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# Supplementary Materials

## **Mechanistic Investigation on Hydrocyanation of Butadiene: A DFT study**

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## Atomic Coordinates

Atomic coordinates of intermediates and transition states are provided.

**Table S1.** Atomic coordinates of the intermediates and transition states.

<b>I<sub>1</sub></b>				<b>TS<sub>1-2</sub></b>			
C	1.217827	0.321165	1.930362	C	-5.85615	-1.90159	-1.07089
H	0.388907	1.056412	1.939687	H	-5.09013	-3.83591	-0.51083
H	2.085715	0.835402	2.385661	H	-6.34034	0.138534	-1.55179
C	0.85681	-0.88566	2.776985	H	-6.81757	-2.29408	-1.41639
H	1.751591	-1.52499	2.892794	C	-2.0084	1.449441	0.586184
H	0.617655	-0.52328	3.794855	C	-2.91588	1.926456	1.530476
C	-0.29091	-1.7497	2.28738	C	-1.25559	2.365575	-0.14053
H	0.010479	-2.30852	1.378529	C	-3.05515	3.284393	1.749214
H	-0.47179	-2.52169	3.056802	H	-3.53958	1.22116	2.093876
C	-1.59353	-1.01412	2.013722	C	-1.38726	3.726769	0.084116
H	-2.44527	-1.6989	2.166844	H	-0.54834	1.99793	-0.89569
H	-1.73519	-0.1988	2.748329	C	-2.28577	4.186467	1.030035
P	-1.74602	-0.32741	0.29522	H	-3.77372	3.646245	2.491776
P	1.556175	-0.09534	0.182724	H	-0.77569	4.431217	-0.48906
C	2.99104	-1.19638	0.344531	H	-2.39319	5.260871	1.209676
C	2.885032	-2.51444	-0.08469	Ni	-0.11223	-0.82789	-0.95228
C	4.183685	-0.76227	0.918917	C	-0.57425	-1.69394	-2.49865
C	3.950798	-3.38664	0.068062	H	-1.33787	-2.11231	-3.17013
H	1.958041	-2.84329	-0.57016	N	0.639042	-1.60342	-2.48575
C	5.246583	-1.63302	1.068165				
H	4.286396	0.282522	1.238656	C	-1.12392	0.254726	-1.99657
C	5.12939	-2.9479	0.644382	H	-0.27844	0.971895	-1.99662
H	3.861096	-4.42061	-0.27918	H	-1.96455	0.776114	-2.49234
H	6.182427	-1.2821	1.515178	C	-0.75929	-0.98427	-2.79281
H	5.973419	-3.63542	0.758312	H	-1.65323	-1.62637	-2.89699
C	2.304468	1.415651	-0.48046	H	-0.50112	-0.6641	-3.82001
C	2.225939	2.660474	0.137337	C	0.381391	-1.8187	-2.24234
C	2.905058	1.323152	-1.73647	H	0.062978	-2.33179	-1.3119
C	2.751194	3.784447	-0.48125	H	0.582608	-2.62924	-2.96478
H	1.740352	2.768397	1.113657	C	1.668189	-1.0478	-1.98447
C	3.439621	2.44304	-2.34281	H	2.543741	-1.6912	-2.17527
H	2.940321	0.350587	-2.24373	H	1.76018	-0.20797	-2.69987
C	3.362497	3.678211	-1.71728	P	1.824881	-0.37364	-0.2616
H	2.685676	4.756991	0.017725	P	-1.5244	-0.10584	-0.25073
H	3.914543	2.353879	-3.32507	C	-2.97143	-1.18907	-0.40885
H	3.780019	4.566284	-2.20148	C	-2.8565	-2.54048	-0.10646
C	-3.40605	-0.89614	-0.18365	C	-4.19203	-0.69181	-0.85879
C	-3.67934	-2.26265	-0.13437	C	-3.94441	-3.38384	-0.26082
C	-4.37492	-0.0457	-0.70712	H	-1.90736	-2.92614	0.284482
C	-4.89401	-2.76039	-0.56459	C	-5.27578	-1.5351	-1.01287
H	-2.91448	-2.95805	0.235948	H	-4.30002	0.379123	-1.07362
C	-5.58879	-0.54677	-1.14632	C	-5.1506	-2.88347	-0.71606
H	-4.18031	1.029881	-0.77485	H	-3.84883	-4.4445	-0.00894

H	-6.23358	-1.13606	-1.36214	H	-2.54124	-0.63381	2.502733
H	-6.01102	-3.55033	-0.8322	H	-1.30449	0.602249	2.552668
C	-2.23671	1.439694	0.368929	P	-1.79495	0.021462	0.281623
C	-2.09492	2.66558	-0.27399	P	1.643904	0.095369	0.364864
C	-2.87751	1.392883	1.607583	C	2.639834	-1.41412	0.28403
C	-2.59549	3.820647	0.304856	C	2.172761	-2.50045	-0.44656
H	-1.57656	2.734629	-1.23672	C	3.848479	-1.51881	0.967889
C	-3.38305	2.546608	2.174734	C	2.900322	-3.6779	-0.4861
H	-2.96447	0.435977	2.138569	H	1.23934	-2.40545	-1.01564
C	-3.24344	3.763245	1.525639	C	4.571797	-2.69555	0.928101
H	-2.48085	4.778791	-0.21306	H	4.239574	-0.6571	1.523591
H	-3.88563	2.495166	3.145581	C	4.095848	-3.77653	0.202353
H	-3.64038	4.676941	1.979398	H	2.532427	-4.52385	-1.07465
C	3.477026	-0.95617	0.225933	H	5.523891	-2.76955	1.463249
C	3.761383	-2.31726	0.133879	H	4.673669	-4.70564	0.165873
C	4.421238	-0.11562	0.805712	C	2.828621	1.417728	-0.00258
C	4.967135	-2.82052	0.582698	C	2.822981	2.615705	0.706736
H	3.014593	-3.00601	-0.28267	C	3.720732	1.262927	-1.06169
C	5.627271	-0.62242	1.259327	C	3.701354	3.632813	0.375813
H	4.213573	0.955346	0.906091	H	2.122925	2.77309	1.534409
C	5.906647	-1.9721	1.145189	C	4.597549	2.281288	-1.38485
H	5.173276	-3.8924	0.49934	H	3.708294	0.345037	-1.65822
H	6.361152	0.053612	1.709647	C	4.592946	3.465978	-0.66822
H	6.860734	-2.36905	1.505135	H	3.686095	4.567687	0.945096
C	2.082709	1.404408	-0.53539	H	5.290199	2.146822	-2.22121
C	2.994579	1.88545	-1.47348	H	5.287761	4.270171	-0.93033
C	1.308097	2.312289	0.177601	C	-2.9806	-1.25392	-0.23798
C	3.11717	3.243505	-1.69797	C	-3.21513	-2.41083	0.496909
H	3.627436	1.182069	-2.02996	C	-3.66292	-1.07419	-1.43948
C	1.422395	3.673667	-0.0547	C	-4.11038	-3.36529	0.041779
H	0.597492	1.938802	0.927579	H	-2.69169	-2.59108	1.441659
C	2.325674	4.138342	-0.99319	C	-4.56574	-2.01954	-1.88384
H	3.83842	3.612409	-2.43444	H	-3.47757	-0.17432	-2.03737
H	0.792068	4.372612	0.505312	C	-4.78939	-3.17101	-1.14589
H	2.418881	5.213076	-1.17987	H	-4.27712	-4.27332	0.629818
Ni	0.108897	-0.78373	0.956345	H	-5.09748	-1.85878	-2.82672
C	-0.6709	-1.33687	2.478445	H	-5.49713	-3.92504	-1.50399
H	0.705214	-1.3521	2.283068	C	-2.79171	1.531469	0.305771
N	-1.33889	-1.6523	3.391964	C	-4.04868	1.567053	0.902528
		<b>I<sub>2</sub></b>		C	-2.27042	2.690435	-0.25839
C	1.396499	0.311957	2.167376	C	-4.76706	2.747148	0.942
H	0.759802	1.207057	2.295927	H	-4.4799	0.650914	1.325502
H	2.363179	0.571738	2.636832	C	-2.99149	3.871645	-0.21687
C	0.787919	-0.87161	2.891877	H	-1.29094	2.652388	-0.75353
H	1.527685	-1.6912	2.935427	C	-4.23735	3.900238	0.384441
H	0.609749	-0.57097	3.941481	H	-5.75726	2.76788	1.408228
C	-0.49994	-1.41036	2.302718	H	-2.57751	4.778249	-0.66893
H	-0.26676	-1.94194	1.356856	H	-4.81059	4.832413	0.412525
H	-0.88748	-2.19387	2.977301	Ni	-0.08474	0.107425	-0.97746
C	-1.56989	-0.3501	2.059679	C	1.001439	-0.00063	-2.44528
				H	-1.1553	0.227706	-1.96385

