

## Supporting Information

# Theoretical Study on Ethylene Polymerization Catalyzed by Half-Titanocenes Bearing Different Ancillary Groups

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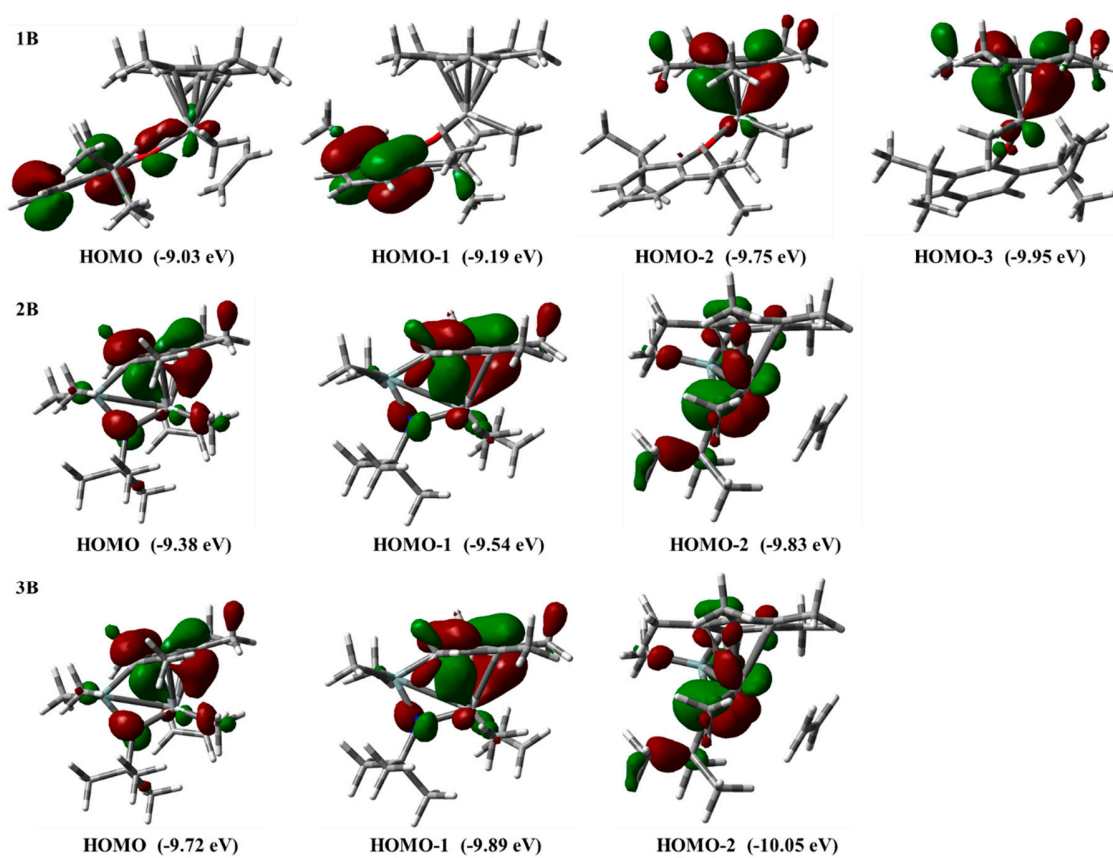
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**Figure S1.** Some occupied HOMOs of **1B**, **2B** and **3B**. The isosurface of MOs is 0.05.

**Table S1.** Cartesian coordinates for all of the calculated structures.

6				H	5.285602	-0.542314	0.092682
<b>C<sub>2</sub>H<sub>4</sub></b>				H	3.229977	-2.324226	2.158695
C	0.000000	0.000000	0.665035	H	3.536848	-3.814623	1.248822
H	0.000000	0.923501	1.237850	H	4.753021	-2.536199	1.286228
H	0.000000	-0.923501	1.237850	H	3.528114	-3.800289	-1.307832
C	0.000000	0.000000	-0.665035	H	3.176692	-2.307601	-2.197188
H	0.000000	-0.923501	-1.237850	H	4.724111	-2.500293	-1.363329
H	0.000000	0.923501	-1.237850	H	0.650232	2.845961	-2.284504
				H	-0.039642	1.317774	-1.911796
60				H	-0.926543	2.825861	-1.491961
<b>1A</b>				H	1.389530	4.022155	1.231261
Ti	-0.985438	-0.173460	-0.501030	H	1.514124	4.460761	-0.481281
O	0.756698	-0.340956	-0.183227	H	-0.066643	4.399843	0.295976
C	-2.736921	0.870281	0.722331				
C	-3.400794	0.090111	-0.284170	66			
C	-3.071133	-1.276169	-0.073129	<b>1B</b>			
C	-2.171023	-1.341407	1.052560	Ti	1.120308	0.130945	0.585949
C	-2.002141	-0.016681	1.569215	O	-0.653513	0.053718	0.458696
C	2.003159	0.226563	-0.082101	C	1.816142	1.016650	-1.448777
C	2.061667	1.638914	-0.085276	C	2.982652	1.086613	-0.617578
C	4.379785	0.053789	0.041259	C	3.367228	-0.247018	-0.296483
C	3.139080	-0.595789	-0.015063	C	2.448758	-1.143180	-0.944854
C	-2.910439	2.350903	0.923425	C	1.505045	-0.362784	-1.671608
C	-4.332951	0.620503	-1.335899	C	-1.978615	-0.004996	0.103328
C	-3.663226	-2.452011	-0.789548	C	-2.698256	1.210616	0.006431
C	-1.623221	-2.604258	1.660184	C	-3.930866	-1.277816	-0.478671
C	0.763656	2.436884	-0.135208	C	-2.576167	-1.265671	-0.130704
C	0.057928	2.345719	-1.511477	C	1.119481	2.182366	-2.090053
C	0.913480	3.915411	0.253230	C	3.769817	2.324838	-0.308692
C	3.038329	-2.114496	-0.016364	C	4.629540	-0.624482	0.428114
C	3.676176	-2.728909	1.244707	C	2.529730	-2.645361	-0.968907
C	3.651951	-2.712635	-1.298188	C	-2.055092	2.551194	0.336032
C	3.324021	2.230568	-0.029514	C	-2.306048	2.913275	1.815826
C	4.475929	1.442259	0.031007	C	-2.510383	3.692936	-0.589358
C	-1.234548	0.350873	2.809259	C	-1.824779	-2.577793	0.054764
H	0.095355	1.990894	0.623977	C	-2.028841	-3.560816	-1.113505
H	1.974299	-2.373443	-0.007940	C	-2.222941	-3.243116	1.390250
C	-1.151499	-1.206756	-2.283421	C	-4.046558	1.128979	-0.352598
H	-2.076616	-1.061215	-2.846827	C	-4.660760	-0.097931	-0.595195
H	-0.290765	-0.874611	-2.879686	C	0.438605	-0.881003	-2.593399
H	-1.024733	-2.279640	-2.087836	H	-0.974382	2.441115	0.205098
H	-4.600601	-2.744286	-0.300896	H	-0.753518	-2.346192	0.100714
H	-3.896601	-2.227908	-1.832671	C	1.426352	1.852265	1.712935
H	-3.002987	-3.321959	-0.769885	H	2.425291	1.884232	2.162069
H	-2.355797	-3.031686	2.355642	H	1.276595	2.780886	1.154423
H	-1.411875	-3.367010	0.905871	H	0.666860	1.809025	2.504165
H	-0.705023	-2.422216	2.222700	H	5.480940	-0.568999	-0.260904
H	-1.861983	0.199587	3.695787	H	4.848392	0.052931	1.258358
H	-0.338998	-0.262674	2.934440	H	4.602968	-1.643947	0.818255
H	-0.924538	1.398505	2.808347	H	2.926685	-2.982483	-1.933747
H	-3.817628	2.537836	1.510881	H	3.197078	-3.036161	-0.197840
H	-2.077363	2.798070	1.470145	H	1.551205	-3.119525	-0.844440
H	-3.029180	2.888454	-0.021345	H	0.232845	-1.938396	-2.418911
H	-5.359512	0.651037	-0.950531	H	-0.502656	-0.334572	-2.492772
H	-4.076657	1.638376	-1.641888	H	0.767170	-0.779687	-3.634738
H	-4.341820	-0.009278	-2.228655	H	1.597193	2.418913	-3.049093
H	3.419399	3.310522	-0.028210	H	0.068224	1.967440	-2.295058
H	5.450652	1.917574	0.074374	H	1.169753	3.082736	-1.473173

H	4.517388	2.491037	-1.093918
H	3.139771	3.215748	-0.267625
H	4.306667	2.248929	0.639895
H	-4.628537	2.040064	-0.439434
H	-5.710287	-0.134241	-0.869763
H	-4.424137	-2.227634	-0.657821
H	-1.791394	-3.102121	-2.077621
H	-1.391077	-4.441501	-0.983903
H	-3.061362	-3.918797	-1.164038
H	-1.630063	-4.146944	1.569690
H	-2.092974	-2.563973	2.239453
H	-3.277243	-3.536602	1.375508
H	-3.376260	3.045437	2.005561
H	-1.945133	2.128493	2.488346
H	-1.799187	3.848246	2.076646
H	-2.377013	3.437824	-1.645413
H	-3.562915	3.950918	-0.437548
H	-1.928226	4.596104	-0.380931
C	0.838012	-1.305139	2.743293
H	0.481756	-0.476442	3.348985
C	2.143378	-1.445000	2.433967
H	2.504890	-2.324997	1.912442
H	2.889472	-0.739971	2.790340
H	0.103916	-2.053138	2.460959

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**1TS(B-C)**

Ti	-1.076683	-0.044076	0.448213
O	0.678261	-0.009600	0.244580
C	-2.062927	-1.045433	-1.387907
C	-3.133936	-0.909383	-0.439657
C	-3.371342	0.480258	-0.237871
C	-2.432086	1.210467	-1.031647
C	-1.635674	0.265022	-1.761821
C	2.043554	0.017199	0.086161
C	2.738102	-1.209252	-0.003601
C	4.085815	1.262247	-0.097192
C	2.692816	1.270389	0.028047
C	-1.550106	-2.339084	-1.959789
C	-3.956761	-2.033893	0.127977
C	-4.482312	1.070056	0.580166
C	-2.374354	2.703907	-1.181630
C	2.033343	-2.558729	0.051990
C	2.377753	-3.317953	1.349291
C	2.339062	-3.420650	-1.188285
C	1.937665	2.590764	0.113399
C	2.260056	3.522841	-1.070522
C	2.203540	3.296631	1.458665
C	4.130071	-1.148976	-0.126047
C	4.802141	0.069992	-0.170282
C	-0.602406	0.595985	-2.802462
H	0.953069	-2.374391	0.056266
H	0.866457	2.368093	0.065268
C	-1.229180	-1.638918	2.367386
H	-1.940003	-2.135565	3.022161
H	-1.375334	-2.063821	1.353680
H	-0.198514	-1.752408	2.692626
H	-5.379612	1.185911	-0.039963
H	-4.759501	0.433236	1.424404
H	-4.235656	2.062355	0.965677

H	-3.026301	3.023545	-2.003739
H	-2.711268	3.222000	-0.280763
H	-1.365925	3.054446	-1.414664
H	-0.129247	1.562567	-2.615479
H	0.187486	-0.156926	-2.850808
H	-1.071622	0.647326	-3.792253
H	-2.149043	-2.626907	-2.832365
H	-0.512263	-2.258529	-2.290336
H	-1.612076	-3.164133	-1.244473
H	-4.834818	-2.211392	-0.504324
H	-3.400986	-2.974287	0.170497
H	-4.324232	-1.812545	1.133584
H	4.697083	-2.072697	-0.187924
H	5.883220	0.090959	-0.264984
H	4.618902	2.206964	-0.137927
H	2.070961	3.032738	-2.031034
H	1.645993	4.428068	-1.019467
H	3.307108	3.840632	-1.063126
H	1.617931	4.219015	1.534148
H	1.947102	2.654898	2.308434
H	3.260200	3.564295	1.560130
H	3.444580	-3.558424	1.393754
H	2.141263	-2.724352	2.238896
H	1.823060	-4.260646	1.405489
H	2.087110	-2.894920	-2.114919
H	3.398703	-3.688501	-1.240311
H	1.767285	-4.353901	-1.156146
C	-1.732865	0.272352	2.872309
H	-2.792202	0.120984	3.058822
C	-1.392263	1.373309	1.948100
H	-0.436937	1.854747	2.159868
H	-2.195391	2.089844	1.800351
H	-1.131883	0.193307	3.774943

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**1C**

Ti	1.120243	-0.020617	0.470141
O	-0.655695	-0.054691	0.420275
C	1.581763	0.641600	-1.714956
C	2.670452	1.118001	-0.918396
C	3.374382	-0.015243	-0.399494
C	2.708772	-1.194370	-0.847626
C	1.589742	-0.785379	-1.653795
C	-1.982002	0.039818	0.078801
C	-2.546984	1.325420	-0.079978
C	-4.070219	-1.023316	-0.424205
C	-2.721930	-1.153261	-0.075193
C	0.642219	1.474083	-2.541532
C	3.058087	2.561607	-0.740849
C	4.638498	0.018010	0.412362
C	3.185208	-2.605619	-0.664681
C	-1.735193	2.585195	0.196453
C	-1.801611	2.946457	1.696644
C	-2.141707	3.788816	-0.669177
C	-2.092296	-2.514733	0.191897
C	-2.640832	-3.634967	-0.707213
C	-2.242683	-2.888797	1.682586
C	-3.900548	1.387719	-0.424575
C	-4.654684	0.228895	-0.601614
C	0.672241	-1.697942	-2.418431
H	-0.686788	2.361638	-0.045080

H	-1.020033	-2.427803	-0.016529
C	1.709934	1.159147	2.598534
H	2.778195	1.221874	2.370555
H	1.139342	1.691312	1.798346
H	1.518879	1.813145	3.452825
H	5.508491	-0.124946	-0.239866
H	4.779610	0.974837	0.921673
H	4.670019	-0.775859	1.164042
H	3.811396	-2.899441	-1.515879
H	3.790952	-2.721835	0.236679
H	2.357304	-3.316493	-0.608655
H	0.587001	-2.680578	-1.949030
H	-0.332738	-1.280367	-2.515940
H	1.062907	-1.854308	-3.431446
H	0.976127	1.484992	-3.586188
H	-0.377222	1.079975	-2.529260
H	0.606835	2.512053	-2.203731
H	3.710420	2.878881	-1.563209
H	2.190189	3.226866	-0.746907
H	3.608237	2.733229	0.187717
H	-4.374727	2.354169	-0.555422
H	-5.703041	0.302881	-0.873128
H	-4.673996	-1.914302	-0.557093
H	-2.580352	-3.371031	-1.767571
H	-2.066151	-4.553375	-0.551472
H	-3.684716	-3.870578	-0.478085
H	-1.746878	-3.842356	1.894614
H	-1.810929	-2.122844	2.335115
H	-3.299047	-2.993109	1.950752
H	-2.828330	3.191344	1.986010
H	-1.474923	2.113464	2.328322
H	-1.174917	3.817884	1.917028
H	-2.140424	3.540960	-1.734842
H	-3.138923	4.157527	-0.410512
H	-1.445243	4.618109	-0.509722
C	1.255877	-0.294232	2.960658
H	1.811767	-0.540735	3.872053
C	1.551841	-1.402234	1.910568
H	0.836562	-2.224103	1.979159
H	2.570517	-1.782853	1.986570
H	0.194883	-0.275149	3.222078

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1D

Ti	1.091946	-0.081484	0.334872
O	-0.679590	-0.084680	0.242842
C	1.738067	0.566443	-1.779681
C	2.645443	1.201902	-0.873290
C	3.432890	0.181924	-0.238259
C	2.986221	-1.082042	-0.713460
C	1.918201	-0.847980	-1.652487
C	-2.027880	0.001627	-0.006401
C	-2.609720	1.280657	-0.138001
C	-4.138722	-1.080972	-0.342012
C	-2.765377	-1.198155	-0.107350
C	0.799435	1.251141	-2.733599
C	2.823720	2.687895	-0.705606
C	4.570565	0.410423	0.714588
C	3.599919	-2.417934	-0.408372
C	-1.795577	2.558798	0.018344

C	-1.966552	3.146639	1.434921
C	-2.117533	3.613139	-1.055791
C	-2.101784	-2.556737	0.079321
C	-2.653643	-3.640047	-0.863090
C	-2.200750	-3.009176	1.551809
C	-3.988972	1.330504	-0.366619
C	-4.747460	0.166513	-0.468343
C	1.216558	-1.904617	-2.462163
H	-0.735556	2.294608	-0.103185
H	-1.036890	-2.438255	-0.157655
C	0.550445	0.521600	3.753166
H	-0.450390	0.323426	3.359083
H	0.707940	-0.127821	4.618568
H	0.589614	1.559525	4.094668
H	5.520795	0.428428	0.167380
H	4.485566	1.365668	1.238278
H	4.647977	-0.383627	1.462451
H	4.339228	-2.671464	-1.177836
H	4.119700	-2.422478	0.552172
H	2.858368	-3.220851	-0.395758
H	1.112851	-2.843773	-1.912194
H	0.220655	-1.584672	-2.776694
H	1.792921	-2.124147	-3.369193
H	1.267107	1.330965	-3.722350
H	-0.136509	0.700826	-2.857835
H	0.552387	2.264419	-2.409779
H	3.541731	3.065170	-1.443662
H	1.890180	3.235985	-0.858394
H	3.210179	2.949540	0.282606
H	-4.477838	2.294156	-0.465468
H	-5.816089	0.231227	-0.647382
H	-4.743016	-1.977803	-0.426025
H	-2.621415	-3.320615	-1.909232
H	-2.062270	-4.556074	-0.767149
H	-3.688693	-3.902133	-0.623369
H	-1.673854	-3.957463	1.702877
H	-1.773520	-2.264733	2.231751
H	-3.246426	-3.156024	1.841215
H	-3.007813	3.435739	1.609093
H	-1.693266	2.421387	2.208139
H	-1.345178	4.039479	1.563569
H	-2.018940	3.204002	-2.065868
H	-3.135441	4.000400	-0.951300
H	-1.439404	4.467673	-0.962152
C	1.629222	0.234409	2.703104
H	1.522107	1.074925	1.917863
C	1.582582	-1.131418	2.044482
H	0.720770	-1.731742	2.348972
H	2.508114	-1.698275	2.105588
H	2.632437	0.457268	3.077016

