222303802
C	-2.831119857	1.848476778	0.457886788	H	-2.338332201	2.676930164	-1.505127750
C	-3.692743657	-0.688230698	-1.114033521	H	-3.982019993	2.984057332	1.895981298
H	4.489186700	0.947425748	2.105883176	H	-3.715987000	1.305015956	2.388129523
H	1.671887176	2.560285266	4.894743000	H	-4.912298326	1.688648293	1.141233277
H	-0.167400527	1.419656650	3.719847541	H	-2.464922942	-0.709873014	-2.930841284
H	0.113970692	-1.341485354	3.897935291	H	-3.595131405	0.649468692	-2.848730211
H	-1.730526737	-2.618018460	4.893748504	H	-4.196012458	-0.973246740	-3.209552454
H	-4.230290530	-1.663485088	1.557330438	H	-5.825575594	-1.017484424	-1.309549912
C	5.574055013	-0.807043325	0.205652458	H	-5.409263271	0.662783673	-0.976248779
C	3.082215417	-3.535571896	0.019766097	H	-5.367495035	-0.528049454	0.324845677
C	-3.125711116	2.750217604	-0.750095185	H	6.447167945	-0.351068533	-0.277238416

H	5.673256482	-1.890870283	0.093835700	C	-0.007388164	-1.661772252	-1.963005986
H	5.629060387	-0.577608263	1.272414399	C	-0.428587015	-3.758610806	-1.058048662
H	5.170202050	-0.265126727	-2.447827694	C	-0.472450132	-4.390030159	-2.298921092
H	3.396995940	-0.202030387	-2.455610809	C	-0.263293102	-3.581471181	-3.417460619
H	4.231807917	-1.725865729	-2.112921525	C	-0.028742925	-2.211827572	-3.253337366
H	3.369071002	-3.637382566	2.791121957	H	0.714197345	1.057296287	-2.227470021
H	3.310312786	-1.897653886	3.108689001	F	-0.608395280	-4.495274120	0.051976503
H	4.634760104	-2.583497336	2.155741694	H	-0.659875551	-5.455565336	-2.367371713
H	2.894033363	-4.539370265	0.418641508	H	-0.284033354	-4.025526318	-4.410064022
H	4.140564251	-3.490186851	-0.257899528	H	0.137633715	-1.576552760	-4.118587082
H	2.487323743	-3.423781755	-0.890669189				
N	-0.211182289	-2.471511286	-0.887750513				

S2 Computed Components.

<i>Table S8a.</i> Computed Components	E(SCF) eV LACVP**	E(SCF) eV cc-pVTZ(-f)	ZPE kcal/mo l	-TS kcal/mo l 298.15K	G(solv) kcal/mol In o-fluoropyridine	G(sol) eV
(PNP)Ti(=CtBu)(CH2tBu)	-59979.53 8 -59978.27	-59992.832	272.3	54.41	-5.88	-59983.63 8 -59982.43
A-TS	2 -54596.64	-59991.509	270.86	55.55	-6.13	8 -54601.23
A	8 -64054.33	-54608.344	225.93	51.76	-10.26	6 -64060.12
A-Pyf	6 -64054.12	-64069.080	277.21	60.33	-10.32	3 -64059.96
B	8 -64054.00	-64068.886	277.14	60.29	-11.05	2 -64059.68
D	4 -64053.82	-64068.723	276.96	58.83	-9.66	3
B-TS	6 -64053.48	-64068.607	276.78	59.09	-7.9	-64059.51
D-TS	2 -64055.04	-64068.207	275.98	60.03	-8.24	-64059.2 -64060.69
C	1 -64054.58	-64069.839	277.78	57.95	-9.01	7 -64060.45
C-TS	4 -64057.44	-64069.509	277.04	57.77	-10.44	3 -64063.08
2 Ea-TS	5 -64054.02	-64072.299 -64068.831	278.25 277.07	56.91 58.91	-8.83 -6.9	4 -64059.67

	6					
	-64054.73					-64060.34
F	3	-64069.543	277.91	58.25	-7.51	3
	-64053.22					-64059.12
F-TS	7	-64068.124	274.44	58.67	-8.32	8
	-64054.50					-64060.43
Ga	1	-64069.402	275.63	59.10	-9.78	6
						-64059.34
H	-64053.58	-64068.404	277.01	59.47	-8.71	8
	-64053.34					-64059.23
Ha-TS	8	-64068.2	274.76	60.31	-7.74	6
						-64058.88
Hb-TS	-64052.98	-64067.885	275.85	59.66	-8.7	7
	-64054.99					-64060.48
Gb	6	-64069.867	281.57	58.21	-6.92	1