N	1.73085	-0.13589	-3.34527	C	-2.48343	2.969222	2.987691
				H	-2.19955	0.888203	3.36634
		<b>I<sub>3</sub></b>		C	-2.31252	3.688476	0.712893
C	1.369973	0.771046	1.763453	H	-1.85703	2.166989	-0.73265
H	0.530644	1.463156	1.577225	C	-2.53382	3.983372	2.048088
C	1.027325	-0.22849	2.861405	H	-2.6618	3.189732	4.044988
H	1.977277	-0.58143	3.30163	H	-2.36076	4.480421	-0.04119
H	0.514792	0.319676	3.675652	H	-2.74904	5.01077	2.358014
C	0.237011	-1.46965	2.492947	Ni	-0.06069	-0.56329	-0.88216
H	0.757545	-2.01607	1.685574	C	-3.14575	0.447513	-3.08294
H	0.281289	-2.15396	3.358937	C	-1.81649	0.480018	-2.97929
C	-1.22978	-1.33993	2.125104	C	-0.96998	-0.66759	-2.74395
H	-1.8399	-1.03713	2.994436	C	-0.0319	-2.42727	-0.69401
P	-1.63482	-0.32538	0.65942	N	-0.04854	-3.5894	-0.58985
P	1.800817	0.043995	0.140962	H	-3.70574	-0.48947	-2.97569
C	3.20137	-1.04244	0.545916	H	-3.72904	1.350623	-3.28087
C	3.242852	-2.35752	0.097563	H	-1.28963	1.441825	-3.08972
C	4.266032	-0.55144	1.303492	H	-1.47083	-1.64648	-2.74617
C	4.322811	-3.16892	0.409508	C	0.412289	-0.62056	-2.84379
H	2.412768	-2.75832	-0.49279	H	-0.10917	0.880842	-0.97106
C	5.340408	-1.36306	1.613859	H	0.981383	-1.53801	-3.0178
H	4.264999	0.492077	1.641986	H	0.904296	0.313374	-3.14382
C	5.368692	-2.67605	1.168455	H	-1.5951	-2.34962	1.86297
H	4.340196	-4.20348	0.053228	H	2.19511	1.418502	2.114101
H	6.168752	-0.9658	2.208882				
H	6.219738	-3.31912	1.415047			<b>TS<sub>3,4</sub></b>	
C	2.629616	1.425855	-0.69832	C	-1.28068	0.952862	-1.79619
C	2.089416	2.710102	-0.64083	H	-0.45608	1.626574	-1.49836
C	3.757993	1.210339	-1.48577	C	-0.83737	0.034543	-2.92479
C	2.682013	3.754102	-1.32766	H	-1.74327	-0.39485	-3.39069
H	1.184662	2.904177	-0.05105	H	-0.37765	0.666259	-3.70947
C	4.341978	2.255614	-2.18128	C	0.084132	-1.1305	-2.61034
H	4.194685	0.207274	-1.55267	H	-0.37334	-1.79118	-1.85326
C	3.810829	3.530768	-2.09952	H	0.127281	-1.74908	-3.52548
H	2.252795	4.759043	-1.26003	C	1.527193	-0.84685	-2.22764
H	5.22944	2.067214	-2.7938	H	2.004356	-0.21637	-3.00082
H	4.276837	4.357844	-2.64437	P	1.852637	-0.10172	-0.56657
C	-3.28953	-0.91271	0.195425	P	-1.82736	0.100882	-0.26155
C	-3.40992	-2.20706	-0.31326	C	-3.1021	-1.03559	-0.88316
C	-4.42171	-0.10468	0.243354	C	-3.03473	-2.39772	-0.61423
C	-4.63329	-2.67923	-0.75091	C	-4.15415	-0.54497	-1.65762
H	-2.52812	-2.85528	-0.37917	C	-4.00097	-3.25444	-1.11954
C	-5.64349	-0.58153	-0.20221	H	-2.20679	-2.79434	-0.016
H	-4.35878	0.917548	0.629452	C	-5.11266	-1.40242	-2.16145
C	-5.75446	-1.86654	-0.70148	H	-4.23172	0.531183	-1.85683
H	-4.70707	-3.69784	-1.14484	C	-5.03536	-2.76086	-1.893
H	-6.52343	0.068603	-0.15712	H	-3.93652	-4.32527	-0.90429
H	-6.72103	-2.23814	-1.05654	H	-5.93313	-1.00763	-2.76875
C	-1.97145	1.358627	1.262687	H	-5.79499	-3.4403	-2.29277
C	-2.21432	1.666663	2.59841	C	-2.81629	1.359877	0.583742
C	-2.02745	2.391426	0.326029	C	-2.37812	2.680998	0.644491