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1E-fsi

Ti	-0.977342	-0.153277	0.300528
O	0.783832	0.121994	0.353359
C	-0.910570	-1.202692	-1.803318
C	-1.798651	-1.992932	-1.022035
C	-2.958123	-1.196781	-0.716163
C	-2.778350	0.086675	-1.305481
C	-1.497611	0.093584	-1.952199

C	2.133638	0.252932	0.136417
C	2.973325	-0.874988	0.294881
C	4.011535	1.642711	-0.427614
C	2.634033	1.529089	-0.217580
C	0.363596	-1.665736	-2.448638
C	-1.606128	-3.453165	-0.713324
C	-4.226338	-1.683748	-0.070775
C	-3.821179	1.155272	-1.450162
C	2.451871	-2.229171	0.759045
C	2.783087	-2.451826	2.250953
C	2.983180	-3.403310	-0.084844
C	1.731504	2.752521	-0.312101
C	2.050231	3.650859	-1.520613
C	1.788589	3.562372	1.000868
C	4.342685	-0.692104	0.076343
C	4.861175	0.548111	-0.286278
C	-0.942741	1.216516	-2.780513
H	1.360023	-2.221589	0.653889
H	0.703310	2.399473	-0.434190
C	-3.308296	3.173879	2.317460
H	-2.482547	3.612199	2.887244
H	-3.504529	3.824936	1.459378
H	-4.198043	3.178649	2.955352
H	-4.947573	-1.974691	-0.844028
H	-4.065273	-2.561056	0.559221
H	-4.704468	-0.912010	0.538531
H	-4.264788	1.097576	-2.451714
H	-4.633568	1.041027	-0.730753
H	-3.409755	2.162021	-1.339848
H	-1.245803	2.196002	-2.402402
H	0.148191	1.190314	-2.826498
H	-1.315163	1.137422	-3.809813
H	0.188390	-1.867631	-3.512301
H	1.159977	-0.920135	-2.383947
H	0.731511	-2.589256	-1.998622
H	-1.747229	-4.047660	-1.623608
H	-0.600421	-3.674914	-0.342229
H	-2.328045	-3.819852	0.019249
H	5.016008	-1.534611	0.196511
H	5.927642	0.663224	-0.452380
H	4.428089	2.606331	-0.701026
H	2.048147	3.086316	-2.458410
H	1.304355	4.448050	-1.601019
H	3.026551	4.135788	-1.425963
H	1.100093	4.413017	0.960791
H	1.522529	2.945809	1.865660
H	2.796958	3.953079	1.172394
H	3.865487	-2.517578	2.399430
H	2.426124	-1.626982	2.876801
H	2.799875	-3.253386	-1.152617
H	4.060281	-3.540967	0.048299
H	2.501324	-4.338210	0.220098
C	-2.968214	1.745654	1.858175
H	-2.837207	1.120170	2.751796
C	-1.704406	1.692366	0.984656
H	-0.833789	2.025912	1.570417
H	-1.789199	2.390396	0.142292
H	-3.829128	1.332236	1.321532
C	-1.866990	-1.645063	2.300358
H	-2.849039	-1.188145	2.378403

C	-0.757701	-1.011277	2.732871
H	-0.802879	-0.014624	3.164674
H	2.341237	-3.385770	2.615767
H	-1.826537	-2.673241	1.956129
H	0.210846	-1.499977	2.736699

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**1TS(E-F)-fsi**

Ti	-0.975737	-0.133706	0.205595
O	0.781823	0.105061	0.358163
C	-0.830739	-1.345778	-1.797114
C	-1.745743	-2.070978	-0.971371
C	-2.921046	-1.259432	-0.790163
C	-2.718325	-0.035687	-1.473245
C	-1.407614	-0.071353	-2.073936
C	2.136598	0.241900	0.153660
C	2.978864	-0.858269	0.432360
C	4.012499	1.591702	-0.498196
C	2.630401	1.481741	-0.311181
C	0.468915	-1.859620	-2.347585
C	-1.593040	-3.513075	-0.573047
C	-4.183902	-1.679488	-0.092562
C	-3.733626	1.051933	-1.684217
C	2.430383	-2.161759	0.998422
C	2.451395	-2.125055	2.541986
C	3.154992	-3.414738	0.477265
C	1.715197	2.678465	-0.536089
C	2.090613	3.515059	-1.771677
C	1.669636	3.564077	0.727525
C	4.351004	-0.684301	0.224914
C	4.867144	0.524042	-0.236823
C	-0.832953	0.970995	-2.993812
H	1.384247	-2.242375	0.680049
H	0.703480	2.293995	-0.706599
C	-3.092435	2.828033	2.983864
H	-2.996767	2.026828	3.722460
H	-2.282040	3.543309	3.158601
H	-4.037393	3.341833	3.180305
H	-4.847721	-2.198557	-0.794665
H	-3.997973	-2.371400	0.733178
H	-4.739087	-0.825022	0.302608
H	-4.257102	0.886572	-2.633734
H	-4.490241	1.073042	-0.897794
H	-3.276881	2.043798	-1.742467
H	-1.161806	1.980836	-2.734610
H	0.259275	0.960797	-2.988895
H	-1.156950	0.780821	-4.024522
H	0.322938	-2.211170	-3.376234
H	1.243400	-1.089124	-2.371058
H	0.851976	-2.701338	-1.767413
H	-1.819573	-4.159585	-1.429294
H	-0.576313	-3.751037	-0.248601
H	-2.278634	-3.797886	0.228005
H	5.027885	-1.506753	0.429219
H	5.936062	0.634336	-0.389904
H	4.427408	2.529678	-0.851370
H	2.165550	2.897834	-2.672322
H	1.332558	4.284978	-1.947740
H	3.045783	4.032499	-1.641163
H	0.962384	4.390862	0.599280

H	1.375705	2.989581	1.612286
H	2.655212	3.994729	0.931871
H	3.480353	-2.061088	2.910091
H	1.912582	-1.255697	2.934073
H	3.190696	-3.437116	-0.616349
H	4.183010	-3.476896	0.846717
H	2.638868	-4.316743	0.821594
C	-3.060820	2.305565	1.540974
H	-3.905610	1.627898	1.365931
C	-1.747798	1.635326	1.155162
H	-0.889632	2.088149	1.659564
H	-1.564801	1.768331	0.041572
H	-3.226150	3.157711	0.867184
C	-1.327316	-1.485450	2.051486
H	-2.039032	-2.251288	1.774436
C	-1.776912	-0.310612	2.617679
H	-2.838926	-0.122644	2.724541
H	2.002747	-3.032159	2.962378
H	-0.303005	-1.806402	2.219376
H	-1.117090	0.307460	3.215348

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**1F-fsi**

Ti	-0.965985	-0.239075	0.139597
O	0.780922	0.060191	0.289483
C	-1.397430	-2.227247	-1.030835
C	-2.690469	-1.744199	-0.654702
C	-2.880233	-0.475282	-1.275791
C	-1.719396	-0.190540	-2.072722
C	-0.807388	-1.277461	-1.931261
C	2.134073	0.223173	0.126673
C	2.995799	-0.769399	0.645725
C	3.992107	1.525602	-0.654444
C	2.606336	1.381304	-0.529548
C	-0.809327	-3.554206	-0.643687
C	-3.717251	-2.496796	0.137975
C	-4.141477	0.344655	-1.235700
C	-1.547249	1.002584	-2.972449
C	2.457328	-1.977424	1.401769
C	2.455150	-1.703774	2.920977
C	3.209798	-3.281161	1.083192
C	1.663067	2.469676	-1.026132
C	2.012696	2.972830	-2.438271
C	1.609517	3.642225	-0.024103
C	4.370288	-0.569587	0.483528
C	4.867734	0.562697	-0.158399
C	0.501129	-1.440694	-2.651067
H	1.415378	-2.122198	1.095791
H	0.655828	2.038748	-1.080113
C	-2.710966	3.341570	3.175454
H	-3.107210	2.595225	3.870172
H	-1.684993	3.578582	3.476665
H	-3.309981	4.247868	3.299277
H	-4.821587	0.024667	-2.034424
H	-4.681329	0.227968	-0.292310
H	-3.950353	1.410126	-1.389280
H	-2.021178	0.809783	-3.942749
H	-2.014123	1.903821	-2.564284
H	-0.495691	1.224869	-3.164431
H	0.958062	-0.479375	-2.895447

H	1.225407	-2.007914	-2.062376
H	0.345846	-1.981448	-3.592288
H	-1.152223	-4.332919	-1.336155
H	0.282140	-3.544553	-0.683058
H	-1.107701	-3.856685	0.363040
H	-4.416376	-2.998450	-0.542100
H	-3.266275	-3.270246	0.762970
H	-4.312362	-1.842545	0.781540
H	5.064061	-1.309200	0.868906
H	5.939262	0.696002	-0.269357
H	4.393316	2.406374	-1.145257
H	2.075749	2.149726	-3.157447
H	1.251755	3.677650	-2.788905
H	2.970996	3.500391	-2.456606
H	0.893882	4.403868	-0.352786
H	1.320392	3.303118	0.976413
H	2.589820	4.121110	0.064974
H	3.475584	-1.558100	3.290356
H	1.885378	-0.801147	3.165665
H	3.250178	-3.473239	0.006132
H	4.238127	-3.263702	1.457004
H	2.710257	-4.128860	1.562914
C	-2.770633	2.874849	1.717243
H	-3.802537	2.629549	1.439472
C	-1.867344	1.656310	1.413943
H	-0.835128	1.899399	1.694951
H	-1.906642	1.605147	0.289908
H	-2.456541	3.695875	1.063654
C	-1.504042	-0.949995	1.971433
H	-2.096445	-1.839261	2.170670
C	-2.343923	0.351069	2.140994
H	-3.387533	0.169115	1.868841
H	2.017118	-2.546690	3.466296
H	-0.610955	-0.939212	2.603596
H	-2.324438	0.610201	3.204397

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**1E-bsi**

Ti	1.073516	-0.173059	0.457679
O	-0.725408	-0.106127	0.388391
C	2.079310	1.164605	-1.198681
C	3.201564	0.641107	-0.456545
C	3.236333	-0.758040	-0.646233
C	2.132830	-1.123784	-1.497346
C	1.435711	0.070456	-1.853052
C	-2.065729	-0.009500	0.049181
C	-2.624022	1.247466	-0.288636
C	-4.189647	-1.087488	-0.344563
C	-2.853407	-1.186240	0.055231
C	1.818435	2.622877	-1.457393
C	4.274444	1.439435	0.228534
C	4.331300	-1.651886	-0.136345
C	1.906912	-2.458236	-2.153744
C	-1.869877	2.568336	-0.199876
C	-2.410295	3.420678	0.968446
C	-1.930838	3.378852	-1.510018
C	-2.309091	-2.542410	0.478189
C	-2.141688	-3.483816	-0.731525
C	-3.166400	-3.203835	1.574954
C	-3.970266	1.278871	-0.672892

C	-4.750021	0.129170	-0.717023
C	0.302168	0.149983	-2.835612
H	-0.818537	2.347233	0.005778
H	-1.324330	-2.370940	0.912920
H	5.288529	-1.353857	-0.580119
H	4.452475	-1.585289	0.950179
H	4.172005	-2.699182	-0.399969
H	2.338869	-2.443560	-3.161698
H	2.379886	-3.281712	-1.616402
H	0.844911	-2.692170	-2.266402
H	-0.312962	1.036843	-2.680013
H	0.694292	0.194831	-3.859049
H	-0.355229	-0.720749	-2.774660
H	2.483975	2.974444	-2.255383
H	0.794801	2.806210	-1.785287
H	2.011016	3.247430	-0.581433
H	5.200722	1.392940	-0.357033
H	4.009113	2.493992	0.320544
H	4.512244	1.057635	1.226683
H	-4.417657	2.231969	-0.936065
H	-5.789624	0.183632	-1.023908
H	-4.802631	-1.983173	-0.356966
H	-1.504487	-3.039023	-1.504460
H	-1.701232	-4.439777	-0.426991
H	-3.108687	-3.699703	-1.196568
H	-2.693895	-4.130402	1.917655
H	-3.289821	-2.542329	2.437890
H	-4.164504	-3.464407	1.210692
H	-3.449951	3.710821	0.787377
H	-2.381277	2.875055	1.915080
H	-1.825695	4.340297	1.080479
H	-1.590817	2.798446	-2.373350
H	-2.949638	3.712583	-1.727625
H	-1.308985	4.276901	-1.432213
C	1.409097	1.795329	2.009255
C	1.787788	0.379666	2.376930
H	1.213297	0.016675	3.228480
H	2.852952	0.206000	2.533033
C	0.422487	2.454785	2.980563
H	-0.474928	1.842292	3.105046
H	0.896326	2.565298	3.960054
H	0.913163	1.836046	0.989229
C	1.057549	-2.267158	2.173140
H	0.060623	-2.034945	2.535384
C	1.274863	-2.740549	0.928022
H	0.460920	-2.955842	0.244187
H	2.259542	-3.084011	0.641022
H	1.863753	-2.203027	2.894813
H	0.116291	3.444756	2.634470
H	2.294041	2.416072	1.850768

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**1TS(E-F)-bsi**

Ti	1.081019	-0.244763	0.396124
O	-0.715363	-0.154760	0.285885
C	2.035006	1.290080	-1.110576
C	3.164674	0.791968	-0.370147
C	3.308518	-0.585197	-0.655538
C	2.263111	-0.962641	-1.567768
C	1.492401	0.204205	-1.863374

C	-2.065259	-0.038596	0.004370
C	-2.632675	1.229534	-0.272407
C	-4.210654	-1.098118	-0.323681
C	-2.860019	-1.213347	0.015095
C	1.689620	2.745500	-1.266768
C	4.130292	1.626477	0.423132
C	4.432433	-1.454470	-0.169086
C	2.136839	-2.279702	-2.279305
C	-1.873202	2.547185	-0.181652
C	-2.402604	3.402266	0.990294
C	-1.947874	3.362195	-1.488773
C	-2.288265	-2.580454	0.362763
C	-1.902291	-3.353269	-0.915828
C	-3.222540	-3.428300	1.245672
C	-3.994152	1.276267	-0.598473
C	-4.779498	0.131301	-0.640777
C	0.386376	0.279985	-2.877702
H	-0.821232	2.320588	0.015467
H	-1.383662	-2.407586	0.950435
H	5.344202	-1.239200	-0.739475
H	4.668896	-1.278242	0.885042
H	4.224320	-2.518776	-0.296882
H	2.653338	-2.227013	-3.245369
H	2.586227	-3.103565	-1.721453
H	1.095669	-2.540763	-2.484270
H	-0.348925	1.045658	-2.627888
H	0.797302	0.523282	-3.865093
H	-0.146507	-0.669063	-2.971422
H	2.430236	3.228312	-1.916115
H	0.713338	2.886039	-1.728998
H	1.696870	3.289778	-0.317542
H	4.998958	1.877804	-0.197927
H	3.690761	2.571286	0.749792
H	4.515918	1.103525	1.303667
H	-4.448203	2.237747	-0.815765
H	-5.830867	0.197418	-0.902044
H	-4.830467	-1.988117	-0.332371
H	-1.209006	-2.780711	-1.541992
H	-1.436028	-4.314271	-0.671295
H	-2.790679	-3.558654	-1.521531
H	-2.703528	-4.334985	1.572908
H	-3.542362	-2.878158	2.135634
H	-4.119566	-3.750437	0.708618
H	-3.429434	3.729613	0.800201
H	-2.406787	2.845346	1.930344
H	-1.790393	4.301570	1.120341
H	-1.605161	2.790432	-2.356469
H	-2.972831	3.681421	-1.699103
H	-1.338505	4.268659	-1.410686
C	1.223834	1.429942	2.281241
C	1.792277	0.037829	2.532553
H	1.518766	-0.281925	3.532751
H	2.875530	-0.024605	2.420704
C	0.032143	1.764262	3.181648
H	-0.794047	1.065528	3.022875
H	0.332813	1.707278	4.231998
H	0.909736	1.629853	1.220623
C	1.198546	-2.024104	2.131125
H	0.231974	-1.950162	2.620097
C	1.275540	-2.418491	0.788014



H	0.381250	-2.751666	0.273682
H	2.200674	-2.865139	0.449634
H	2.029549	-2.244614	2.790741
H	-0.335275	2.774245	2.990683
H	2.032145	2.161299	2.391311

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**1F-bsi**

Ti	1.061061	-0.045135	0.160428
O	-0.714347	0.006065	0.325437
C	2.450728	0.815844	-1.559550
C	3.186937	-0.276212	-0.991501
C	2.428826	-1.465622	-1.182127
C	1.215848	-1.108636	-1.873251
C	1.249550	0.296636	-2.131519
C	-2.070753	-0.003440	0.090624
C	-2.725271	1.210954	-0.214939
C	-4.132684	-1.226432	-0.065138
C	-2.757724	-1.237139	0.187381
C	2.899417	2.250764	-1.628112
C	4.548582	-0.197019	-0.362816
C	2.880988	-2.864073	-0.882227
C	0.182900	-2.066893	-2.395645
C	-2.009328	2.556212	-0.211826
C	-2.333282	3.331293	1.083204
C	-2.334792	3.417845	-1.446293
C	-2.047213	-2.514850	0.616724
C	-2.599523	-3.784865	-0.052147
C	-2.079548	-2.652317	2.154174
C	-4.104246	1.154200	-0.448979
C	-4.802993	-0.047478	-0.385013
C	0.237005	1.061658	-2.934190
H	-0.928790	2.363821	-0.222704
H	-0.997324	-2.424716	0.317216
H	3.349227	-3.298834	-1.773696
H	3.621326	-2.894797	-0.080300
H	2.050964	-3.516343	-0.600181
H	0.420426	-2.336894	-3.432028
H	0.154100	-2.992898	-1.817755
H	-0.819895	-1.633154	-2.391099
H	0.252761	2.129426	-2.705929
H	0.454917	0.955454	-4.004004
H	-0.778894	0.694931	-2.769512
H	3.395009	2.443085	-2.587322
H	2.061533	2.950734	-1.558008
H	3.615020	2.498974	-0.840946
H	5.320090	-0.427487	-1.107468
H	4.767193	0.800064	0.026750
H	4.666426	-0.912965	0.454751
H	-4.640289	2.069122	-0.679687
H	-5.871562	-0.065240	-0.574856
H	-4.691056	-2.154121	-0.005409
H	-2.629230	-3.691298	-1.142153
H	-1.968878	-4.643403	0.199809
H	-3.610632	-4.022918	0.291981
H	-1.524694	-3.540361	2.476273
H	-1.644144	-1.777046	2.645871
H	-3.110148	-2.753564	2.509521
H	-3.398956	3.577459	1.127485
H	-2.096242	2.745354	1.976444