C	-3.95214	1.002	1.304302	C	-0.62728	0.14707	-3.05726
C	-3.06483	3.619551	1.3931	H	-1.53753	-0.3025	-3.49229
H	-1.47706	2.986233	0.0982	H	-0.19144	0.768498	-3.86305
C	-4.63291	1.940026	2.059992	C	0.33466	-0.97566	-2.72562
H	-4.31042	-0.03327	1.274658	H	-0.11175	-1.67473	-1.99433
C	-4.19283	3.25159	2.106594	H	0.463961	-1.5739	-3.64483
H	-2.71135	4.655258	1.420198	C	1.716609	-0.54559	-2.26712
H	-5.52355	1.639566	2.621368	H	2.059104	0.310838	-2.87734
H	-4.73235	3.992523	2.703929	P	1.910758	-0.07716	-0.49054
C	3.395475	-0.88117	-0.02238	P	-1.63034	0.250275	-0.41106
C	3.470223	-2.27292	0.051992	C	-2.92985	-0.86436	-1.0124
C	4.442424	-0.12636	0.505772	C	-3.06192	-2.14581	-0.49002
C	4.57419	-2.88579	0.615712	C	-3.84849	-0.42148	-1.96416
H	2.635764	-2.89251	-0.29413	C	-4.08934	-2.97198	-0.91945
C	5.542418	-0.74665	1.071958	H	-2.34768	-2.50453	0.257774
H	4.400775	0.967588	0.48096	C	-4.86759	-1.24971	-2.39496
C	5.614148	-2.12757	1.127579	H	-3.77508	0.595484	-2.36876
H	4.612752	-3.97822	0.666416	C	-4.98871	-2.52772	-1.87121
H	6.356182	-0.1367	1.476557	H	-4.18062	-3.97985	-0.5027
H	6.48334	-2.61612	1.578444	H	-5.58042	-0.89204	-3.14497
C	2.41243	1.581654	-0.99029	H	-5.79674	-3.18338	-2.21129
C	3.408133	1.751772	-1.9529	C	-2.60345	1.557243	0.388635
C	1.896339	2.713399	-0.36945	C	-2.07833	2.845045	0.49107
C	3.85087	3.012842	-2.30311	C	-3.83457	1.290915	0.982205
H	3.867623	0.873913	-2.42302	C	-2.77248	3.842214	1.15013
C	2.339525	3.979454	-0.71993	H	-1.10429	3.079486	0.043753
H	1.134272	2.598928	0.40941	C	-4.52291	2.28918	1.651523
C	3.310549	4.132693	-1.69103	H	-4.26408	0.284548	0.923593
H	4.632702	3.123551	-3.06127	C	-3.99845	3.567227	1.734386
H	1.918767	4.857678	-0.22069	H	-2.34911	4.850155	1.20808
H	3.658604	5.132044	-1.96944	H	-5.48959	2.061365	2.112
Ni	0.065988	-0.44417	0.590898	H	-4.54745	4.355427	2.259156
C	1.955644	-1.20133	3.108971	C	3.300767	-1.08778	0.088247
C	0.945077	-0.34182	3.261665	C	3.384892	-2.43912	-0.24183
C	-0.43735	-0.7356	3.407934	C	4.230936	-0.55567	0.979643
C	0.154599	-2.29624	0.491538	C	4.393713	-3.22726	0.283049
N	0.225817	-3.46066	0.456125	H	2.635393	-2.89851	-0.89436
H	1.775594	-2.28007	3.036257	C	5.23692	-1.34853	1.503105
H	2.992377	-0.86702	3.009056	H	4.176257	0.50165	1.263844
H	1.150249	0.738588	3.306206	C	5.324206	-2.68515	1.152462
H	-0.63616	-1.81715	3.379286	H	4.444115	-4.28655	0.012396
C	-1.4479	0.115906	3.592889	H	5.964433	-0.91158	2.195
H	0.009234	1.001123	0.754597	H	6.120654	-3.31103	1.566409
H	-2.47755	-0.22839	3.713618	C	2.692929	1.566271	-0.61429
H	-1.29063	1.201506	3.604002	C	3.820653	1.712672	-1.42558
H	2.073825	-1.80642	-2.24239	C	2.218127	2.681219	0.067027
H	-2.08669	1.614037	-2.16895	C	4.438216	2.94035	-1.56599
		<b>I<sub>4</sub></b>		H	4.232509	0.841501	-1.94965
C	-1.02858	1.079961	-1.92994	C	2.838934	3.913599	-0.07284
H	-0.16366	1.697952	-1.61762	H	1.348835	2.587264	0.727158
				C	3.945074	4.046899	-0.89129



H	0.142481	-1.94784	-3.49222	C	2.169394	-0.96951	2.758207
C	1.269124	-0.51922	-2.36855	C	0.732469	-0.86977	2.666102
H	1.319469	0.374284	-3.01955	C	-0.01215	-2.46344	0.69224
P	1.60566	0.037412	-0.62007	N	0.07104	-3.61591	0.515487
P	-1.8447	-0.01242	-0.27188	H	2.345267	-3.0431	3.164523
C	-3.28661	-1.07321	-0.58227	H	3.948072	-2.09289	3.029309
C	-3.19566	-2.45508	-0.45693	H	2.727812	-0.03721	2.570825
C	-4.48577	-0.50608	-1.0149	H	0.182024	-1.69638	3.132674
C	-4.28732	-3.25379	-0.75978	C	0.099476	0.448848	2.755806
H	-2.26145	-2.91409	-0.11594	H	-0.23987	0.842093	1.727208
C	-5.57217	-1.30664	-1.31245	H	-0.81371	0.48583	3.368473
H	-4.57413	0.583493	-1.1089	H	0.7942	1.25304	3.054036
C	-5.47302	-2.68394	-1.18637	H	2.126624	-1.14564	-2.66823
H	-4.20426	-4.34039	-0.65653	H	-2.41195	1.260956	-2.26991
H	-6.50972	-0.85006	-1.64585				
H	-6.33413	-3.31798	-1.42167				
C	-2.5795	1.394639	0.605991	C	-1.56975	0.578157	-2.07607
C	-2.29109	2.716562	0.274864	H	-0.74706	1.318768	-2.08115
C	-3.3581	1.143357	1.737019	C	-1.25509	-0.57467	-3.02265
C	-2.77188	3.758592	1.052671	H	-2.14182	-1.23612	-3.13792
H	-1.67961	2.950676	-0.60382	H	-1.08304	-0.14252	-4.03208
C	-3.84003	2.185635	2.507154	C	-0.04697	-1.44335	-2.64023
H	-3.59517	0.10817	2.013994	H	-0.27596	-2.08286	-1.76212
C	-3.54557	3.497155	2.169247	H	0.112144	-2.17407	-3.46369
H	-2.54137	4.791912	0.773217	C	1.239944	-0.65427	-2.43645
H	-4.4557	1.969428	3.38621	H	1.259086	0.221745	-3.11316
H	-3.92522	4.320896	2.781137	P	1.572064	-0.05624	-0.6445
C	3.218623	-0.75061	-0.34102	P	-1.83101	-0.04363	-0.3032
C	3.31101	-2.13179	-0.51268	C	-3.31743	-1.13928	-0.55176
C	4.323989	-0.06574	0.158523	C	-3.22722	-2.52421	-0.42987
C	4.483925	-2.80249	-0.21863	C	-4.52786	-0.54319	-0.92816
H	2.4393	-2.70367	-0.85428	C	-4.35557	-3.31859	-0.67663
C	5.49808	-0.73987	0.448834	H	-2.29699	-3.02449	-0.13885
H	4.272643	1.016111	0.324982	C	-5.6496	-1.33713	-1.17339
C	5.585031	-2.10854	0.256535	H	-4.62473	0.540763	-1.02318
H	4.533437	-3.88719	-0.35627	C	-5.56362	-2.72842	-1.0467
H	6.360726	-0.18247	0.828775	H	-4.28208	-4.40115	-0.57043
H	6.514204	-2.63953	0.486194	H	-6.59243	-0.87444	-1.45955
C	2.062495	1.782946	-0.88322	H	-6.44049	-3.34751	-1.2343
C	3.007909	2.168289	-1.83524	C	-2.55249	1.441751	0.559448
C	1.426025	2.775505	-0.1449	C	-2.26294	2.742837	0.143745
C	3.300007	3.503655	-2.04157	C	-3.31912	1.223037	1.708422
H	3.533899	1.403374	-2.41989	C	-2.74828	3.830697	0.878138
C	1.713396	4.115788	-0.3528	H	-1.66655	2.944111	-0.7472
H	0.678866	2.495103	0.608702	C	-3.8034	2.313183	2.438096
C	2.650802	4.481238	-1.30194	H	-3.5564	0.210577	2.052225
H	4.045922	3.788204	-2.79056	C	-3.51685	3.61726	2.025095
H	1.19881	4.88069	0.237502	H	-2.52836	4.845941	0.551813
H	2.882159	5.538149	-1.46773	H	-4.40387	2.142782	3.331606
Ni	-0.02938	-0.6471	0.875775	H	-3.89218	4.465308	2.596955
C	2.855076	-2.0853	3.009886	C	3.18449	-0.94885	-0.35669

TS<sub>5-6</sub>

C	3.17324	-2.34445	-0.44049	C	2.919798	-1.13901	0.474694
C	4.342945	-0.27705	0.039946	C	2.696514	-2.47863	0.182475
C	4.329328	-3.06791	-0.13095	C	4.166049	-0.74563	0.956999
H	2.269356	-2.89582	-0.71237	C	3.700978	-3.41202	0.370367
C	5.497204	-1.0049	0.347332	H	1.718842	-2.78983	-0.20672
H	4.374005	0.811769	0.122863	C	5.169055	-1.67873	1.138356
C	5.491023	-2.39937	0.263807	H	4.359203	0.311298	1.178676
H	4.316928	-4.15596	-0.18403	C	4.936731	-3.01332	0.846581
H	6.400369	-0.48174	0.657666	H	3.51701	-4.46322	0.128055
H	6.388635	-2.96516	0.510778	H	6.148528	-1.35968	1.508323
C	2.076951	1.715656	-0.95736	H	5.73437	-3.74996	0.986247
C	3.044514	2.034294	-1.91479	C	2.38214	1.543883	-0.28519
C	1.442905	2.7264	-0.23537	C	2.195196	2.786445	0.315316
C	3.373521	3.371484	-2.15203	C	3.20043	1.457176	-1.41244
H	3.562171	1.256145	-2.48098	C	2.807487	3.917131	-0.197
C	1.773223	4.06611	-0.47485	H	1.543282	2.896348	1.188383
H	0.687023	2.500173	0.527346	C	3.811514	2.590751	-1.91627
C	2.736345	4.388252	-1.4328	H	3.343481	0.494186	-1.91264
H	4.128569	3.622647	-2.89601	C	3.619149	3.821951	-1.31293
H	1.280387	4.855588	0.091408	H	2.64426	4.884901	0.288404
H	2.995078	5.430746	-1.61855	H	4.447703	2.505817	-2.80238
Ni	0.001829	-0.55299	0.856335	H	4.105276	4.715272	-1.71725
C	3.004473	-1.7026	3.015222	C	-3.48277	-0.2272	0.302312
C	2.389662	-0.58788	2.619585	C	-4.21653	-1.31654	0.768334
C	0.958608	-0.39619	2.556184	C	-4.14684	0.729955	-0.46498
C	-0.33726	-2.28909	1.316402	C	-5.56577	-1.43999	0.488179
N	-0.42181	-3.43216	1.517408	H	-3.73466	-2.10661	1.35431
H	2.428073	-2.58321	3.320137	C	-5.49437	0.604435	-0.74629
H	4.093347	-1.79664	2.994555	H	-3.59956	1.590582	-0.86164
H	3.006816	0.263712	2.285871	C	-6.21049	-0.48045	-0.27172
H	0.427032	-1.07229	3.241233	H	-6.11746	-2.30575	0.866674
C	0.481326	1.019499	2.669923	H	-5.99112	1.369392	-1.35072
H	-0.4827	1.195635	2.152969	H	-7.27614	-0.58062	-0.49735
H	0.294493	1.304584	3.724083	C	-1.50678	1.715446	0.530984
H	1.216416	1.733826	2.259042	C	-2.02745	2.525032	1.538849
H	2.104976	-1.27582	-2.74468	C	-0.91701	2.31566	-0.57668
H	-2.46218	1.128694	-2.4287	C	-1.92711	3.901004	1.453452
		<b>I<sub>6</sub></b>		H	-2.54161	2.07637	2.396808
C	1.317012	0.473495	2.10442	C	-0.83289	3.695849	-0.67028
H	0.522227	1.239221	2.175166	H	-0.51329	1.68278	-1.37988
C	0.975268	-0.70905	2.98585	C	-1.32819	4.488454	0.348692
H	1.839396	-1.39544	3.037637	H	-2.33433	4.526249	2.253977
H	0.831772	-0.32865	4.01492	H	-0.35433	4.149856	-1.54316
C	-0.2547	-1.48827	2.571045	H	-1.25625	5.578583	0.281615
H	-0.03704	-2.11509	1.683934	Ni	-0.1262	-0.85402	-0.85463
H	-0.49257	-2.20516	3.375995	C	-0.66489	-4.11627	-0.45905
C	-1.47875	-0.62917	2.295213	C	-1.44158	-3.08117	-0.81025
H	-1.49365	0.254794	2.960472	C	-1.19076	-2.151	-1.89513
P	-1.67649	-0.09607	0.537918	C	1.049922	-0.91133	-2.26005
P	1.560507	0.052644	0.338904	N	1.807892	-0.93092	-3.14684
				H	0.216722	-4.3857	-1.05343