H	-1.771660	4.270639	1.126044
H	-2.151476	2.879876	-2.380583
H	-3.380739	3.738682	-1.449165
H	-1.722088	4.325413	-1.446064
C	2.341794	1.690207	2.192551
C	2.382654	0.546383	3.218625
H	2.232069	0.977593	4.215279
H	3.385486	0.102963	3.221633
C	1.145145	2.639949	2.315655
H	0.182971	2.121139	2.272134
H	1.188754	3.155926	3.279578
H	2.423173	1.266704	1.154426
C	1.350921	-0.562904	2.963898
H	0.334050	-0.146877	2.967708
C	1.629737	-1.357455	1.667769
H	0.971976	-2.232566	1.591958
H	2.664323	-1.709346	1.644396
H	1.370258	-1.266312	3.807518
H	1.155269	3.405690	1.533903
H	3.268769	2.272855	2.243299

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**1TS<sub>E</sub>**

Ti	-1.122061	0.062238	0.376366
O	0.646784	0.004855	0.290869
C	-1.613026	-0.481668	-1.809835
C	-2.508322	-1.251187	-0.997795
C	-3.403614	-0.336620	-0.338177
C	-3.035357	0.982430	-0.706475
C	-1.910509	0.900587	-1.603037
C	1.992514	0.046037	0.014410
C	2.687505	-1.169487	-0.159245
C	3.990994	1.328035	-0.326362
C	2.617717	1.310478	-0.065686
C	-0.583794	-1.026399	-2.759986
C	-2.624395	-2.749911	-0.995584
C	-4.555707	-0.731895	0.539780
C	-3.730920	2.255311	-0.307923
C	2.001149	-2.523525	-0.030775
C	2.323234	-3.170283	1.332546
C	2.350445	-3.479375	-1.186450
C	1.844946	2.599546	0.185112
C	2.248255	3.747900	-0.755673
C	1.974592	3.030099	1.661800
C	4.060724	-1.084139	-0.415668
C	4.708485	0.145615	-0.499873
C	-1.269778	2.060441	-2.316245
H	0.919481	-2.353810	-0.063167
H	0.783192	2.391959	-0.007417
C	-0.555474	-0.962022	3.661918
H	0.412812	-0.512016	3.431995
H	-0.748147	-0.825479	4.734688
H	-0.512946	-2.036064	3.471734
H	-5.453728	-0.898018	-0.067605
H	-4.356303	-1.661438	1.078813
H	-4.805065	0.041681	1.271176
H	-4.404933	2.578971	-1.110121
H	-4.340331	2.129872	0.590285
H	-3.030935	3.078188	-0.132877
H	-1.281523	2.974216	-1.715683

H	-0.233332	1.849752	-2.589447
H	-1.814722	2.278554	-3.242857
H	-1.000763	-1.074309	-3.773137
H	0.310995	-0.400446	-2.802483
H	-0.272938	-2.036962	-2.487664
H	-3.268440	-3.075386	-1.821447
H	-1.654692	-3.235215	-1.127422
H	-3.059906	-3.123343	-0.066751
H	4.632450	-1.996737	-0.549947
H	5.774597	0.184074	-0.700266
H	4.509424	2.278700	-0.392168
H	2.187180	3.449059	-1.806474
H	1.587943	4.607923	-0.605056
H	3.269141	4.091683	-0.564028
H	1.367902	3.919343	1.865385
H	1.662785	2.231821	2.344282
H	3.014671	3.272498	1.902094
H	3.395313	-3.371869	1.426046
H	2.035723	-2.517580	2.162952
H	1.792321	-4.121730	1.443666
H	2.143878	-3.027184	-2.161557
H	3.405868	-3.768050	-1.172104
H	1.764393	-4.400569	-1.104181
C	-1.677398	-0.304183	2.917099
H	-1.489692	-1.325443	1.250286
C	-1.631341	0.980577	2.418427
H	-0.733288	1.582543	2.563931
H	-2.556574	1.509669	2.202826
H	-2.646320	-0.795109	2.978888

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# 1H-E

Ti	-1.139276	-0.010215	0.381539
O	0.630250	-0.006814	0.303913
C	-1.639483	-0.715495	-1.751015
C	-2.645091	-1.285515	-0.900246
C	-3.422314	-0.205009	-0.358709
C	-2.889904	1.015658	-0.857452
C	-1.778082	0.705416	-1.712275
C	1.969198	0.036964	-0.002638
C	2.674323	-1.179011	-0.133504
C	3.944622	1.321674	-0.452040
C	2.578804	1.302767	-0.154375
C	-0.666395	-1.479148	-2.604833
C	-2.972254	-2.746964	-0.780216
C	-4.619294	-0.368996	0.534135
C	-3.417920	2.400222	-0.598485
C	2.006975	-2.529794	0.092721
C	2.303508	-3.045568	1.516773
C	2.399987	-3.579829	-0.961865
C	1.800447	2.593995	0.067478
C	2.190422	3.721562	-0.903329
C	1.939714	3.062251	1.531980
C	4.038996	-1.091451	-0.430813
C	4.669889	0.139654	-0.591333
C	-0.989791	1.690564	-2.530433
H	0.924312	-2.384028	0.020047
H	0.739154	2.375171	-0.110777
C	-0.436743	-0.571841	3.835614
H	0.472268	-0.009457	3.611974

H	-0.627912	-0.510456	4.915558
H	-0.280775	-1.629149	3.603727
H	-5.513473	-0.578454	-0.065414
H	-4.497044	-1.204912	1.228515
H	-4.830989	0.531468	1.116543
H	-4.019408	2.734660	-1.452245
H	-4.063429	2.440430	0.281962
H	-2.617953	3.135859	-0.468669
H	-0.969963	2.683389	-2.074138
H	0.043092	1.366340	-2.677869
H	-1.443696	1.800224	-3.522924
H	-1.082262	-1.619106	-3.609983
H	0.284870	-0.952595	-2.713925
H	-0.457338	-2.470724	-2.197976
H	-3.657799	-3.039750	-1.584821
H	-2.081020	-3.372134	-0.862641
H	-3.455210	-2.979102	0.170852
H	4.617966	-2.002988	-0.536342
H	5.729665	0.179272	-0.822791
H	4.451071	2.273130	-0.574129
H	2.126830	3.396720	-1.946155
H	1.523744	4.579705	-0.770693
H	3.209031	4.078984	-0.724924
H	1.330486	3.953773	1.718241
H	1.637309	2.279679	2.236681
H	2.980371	3.315473	1.758116
H	3.375901	-3.219295	1.653503
H	1.985296	-2.324788	2.276762
H	1.783110	-3.991441	1.700852
H	2.218691	-3.219269	-1.979183
H	3.456087	-3.857371	-0.890191
H	1.817952	-4.495307	-0.814490
C	-1.631687	-0.035392	3.121410
H	-1.451876	-1.458756	1.128079
C	-1.679739	1.132509	2.423329
H	-0.813255	1.795679	2.401871
H	-2.637112	1.546544	2.116345
H	-2.553749	-0.603529	3.236209

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# 1G

Ti	-0.977359	-0.153220	0.300409
O	0.783810	0.122060	0.353356
C	-1.798681	-1.992962	-1.022089
C	-2.958129	-1.196791	-0.716241
C	-2.778346	0.086650	-1.305603
C	-1.497616	0.093520	-1.952335
C	-0.910583	-1.202753	-1.803392
C	2.133631	0.252998	0.136424
C	2.973310	-0.874935	0.294855
C	4.011514	1.642761	-0.427680
C	2.634019	1.529155	-0.217584
C	-1.606107	-3.453152	-0.713201
C	-4.226308	-1.683633	-0.070699
C	-3.821183	1.155237	-1.450214
C	-0.942649	1.216434	-2.780612
C	2.451877	-2.229122	0.759013
C	2.783283	-2.451857	2.250871
C	2.983057	-3.403226	-0.084998
C	1.731486	2.752586	-0.311994

C	2.050311	3.651183	-1.520278
C	1.788428	3.562175	1.001148
C	4.342662	-0.692058	0.076263
C	4.861145	0.548153	-0.286380
C	0.363607	-1.665789	-2.448684
H	1.360017	-2.221509	0.654000
H	0.703311	2.399543	-0.434266
C	-3.308933	3.173532	2.317128
H	-2.483247	3.612806	2.886265
H	-3.506043	3.823919	1.458739
H	-4.198390	3.178033	2.955427
H	-4.265971	1.096538	-2.451188
H	-4.632764	1.041943	-0.729741
H	-3.409429	2.162018	-1.341481
H	-1.315356	1.137629	-3.809831
H	-1.245319	2.195953	-2.402269
H	0.148263	1.189913	-2.826873
H	1.160237	-0.920513	-2.383290
H	0.731078	-2.589728	-1.999165
H	0.188625	-1.866933	-3.512523
H	-1.747255	-4.047784	-1.623390
H	-0.600371	-3.674818	-0.342142
H	-2.327966	-3.819758	0.019468
H	-4.947741	-1.974342	-0.843856
H	-4.065272	-2.561057	0.559142
H	-4.704215	-0.911898	0.538791
H	5.015991	-1.534564	0.196406
H	5.927607	0.663250	-0.452526
H	4.428065	2.606374	-0.701118
H	2.048379	3.086830	-2.458189
H	1.304388	4.448336	-1.600614
H	3.026578	4.136175	-1.425408
H	1.099908	4.412806	0.961190
H	1.522328	2.945429	1.865796
H	2.796773	3.952876	1.172824
H	3.865700	-2.517647	2.399200
H	2.426427	-1.627031	2.876804
H	2.341455	-3.385805	2.615699
H	2.799594	-3.253260	-1.152737
H	4.060179	-3.540891	0.047976
H	2.501248	-4.338139	0.219977
C	-2.967997	1.745282	1.858558
H	-2.836173	1.120444	2.752510
C	-1.704483	1.692425	0.984535
H	-0.833804	2.026418	1.569924
H	-1.790008	2.390361	0.142176
H	-3.828848	1.330927	1.322525
C	-1.866646	-1.645060	2.300627
C	-0.757377	-1.011203	2.733072
H	-1.826208	-2.673332	1.956677
H	-2.848688	-1.188089	2.378489
H	-0.802566	-0.014439	3.164614
H	0.211157	-1.499921	2.737064
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<b>1TSr</b>			
Ti	-0.983267	-0.379618	0.133421
O	0.763522	-0.120703	-0.182794
C	-2.613567	-0.097158	-1.611782
C	-3.393445	-0.531338	-0.488804

C	-3.283395	0.452295	0.528836
C	-2.449636	1.513800	0.037793
C	-2.033649	1.164499	-1.282770
C	2.114453	0.162213	-0.157564
C	3.037241	-0.912318	-0.227862
C	3.930850	1.739292	-0.001664
C	2.551043	1.503837	-0.045916
C	-2.609367	-0.683786	-2.997068
C	-4.288132	-1.738189	-0.445621
C	-4.045773	0.460188	1.824710
C	-2.288620	2.868962	0.670086
C	2.591154	-2.357734	-0.397428
C	3.392017	-3.354239	0.460384
C	2.631699	-2.765125	-1.885857
C	1.605801	2.695690	0.008693
C	1.812824	3.627293	-1.203449
C	1.749515	3.487891	1.324361
C	4.400825	-0.609291	-0.183584
C	4.852933	0.702183	-0.069514
C	-1.303026	2.041287	-2.261293
H	1.553585	-2.414815	-0.060833
H	0.584369	2.309977	-0.038774
C	0.303043	-1.674841	3.178440
H	1.219235	-1.519464	2.602445
H	0.511585	-1.394843	4.217202
H	0.048765	-2.737522	3.175292
H	-4.991307	1.002326	1.701614
H	-4.298403	-0.548746	2.160716
H	-3.502814	0.958047	2.632661
H	-2.977340	3.576836	0.193032
H	-2.534190	2.863410	1.734481
H	-1.280300	3.273516	0.559262
H	-0.846071	2.903484	-1.776449
H	-0.518835	1.501500	-2.799822
H	-2.007684	2.422095	-3.011083
H	-3.216827	-0.056378	-3.660555
H	-1.605499	-0.730467	-3.429113
H	-3.042068	-1.685973	-3.030188
H	-5.275672	-1.486096	-0.850958
H	-3.908086	-2.570331	-1.044101
H	-4.445743	-2.100142	0.573680
H	5.123305	-1.416422	-0.240711
H	5.917181	0.912670	-0.036459
H	4.285984	2.761480	0.084484
H	1.707156	3.087661	-2.148951
H	1.085917	4.447026	-1.190584
H	2.809864	4.077951	-1.190186
H	1.023437	4.307330	1.361844
H	1.594243	2.855465	2.204328
H	2.745541	3.931904	1.414669
H	4.429505	-3.444674	0.125603
H	3.406843	-3.060930	1.514897
H	2.947179	-4.352261	0.388849
H	2.038450	-2.086258	-2.508044
H	3.658723	-2.735937	-2.263590
H	2.253307	-3.783907	-2.024647
C	-0.827770	-0.798549	2.677621
H	-1.152636	-1.671537	1.413796
C	-0.600027	0.515533	2.258306
H	0.422893	0.864436	2.160340

H	-1.348145	1.273530	2.432253
H	-1.810573	-1.015677	3.098276
C	-0.982651	-2.471859	-0.908981
C	-1.087289	-2.884549	0.419195
H	-0.013428	-2.429767	-1.390577
H	-1.832110	-2.574500	-1.564502
H	-2.032010	-3.286099	0.779613
H	-0.205941	-3.246604	0.942268

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# **1H-T**

C	1.835537	-0.746146	-1.662416
C	2.970581	-0.098552	-1.068023
C	1.736432	-2.201834	-2.027751
H	2.088642	-2.352881	-3.055653
H	0.709597	-2.572330	-1.983780
H	2.352751	-2.835715	-1.385618
C	4.292748	-0.742123	-0.750275
H	4.975639	-0.620756	-1.600068
H	4.199903	-1.814679	-0.569100
H	4.781841	-0.289346	-1.16558
C	1.412987	1.523825	-1.587569
C	2.710828	1.302883	-1.036679
C	0.784280	2.860704	-1.849357
H	-0.306562	2.812665	-1.829106
H	1.104878	3.616316	-1.128824
H	1.074992	3.217671	-2.845513
C	3.688035	2.374470	-0.654213
H	4.170177	2.772400	-1.555647
H	3.205789	3.218722	-0.154015
H	4.480923	1.998824	-0.004209
C	0.879342	0.259221	-1.995646
Ti	0.996594	0.177799	0.332214
C	3.582921	-2.070130	2.663853
H	3.370476	-1.370679	3.474877
H	3.878937	-3.029404	3.108017
H	4.451216	-1.719421	2.095691
C	2.400307	-2.301419	1.781775
C	1.155349	-1.813239	1.976652
H	0.917238	-1.213134	2.854207
H	0.317673	-2.202504	1.408844
H	2.902249	0.448361	1.817141
H	2.553843	-2.985476	0.947433
C	1.219703	1.871208	1.507727
C	2.462515	1.370202	2.253792
H	0.326103	1.866067	2.137348
H	2.252108	1.127549	3.298965
H	3.276377	2.097429	2.219074
H	1.343098	2.861895	1.075043
C	-0.394645	0.058887	-2.763539
H	-0.217048	0.246725	-3.829512
H	-0.773900	-0.959872	-2.669490
H	-1.185712	0.737382	-2.437126
O	-0.772172	-0.039802	0.424096
C	-2.131283	-0.118271	0.216914
C	-2.715075	-1.368342	-0.097184
C	-2.905341	1.060836	0.343477
C	-4.102397	-1.410015	-0.273460
C	-4.286218	0.952212	0.150436
C	-4.885924	-0.266643	-0.153735

H	-4.577790	-2.357439	-0.506004
H	-4.904394	1.838616	0.244741
H	-5.960571	-0.325177	-0.294696
C	-2.288277	2.398177	0.731149
H	-1.221993	2.351241	0.494311
C	-1.907363	-2.656368	-0.193169
H	-0.849938	-2.378523	-0.264306
C	-2.420166	2.628386	2.251824
H	-3.473626	2.698534	2.542115
H	-1.978101	1.806059	2.824342
H	-1.927071	3.560181	2.549203
C	-2.872331	3.589202	-0.049935
H	-3.916489	3.783368	0.213367
H	-2.310490	4.499772	0.181691
H	-2.827470	3.426733	-1.131773
C	-2.236423	-3.483941	-1.450434
H	-1.562416	-4.343867	-1.524950
H	-3.256230	-3.878571	-1.421501
H	-2.139525	-2.891641	-2.365798
C	-2.093697	-3.512669	1.077868
H	-1.467390	-4.410935	1.040895
H	-1.845248	-2.953506	1.985802
H	-3.134710	-3.836939	1.173057