H	-0.88897	-4.74544	0.40658	H	4.091407	1.129683	0.190556
H	-2.34097	-2.89098	-0.19964	C	5.901339	-1.73491	0.164874
H	-0.46773	-2.5951	-2.59642	H	5.135136	-3.69137	-0.31492
C	-2.37345	-1.62738	-2.65513	H	6.377316	0.316086	0.604694
H	-3.20205	-1.30286	-2.00707	H	6.917746	-2.09307	0.353051
H	-2.09338	-0.77345	-3.29274	C	1.802574	1.50456	-0.82469
H	-2.78832	-2.40308	-3.32767	C	2.48184	2.05435	-1.91175
H	-2.38877	-1.19001	2.55903	C	1.314877	2.353088	0.163944
H	2.236623	0.96219	2.476338	C	2.636651	3.423515	-2.02096
		<b>TS<sub>6-7</sub></b>		H	2.916815	1.403016	-2.67911
C	-1.29219	0.339462	-2.10378	C	1.475814	3.725448	0.055488
H	-0.42767	1.021988	-2.19946	H	0.78742	1.91897	1.024647
C	-1.08866	-0.88924	-2.96358	C	2.129346	4.261769	-1.03878
H	-2.01829	-1.48438	-2.99625	H	3.165982	3.84412	-2.88155
H	-0.90996	-0.54934	-4.00125	H	1.075666	4.378907	0.836895
C	0.06295	-1.76107	-2.5211	H	2.252835	5.345712	-1.12948
H	-0.2015	-2.31679	-1.5999	Ni	0.037833	-0.75894	0.907652
H	0.240804	-2.53176	-3.29095	C	0.6874	-2.68185	1.744356
C	1.342811	-0.98143	-2.29543	C	1.445869	-1.58848	2.189856
H	1.422918	-0.16098	-3.03304	C	1.1078	-0.43507	2.900545
P	1.595168	-0.28568	-0.59275	C	-1.3712	-0.93384	2.067609
P	-1.58382	-0.02513	-0.32881	N	-2.27912	-1.07106	2.785542
C	-2.98705	-1.16395	-0.49015	H	-0.18946	-3.02584	2.29734
C	-4.18626	-0.72013	-1.03844	H	1.234603	-3.4649	1.209197
C	-2.8367	-2.50805	-0.17159	H	2.466575	-1.55074	1.781525
C	-5.22421	-1.60795	-1.25595	H	0.248834	-0.45559	3.57637
H	-4.31947	0.34129	-1.28107	C	2.145865	0.580588	3.217499
C	-3.87491	-3.3944	-0.39653	H	2.589744	0.427851	4.222748
H	-1.8935	-2.84914	0.275919	H	2.983923	0.555605	2.49847
C	-5.06813	-2.9464	-0.93589	H	1.750695	1.611291	3.221123
H	-6.16985	-1.24839	-1.67414	H	2.214733	-1.62709	-2.48566
H	-3.75463	-4.44865	-0.12989	H	-2.16303	0.915828	-2.46607
H	-5.89194	-3.64734	-1.10329			<b>I<sub>7</sub></b>	
C	-2.33481	1.530325	0.227839	C	-1.22591	-0.09622	-2.17548
C	-1.91687	2.744118	-0.31533	H	-0.36513	0.578659	-2.33708
C	-3.29662	1.541828	1.238583	C	-0.96848	-1.45007	-2.80951
C	-2.42984	3.940916	0.151076	H	-1.9193	-2.00989	-2.86323
H	-1.16835	2.770892	-1.1136	H	-0.65594	-1.28672	-3.85803
C	-3.81233	2.741623	1.692323	C	0.060718	-2.31572	-2.11433
H	-3.62887	0.600507	1.687005	H	-0.31101	-2.62977	-1.1191
C	-3.37889	3.943361	1.158427	H	0.161005	-3.25115	-2.69238
H	-2.08516	4.883139	-0.28763	C	1.436942	-1.69772	-1.9592
H	-4.56495	2.733521	2.486488	H	1.713087	-1.13904	-2.87362
H	-3.78645	4.88981	1.52813	P	1.691459	-0.59687	-0.4909
C	3.312509	-0.81912	-0.31788	P	-1.56091	-0.21597	-0.38179
C	3.626016	-2.17236	-0.44943	C	-3.00843	-1.31287	-0.41682
C	4.313818	0.064768	0.069005	C	-4.19072	-0.86445	-1.00157
C	4.908771	-2.62603	-0.2112	C	-2.93068	-2.62433	0.03534
H	2.841118	-2.88912	-0.72215	C	-5.27711	-1.71058	-1.12474
C	5.599581	-0.39278	0.30527	H	-4.26951	0.1731	-1.34994