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# **2A**

Ti	0.914507	-0.145536	-0.654783
C	2.310509	1.264928	0.558288
C	1.709549	0.380504	1.510423
N	-0.855207	-0.046463	-0.213485
C	2.114949	-0.944857	1.182562
C	3.176642	0.490861	-0.298719
C	2.200028	2.765349	0.541341
H	1.290371	3.116291	1.033192
H	3.050218	3.209511	1.073319
H	2.213363	3.169882	-0.474903
C	-2.132125	-0.024571	-0.145293
C	3.038715	-0.871600	0.075631
C	-2.832188	1.364699	-0.054966
C	4.118590	1.051213	-1.323498
H	4.349824	0.327971	-2.108227
H	3.720090	1.949439	-1.801572
H	5.065541	1.330760	-0.845751
C	0.841434	0.778228	2.668666
H	0.084604	0.022973	2.892864
H	1.455581	0.904683	3.568383
H	0.329778	1.726108	2.489333
C	-2.870187	-1.398346	-0.156315
C	1.759153	-2.199313	1.933979
H	1.644123	-3.063872	1.273255
H	2.553969	-2.448651	2.647466
H	0.834121	-2.084871	2.502914
C	-3.453295	-1.631288	-1.577378
H	-4.266069	-0.949160	-1.823352
H	-2.678538	-1.538002	-2.345386
H	-3.849339	-2.650338	-1.627401
C	-1.872801	-2.541450	0.128714
H	-1.111773	-2.627512	-0.654196
H	-1.370230	-2.412160	1.091480
H	-2.414285	-3.491207	0.156309

C	-4.145008	1.466944	-0.863421
H	-4.551226	2.474280	-0.731378
H	-3.972485	1.323191	-1.933719
H	-4.914636	0.766873	-0.538100
C	3.754623	-2.043782	-0.534041
H	3.134127	-2.944966	-0.554048
H	4.084631	-1.836970	-1.554125
H	4.646052	-2.287912	0.056854
C	-3.994264	-1.493353	0.901207
H	-4.790053	-0.762889	0.755826
H	-4.450776	-2.485440	0.833492
H	-3.601962	-1.381715	1.916354
C	-1.885946	2.467338	-0.577012
H	-2.397461	3.432669	-0.526817
H	-0.975352	2.543176	0.021637
H	-1.603788	2.294177	-1.620786
C	-3.117662	1.650455	1.446061
H	-3.504104	2.670222	1.538980
H	-3.860432	0.975483	1.872057
H	-2.204260	1.581640	2.044188
C	1.289424	-0.071147	-2.673164
H	1.279629	0.988669	-2.975339
H	2.187339	-0.532457	-3.091734
H	0.399877	-0.547707	-3.119843

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**2B**

Ti	-0.890338	-0.050693	-0.599339
C	-2.255980	-0.856873	1.221564
C	-1.461200	0.225616	1.699485
N	0.886368	-0.014206	-0.137325
C	-1.851540	1.405390	0.988200
C	-3.145879	-0.345000	0.220220
C	-2.247732	-2.252746	1.782490
H	-1.239518	-2.589122	2.040665
H	-2.841776	-2.289713	2.703560
H	-2.680878	-2.981904	1.094231
C	2.162306	0.013873	-0.031718
C	-2.893812	1.053319	0.073169
C	2.902895	-1.315320	0.323447
C	-4.269507	-1.081402	-0.455983
H	-4.304805	-0.895459	-1.534425
H	-4.216537	-2.159897	-0.293565
H	-5.229756	-0.745239	-0.046874
C	-0.484217	0.165623	2.837695
H	0.335457	0.875836	2.708880
H	-0.987925	0.410465	3.780673
H	-0.050713	-0.830925	2.949810
C	2.900066	1.362850	-0.312171
C	-1.394192	2.807402	1.268087
H	-1.259926	3.392231	0.354297
H	-2.149249	3.323692	1.873953
H	-0.457483	2.829405	1.825506
C	3.242490	1.371393	-1.829440
H	3.959051	0.596809	-2.106836
H	2.341384	1.246349	-2.437135
H	3.685974	2.339343	-2.083388
C	1.963797	2.554272	-0.030965
H	1.058915	2.518319	-0.637960
H	1.675100	2.588994	1.023438

H	2.489688	3.485217	-0.261852
C	4.091376	-1.621716	-0.617859
H	4.544108	-2.569815	-0.311415
H	3.761003	-1.737190	-1.654906
H	4.876673	-0.867061	-0.591663
C	-3.718503	2.012659	-0.733937
H	-3.141333	2.883293	-1.052940
H	-4.139240	1.544084	-1.626994
H	-4.558453	2.380721	-0.131652
C	4.187188	1.604077	0.507199
H	4.959630	0.850856	0.353894
H	4.612317	2.563680	0.197650
H	3.977386	1.675089	1.578026
C	1.938944	-2.514968	0.238598
H	2.474459	-3.425506	0.521812
H	1.087260	-2.401838	0.913976
H	1.564978	-2.659043	-0.779153
C	3.393365	-1.230158	1.795903
H	3.780224	-2.210759	2.090629
H	4.192431	-0.505554	1.941705
H	2.571563	-0.979734	2.473954
C	-1.047954	1.170859	-2.276651
H	-0.197690	0.937913	-2.933213
H	-1.979760	1.004549	-2.831783
H	-0.992899	2.236793	-2.028325
C	-0.695919	-1.908741	-2.551693
C	-1.332326	-2.550212	-1.555120
H	-1.235729	-1.500738	-3.400660
H	0.387330	-1.823821	-2.577313
H	-2.405806	-2.700394	-1.580749
H	-0.784588	-3.016428	-0.740229

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**2TS(B-C)**

Ti	-0.902470	-0.178456	0.546456
C	-2.264252	1.334208	-0.735587
C	-1.464830	0.566071	-1.641467
N	0.892574	-0.045555	0.154230
C	-1.841736	-0.803932	-1.509424
C	-3.172046	0.438218	-0.082273
C	-2.268225	2.833209	-0.625416
H	-1.283111	3.261292	-0.826420
H	-2.964327	3.265074	-1.354814
H	-2.584519	3.175817	0.362918
C	2.168745	-0.010117	0.043627
C	-2.902528	-0.880211	-0.543877
C	2.886707	1.377550	0.012187
C	-4.286845	0.821445	0.849565
H	-4.402658	0.116390	1.678522
H	-4.151890	1.821115	1.268268
H	-5.239039	0.831377	0.305308
C	-0.499258	1.115746	-2.650573
H	0.322114	0.423445	-2.848407
H	-1.014220	1.295044	-3.602289
H	-0.070219	2.067370	-2.330020
C	2.936081	-1.372755	-0.024271
C	-1.354150	-1.945968	-2.358050
H	-1.296568	-2.885867	-1.801827
H	-2.043268	-2.110129	-3.195631
H	-0.368466	-1.746477	-2.782711

C	3.393840	-1.726172	1.418104
H	4.148783	-1.041626	1.805705
H	2.545713	-1.732698	2.110455
H	3.828169	-2.730950	1.413274
C	1.997968	-2.497772	-0.508386
H	1.180976	-2.683906	0.189763
H	1.570435	-2.270787	-1.488546
H	2.570401	-3.425386	-0.598713
C	4.136343	1.445026	0.922538
H	4.555571	2.453801	0.857479
H	3.878693	1.267071	1.970946
H	4.927224	0.751159	0.639803
C	-3.692112	-2.113977	-0.205444
H	-3.080891	-3.020343	-0.236846
H	-4.152003	-2.051189	0.784454
H	-4.504871	-2.250609	-0.929022
C	4.157505	-1.380299	-0.972677
H	4.927587	-0.656124	-0.710100
H	4.620667	-2.370599	-0.925749
H	3.860856	-1.210499	-2.011610
C	1.933682	2.491103	0.489222
H	2.441370	3.456331	0.407349
H	1.020492	2.537171	-0.106860
H	1.659759	2.354084	1.539589
C	3.285424	1.700334	-1.454761
H	3.685306	2.718684	-1.489373
H	4.051794	1.033939	-1.848064
H	2.418592	1.660756	-2.120106
C	-1.064757	-1.802313	1.925696
H	-0.308070	-2.261342	2.559602
H	-2.059432	-2.144263	2.212369
H	-0.861759	-2.193247	0.888901
C	-0.942477	0.082259	3.025862
C	-1.155123	1.232986	2.254676
H	-1.743917	-0.325773	3.631560
H	0.058695	-0.146294	3.374967
H	-2.142805	1.678381	2.249401
H	-0.322585	1.906899	2.079197

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**2C**

Ti	0.899544	-0.292707	-0.360904
C	2.812454	1.123034	-0.301861
C	1.757431	1.699487	0.489944
N	-0.905319	-0.076553	-0.083940
C	1.514637	0.838716	1.606813
C	3.195206	-0.101166	0.314143
C	3.484605	1.781939	-1.471344
H	2.785104	2.372546	-2.068223
H	4.268294	2.463696	-1.118627
H	3.960679	1.055506	-2.133594
C	-2.180678	-0.008167	-0.042025
C	2.376668	-0.289982	1.479196
C	-2.875812	1.263199	-0.626098
C	4.309057	-1.002289	-0.137097
H	4.163299	-2.036204	0.185991
H	4.428900	-0.998018	-1.223534
H	5.260401	-0.665862	0.293313
C	1.180175	3.072029	0.286934
H	0.206280	3.182971	0.767018

H	1.848903	3.822934	0.725881
H	1.068909	3.322492	-0.771339
C	-2.944514	-1.204409	0.612716
C	0.580720	1.115426	2.750047
H	0.243158	0.196269	3.234896
H	1.089134	1.717057	3.513251
H	-0.303791	1.670610	2.430778
C	-3.607362	-2.065417	-0.495292
H	-4.425656	-1.556933	-1.002871
H	-2.875761	-2.377116	-1.248392
H	-4.015324	-2.971893	-0.037088
C	-1.960165	-2.113558	1.377954
H	-1.237321	-2.588600	0.709692
H	-1.411318	-1.560245	2.145658
H	-2.521167	-2.910937	1.873688
C	-4.234257	0.996629	-1.313252
H	-4.624049	1.951186	-1.679697
H	-4.126904	0.337512	-2.179182
H	-4.990476	0.577973	-0.649380
C	2.477932	-1.433100	2.454261
H	1.517098	-1.661911	2.923359
H	2.849474	-2.347327	1.984029
H	3.177426	-1.180849	3.260398
C	-4.010565	-0.733685	1.631304
H	-4.797842	-0.123910	1.188898
H	-4.490615	-1.616535	2.064544
H	-3.557488	-0.170541	2.452768
C	-1.962240	1.918202	-1.684513
H	-2.461946	2.800545	-2.094642
H	-1.009640	2.239536	-1.262381
H	-1.759987	1.233606	-2.514538
C	-3.075298	2.272952	0.536549
H	-3.469688	3.208778	0.128139
H	-3.780176	1.917224	1.289353
H	-2.126909	2.498388	1.033052
C	1.212568	-2.904354	-1.168325
H	0.694690	-3.866415	-1.134838
H	2.281641	-3.084725	-1.304786
H	1.090667	-2.520307	-0.128206
C	0.647386	-2.003553	-2.291822
C	1.319658	-0.609802	-2.346425
H	0.804736	-2.527703	-3.242626
H	-0.440417	-1.916271	-2.183532
H	2.357311	-0.671500	-2.679722
H	0.771980	0.087619	-2.990888

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**2D**

Ti	-0.886893	0.231233	-0.331968
C	-2.868598	-1.089615	-0.489241
C	-1.836600	-1.807656	0.215592
N	0.922674	0.034220	-0.095661
C	-1.576943	-1.119675	1.443329
C	-3.218586	0.046445	0.286465
C	-3.523314	-1.535549	-1.765903
H	-2.820232	-2.032463	-2.439908
H	-4.322109	-2.254901	-1.547208
H	-3.975767	-0.701675	-2.307179
C	2.198583	-0.043291	-0.048954
C	-2.394401	0.051870	1.466884

C	2.883647	-1.205550	-0.835451
C	-4.308858	1.028690	-0.029862
H	-4.147074	1.995616	0.452513
H	-4.416090	1.195693	-1.104989
H	-5.271497	0.648835	0.333748
C	-1.290492	-3.150756	-0.185922
H	-0.323483	-3.356050	0.277296
H	-1.979546	-3.943717	0.129952
H	-1.173402	-3.243175	-1.269286
C	2.960737	1.011593	0.811874
C	-0.662600	-1.583476	2.541647
H	-0.271882	-0.749999	3.130122
H	-1.208407	-2.239626	3.230523
H	0.187443	-2.149938	2.155495
C	3.669052	2.028211	-0.123991
H	4.501907	1.595081	-0.675806
H	2.968515	2.464528	-0.843418
H	4.066030	2.845273	0.486428
C	1.968919	1.802256	1.690193
H	1.271592	2.392348	1.090130
H	1.390819	1.140837	2.341996
H	2.528093	2.496035	2.324494
C	4.257550	-0.852361	-1.447816
H	4.636980	-1.736250	-1.969475
H	4.178029	-0.049812	-2.186247
H	5.008378	-0.572034	-0.708905
C	-2.491509	1.035913	2.603038
H	-1.545387	1.140562	3.140112
H	-2.796172	2.029625	2.264918
H	-3.240222	0.698842	3.330025
C	3.993056	0.356935	1.761239
H	4.779334	-0.188900	1.240094
H	4.478495	1.146338	2.343200
H	3.509727	-0.323155	2.469176
C	1.973741	-1.658517	-1.998539
H	2.472986	-2.456348	-2.555748
H	1.018890	-2.050993	-1.643490
H	1.775731	-0.838000	-2.695827
C	3.046078	-2.401121	0.142985
H	3.426545	-3.263135	-0.413946
H	3.747553	-2.193625	0.952338
H	2.085603	-2.684403	0.583590
C	-0.295306	3.630430	-1.459941
H	-0.255684	4.421331	-0.705413
H	0.707615	3.208178	-1.571507
H	-0.577503	4.083002	-2.414473
C	-1.313585	2.545730	-1.089136
C	-1.370617	1.330109	-1.999935
H	-1.037052	2.240737	-0.015814
H	-2.311174	2.968306	-0.946497
H	-2.305246	1.206416	-2.542466
H	-0.509137	1.260266	-2.676951

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## 2E-fsi

Ti	0.876948	0.205516	-0.257434
C	2.111561	-0.478372	1.686137
C	1.331049	-1.592989	1.227076
N	-0.925304	-0.167435	-0.123161
C	1.816278	-1.968832	-0.058710

C	3.087030	-0.181307	0.689948
C	2.030615	0.153101	3.046494
H	1.010507	0.176258	3.435380
H	2.637332	-0.419696	3.758793
H	2.412631	1.176227	3.046252
C	-2.196937	-0.219246	0.010471
C	2.902428	-1.101279	-0.391672
C	-2.850488	0.229253	1.355727
C	4.194166	0.825659	0.814311
H	4.516278	1.210379	-0.157164
H	3.903939	1.679081	1.430928
H	5.071240	0.366147	1.286407
C	0.332019	-2.377518	2.027335
H	-0.522567	-2.692138	1.423124
H	0.806678	-3.284686	2.420875
H	-0.043929	-1.815321	2.883466
C	-3.027259	-0.668494	-1.244410
C	1.358571	-3.157822	-0.857394
H	1.524628	-3.026802	-1.930480
H	1.916795	-4.053438	-0.556997
H	0.297850	-3.368964	-0.704919
C	-3.241177	0.591565	-2.125329
H	-3.893566	1.325327	-1.647414
H	-2.292780	1.085789	-2.355021
H	-3.709196	0.295671	-3.069540
C	-2.224317	-1.715399	-2.047973
H	-1.260110	-1.334019	-2.380199
H	-2.045912	-2.616169	-1.452193
H	-2.797118	-2.009731	-2.932209
C	-3.899078	1.345093	1.115957
H	-4.301105	1.656913	2.084909
H	-3.444664	2.225211	0.650392
H	-4.742849	1.030095	0.502647
C	3.833375	-1.294198	-1.558246
H	3.311479	-1.549180	-2.485732
H	4.456502	-0.415888	-1.742859
H	4.516860	-2.125446	-1.346389
C	-4.402004	-1.312136	-0.955717
H	-5.092729	-0.663719	-0.417533
H	-4.870966	-1.547995	-1.916105
H	-4.304150	-2.252108	-0.406937
C	-1.791020	0.806103	2.312992
H	-2.283361	1.127488	3.235321
H	-1.040374	0.061028	2.576804
H	-1.278968	1.671160	1.887445
C	-3.507634	-0.979529	2.074814
H	-3.811017	-0.661994	3.077225
H	-4.395652	-1.354047	1.570103
H	-2.801050	-1.806856	2.192253
C	1.139867	2.206913	0.274837
C	0.050181	3.103199	-0.345447
H	-0.153348	2.828366	-1.391960
H	-0.897733	2.945031	0.180239
C	0.409365	4.598622	-0.301274
H	1.329366	4.802377	-0.860185
H	-0.389330	5.210072	-0.733956
H	0.568906	4.929719	0.729768
C	0.813393	0.335748	-2.921210
C	1.837733	1.178829	-2.699183
H	0.975681	-0.731125	-3.059562

H	-0.197642	0.699418	-3.071209
H	1.681362	2.250766	-2.632139
H	2.862073	0.829800	-2.640082
H	1.172691	2.337126	1.363421
H	2.135309	2.498787	-0.096488