C	-4.01782	-3.4713	-0.09634	H	1.321037	3.50113	1.955637
H	-2.02125	-2.97535	0.532773	H	-0.46343	3.484885	1.852838
C	-5.19018	-3.01694	-0.67317	H	2.187696	-2.50091	-1.87054
H	-6.20537	-1.34317	-1.5736	H	-2.08695	0.385611	-2.67557
H	-3.95048	-4.49751	0.27668				
H	-6.05155	-3.6859	-0.76437			<b>TS<sub>7-8</sub></b>	
C	-2.27861	1.391538	0.044521	C	1.199586	0.282585	2.070976
C	-2.13608	2.525096	-0.75149	H	0.364584	1.007542	2.096266
C	-2.95764	1.49863	1.26039	C	0.857299	-0.96337	2.883694
C	-2.66478	3.740541	-0.34418	H	1.782528	-1.55222	3.075035
H	-1.60096	2.47235	-1.70601	H	0.526315	-0.62311	3.890084
C	-3.48303	2.713227	1.658328	C	-0.21041	-1.91832	2.323915
H	-3.06567	0.616359	1.904046	H	0.156499	-2.45183	1.41952
C	-3.34083	3.837051	0.858781	H	-0.33437	-2.74153	3.065582
H	-2.55029	4.621007	-0.98446	C	-1.5787	-1.28737	2.09825
H	-4.01504	2.78147	2.612095	H	-1.81718	-0.60157	2.932522
H	-3.75899	4.796782	1.178022	P	-1.74444	-0.33572	0.431401
C	3.345479	-1.10608	0.059935	P	1.660176	-0.11115	0.255354
C	3.561867	-2.45141	0.355705	C	3.170475	-1.18583	0.542653
C	4.356604	-0.19304	0.340094	C	4.451333	-0.62416	0.543121
C	4.768227	-2.87751	0.87556	C	3.005027	-2.54167	0.830429
H	2.755155	-3.18035	0.206075	C	5.568066	-1.42863	0.793694
C	5.563904	-0.62126	0.867158	H	4.622093	0.438242	0.357098
H	4.20443	0.873605	0.144415	C	4.12533	-3.34665	1.07828
C	5.776617	-1.96185	1.128831	H	2.018194	-3.01844	0.861324
H	4.91773	-3.93806	1.099313	C	5.407025	-2.79356	1.054652
H	6.349641	0.110716	1.078444	H	6.564336	-0.99125	0.783452
H	6.731065	-2.29672	1.546298	H	3.988775	-4.40989	1.274042
C	2.021286	1.025616	-1.25099	H	6.277777	-3.42135	1.237772
C	2.969284	1.188292	-2.25949	C	2.411388	1.500236	-0.34582
C	1.291163	2.132504	-0.83488	C	2.168707	2.710907	0.302705
C	3.174578	2.427525	-2.83643	C	3.207658	1.460547	-1.49623
H	3.573987	0.332551	-2.58505	C	2.739439	3.890981	-0.19415
C	1.487603	3.372256	-1.41988	H	1.543549	2.778834	1.193993
H	0.551692	2.017339	-0.03342	C	3.779053	2.639976	-1.98596
C	2.430512	3.521253	-2.42082	H	3.398183	0.525626	-2.03189
H	3.927334	2.543417	-3.6228	C	3.54644	3.856023	-1.33395
H	0.894453	4.228309	-1.07933	H	2.554416	4.836505	0.312459
H	2.593878	4.500184	-2.88286	H	4.402957	2.610814	-2.87839
Ni	0.094306	-0.67045	1.006093	H	3.99289	4.773065	-1.71614
C	1.335655	-0.56284	2.511686	C	-3.40222	-0.98127	-0.17516
C	1.368468	0.879655	2.367687	C	-3.557	-2.36224	-0.32999
C	0.401628	1.733053	2.750323	C	-4.43494	-0.11014	-0.52467
C	-1.15892	-1.22128	2.240172	C	-4.76618	-2.87376	-0.81477
N	-1.99435	-1.49263	3.008396	H	-2.74982	-3.06352	-0.09989
H	0.860542	-0.91472	3.433859	C	-5.64277	-0.6265	-1.01154
H	2.303244	-1.06118	2.36443	H	-4.33288	0.972962	-0.43206
H	2.213046	1.311033	1.79683	C	-5.81053	-2.0068	-1.15274
H	-0.4652	1.32189	3.2909	H	-4.88897	-3.94886	-0.93739
C	0.401522	3.184127	2.477843	H	-6.45026	0.050394	-1.28383
H	0.321587	3.784268	3.401453	H	-6.74954	-2.40689	-1.53164

C	-2.21675	1.373616	1.105264	H	-5.98504	-3.56648	-1.15241
C	-3.2351	1.502302	2.055352	C	-2.50272	1.462718	0.422197
C	-1.52674	2.498283	0.662852	C	-2.22906	2.763622	0.000015
C	-3.54843	2.762408	2.575267	C	-3.39695	1.29201	1.481079
H	-3.80771	0.639024	2.401234	C	-2.82269	3.850889	0.618472
C	-1.83935	3.761761	1.184541	H	-1.55079	2.942026	-0.84184
H	-0.7472	2.437082	-0.11337	C	-3.98629	2.379178	2.09874
C	-2.84647	3.893649	2.142844	H	-3.66602	0.279466	1.804873
H	-4.34078	2.864595	3.314752	C	-3.69761	3.66518	1.673842
H	-1.29993	4.640547	0.836079	H	-2.60383	4.861961	0.258698
H	-3.09007	4.874078	2.549581	H	-4.69061	2.217073	2.92102
Ni	-0.03347	-0.73553	-1.01618	H	-4.16625	4.525835	2.16084
C	-1.12461	-1.18442	-2.59776	C	3.362092	-0.80443	-0.0175
C	-1.09092	0.262363	-2.55401	C	3.665162	-2.16348	0.078522
C	0.085673	0.963181	-2.63075	C	4.33029	0.125218	0.357431
C	0.610375	-2.44412	-1.203	C	4.914835	-2.57121	0.507496
N	0.922831	-3.5632	-1.28637	H	2.903029	-2.91739	-0.14856
H	-0.51817	-1.71515	-3.33886	C	5.57662	-0.29114	0.791833
H	-2.07493	-1.70051	-2.48061	H	4.112789	1.197695	0.313656
H	-2.03516	0.799921	-2.38157	C	5.875766	-1.63965	0.861422
H	1.009247	0.535181	-3.03163	H	5.134596	-3.64137	0.574275
C	0.116136	2.454114	-2.48549	H	6.324756	0.455158	1.07827
H	-0.88644	2.854015	-2.28255	H	6.863092	-1.96781	1.201657
H	0.773861	2.77805	-1.66221	C	1.937888	1.437834	-0.99863
H	0.481476	2.94416	-3.3969	C	2.853954	1.769598	-1.99555
H	-2.35548	-2.07663	2.125972	C	1.202344	2.457877	-0.40846
H	2.055224	0.797844	2.55315	C	3.019667	3.083472	-2.39289
				H	3.468139	0.986729	-2.45721
		<b>I<sub>s</sub></b>		C	1.362337	3.774351	-0.80791
C	-1.30749	0.554609	-1.97811	H	0.476191	2.206775	0.374465
H	-0.47908	1.283034	-1.94316	C	2.271175	4.089084	-1.80201
C	-0.96785	-0.56546	-2.94292	H	3.74484	3.327229	-3.17578
H	-1.90065	-1.09504	-3.21059	H	0.767282	4.560834	-0.3312
H	-0.60953	-0.10389	-3.88309	H	2.402195	5.128246	-2.12002
C	0.019888	-1.61115	-2.47341	Ni	0.112879	-0.77025	0.940513
H	-0.40644	-2.19534	-1.64075	C	-0.89356	-1.24078	2.581178
H	0.129684	-2.34505	-3.29196	C	0.35417	-0.67704	2.896932
C	1.424495	-1.16963	-2.10139	C	0.580435	0.634279	2.492905
H	1.865223	-0.55466	-2.9087	C	0.396614	-2.58597	0.569881
P	1.681197	-0.29661	-0.49536	N	0.583282	-3.71614	0.340665
P	-1.64164	0.012104	-0.25456	H	-1.77919	-0.59619	2.654194
C	-3.04225	-1.12489	-0.51162	H	-1.07481	-2.30198	2.770613
C	-2.94035	-2.46028	-0.1396	H	1.194177	-1.3069	3.220846
C	-4.21659	-0.67613	-1.11482	H	-0.29993	1.298533	2.45456
C	-3.99382	-3.33104	-0.37142	C	1.895682	1.285907	2.733355
H	-2.01762	-2.82686	0.325041	H	2.145176	2.063745	1.994418
C	-5.2652	-1.54622	-1.34296	H	1.912534	1.784653	3.719924
H	-4.31754	0.380182	-1.3952	H	2.715391	0.548363	2.727348
C	-5.15378	-2.87721	-0.97135	H	2.05099	-2.07594	-2.03808
H	-3.89978	-4.38119	-0.0776	H	-2.17916	1.117072	-2.36316
H	-6.18387	-1.18182	-1.81426				