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**2TS(E-F)-fsi**

Ti	-0.902470	-0.178456	0.546456
C	-2.264252	1.334208	-0.735587
C	-1.464830	0.566071	-1.641467
N	0.892574	-0.045555	0.154230
C	-1.841736	-0.803932	-1.509424
C	-3.172046	0.438218	-0.082273
C	-2.268225	2.833209	-0.625416
H	-1.283111	3.261292	-0.826420
H	-2.964327	3.265074	-1.354814
H	-2.584519	3.175817	0.362918
C	2.168745	-0.010117	0.043627
C	-2.902528	-0.880211	-0.543877
C	2.886707	1.377550	0.012187
C	-4.286845	0.821445	0.849565
H	-4.402658	0.116390	1.678522
H	-4.151890	1.821115	1.268268
H	-5.239039	0.831377	0.305308
C	-0.499258	1.115746	-2.650573
H	0.322114	0.423445	-2.848407
H	-1.014220	1.295044	-3.602289
H	-0.070219	2.067370	-2.330020
C	2.936081	-1.372755	-0.024271
C	-1.354150	-1.945968	-2.358050
H	-1.296568	-2.885867	-1.801827
H	-2.043268	-2.110129	-3.195631
H	-0.368466	-1.746477	-2.782711
C	3.393840	-1.726172	1.418104
H	4.148783	-1.041626	1.805705
H	2.545713	-1.732698	2.110455
H	3.828169	-2.730950	1.413274
C	1.997968	-2.497772	-0.508386
H	1.180976	-2.683906	0.189763
H	1.570435	-2.270787	-1.488546
H	2.570401	-3.425386	-0.598713
C	4.136343	1.445026	0.922538
H	4.555571	2.453801	0.857479
H	3.878693	1.267071	1.970946
H	4.927224	0.751159	0.639803
C	-3.692112	-2.113977	-0.205444
H	-3.080891	-3.020343	-0.236846
H	-4.152003	-2.051189	0.784454
H	-4.504871	-2.250609	-0.929022
C	4.157505	-1.380299	-0.972677
H	4.927587	-0.656124	-0.710100
H	4.620667	-2.370599	-0.925749
H	3.860856	-1.210499	-2.011610
C	1.933682	2.491103	0.489222
H	2.441370	3.456331	0.407349
H	1.020492	2.537171	-0.106860
H	1.659759	2.354084	1.539589
C	3.285424	1.700334	-1.454761
H	3.685306	2.718684	-1.489373

H	4.051794	1.033939	-1.848064
H	2.418592	1.660756	-2.120106
C	-1.064757	-1.802313	1.925696
H	-0.308070	-2.261342	2.559602
H	-2.059432	-2.144263	2.212369
H	-0.861759	-2.193247	0.888901
C	-0.942477	0.082259	3.025862
C	-1.155123	1.232986	2.254676
H	-1.743917	-0.325773	3.631560
H	0.058695	-0.146294	3.374967
H	-2.142805	1.678381	2.249401
H	-0.322585	1.906899	2.079197

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**2F-fsi**

Ti	0.841091	-0.099263	-0.211029
C	1.902885	-1.099049	1.638411
C	1.090105	-2.099235	1.032407
N	-0.984152	-0.168689	-0.009882
C	1.594078	-2.330137	-0.289567
C	2.931742	-0.735311	0.705760
C	1.761530	-0.569995	3.040383
H	0.733864	-0.643934	3.404214
H	2.391365	-1.146696	3.728729
H	2.073947	0.475021	3.124180
C	-2.257772	-0.059914	0.002180
C	2.750270	-1.505925	-0.481875
C	-2.893351	0.832916	1.116298
C	4.072967	0.205358	0.978246
H	4.432543	0.693545	0.068527
H	3.807744	0.982340	1.700035
H	4.920185	-0.348139	1.401685
C	-0.029305	-2.847064	1.696465
H	-0.779486	-3.182507	0.977883
H	0.362884	-3.737682	2.202156
H	-0.535228	-2.240087	2.450802
C	-3.080010	-0.785796	-1.108694
C	1.116562	-3.374696	-1.258265
H	1.153755	-3.024297	-2.293582
H	1.760268	-4.260800	-1.194349
H	0.096376	-3.696063	-1.045989
C	-3.301606	0.244324	-2.252274
H	-3.935258	1.080752	-1.955444
H	-2.348381	0.642430	-2.614345
H	-3.791578	-0.261929	-3.089997
C	-2.273685	-1.963269	-1.690556
H	-1.324926	-1.640002	-2.122837
H	-2.067295	-2.718310	-0.926685
H	-2.857629	-2.441596	-2.482169
C	-3.964455	1.814330	0.587634
H	-4.349269	2.397485	1.429964
H	-3.540250	2.520895	-0.132305
H	-4.817646	1.321082	0.122497
C	3.689685	-1.580395	-1.649587
H	3.164845	-1.785201	-2.585882
H	4.261085	-0.657973	-1.778200
H	4.413363	-2.390526	-1.496350
C	-4.441614	-1.352812	-0.649315
H	-5.129043	-0.596142	-0.271464
H	-4.925940	-1.823385	-1.510371



H	-4.319435	-2.124675	0.115776
C	-1.807875	1.676137	1.815677
H	-2.276476	2.297030	2.584618
H	-1.055036	1.052607	2.304878
H	-1.301811	2.344251	1.112710
C	-3.512251	-0.103075	2.191567
H	-3.831543	0.506889	3.042511
H	-4.383210	-0.650210	1.833517
H	-2.776750	-0.826262	2.558051
C	1.533313	2.551908	-0.250498
C	1.167716	3.981012	0.197244
H	0.075891	4.075865	0.245549
H	1.536647	4.131587	1.218057
C	1.745943	5.071431	-0.712744
H	1.346188	5.019655	-1.729899
H	1.500396	6.061055	-0.317526
H	2.837284	5.000341	-0.773577
C	1.324568	0.691669	-2.045222
C	0.879830	2.104250	-1.581765
H	2.364747	0.686765	-2.376097
H	0.688934	0.307524	-2.850898
H	-0.212091	2.172979	-1.492946
H	1.159492	2.834250	-2.350511
H	1.243558	1.900294	0.616795
H	2.622354	2.456404	-0.331359

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#### 2E-bsi

Ti	-0.874641	0.089056	-0.485238
C	-1.935890	-1.635054	0.867278
C	-1.271227	-0.722097	1.740420
N	0.954571	-0.076551	-0.177067
C	-1.902024	0.551514	1.611682
C	-3.011790	-0.926612	0.226891
C	-1.716540	-3.122978	0.856718
H	-0.657853	-3.387442	0.924286
H	-2.214544	-3.575703	1.722877
H	-2.127263	-3.602528	-0.033557
C	2.224444	-0.095060	-0.000541
C	-2.990812	0.415400	0.678525
C	3.016679	-1.415685	-0.277696
C	-4.097582	-1.503126	-0.638476
H	-4.212779	-0.963498	-1.584256
H	-3.935076	-2.559005	-0.862238
H	-5.058966	-1.432716	-0.115535
C	-0.203549	-1.084128	2.730723
H	0.462091	-0.245012	2.942810
H	-0.660523	-1.387799	3.680776
H	0.407036	-1.919550	2.381634
C	2.945797	1.229787	0.433002
C	-1.644588	1.746829	2.487302
H	-1.877777	2.689910	1.987284
H	-2.277107	1.691428	3.381869
H	-0.607670	1.793365	2.824886
C	3.310746	1.986579	-0.874424
H	4.075801	1.471362	-1.457289
H	2.432441	2.125664	-1.510204
H	3.701477	2.975907	-0.615793
C	1.997436	2.118171	1.262503
H	1.108673	2.410695	0.707263

H	1.683491	1.611721	2.180054
H	2.523851	3.032039	1.552585
C	4.202910	-1.203215	-1.249850
H	4.685913	-2.169518	-1.425369
H	3.861050	-0.827195	-2.219234
H	4.967667	-0.526436	-0.870633
C	-4.065091	1.426935	0.389111
H	-3.834313	2.405690	0.813119
H	-4.250170	1.553431	-0.682496
H	-5.010759	1.100079	0.838673
C	4.224258	1.060588	1.285770
H	5.012944	0.488217	0.799182
H	4.631697	2.057071	1.482397
H	4.008582	0.604345	2.255528
C	2.102484	-2.474322	-0.916902
H	2.676660	-3.389517	-1.086651
H	1.262197	-2.722025	-0.264587
H	1.717298	-2.143111	-1.883966
C	3.523091	-2.015133	1.063565
H	3.915691	-3.017746	0.867229
H	4.321048	-1.437889	1.524974
H	2.708638	-2.116313	1.787635
C	-1.467842	1.473055	-1.959929
H	-0.793382	1.533480	-2.817665
H	-2.500549	1.403620	-2.306468
C	-1.204825	2.581936	-0.959462
H	-2.139510	2.980534	-0.561416
H	-0.696656	2.169719	-0.037102
C	-0.307676	3.719063	-1.467693
H	-0.819668	4.255138	-2.271921
H	-0.074772	4.435994	-0.674781
H	0.634285	3.336586	-1.869951
C	-1.127554	-2.039419	-2.163554
H	-0.419036	-2.619740	-1.587789
H	-2.158248	-2.371134	-2.162455
C	-0.733161	-1.043436	-2.978322
H	-1.429698	-0.553166	-3.648233
H	0.311710	-0.759897	-3.070609

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#### 2TS(E-F)-bsi

Ti	-0.912111	0.107958	-0.472074
C	-1.894056	-1.813471	0.592099
C	-1.189435	-1.074636	1.593317
N	0.922404	-0.054241	-0.178608
C	-1.821915	0.196690	1.733108
C	-2.992934	-1.008853	0.147235
C	-1.658816	-3.252324	0.230406
H	-0.619455	-3.549170	0.386442
H	-2.279226	-3.904330	0.857455
H	-1.914153	-3.467366	-0.809958
C	2.195886	-0.101528	-0.027217
C	-2.946120	0.228652	0.841704
C	2.987655	-1.372481	-0.488487
C	-4.098243	-1.431283	-0.778621
H	-4.358529	-0.655405	-1.506017
H	-3.854131	-2.343635	-1.326174
H	-5.006196	-1.639689	-0.199302
C	-0.088522	-1.602342	2.464569
H	0.639416	-0.830088	2.722565

H	-0.506754	-1.986706	3.402893
H	0.446427	-2.424645	1.986602
C	2.931985	1.150192	0.573503
C	-1.515030	1.223537	2.787929
H	-1.690291	2.246466	2.442981
H	-2.159670	1.065704	3.661286
H	-0.481466	1.159607	3.131115
C	3.340862	2.062571	-0.615267
H	4.126360	1.622698	-1.230811
H	2.486134	2.282622	-1.260252
H	3.720087	3.011530	-0.222731
C	1.985200	1.943358	1.495516
H	1.103456	2.308901	0.974164
H	1.657578	1.334159	2.342636
H	2.518007	2.809931	1.897723
C	4.197546	-1.026496	-1.391998
H	4.665925	-1.962128	-1.713059
H	3.882313	-0.493570	-2.294340
H	4.967745	-0.437194	-0.896226
C	-4.015660	1.285228	0.793465
H	-3.705287	2.210999	1.281972
H	-4.333510	1.525285	-0.226488
H	-4.908192	0.930387	1.323375
C	4.187259	0.845897	1.424944
H	4.978587	0.327530	0.885641
H	4.605320	1.799699	1.761608
H	3.939768	0.269253	2.320293
C	2.086785	-2.307876	-1.313188
H	2.650580	-3.206621	-1.578955
H	1.201011	-2.617996	-0.756254
H	1.772853	-1.831949	-2.246095
C	3.467770	-2.177891	0.750182
H	3.893081	-3.124532	0.402246
H	4.236002	-1.669679	1.329215
H	2.635672	-2.416192	1.418413
C	-1.647813	1.787655	-1.832821
H	-1.398365	2.313692	-2.749119
H	-2.718578	1.571984	-1.831080
C	-1.205142	2.619161	-0.630264
H	-2.086753	3.021434	-0.123720
H	-0.716109	2.026260	0.191349
C	-0.233036	3.743867	-1.003794
H	-0.737302	4.462561	-1.656354
H	0.119578	4.281327	-0.119771
H	0.638669	3.358311	-1.538398
C	-1.078513	-1.145055	-2.291650
H	-0.203498	-1.770249	-2.189126
H	-2.023216	-1.668823	-2.379528
C	-0.968242	0.092507	-2.952812
H	-1.756399	0.402606	-3.628766
H	0.017300	0.471160	-3.212696

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# **2F-bsi**

Ti	-0.838971	-0.010952	-0.220455
C	-1.457082	-2.219564	0.196027
C	-1.239028	-1.604328	1.468950
N	0.990758	-0.080036	-0.037663
C	-2.206384	-0.568611	1.620868
C	-2.609562	-1.602461	-0.409535

C	-0.767999	-3.451349	-0.320621
H	0.243513	-3.553265	0.077043
H	-1.329959	-4.343869	-0.018111
H	-0.708104	-3.465950	-1.412018
C	2.268857	-0.062520	-0.036904
C	-3.070009	-0.586554	0.470644
C	3.029734	-1.062996	-0.964362
C	-3.278718	-2.064144	-1.671152
H	-3.905414	-1.285910	-2.111679
H	-2.557963	-2.384023	-2.428333
H	-3.927605	-2.922274	-1.457243
C	-0.224249	-2.029658	2.490764
H	0.032617	-1.217593	3.174662
H	-0.625330	-2.850748	3.097400
H	0.699040	-2.385180	2.027995
C	2.975097	0.969549	0.901188
C	-2.361585	0.319230	2.826991
H	-2.842581	1.269336	2.581484
H	-2.988663	-0.173106	3.580196
H	-1.402126	0.540604	3.302256
C	3.416895	2.193308	0.054661
H	4.217181	1.960215	-0.647362
H	2.576068	2.609696	-0.509628
H	3.784625	2.973552	0.728546
C	1.987526	1.469229	1.976761
H	1.136214	1.995801	1.541286
H	1.609079	0.643335	2.586246
H	2.504391	2.168109	2.640873
C	4.275443	-0.455178	-1.650498
H	4.728266	-1.225227	-2.282503
H	4.007141	0.382173	-2.301032
H	5.044340	-0.120496	-0.954786
C	-4.284317	0.273147	0.266371
H	-4.206386	1.229553	0.789013
H	-4.469031	0.478588	-0.790853
H	-5.173925	-0.234407	0.659442
C	4.192533	0.381265	1.653004
H	4.992220	0.039740	0.996582
H	4.613247	1.163654	2.292113
H	3.899919	-0.448244	2.303432
C	2.097225	-1.551344	-2.092635
H	2.648763	-2.237408	-2.741966
H	1.228753	-2.085669	-1.705647
H	1.746464	-0.717937	-2.709260
C	3.447457	-2.295294	-0.117634
H	3.881663	-3.048766	-0.782361
H	4.191836	-2.056746	0.642370
H	2.582916	-2.747707	0.378053
C	-1.827486	3.057162	-1.600700
H	-1.630374	4.070161	-1.970215
H	-2.858300	2.820355	-1.888742
C	-1.703113	3.075782	-0.066018
H	-2.657863	3.347995	0.396951
H	-1.527333	2.035606	0.317762
C	-0.599703	3.993939	0.463111
H	-0.843060	5.033297	0.220827
H	-0.496208	3.923004	1.549692
H	0.371457	3.770353	0.011135
C	-1.378510	0.598807	-2.119658
H	-0.769829	-0.095465	-2.725972

H	-2.414916	0.500853	-2.450543
C	-0.885225	2.052621	-2.281367
H	-0.806707	2.285424	-3.352121
H	0.137238	2.179545	-1.890870

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**2TS<sub>E</sub>**

Ti	-0.920157	0.294629	-0.333586
C	-2.905259	-0.980220	-0.493150
C	-1.841193	-1.803247	0.013529
N	0.868882	0.019409	-0.053798
C	-1.475118	-1.303270	1.300501
C	-3.171112	0.036174	0.464840
C	-3.654362	-1.228022	-1.775107
H	-2.998518	-1.560558	-2.586039
H	-4.399226	-2.019348	-1.627574
H	-4.194779	-0.341704	-2.116903
C	2.146238	-0.045991	-0.014797
C	-2.267008	-0.141361	1.566815
C	2.853021	-0.943124	-1.082211
C	-4.242969	1.084872	0.379629
H	-3.953630	2.004944	0.893660
H	-4.499467	1.335107	-0.653587
H	-5.162332	0.724166	0.857074
C	-1.336588	-3.067573	-0.626614
H	-0.335490	-3.328881	-0.277225
H	-1.998551	-3.906796	-0.379685
H	-1.305480	-2.998006	-1.718092
C	2.898012	0.763538	1.086673
C	-0.515657	-1.955482	2.252876
H	-0.147498	-1.252237	3.001903
H	-1.019415	-2.769255	2.788621
H	0.347060	-2.386043	1.739106
C	3.480798	2.049606	0.438708
H	4.268646	1.848662	-0.286540
H	2.695824	2.633001	-0.052900
H	3.909619	2.673549	1.229097
C	1.919212	1.206560	2.193311
H	1.123350	1.845976	1.807455
H	1.457337	0.345900	2.684305
H	2.472370	1.768317	2.951650
C	4.171804	-0.360930	-1.639192
H	4.580047	-1.067158	-2.368674
H	4.005995	0.585891	-2.161331
H	4.938380	-0.206960	-0.880167
C	-2.283908	0.633567	2.854519
H	-1.288887	0.705454	3.299140
H	-2.655814	1.649938	2.710970
H	-2.936989	0.139045	3.583940
C	4.029524	-0.039316	1.771306
H	4.821704	-0.351280	1.090711
H	4.491145	0.596345	2.532972
H	3.639938	-0.926125	2.279821
C	1.917628	-1.172207	-2.289132
H	2.430849	-1.791379	-3.030501
H	0.998434	-1.689903	-2.005156
H	1.653694	-0.226962	-2.775579
C	3.127576	-2.325706	-0.428343
H	3.521431	-3.004232	-1.191697
H	3.858623	-2.275371	0.378778

H	2.206953	-2.766026	-0.033023
C	-0.254544	3.682246	-1.186080
H	-0.213329	4.069099	-0.166226
H	0.718755	3.268693	-1.460297
H	-0.459585	4.530355	-1.853168
C	-1.361135	2.687667	-1.363894
C	-1.296981	1.594567	-2.196208
H	-1.104697	1.794748	0.425059
H	-2.333079	2.981326	-0.973759
H	-2.211953	1.117136	-2.542286
H	-0.388045	1.398785	-2.766232

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**2H-E**

Ti	-0.923182	0.376114	-0.186225
C	-2.886530	-0.833477	-0.716751
C	-1.826192	-1.750655	-0.409139
N	0.860181	-0.000761	-0.027704
C	-1.490713	-1.585333	0.969717
C	-3.183600	-0.090066	0.459900
C	-3.606221	-0.757224	-2.036715
H	-2.929986	-0.870705	-2.890092
H	-4.342266	-1.567039	-2.108613
H	-4.154036	0.180809	-2.157676
C	2.138295	-0.064772	-0.001636
C	-2.306539	-0.537522	1.503864
C	2.858194	-0.616815	-1.274295
C	-4.250429	0.956048	0.613506
H	-3.949230	1.741932	1.311148
H	-4.513009	1.424940	-0.338816
H	-5.168503	0.505566	1.010498
C	-1.293650	-2.813397	-1.330185
H	-0.288285	-3.130757	-1.045358
H	-1.938476	-3.700340	-1.296601
H	-1.260723	-2.482855	-2.372491
C	2.880742	0.417077	1.283558
C	-0.548950	-2.457963	1.747508
H	-0.235886	-1.984894	2.679645
H	-1.046520	-3.399530	2.009851
H	0.347999	-2.708953	1.176050
C	3.388533	1.862858	1.024581
H	4.156176	1.918177	0.252788
H	2.562260	2.523376	0.743342
H	3.822110	2.250720	1.951681
C	1.911401	0.474323	2.481929
H	1.075488	1.152687	2.304494
H	1.507472	-0.514938	2.712681
H	2.457981	0.825779	3.361984
C	4.146105	0.145732	-1.660163
H	4.570321	-0.321816	-2.554071
H	3.935836	1.190290	-1.908372
H	4.917139	0.123354	-0.890780
C	-2.368140	-0.119044	2.945403
H	-1.386450	-0.158465	3.422056
H	-2.748030	0.898411	3.054885
H	-3.035006	-0.788256	3.502863
C	4.063682	-0.488753	1.699162
H	4.853857	-0.556265	0.951510
H	4.513621	-0.071747	2.605200
H	3.726902	-1.501096	1.940624

C	1.915487	-0.551216	-2.494804
H	2.437582	-0.940153	-3.373751
H	1.013281	-1.149886	-2.351749
H	1.621929	0.480279	-2.717445
C	3.189670	-2.113233	-1.017207
H	3.588418	-2.548253	-1.939147
H	3.935273	-2.255237	-0.235078
H	2.291561	-2.676103	-0.744098
C	-0.198107	3.939032	-0.484559
H	-0.112153	3.995974	0.603842
H	0.754657	3.619415	-0.913055
H	-0.412190	4.955191	-0.841782
C	-1.328655	3.052093	-0.889223
C	-1.269365	2.084500	-1.842636
H	-1.062297	1.535562	1.010942
H	-2.291429	3.263125	-0.426081
H	-2.182491	1.633465	-2.227355
H	-0.354282	1.925883	-2.413679

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## 2G

Ti	-0.763725	0.281715	-0.008807
C	-2.224078	-1.411031	-0.964467
C	-1.679871	-1.886725	0.268389
N	1.075131	0.047327	0.153532
C	-2.196544	-1.071062	1.321816
C	-3.090230	-0.312311	-0.668345
C	-2.083602	-2.088481	-2.296659
H	-1.079237	-2.488737	-2.455291
H	-2.783621	-2.931198	-2.359756
H	-2.314479	-1.418704	-3.127682
C	2.339347	-0.127161	0.038741
C	-3.068221	-0.094968	0.738007
C	2.846879	-1.557801	-0.358227
C	-3.985620	0.380155	-1.654545
H	-4.336815	1.346962	-1.286216
H	-3.500928	0.538585	-2.622217
H	-4.875474	-0.232783	-1.844094
C	-0.990657	-3.205581	0.480786
H	-0.320750	-3.190980	1.342704
H	-1.747842	-3.976813	0.674275
H	-0.419092	-3.530498	-0.389314
C	3.302320	1.058564	0.353818
C	-2.047774	-1.405586	2.783323
H	-2.559340	-0.686750	3.426417
H	-2.502186	-2.383378	2.982692
H	-1.003266	-1.469225	3.104869
C	4.131459	1.446684	-0.899250
H	4.896071	0.718475	-1.158237
H	3.488496	1.599387	-1.772794
H	4.640028	2.394558	-0.698511
C	2.515994	2.312982	0.773626
H	1.818456	2.631927	-0.004198
H	1.960862	2.151554	1.698888
H	3.218735	3.131963	0.951307
C	4.294479	-1.689578	-0.881617
H	4.492719	-2.754567	-1.038573
H	4.429734	-1.197016	-1.846833
H	5.056637	-1.327045	-0.192215
C	-3.948664	0.875903	1.477797

H	-3.564822	1.117412	2.471369
H	-4.083064	1.814228	0.932215
H	-4.946807	0.444013	1.619836
C	4.233158	0.692091	1.538315
H	4.886292	-0.155855	1.335726
H	4.873354	1.551560	1.760976
H	3.654069	0.469013	2.440288
C	1.941228	-2.114616	-1.478969
H	2.226126	-3.147865	-1.699365
H	0.890809	-2.095803	-1.198564
H	2.058950	-1.534014	-2.400052
C	2.713203	-2.428188	0.920046
H	2.946939	-3.469622	0.677228
H	3.407320	-2.106428	1.701612
H	1.700363	-2.387159	1.324517
C	-0.320655	3.500842	-2.038698
H	-0.685929	4.439725	-1.611165
H	0.732414	3.384976	-1.767201
H	-0.375026	3.581065	-3.127985
C	-1.159023	2.301862	-1.568155
C	-0.672255	0.936093	-2.002276
H	-1.181183	2.372995	-0.438579
H	-2.208886	2.441010	-1.837926
H	-1.259234	0.474205	-2.790510
H	0.388913	0.924577	-2.261932
C	-0.877421	2.648163	1.828959
C	-0.605836	1.558134	2.564892
H	-0.091071	3.217188	1.344123
H	-1.885108	3.049242	1.766221
H	-1.379542	1.057850	3.131550
H	0.406760	1.192658	2.697594

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## 2TSr

Ti	-0.770836	0.245367	0.213709
C	-2.135697	-1.167832	-1.166279
C	-1.784340	-1.876829	0.022423
N	1.071388	0.032184	0.098172
C	-2.445249	-1.245842	1.123044
C	-3.010017	-0.094958	-0.793783
C	-1.854368	-1.634974	-2.569676
H	-0.809436	-1.915212	-2.724290
H	-2.461991	-2.520288	-2.793674
H	-2.115319	-0.881318	-3.316651
C	2.338299	-0.155135	0.055877
C	-3.197013	-0.142284	0.616521
C	2.858541	-1.530133	-0.492546
C	-3.773377	0.785705	-1.744662
H	-4.064588	1.735196	-1.287994
H	-3.219511	1.003240	-2.661536
H	-4.699810	0.283452	-2.049692
C	-1.115551	-3.222013	0.096953
H	-0.498059	-3.331414	0.992103
H	-1.881869	-4.006884	0.138946
H	-0.491369	-3.428576	-0.773094
C	3.294890	0.950266	0.603240
C	-2.521256	-1.824514	2.508153
H	-2.959359	-1.128748	3.226707
H	-3.161223	-2.715452	2.497861
H	-1.543315	-2.134506	2.887623

C	4.161402	1.540036	-0.540833
H	4.908671	0.848237	-0.922532
H	3.541262	1.873853	-1.380161
H	4.693135	2.416985	-0.158695
C	2.496023	2.117504	1.210441
H	1.824042	2.571168	0.480150
H	1.908162	1.799079	2.073548
H	3.193767	2.887478	1.552324
C	4.312935	-1.583929	-1.011818
H	4.522979	-2.617235	-1.305498
H	4.452600	-0.966299	-1.902250
H	5.065405	-1.308164	-0.273746
C	-4.126565	0.726578	1.415989
H	-3.762232	0.896911	2.433148
H	-4.284960	1.701495	0.947835
H	-5.110161	0.249951	1.508113
C	4.193534	0.389508	1.735184
H	4.860672	-0.408977	1.413362
H	4.819341	1.201218	2.119478
H	3.590449	0.016288	2.568977
C	1.970249	-1.968352	-1.675871
H	2.282173	-2.958493	-2.021547
H	0.922043	-2.014544	-1.391793
H	2.068534	-1.275735	-2.518845
C	2.709832	-2.548171	0.670093
H	2.965625	-3.549694	0.309677
H	3.376419	-2.316163	1.504668
H	1.684502	-2.571280	1.046636
C	-0.134420	3.864961	-1.255107
H	-0.498094	4.280945	-0.310654
H	0.945598	3.716926	-1.192176
H	-0.325117	4.625982	-2.022445
C	-0.859467	2.611829	-1.648501
C	-0.272459	1.494591	-2.141910
H	-1.175904	2.080869	0.358473
H	-1.943993	2.688989	-1.690937
H	-0.849016	0.725947	-2.638882
H	0.807068	1.416443	-2.207136
C	-0.989706	2.161785	1.794185
C	-0.743558	0.832089	2.307016
H	-0.167117	2.872317	1.772036
H	-1.949564	2.620634	2.023419
H	-1.506364	0.418356	2.953148
H	0.268602	0.614340	2.638390

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## 2H-T

Ti	0.767007	0.146595	-0.256497
C	2.077139	-1.104107	1.278349
C	1.758164	-1.937461	0.161286
N	-1.072006	-0.030519	-0.084582
C	2.453362	-1.426618	-0.982281
C	2.968120	-0.080472	0.818672
C	1.727599	-1.394644	2.713342
H	0.686464	-1.700301	2.841299
H	2.353814	-2.212351	3.091104
H	1.907982	-0.535956	3.364615
C	-2.344883	-0.171051	-0.045465
C	3.197180	-0.279910	-0.573431
C	-2.915967	-1.521501	0.508270

C	3.710114	0.894198	1.691754
H	3.999104	1.799783	1.152240
H	3.141253	1.188419	2.577074
H	4.636753	0.430996	2.052930
C	1.085377	-3.282189	0.206760
H	0.435165	-3.456319	-0.654550
H	1.849789	-4.069622	0.195357
H	0.494264	-3.421720	1.112259
C	-3.249562	0.967595	-0.611302
C	2.549785	-2.133988	-2.303399
H	2.963664	-1.496245	-3.086938
H	3.217432	-2.999510	-2.208819
H	1.581171	-2.508375	-2.646070
C	-4.125744	1.588019	0.508388
H	-4.908244	0.923439	0.867426
H	-3.519331	1.899523	1.366001
H	-4.614628	2.483215	0.111725
C	-2.395064	2.103421	-1.203258
H	-1.720197	2.536383	-0.462449
H	-1.801531	1.758602	-2.051924
H	-3.057058	2.896958	-1.562118
C	-4.385614	-1.530679	0.984086
H	-4.630760	-2.554178	1.284678
H	-4.535458	-0.897722	1.861835
H	-5.108293	-1.246088	0.219943
C	4.150268	0.498097	-1.435704
H	3.806272	0.567845	-2.471570
H	4.309217	1.513645	-1.064163
H	5.130659	0.006753	-1.458808
C	-4.136364	0.430172	-1.764353
H	-4.836241	-0.345395	-1.456141
H	-4.725947	1.259826	-2.167214
H	-3.524166	0.034242	-2.580781
C	-2.071405	-1.956934	1.724651
H	-2.419208	-2.930312	2.083389
H	-1.018420	-2.038524	1.467829
H	-2.171909	-1.242185	2.548549
C	-2.757601	-2.562591	-0.632387
H	-3.051991	-3.550565	-0.264396
H	-3.390827	-2.326333	-1.491667
H	-1.721676	-2.618711	-0.975539
C	0.333428	4.229726	0.942049
H	0.765806	4.472428	-0.035702
H	-0.753521	4.178901	0.847472
H	0.580310	5.070935	1.601490
C	0.916802	2.972717	1.509635
C	0.215321	1.908400	1.946729
H	1.199190	2.133692	-0.816371
H	1.998978	2.966754	1.627029
H	0.693656	1.100141	2.489427
H	-0.868602	1.895628	1.908914
C	1.082447	1.984707	-1.931707
C	0.769134	0.552695	-2.310456
H	0.294493	2.695753	-2.186223
H	2.039759	2.327879	-2.327762
H	1.493978	0.109555	-2.984781
H	-0.243500	0.402059	-2.684932

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## 3A

C	-1.213976	-1.073358	-1.122777
C	-2.384879	-0.266613	-0.982455
C	-0.660477	-1.545750	-2.445077
H	-0.433615	-2.613807	-2.399824
H	0.263900	-1.034609	-2.740303
H	-1.386514	-1.398023	-3.246556
C	-3.281367	0.212224	-2.092875
H	-4.073238	-0.522900	-2.282051
H	-2.745027	0.354171	-3.034841
H	-3.775788	1.154303	-1.841453
C	2.063260	-2.663062	-0.751129
H	1.970084	-2.407377	-1.807812
H	1.632601	-3.661448	-0.606566
H	3.130216	-2.738287	-0.517294
C	3.503405	0.547034	-1.156345
H	3.982422	-0.259329	-0.593805
H	4.280607	1.268614	-1.427008
H	3.091230	0.127364	-2.078919
C	-1.555224	-0.684553	1.130909
C	-2.606429	-0.044071	0.412279
C	-1.487958	-0.767212	2.627814
H	-2.071757	-1.633746	2.962712
H	-0.472189	-0.901350	2.995700
H	-1.912957	0.115438	3.110144
C	-3.791763	0.652215	1.010287
H	-4.594699	-0.072348	1.194007
H	-3.555029	1.120853	1.967657
H	-4.196208	1.421792	0.348360
C	1.841070	-1.819046	2.161401
H	1.642115	-1.014741	2.873540
H	1.397480	-2.742796	2.549645
H	2.925861	-1.972113	2.133355
C	3.021257	1.786062	0.987033
H	3.457491	0.975870	1.578123
H	3.815052	2.506671	0.766077
H	2.265567	2.283719	1.600903
Si	1.226919	-1.453993	0.421836
N	1.323765	0.269699	-0.012954
C	-0.660436	-1.314226	0.186049
C	2.413682	1.234788	-0.314170
C	1.787823	2.377958	-1.151984
H	1.368389	1.994385	-2.095715
H	1.023449	2.943702	-0.596193
H	2.535042	3.125183	-1.435265
Ti	-0.437278	0.896581	-0.224989
C	-0.888683	2.390349	1.137393
H	-1.452850	2.189717	2.048403
H	-0.000417	2.974276	1.402866
H	-1.530160	3.023611	0.488732

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### 3B

C	1.466081	-0.839408	1.258228
C	2.580776	-0.356159	0.506439
C	1.350420	-0.777421	2.759234
H	1.473986	-1.784233	3.173567
H	0.383141	-0.409687	3.106190
H	2.131188	-0.155031	3.201655
C	3.808340	0.316326	1.054266
H	4.576371	-0.430964	1.288835

H	3.609803	0.867627	1.976674
H	4.251143	1.009823	0.334200
C	-1.922584	-1.638681	2.364033
H	-1.741155	-0.762046	2.990707
H	-1.431458	-2.498537	2.833359
H	-2.999463	-1.833877	2.377859
C	-3.772228	0.659982	0.504486
H	-4.047294	-0.395917	0.425210
H	-4.656655	1.244483	0.233408
H	-3.529255	0.880477	1.548010
C	1.149021	-1.420511	-0.954154
C	2.393586	-0.731447	-0.859738
C	0.603606	-2.028441	-2.219219
H	0.496486	-3.111133	-2.097384
H	-0.376804	-1.631147	-2.493994
H	1.275209	-1.854631	-3.061311
C	3.393742	-0.536656	-1.960835
H	4.052213	-1.411154	-2.029419
H	2.918131	-0.407360	-2.935030
H	4.030687	0.333466	-1.784093
C	-2.256151	-2.712010	-0.454551
H	-2.092659	-2.633428	-1.530063
H	-1.934623	-3.712704	-0.140242
H	-3.333851	-2.651021	-0.271320
C	-2.966155	0.652352	-1.885057
H	-3.171750	-0.416609	-1.984160
H	-3.863254	1.195461	-2.198726
H	-2.154184	0.912426	-2.570429
Si	-1.334509	-1.440528	0.584162
N	-1.373542	0.255420	-0.023242
C	0.547573	-1.480024	0.360926
C	-2.601819	1.017843	-0.431943
C	-2.353168	2.534460	-0.330445
H	-2.134009	2.830714	0.700265
H	-1.535969	2.861731	-0.980730
H	-3.244940	3.084117	-0.645157
Ti	0.458229	0.686696	-0.276295
C	0.803625	1.518720	-2.145776
H	0.681383	0.831867	-2.989455
H	0.092514	2.345799	-2.279964
H	1.821874	1.928595	-2.195831
C	1.219320	2.982152	0.717245
C	0.691429	2.498351	1.856356
H	-0.348211	2.667329	2.119376
H	1.296028	1.959942	2.578463
H	2.277633	2.871735	0.492235
H	0.632135	3.589451	0.033246

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### 3TS(B-C)

C	-1.380755	-1.170597	-1.080943
C	-2.561094	-0.592305	-0.522525
C	-1.202677	-1.466783	-2.544109
H	-1.602985	-2.463854	-2.765059
H	-0.158298	-1.462119	-2.851508
H	-1.743219	-0.758155	-3.176206
C	-3.778473	-0.158443	-1.285131
H	-4.467372	-1.003709	-1.405857
H	-3.538001	0.195853	-2.290670
H	-4.330716	0.631087	-0.768621