TS <sub>8-9</sub>				I <sub>9</sub>			
C	-1.34156	0.28461	-2.0219	C	1.757517	3.847925	-0.97444
H	-0.50501	1.011313	-2.04686	H	0.564217	2.347578	0.013662
C	-1.0035	-0.9203	-2.87972	C	2.867884	4.093595	-1.76165
H	-1.8924	-1.57407	-2.94979	H	4.538908	3.229136	-2.81012
H	-0.82818	-0.54815	-3.9076	H	1.131074	4.675785	-0.62676
C	0.184148	-1.76071	-2.45416	H	3.126904	5.119199	-2.04335
H	-0.04951	-2.34036	-1.54316	Ni	0.096485	-0.52106	0.863349
H	0.343639	-2.52062	-3.23996	C	0.741539	-1.59704	2.537611
C	1.481147	-0.99221	-2.26362	C	0.968047	-0.16502	2.588917
H	1.572696	-0.19498	-3.02657	C	-0.09289	0.714888	2.60635
P	1.709817	-0.20996	-0.59534	C	0.27774	-2.3675	1.01179
P	-1.69519	-0.09574	-0.25923	N	0.241463	-3.49301	0.672022
C	-3.12762	-1.20174	-0.45413	H	-0.06935	-1.96761	3.18107
C	-3.004	-2.56015	-0.17924	H	1.65932	-2.18161	2.674562
C	-4.33803	-0.71672	-0.94765	H	1.998333	0.209945	2.506112
C	-4.07504	-3.41387	-0.39499	H	-1.06648	0.327863	2.945179
H	-2.05561	-2.95641	0.200195	C	0.078523	2.186366	2.695369
C	-5.40458	-1.57105	-1.15475	H	-0.65983	2.735871	2.086322
H	-4.45234	0.352739	-1.16261	H	-0.05431	2.543028	3.732717
C	-5.27338	-2.92318	-0.87882	H	1.085209	2.496196	2.368218
H	-3.96534	-4.48046	-0.17627	H	2.341902	-1.66199	-2.43602
H	-6.35246	-1.17686	-1.53601	H	-2.21246	0.806543	-2.46396
H	-6.1186	-3.59897	-1.04301				
C	-2.49588	1.430971	0.306404	C	-1.45864	0.626372	-2.08403
C	-2.27484	2.674161	-0.28014	H	-0.73247	1.462907	-2.07342
C	-3.28203	1.374507	1.457759	C	-0.97887	-0.46187	-3.02489
C	-2.8224	3.82407	0.268951	H	-1.77575	-1.21834	-3.14586
H	-1.66547	2.760539	-1.18656	H	-0.85065	-0.00396	-4.02473
C	-3.82908	2.519426	2.002081	C	0.314037	-1.1614	-2.64701
H	-3.47524	0.402315	1.929336	H	0.15103	-1.82876	-1.77592
C	-3.59878	3.752157	1.410193	H	0.587491	-1.83625	-3.47714
H	-2.64076	4.790941	-0.21181	C	1.466335	-0.20716	-2.36463
H	-4.44861	2.450196	2.901949	H	1.315152	0.746782	-2.90355
H	-4.03016	4.659924	1.842718	P	1.680188	0.184759	-0.5699
C	3.259815	-0.94394	-0.01269	P	-1.69098	0.090705	-0.34227
C	3.444024	-2.3254	-0.09574	C	-2.8739	-1.26706	-0.5887
C	4.19926	-0.18947	0.690904	C	-2.49333	-2.5614	-0.25292
C	4.551869	-2.92361	0.477236	C	-4.11344	-1.06296	-1.1932
H	2.691869	-2.95133	-0.58921	C	-3.33643	-3.63074	-0.51184
C	5.305576	-0.79266	1.262569	H	-1.51214	-2.7376	0.204495
H	4.069406	0.895718	0.781821	C	-4.95652	-2.12938	-1.4436
C	5.489717	-2.16057	1.152671	H	-4.43052	-0.04728	-1.46167
H	4.678507	-4.00801	0.39827	C	-4.5678	-3.41632	-1.10289
H	6.037837	-0.18108	1.799134	H	-3.01792	-4.64361	-0.24739
H	6.365951	-2.63641	1.60332	H	-5.93043	-1.95584	-1.91331
C	2.218443	1.478367	-1.04446	H	-5.23551	-4.26008	-1.3043
C	3.334021	1.739629	-1.83858	C	-2.73776	1.443958	0.274981
C	1.440077	2.547646	-0.61651	C	-2.4027	2.767884	-0.00498
C	3.657104	3.036774	-2.19041	C	-3.83226	1.202529	1.103803
H	3.968186	0.910526	-2.17562	C	-3.14807	3.814383	0.509135