C	2.072707	-2.239528	-1.745165
H	1.949300	-1.577227	-2.605583
H	1.578544	-3.190546	-1.973534
H	3.142154	-2.446505	-1.640196
C	3.835490	0.457041	-0.628552
H	4.101288	-0.492542	-0.154627
H	4.714708	1.105192	-0.564456
H	3.628028	0.276601	-1.686686
C	-1.164109	-1.174094	1.220150
C	-2.427944	-0.585065	0.892608
C	-0.670213	-1.405574	2.628114
H	-0.479485	-2.470461	2.791269
H	0.259101	-0.874067	2.854674
H	-1.414482	-1.091287	3.362354
C	-3.485185	-0.139026	1.864225
H	-4.152013	-0.974716	2.108474
H	-3.065250	0.220383	2.807234
H	-4.109197	0.657902	1.451600
C	2.262177	-2.420992	1.280759
H	2.095967	-1.984372	2.266800
H	1.913860	-3.460615	1.311625
H	3.342628	-2.452648	1.105918
C	2.967860	1.332787	1.563375
H	3.144225	0.375195	2.060633
H	3.869427	1.942949	1.677676
H	2.152030	1.842133	2.087823
Si	1.397111	-1.527408	-0.135403
N	1.410983	0.270191	-0.041443
C	-0.496391	-1.545022	-0.002367
C	2.638759	1.130525	0.070288
C	2.407747	2.495380	-0.604323
H	2.222146	2.376901	-1.675652
H	1.567321	3.042774	-0.163772
H	3.292934	3.127309	-0.487303
Ti	-0.434516	0.683079	0.044101
C	-0.947084	2.404288	1.265316
H	-1.035089	1.445734	1.836694
H	0.045805	2.840054	1.403718
H	-1.697658	3.055144	1.708361
C	-1.462987	2.814011	-0.686493
C	-0.929514	1.897120	-1.658457
H	-0.002259	2.191458	-2.143798
H	-1.645442	1.419086	-2.317112
H	-2.539220	2.836707	-0.544143
H	-0.985740	3.782644	-0.565163

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3C

C	-1.204770	-1.299637	-1.100541
C	-2.445479	-0.764646	-0.649844
C	-0.877638	-1.578696	-2.540955
H	-1.096592	-2.628310	-2.771999
H	0.172770	-1.408066	-2.773449
H	-1.472977	-0.962259	-3.217195
C	-3.630903	-0.419067	-1.499929
H	-4.312045	-1.276968	-1.559866
H	-3.346321	-0.163477	-2.522467
H	-4.205741	0.415249	-1.088345
C	2.297718	-2.331673	-1.466098
H	2.227122	-1.761559	-2.395009

H	1.819787	-3.304281	-1.629652
H	3.358740	-2.517869	-1.273712
C	3.804440	0.598876	-0.741703
H	4.130016	-0.308525	-0.224090
H	4.650023	1.293138	-0.735187
H	3.583141	0.348619	-1.782638
C	-1.154886	-1.232350	1.210916
C	-2.411059	-0.707652	0.776134
C	-0.736143	-1.363950	2.655309
H	-0.342169	-2.364925	2.847851
H	0.043546	-0.651428	2.949834
H	-1.585429	-1.211099	3.323899
C	-3.557052	-0.276197	1.649226
H	-4.248892	-1.113304	1.802739
H	-3.230704	0.056264	2.637424
H	-4.135877	0.533238	1.195742
C	2.351537	-2.158887	1.566361
H	2.086094	-1.642178	2.490220
H	2.096322	-3.218806	1.685679
H	3.439790	-2.105466	1.454475
C	2.945841	1.563464	1.417771
H	3.194855	0.653347	1.969797
H	3.809181	2.234704	1.466840
H	2.111392	2.054411	1.931324
Si	1.511500	-1.481090	0.022375
N	1.413221	0.312647	-0.063113
C	-0.382840	-1.599075	0.054144
C	2.590443	1.248540	-0.050634
C	2.266729	2.555463	-0.794443
H	2.007479	2.360459	-1.838990
H	1.443773	3.108422	-0.328238
H	3.136874	3.218116	-0.781324
Ti	-0.463213	0.624350	-0.010579
C	-1.209793	2.611735	1.153378
H	-1.323046	1.633758	1.679913
H	-0.157870	2.923729	1.182408
H	-1.744950	3.278658	1.833401
C	-1.844614	2.721418	-0.278644
C	-1.154895	1.922941	-1.425239
H	-0.303476	2.476756	-1.831622
H	-1.849360	1.678173	-2.225583
H	-2.900179	2.450143	-0.203320
H	-1.797969	3.788722	-0.518853

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3D

C	-1.088903	-1.649085	-0.893513
C	-2.379821	-1.035788	-0.749520
C	-0.611095	-2.247051	-2.192482
H	-1.211092	-3.134949	-2.425182
H	0.429782	-2.558831	-2.149311
H	-0.728672	-1.560919	-3.039156
C	-3.432100	-0.946911	-1.815974
H	-4.055486	-1.849644	-1.806530
H	-2.998132	-0.865441	-2.815501
H	-4.097520	-0.093378	-1.665450
C	2.419160	-2.748491	-0.508241
H	2.454725	-2.532330	-1.578123
H	1.958592	-3.734290	-0.375601
H	3.452084	-2.822209	-0.154379

C	3.781616	0.289100	-0.954599
H	4.143628	-0.410071	-0.194827
H	4.606408	0.969284	-1.187101
H	3.544517	-0.272875	-1.862206
C	-1.310167	-0.978453	1.299265
C	-2.514948	-0.625305	0.600365
C	-1.092868	-0.759420	2.779645
H	-0.630056	-1.640517	3.228982
H	-0.452170	0.098130	3.011459
H	-2.046179	-0.595182	3.286224
C	-3.737197	0.002757	1.202656
H	-4.433688	-0.776211	1.537033
H	-3.502959	0.619796	2.073188
H	-4.274792	0.622132	0.479823
C	2.145294	-1.542804	2.271346
H	1.760575	-0.758608	2.925922
H	1.910873	-2.512843	2.725355
H	3.237233	-1.456341	2.252049
C	2.942694	1.850576	0.833823
H	3.236306	1.157992	1.627179
H	3.783703	2.526104	0.648289
H	2.100168	2.448057	1.196803
Si	1.475650	-1.476348	0.514921
N	1.405638	0.199286	-0.164980
C	-0.418784	-1.648103	0.387389
C	2.568051	1.095405	-0.458090
C	2.166863	2.103261	-1.550410
H	1.860083	1.589937	-2.468807
H	1.350197	2.752502	-1.218301
H	3.008268	2.755819	-1.800865
Ti	-0.461751	0.449904	-0.341070
C	-0.848947	4.014776	0.567736
H	0.146134	4.108734	0.124722
H	-1.499816	4.750543	0.087863
H	-0.776206	4.263402	1.630333
C	-1.435430	2.611073	0.360726
C	-1.498162	2.085287	-1.061739
H	-0.857995	2.637196	-1.760407
H	-2.503834	1.975439	-1.463491
H	-0.778214	1.928648	1.018871
H	-2.408056	2.521966	0.850352

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### 3E-fsi

C	0.573069	-1.071328	1.581499
C	1.924645	-1.155933	1.136264
C	0.157985	-0.508666	2.915637
H	-0.215603	-1.312862	3.559100
H	-0.632008	0.241270	2.836288
H	1.002626	-0.043280	3.426392
C	3.141123	-0.765083	1.922893
H	3.359263	-1.527240	2.681049
H	3.010468	0.184529	2.448006
H	4.026076	-0.677713	1.289354
C	-3.078654	-1.176335	1.940608
H	-2.692371	-0.573231	2.763243
H	-3.096092	-2.220841	2.276153
H	-4.116933	-0.880734	1.761606
C	-2.371358	2.404916	1.184397
H	-2.785058	1.720924	1.929987

H	-2.996065	3.303680	1.174654
H	-1.366062	2.696506	1.503196
C	0.575939	-2.165563	-0.450622
C	1.929926	-1.827278	-0.120418
C	0.150888	-2.963993	-1.656787
H	-0.363839	-3.875598	-1.338098
H	-0.539101	-2.424958	-2.312440
H	1.009020	-3.272876	-2.256998
C	3.173177	-2.250706	-0.850534
H	3.939257	-1.470058	-0.846622
H	3.611014	-3.128232	-0.359303
H	2.981393	-2.529289	-1.888185
C	-3.024732	-2.028848	-0.976789
H	-2.667408	-1.835461	-1.991263
H	-2.976503	-3.109262	-0.800324
H	-4.080251	-1.742084	-0.939565
C	-3.777162	1.378388	-0.641042
H	-4.259685	0.717924	0.084580
H	-4.393143	2.279872	-0.712219
H	-3.783273	0.890178	-1.619956
Si	-2.064635	-1.103251	0.353704
N	-1.479573	0.525015	-0.170973
C	-0.283673	-1.698832	0.593683
C	-2.344798	1.758488	-0.215176
C	-1.812268	2.776069	-1.240810
H	-0.799118	3.113318	-1.005374
H	-1.824712	2.359954	-2.252184
H	-2.449795	3.664905	-1.244199
Ti	0.398504	0.248250	-0.301419
C	1.469093	1.856889	0.473239
C	1.605025	-0.007988	-2.687338
C	0.594936	0.882004	-2.760909
H	2.594319	0.282008	-2.344382
H	1.488049	-1.022796	-3.048832
H	-0.368548	0.613985	-3.182945
H	0.744526	1.928460	-2.504436
H	1.525904	1.798362	1.567760
H	0.769240	2.681694	0.251326
C	2.853282	2.189575	-0.116424
H	3.539037	1.346234	0.031385
H	2.777399	2.335991	-1.203094
C	3.478563	3.452643	0.497853
H	3.621175	3.333244	1.576784
H	4.454403	3.665850	0.049548
H	2.837173	4.326023	0.340830

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### 3TS(E-F)-fsi

C	0.674899	-1.325264	1.499248
C	1.954692	-1.519869	0.888090
C	0.480168	-0.842923	2.914813
H	0.221562	-1.686352	3.565041
H	-0.319725	-0.106839	3.009362
H	1.392357	-0.393578	3.312962
C	3.287534	-1.291724	1.540415
H	3.569696	-2.165027	2.140732
H	3.280865	-0.431110	2.215167
H	4.083487	-1.138112	0.807051
C	-2.864736	-0.923319	2.286199
H	-2.453186	-0.159205	2.947984



H	-2.741513	-1.895369	2.778369
H	-3.940389	-0.740919	2.197870
C	-3.058224	2.169707	0.850407
H	-3.821549	1.413168	1.050281
H	-3.577292	3.112541	0.651775
H	-2.454635	2.298711	1.753875
C	0.335328	-2.214466	-0.604527
C	1.745755	-2.056594	-0.407869
C	-0.276601	-2.905783	-1.793378
H	-0.499213	-3.947668	-1.534745
H	-1.209623	-2.448078	-2.121471
H	0.404323	-2.930254	-2.647195
C	2.823329	-2.480890	-1.363850
H	3.751697	-1.925334	-1.210040
H	3.057254	-3.543495	-1.223781
H	2.528561	-2.360124	-2.409836
C	-3.317246	-1.834459	-0.566139
H	-3.112826	-1.706263	-1.630994
H	-3.349338	-2.909207	-0.352423
H	-4.320456	-1.440276	-0.371715
C	-3.070302	1.560255	-1.593735
H	-3.804184	0.770413	-1.418342
H	-3.618700	2.475995	-1.836003
H	-2.474686	1.283194	-2.469025
Si	-2.072322	-0.996379	0.575105
N	-1.397108	0.549317	-0.061573
C	-0.346703	-1.773640	0.583218
C	-2.178439	1.790786	-0.356622
C	-1.216865	2.956931	-0.638600
H	-0.593714	3.170674	0.235701
H	-0.571862	2.749604	-1.499222
H	-1.776111	3.867368	-0.872362
Ti	0.450461	0.143660	-0.277615
C	1.981386	1.592160	0.070062
C	1.705345	1.171032	-2.191020
C	0.715499	0.259841	-2.537678
H	1.521223	2.235190	-2.270975
H	2.749564	0.875451	-2.195205
H	0.990637	-0.732490	-2.870665
H	-0.250812	0.625751	-2.872452
H	2.854319	0.984828	0.321453
H	1.252234	1.494373	0.941361
C	2.386217	3.055149	-0.050174
H	3.163421	3.133027	-0.819695
H	1.542673	3.664740	-0.390251
C	2.935489	3.629974	1.266642
H	3.808911	3.068675	1.613567
H	3.239492	4.671443	1.127913
H	2.180539	3.606701	2.059991

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### 3F-fsi

C	0.578478	-1.421813	1.450474
C	1.739121	-1.733075	0.678315
C	0.607518	-0.898457	2.866116
H	-0.121123	-1.427283	3.484565
H	0.374339	0.170733	2.941262
H	1.591144	-1.047847	3.315731
C	3.167773	-1.686010	1.146175
H	3.470671	-2.666812	1.532688

H	3.321034	-0.961892	1.949703
H	3.857481	-1.438999	0.334366
C	-2.667552	-0.300416	2.593650
H	-1.981458	0.378533	3.104428
H	-2.712998	-1.232889	3.168509
H	-3.665348	0.147539	2.627968
C	-3.213210	2.342244	0.438625
H	-3.985552	1.576751	0.558961
H	-3.712857	3.250417	0.087959
H	-2.775423	2.553778	1.418457
C	-0.114937	-2.180494	-0.621406
C	1.308607	-2.217961	-0.594252
C	-0.962849	-2.657843	-1.770208
H	-1.538731	-3.539885	-1.470024
H	-1.673516	-1.902752	-2.112436
H	-0.348816	-2.940432	-2.626653
C	2.212180	-2.766066	-1.658236
H	3.181946	-2.261333	-1.674141
H	2.408771	-3.829284	-1.472886
H	1.775349	-2.687918	-2.655730
C	-3.681435	-1.455877	-0.022617
H	-3.578627	-1.612545	-1.097288
H	-3.870629	-2.431394	0.441813
H	-4.574230	-0.844190	0.144672
C	-2.798135	1.585870	-1.929087
H	-3.528670	0.779474	-1.827284
H	-3.321946	2.465161	-2.317539
H	-2.052852	1.279847	-2.669371
Si	-2.184858	-0.673041	0.810724
N	-1.417045	0.693010	-0.069768
C	-0.588328	-1.683244	0.653453
C	-2.135339	1.911481	-0.575693
C	-1.156372	3.086373	-0.753395
H	-0.668769	3.337805	0.195216
H	-0.392371	2.875529	-1.508820
H	-1.693704	3.977071	-1.091766
Ti	0.368715	0.082075	-0.323487
C	2.226605	1.667878	-0.225561
C	2.322373	1.014356	-1.647979
C	1.027423	0.375396	-2.230944
H	2.635925	1.832140	-2.306998
H	3.133646	0.281712	-1.631864
H	1.242650	-0.399604	-2.963027
H	0.382050	1.135824	-2.686336
H	2.064035	0.932373	0.604755
H	1.413368	2.407569	-0.189931
C	3.533959	2.377525	0.181891
H	4.355112	1.652929	0.134069
H	3.746693	3.141008	-0.575179
C	3.470571	3.016976	1.570450
H	3.290832	2.269695	2.351808
H	4.414104	3.516311	1.805589
H	2.675351	3.767637	1.631064

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### 3E-bsi

C	1.462208	-1.771080	0.106421
C	2.604027	-0.913817	-0.000685
C	1.416122	-2.970893	1.014243
H	2.031192	-3.766174	0.575479

H	0.412360	-3.376439	1.128626
H	1.827735	-2.771305	2.007888
C	3.875272	-1.003659	0.793259
H	4.660963	-1.480801	0.194002
H	3.761353	-1.604006	1.698638
H	4.249924	-0.016376	1.080379
C	-1.976574	-3.033205	0.244678
H	-1.746304	-2.979526	1.311711
H	-1.552290	-3.962485	-0.151853
H	-3.064170	-3.114276	0.152307
C	-3.826200	-0.159913	0.883382
H	-4.116201	-0.858174	0.092650
H	-4.715894	0.421763	1.143252
H	-3.531107	-0.736925	1.764736
C	1.112468	-0.328568	-1.659610
C	2.400553	-0.040355	-1.094443
C	0.578791	0.301593	-2.922111
H	0.709004	-0.387209	-3.764294
H	-0.482474	0.545537	-2.860089
H	1.111515	1.221873	-3.168894
C	3.440937	0.909037	-1.613075
H	4.289554	0.345430	-2.019325
H	3.067081	1.546096	-2.415987
H	3.838478	1.553316	-0.821596
C	-2.282891	-1.623625	-2.399906
H	-2.104622	-0.787335	-3.076591
H	-1.970873	-2.540020	-2.916281
H	-3.362685	-1.702060	-2.235446
C	-3.123529	1.519319	-0.859828
H	-3.330167	0.819427	-1.672354
H	-4.034751	2.097610	-0.677543
H	-2.346424	2.214220	-1.193170
Si	-1.367512	-1.552557	-0.754461
N	-1.444299	0.009621	0.157198
C	0.519599	-1.424803	-0.923818
C	-2.695976	0.783597	0.428636
C	-2.451664	1.825697	1.535600
H	-2.264517	1.353799	2.503819
H	-1.607404	2.478246	1.295304
H	-3.330113	2.466839	1.653099
Ti	0.409548	0.365965	0.425049
C	0.152965	4.163209	-0.297282
H	-0.674250	4.199926	0.416639
H	0.902792	4.890391	0.026278
H	-0.226363	4.475065	-1.275094
C	0.793300	2.765299	-0.367473
C	1.278330	2.193871	0.958457
H	0.741182	2.629248	1.808870
H	2.353471	2.272490	1.120343
H	0.010928	2.095241	-0.834121
H	1.600533	2.765248	-1.101209
C	1.184315	0.078917	3.008068
C	-0.002264	-0.550848	2.884655
H	-0.927050	-0.071503	3.182807
H	-0.070081	-1.594701	2.602636
H	1.252866	1.082269	3.411289
H	2.123273	-0.426131	2.809087

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3 TS(E-F)-bsi

C	-1.281641	-1.842319	-0.476271
C	-2.493116	-1.115926	-0.257811
C	-1.070362	-2.807091	-1.611527
H	-1.194838	-3.832322	-1.244206
H	-0.076991	-2.740161	-2.054864
H	-1.804074	-2.662351	-2.407180
C	-3.702432	-1.115123	-1.147781
H	-4.338011	-1.982130	-0.928594
H	-3.442403	-1.174190	-2.208159
H	-4.316734	-0.222991	-1.001203
C	2.177527	-2.928232	-0.629790
H	2.033300	-2.703788	-1.689170
H	1.713104	-3.898877	-0.422714
H	3.252786	-3.042261	-0.461157
C	3.773095	0.056110	-1.041948
H	4.138675	-0.703237	-0.344366
H	4.621515	0.700427	-1.292392
C	3.445839	-0.442994	-1.958412
C	-1.120290	-0.765544	1.563546
C	-2.402133	-0.466923	1.001513
C	-0.676341	-0.356977	2.945096
H	-0.761374	-1.207819	3.630268
H	0.360807	-0.020020	2.975547
H	-1.296300	0.445436	3.350196
C	-3.524458	0.284539	1.659564
H	-4.273303	-0.420624	2.040002
H	-3.189521	0.880294	2.510701
H	-4.047015	0.949898	0.964656
C	2.381340	-1.822011	2.174168
H	2.188296	-1.045392	2.915697
H	2.092422	-2.784065	2.614914
H	3.462821	-1.861682	2.004581
C	3.127138	1.528252	0.894448
H	3.406725	0.761220	1.620601
H	4.006170	2.155427	0.714185
H	2.351917	2.156746	1.343606
Si	1.477909	-1.616147	0.532221
N	1.441059	0.046205	-0.149542
C	-0.410692	-1.629369	0.651967
C	2.639046	0.898486	-0.426961
C	2.276233	2.017980	-1.419900
H	2.026822	1.613382	-2.404995
H	1.432793	2.616950	-1.059437
H	3.119719	2.702200	-1.550175
Ti	-0.427504	0.375000	-0.357398
C	-0.143659	3.868829	1.063839
H	0.602818	4.049370	0.286351
H	-0.872495	4.683257	1.025396
H	0.359709	3.911604	2.033588
C	-0.862702	2.524455	0.875610
C	-1.545310	2.376140	-0.492368
H	-1.527635	3.329420	-1.011131
H	-2.578309	2.040142	-0.408406
H	-0.098327	1.732794	1.121800
H	-1.603292	2.379125	1.665539
C	-1.058869	1.627995	-2.425329
C	-0.613749	0.290582	-2.544266
H	0.402967	0.112532	-2.879625
H	-1.336126	-0.452452	-2.858592
H	-0.358207	2.428340	-2.634869

H -2.089065 1.858305 -2.674318

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**3F-bsi**

C -0.313909 -2.201118 -0.617509  
C -1.733849 -2.024357 -0.506602  
C 0.347390 -2.805350 -1.828830  
H 0.199735 -3.892303 -1.819041  
H 1.419869 -2.624308 -1.854803  
H -0.083777 -2.434520 -2.763893  
C -2.760139 -2.451495 -1.512608  
H -3.112308 -3.465102 -1.284273  
H -2.356179 -2.472392 -2.527286  
H -3.634450 -1.795704 -1.510212  
C 3.357332 -2.089886 -0.198290  
H 3.348935 -2.041359 -1.288912  
H 3.215979 -3.136309 0.096318  
H 4.356108 -1.791510 0.135868  
C 3.584639 1.039808 -1.442248  
H 4.230614 0.489168 -0.753362  
H 4.164275 1.884240 -1.827026  
H 3.338888 0.387490 -2.285385  
C -0.752637 -1.331795 1.468782  
C -2.001153 -1.484298 0.777791  
C -0.626958 -0.812681 2.882089  
H 0.132392 -1.373003 3.430245  
H -0.352599 0.247551 2.939463  
H -1.571841 -0.928205 3.417608  
C -3.366800 -1.228130 1.346073  
H -3.740950 -2.136082 1.836022  
H -3.368366 -0.435742 2.098376  
H -4.089098 -0.962063 0.570764  
C 2.684193 -0.632479 2.377915  
H 2.096044 0.117127 2.910628  
H 2.703282 -1.546557 2.983311  
H 3.715910 -0.269621 2.320369  
C 2.694540 2.420415 0.471483  
H 3.283235 1.855088 1.197820  
H 3.295531 3.276502 0.149190  
H 1.802416 2.803032 0.977505  
Si 2.048789 -1.028605 0.650619  
N 1.462314 0.413168 -0.274937  
C 0.310487 -1.799346 0.624167  
C 2.310299 1.555990 -0.747955  
C 1.530368 2.424640 -1.748674  
H 1.257927 1.856167 -2.643789  
H 0.620997 2.842842 -1.302463  
H 2.145097 3.269836 -2.070866  
Ti -0.400108 0.057094 -0.399547  
C -1.515872 3.418183 1.836641  
H -0.971452 4.257684 1.393970  
H -2.473415 3.797436 2.206060  
H -0.944790 3.055909 2.696460  
C -1.755534 2.311163 0.802942  
C -2.520366 2.758328 -0.450334  
H -1.923524 3.505184 -0.990077  
H -3.434755 3.271556 -0.130016  
H -0.730015 1.963385 0.512854  
H -2.283179 1.474259 1.278500  
C -2.883355 1.598838 -1.388587

C -1.660963 0.796433 -1.874646  
H -3.428903 2.000790 -2.252572  
H -3.587382 0.929454 -0.876917  
H -1.963209 0.026186 -2.594047  
H -0.960176 1.468945 -2.400053

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**3TSe**

C -0.967838 -1.636697 -0.940548  
C -2.290955 -1.099190 -0.811882  
C -0.401313 -2.189144 -2.227147  
H -0.204039 -3.260840 -2.123505  
H 0.538546 -1.715700 -2.524627  
H -1.106422 -2.066422 -3.051421  
C -3.315534 -0.998983 -1.908355  
H -3.823298 -1.962137 -2.039611  
H -2.874128 -0.737782 -2.874341  
H -4.088194 -0.260460 -1.680348  
C 2.486613 -2.689281 -0.533558  
H 2.402091 -2.541077 -1.611344  
H 2.111195 -3.693685 -0.303004  
H 3.550197 -2.675410 -0.276490  
C 3.709831 0.464747 -1.096093  
H 4.148818 -0.286020 -0.432813  
H 4.497736 1.183861 -1.340337  
H 3.402674 -0.028656 -2.022912  
C -1.298718 -1.059543 1.275760  
C -2.492124 -0.745478 0.546302  
C -1.189225 -0.977702 2.773213  
H -1.622734 -1.882735 3.216234  
H -0.156962 -0.912421 3.111139  
H -1.730725 -0.120103 3.178294  
C -3.763832 -0.216027 1.142524  
H -4.410612 -1.046765 1.451092  
H -3.577783 0.388232 2.033917  
H -4.338372 0.385306 0.432317  
C 2.245351 -1.501654 2.252233  
H 1.935344 -0.666769 2.884572  
H 1.956338 -2.436193 2.746453  
H 3.339881 -1.491902 2.203805  
C 2.988007 1.833409 0.894827  
H 3.379880 1.082452 1.585461  
H 3.783684 2.560980 0.704928  
H 2.157597 2.347931 1.387323  
Si 1.540330 -1.435590 0.507870  
N 1.414743 0.231648 -0.154254  
C -0.342841 -1.635900 0.363045  
C 2.526789 1.189616 -0.427758  
C 2.018487 2.285696 -1.382416  
H 1.653838 1.855419 -2.323429  
H 1.218463 2.874616 -0.920316  
H 2.819285 2.987495 -1.632952  
Ti -0.456451 0.481027 -0.300177  
C -1.029576 3.868805 0.821849  
H -0.115306 4.122751 0.281781  
H -1.703048 4.733887 0.756451  
H -0.797901 3.712039 1.877022  
C -1.751461 2.697328 0.224244  
C -1.641249 2.286248 -1.089433  
H -0.956375 2.797217 -1.765361

H	-2.451867	1.720982	-1.546422
H	-0.709471	1.339522	1.130153
H	-2.596707	2.329029	0.800929

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### 3H-E

C	-0.768413	-1.620478	-1.069540
C	-2.128601	-1.301431	-0.751475
C	-0.261342	-1.896282	-2.463628
H	0.018347	-2.950592	-2.561848
H	0.619708	-1.304512	-2.723813
H	-1.027703	-1.692907	-3.214015
C	-3.274651	-1.220147	-1.722524
H	-3.735497	-2.208282	-1.840803
H	-2.961304	-0.896916	-2.718599
H	-4.061132	-0.542729	-1.379177
C	2.843334	-2.143306	-1.126766
H	2.664373	-1.771505	-2.137257
H	2.624338	-3.217931	-1.119767
H	3.911947	-2.032158	-0.915500
C	3.417684	1.366195	-1.222464
H	4.057711	0.521334	-0.952960
H	4.057759	2.249607	-1.310017
H	2.978869	1.165014	-2.204887
C	-0.944783	-1.419279	1.229814
C	-2.232304	-1.172864	0.658834
C	-0.699424	-1.527764	2.708118
H	-0.895037	-2.557484	3.032187
H	0.326335	-1.288483	2.980792
H	-1.359010	-0.868634	3.275772
C	-3.486381	-0.909396	1.440075
H	-3.884825	-1.849058	1.842355
H	-3.304268	-0.248637	2.292091
H	-4.274415	-0.469577	0.823780
C	2.686035	-1.618068	1.856220
H	2.369718	-0.956006	2.664685
H	2.508576	-2.653210	2.170123
H	3.768522	-1.501375	1.735824
C	2.967135	1.854914	1.214834
H	3.596348	1.015270	1.519727
H	3.600842	2.746823	1.177979
H	2.199655	2.006088	1.979285
Si	1.828020	-1.289838	0.212402
N	1.416814	0.426846	-0.096956
C	-0.020925	-1.715273	0.161700
C	2.324989	1.606975	-0.163846
C	1.501161	2.844021	-0.563528
H	1.076221	2.727895	-1.568315
H	0.698211	3.032511	0.161934
H	2.126364	3.741428	-0.582726
Ti	-0.474469	0.446832	-0.133096
C	-2.243396	3.671144	0.800095
H	-1.443047	4.280524	0.375279
H	-3.158434	4.276741	0.832644
H	-1.999906	3.414671	1.835991
C	-2.514960	2.442616	-0.001194
C	-1.933467	2.120841	-1.183404
H	-1.232810	2.802039	-1.661174
H	-2.337888	1.311513	-1.791992
H	-0.705894	1.004450	1.414695

H	-3.284478	1.779075	0.392941
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### 3G

C	-0.930227	-1.366387	-1.371795
C	-2.238330	-1.101662	-0.879140
C	-0.544245	-1.349896	-2.826066
H	-0.333116	-2.369962	-3.165200
H	0.344356	-0.747500	-3.022124
H	-1.351818	-0.960358	-3.448620
C	-3.440696	-0.764547	-1.710990
H	-3.851228	-1.678162	-2.158524
H	-3.202424	-0.086806	-2.535405
H	-4.238939	-0.313116	-1.117698
C	2.693051	-1.918649	-1.767840
H	2.361824	-1.417282	-2.678202
H	2.578441	-2.999110	-1.918866
H	3.764386	-1.725463	-1.647299
C	2.869851	1.677578	-1.504057
H	3.301928	0.789647	-1.970884
H	3.615484	2.477521	-1.554736
H	2.002517	1.984216	-2.094656
C	-0.943394	-1.791736	0.902706
C	-2.241270	-1.333851	0.530420
C	-0.605114	-2.390453	2.242040
H	0.391460	-2.129880	2.598075
H	-1.331376	-2.115825	3.010577
H	-0.635750	-3.483297	2.156758
C	-3.447588	-1.250551	1.424641
H	-4.002042	-2.196924	1.410087
H	-3.178662	-1.054197	2.465610
H	-4.141064	-0.468040	1.105493
C	2.657477	-2.256891	1.236405
H	2.469418	-1.788232	2.205579
H	2.366468	-3.311009	1.307138
H	3.738505	-2.231924	1.066804
C	3.735806	0.972594	0.750747
H	4.217150	0.100941	0.297619
H	4.472198	1.782142	0.756555
H	3.493015	0.730437	1.789905
Si	1.761500	-1.429372	-0.205208
N	1.444531	0.324330	0.012071
C	-0.098022	-1.777210	-0.263095
C	2.482294	1.405263	-0.035531
C	1.949223	2.707453	0.595048
H	1.037682	3.061470	0.103109
H	1.753503	2.587717	1.664852
H	2.691095	3.504805	0.493114
Ti	-0.460124	0.402714	0.120114
C	-2.145096	3.718482	-0.441974
H	-1.222228	4.062040	0.036944
H	-2.231830	4.245903	-1.395945
H	-2.988273	4.016888	0.188407
C	-2.129992	2.203308	-0.689535
C	-0.942459	1.667290	-1.471772
H	-0.129347	2.393395	-1.559925
H	-1.185625	1.277180	-2.456701
H	-2.194492	1.718057	0.332928
H	-3.067363	1.877286	-1.146374
C	-0.199509	0.837250	2.868426

C	-1.056304	1.784405	2.446707
H	0.875172	0.971175	2.821025
H	-0.707416	2.739113	2.061418
H	-2.127841	1.675748	2.589613
H	-0.556471	-0.068156	3.343374

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### 3TS<sub>T</sub>

C	1.141337	-1.332843	1.292338
C	2.380920	-0.989016	0.675799
C	0.929827	-1.439230	2.778851
H	0.965551	-2.494797	3.072192
H	-0.032940	-1.046891	3.107672
H	1.715495	-0.929853	3.342189
C	3.637152	-0.578471	1.391142
H	4.187353	-1.463295	1.734355
H	3.433721	0.028995	2.277880
H	4.314176	-0.014533	0.744097
C	-2.380328	-1.858106	2.070594
H	-2.162694	-1.092882	2.819041
H	-1.999861	-2.816094	2.443071
H	-3.468922	-1.950691	2.001076
C	-3.520067	1.206425	0.998927
H	-4.020606	0.241375	1.113149
H	-4.298637	1.967353	0.884957
H	-2.969730	1.418346	1.920605
C	0.945703	-1.719093	-0.977802
C	2.261240	-1.227716	-0.722850
C	0.480600	-2.285003	-2.294110
H	-0.484854	-1.891760	-2.616836
H	1.203325	-2.099139	-3.092025
H	0.376259	-3.371985	-2.206675
C	3.371550	-1.103704	-1.728029
H	3.882591	-2.066241	-1.852626
H	3.011814	-0.807588	-2.717526
H	4.128415	-0.379543	-1.415864
C	-2.633922	-2.525609	-0.871273
H	-2.483958	-2.248388	-1.916092
H	-2.357094	-3.580863	-0.759097
H	-3.705234	-2.452275	-0.656164
C	-3.384028	0.851132	-1.490489
H	-3.856027	-0.128927	-1.394250
H	-4.177046	1.586140	-1.660979
H	-2.745054	0.833019	-2.378607
Si	-1.650360	-1.498389	0.367356
N	-1.465814	0.245555	-0.029829
C	0.221529	-1.756586	0.268062
C	-2.582495	1.220982	-0.224831
C	-2.031470	2.651318	-0.389325
H	-1.534183	2.994551	0.521599
H	-1.334132	2.731482	-1.230153
H	-2.848285	3.350236	-0.591254
Ti	0.427454	0.439411	-0.143706
C	1.506177	3.852899	0.671810
H	0.469974	4.121487	0.452819
H	1.812335	4.417334	1.559214
H	2.142063	4.177380	-0.155975
C	1.664358	2.374338	0.985586
C	0.733899	1.676853	1.781028
H	-0.219975	2.143587	2.007196

H	1.086005	0.967170	2.514009
H	1.539105	1.920168	-0.429636
H	2.701465	2.046408	1.071649
C	0.496725	0.963261	-2.412196
C	1.395260	1.919522	-1.928627
H	-0.524001	1.248686	-2.636861
H	1.083455	2.961306	-1.879994
H	2.462331	1.772988	-2.086279
H	0.865734	0.091147	-2.930163

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C	1.076565	-1.090862	1.405346
C	2.243679	-1.130988	0.585322
C	1.047594	-0.682585	2.856848
H	0.667744	-1.505954	3.469191
H	0.405600	0.180088	3.056422
H	2.048442	-0.445674	3.223417
C	3.657756	-0.832185	0.999932
H	4.182655	-1.765940	1.236102
H	3.711722	-0.201978	1.889257
H	4.227167	-0.343076	0.204253
C	-2.302255	-0.763114	2.683232
H	-1.830773	0.115106	3.130550
H	-2.032840	-1.636131	3.288668
H	-3.385575	-0.633828	2.768598
C	-3.688936	1.525539	0.495828
H	-4.204448	0.581707	0.696973
H	-4.444319	2.235125	0.144321
H	-3.280908	1.906783	1.436665
C	0.488294	-1.989094	-0.646153
C	1.877114	-1.691572	-0.676940
C	-0.258302	-2.695240	-1.745416
H	-1.164540	-2.167403	-2.047616
H	0.364304	-2.817135	-2.633617
H	-0.552992	-3.696292	-1.411934
C	2.827991	-2.017975	-1.790794
H	3.123777	-3.073038	-1.738278
H	2.382012	-1.861140	-2.776722
H	3.743610	-1.424798	-1.735294
C	-3.092749	-2.256597	0.171508
H	-2.993927	-2.453427	-0.896749
H	-2.989352	-3.213125	0.698681
H	-4.110960	-1.898767	0.356468
C	-3.197701	0.764505	-1.852609
H	-3.650493	-0.210866	-1.659581
H	-3.980688	1.424665	-2.239484
H	-2.442385	0.640998	-2.633232
Si	-1.827144	-1.053830	0.880447
N	-1.511115	0.441481	-0.061398
C	-0.033230	-1.605472	0.648045
C	-2.585332	1.361742	-0.568592
C	-2.022435	2.762418	-0.877303
H	-1.688045	3.265915	0.033786
H	-1.193396	2.729652	-1.591843
H	-2.801997	3.385794	-1.324869
Ti	0.374828	0.344318	-0.355117
C	3.351802	2.916229	0.684017
H	3.120924	3.462983	-0.232906
H	3.819913	3.614262	1.390137

H	4.104596	2.149065	0.472914
C	2.134908	2.333750	1.325615
C	0.860856	2.535010	0.923602
H	0.643800	3.197584	0.087978
H	0.022844	2.237021	1.547397
H	2.260180	1.234172	-1.193431
H	2.301829	1.754059	2.231555
C	0.533174	0.528657	-2.411846
C	1.868132	1.256395	-2.242915
H	-0.266068	1.186868	-2.759213
H	1.816839	2.318180	-2.497842
H	2.672146	0.788313	-2.814736
H	0.583650	-0.342875	-3.060239