H	-1.53952	2.994856	-0.64221	H	-0.74145	0.472898	-3.91238
C	-4.57587	2.249737	1.618154	C	0.291568	-1.02712	-2.78006
H	-4.11299	0.170709	1.345582	H	0.072577	-1.79914	-2.01992
C	-4.23992	3.559076	1.320404	H	0.462642	-1.5907	-3.71377
H	-2.87269	4.84596	0.266242	C	1.580402	-0.30926	-2.41452
H	-5.43604	2.036655	2.260964	H	1.692689	0.616714	-3.01054
H	-4.83209	4.385441	1.724511	P	1.751864	0.095493	-0.6274
C	3.262449	-0.62902	-0.21146	P	-1.59184	0.122642	-0.22669
C	3.496278	-1.91675	-0.69151	C	-2.81789	-1.13795	-0.68777
C	4.174896	-0.07728	0.685612	C	-2.48757	-2.48566	-0.58112
C	4.614753	-2.62766	-0.29606	C	-4.03978	-0.78381	-1.26178
H	2.77113	-2.3968	-1.35982	C	-3.36956	-3.45867	-1.02339
C	5.29588	-0.78813	1.076573	H	-1.51673	-2.77743	-0.16237
H	4.004186	0.929828	1.084444	C	-4.91844	-1.75759	-1.69634
C	5.519518	-2.06544	0.588321	H	-4.31198	0.273814	-1.36227
H	4.7755	-3.64024	-0.67894	C	-4.58533	-3.09802	-1.57478
H	6.007587	-0.33574	1.775119	H	-3.09454	-4.51383	-0.93481
H	6.404568	-2.62754	0.902323	H	-5.87651	-1.46716	-2.13883
C	2.144037	1.941197	-0.6137	H	-5.28238	-3.8683	-1.91972
C	3.190915	2.410038	-1.40555	C	-2.63264	1.458858	0.449892
C	1.41183	2.853063	0.140165	C	-2.27301	2.792423	0.25513
C	3.493308	3.758206	-1.4443	C	-3.76558	1.191146	1.217916
H	3.786787	1.701123	-1.9939	C	-3.01538	3.819018	0.812514
C	1.71294	4.205334	0.099825	H	-1.39704	3.047576	-0.35096
H	0.594134	2.484227	0.775721	C	-4.508	2.217866	1.771387
C	2.75276	4.657846	-0.69287	H	-4.08732	0.154743	1.371739
H	4.319483	4.114559	-2.0677	C	-4.13495	3.536751	1.573917
H	1.130459	4.911595	0.699709	H	-2.71462	4.857206	0.638535
H	2.99455	5.725007	-0.72419	H	-5.39728	1.981181	2.364215
Ni	0.088426	-0.30635	0.763698	H	-4.72419	4.347603	2.012272
C	1.647475	-2.24782	2.286541	C	3.464539	-0.36753	-0.23641
C	0.916833	-0.935	2.396864	C	3.961226	-1.60885	-0.63066
C	-0.48181	-0.87826	2.529426	C	4.274269	0.467708	0.530001
C	1.115985	-3.10854	1.245864	C	5.247573	-1.98408	-0.29127
N	0.700101	-3.79257	0.410072	H	3.323501	-2.31675	-1.16883
H	1.625395	-2.8219	3.236449	C	5.557978	0.081605	0.873198
H	2.717373	-2.0901	2.059676	H	3.902707	1.441544	0.866535
H	1.516589	-0.15973	2.90055	C	6.051077	-1.14152	0.457105
H	-1.03603	-1.83259	2.487553	H	5.619983	-2.96322	-0.60703
C	-1.12258	0.186136	3.357669	H	6.180708	0.753207	1.472666
H	-2.16199	0.395938	3.058071	H	7.067367	-1.4456	0.726023
H	-1.14706	-0.08214	4.432551	C	1.849097	1.907698	-0.53935
H	-0.57054	1.139697	3.280914	C	2.645711	2.647242	-1.41131
H	2.417642	-0.60968	-2.75435	C	1.161115	2.575197	0.467087
H	-2.40155	1.055128	-2.47307	C	2.729803	4.021639	-1.29196
				H	3.230959	2.13386	-2.1836
				C	1.244801	3.953087	0.589147
C	-1.23356	0.8486	-1.88616	H	0.538239	2.0017	1.168543
H	-0.41055	1.578062	-1.76899	C	2.025963	4.677192	-0.29335
C	-0.90422	-0.12711	-2.99609	H	3.358718	4.590772	-1.98352
H	-1.78808	-0.75586	-3.20744	H	0.690528	4.461894	1.384616

H	2.094189	5.765623	-0.20074	H	4.77157	2.366237	-2.60967
Ni	0.205841	-0.87211	0.663884	H	4.009733	4.692468	-2.17567
C	-1.2086	-0.40666	2.98219	C	-3.49289	-0.73348	0.059037
C	-0.57948	-1.59381	2.300469	C	-3.84131	-2.05917	0.314158
C	0.565264	-2.07399	3.082534	C	-4.38122	0.071349	-0.65143
C	0.952175	-2.50824	0.27583	C	-5.0608	-2.55356	-0.10711
N	1.304144	-3.52153	-0.18744	H	-3.13046	-2.73444	0.800765
H	-0.59389	0.512887	2.882689	C	-5.5977	-0.43241	-1.07621
H	-1.31855	-0.57262	4.072151	H	-4.12544	1.111327	-0.88
H	-1.30992	-2.40324	2.121825	C	-5.9437	-1.74267	-0.79992
H	1.257602	-1.28498	3.427716	H	-5.31501	-3.59827	0.095632
C	0.829418	-3.33028	3.43038	H	-6.28551	0.21376	-1.63039
H	-2.20531	-0.16482	2.591949	H	-6.90615	-2.1399	-1.13744
H	1.718381	-3.59378	4.009216	C	-2.10662	1.671211	0.506331
H	0.188898	-4.15634	3.103098	C	-2.96009	2.328775	1.390703
H	2.444108	-0.94108	-2.68114	C	-1.46134	2.414297	-0.4764
H	-2.11438	1.44611	-2.18663	C	-3.13988	3.697033	1.306875
				H	-3.51253	1.757856	2.146248
		<b>I<sub>10</sub></b>		C	-1.64364	3.785094	-0.56429
C	0.951546	0.977274	2.008921	H	-0.78912	1.907383	-1.18221
H	0.074926	1.637522	1.872956	C	-2.47872	4.428073	0.33152
C	0.666876	-0.06318	3.074884	H	-3.81152	4.201238	2.008468
H	1.609189	-0.57429	3.342223	H	-1.11989	4.352893	-1.34015
H	0.35381	0.478396	3.988061	H	-2.62272	5.511125	0.268471
C	-0.37172	-1.11562	2.747029	Ni	-0.12446	-0.83571	-0.64146
H	0.002553	-1.8044	1.964503	C	2.8726	-2.70088	-2.51367
H	-0.50503	-1.74549	3.643919	C	1.565376	-2.44426	-2.48209
C	-1.73214	-0.58422	2.327417	C	0.96849	-1.14199	-2.22804
H	-2.03032	0.274673	2.958407	C	-0.77892	-2.5695	-0.69008
P	-1.85426	-0.12823	0.549436	N	-1.12839	-3.67452	-0.54646
P	1.423245	0.294859	0.372195	H	3.616921	-1.90998	-2.35122
C	2.785116	-0.80762	0.847021	H	3.262517	-3.7084	-2.67978
C	2.623566	-2.18451	0.742036	H	0.858863	-3.27519	-2.6284
C	3.961486	-0.29782	1.395126	H	1.742193	-0.35268	-2.28055
C	3.626096	-3.03694	1.176324	C	-0.19293	-0.7844	-3.12028
H	1.705686	-2.59174	0.299084	H	-0.84471	0.010113	-2.69282
C	4.959234	-1.15145	1.825116	H	0.147255	-0.38396	-4.09515
H	4.101832	0.787349	1.477483	H	-0.84335	-1.65297	-3.30917
C	4.791361	-2.52373	1.714504	H	-2.49803	-1.35908	2.499728
H	3.491938	-4.11859	1.079636	H	1.76806	1.636191	2.359536
H	5.880869	-0.7421	2.251063				
H	5.58412	-3.19915	2.051623			<b>TS<sub>10-11</sub></b>	
C	2.288355	1.701832	-0.3808	C	-1.10106	1.038942	-1.90961
C	1.875072	3.01239	-0.14299	H	-0.2552	1.723551	-1.70862
C	3.337107	1.491056	-1.27694	C	-0.7314	0.083955	-3.02751
C	2.489104	4.074786	-0.78163	H	-1.62977	-0.4883	-3.32444
H	1.06058	3.217594	0.559442	H	-0.46734	0.697869	-3.91009
C	3.946573	2.554812	-1.91604	C	0.392339	-0.90066	-2.76722
H	3.701237	0.473165	-1.45829	H	0.080612	-1.6695	-2.0354
C	3.523658	3.850626	-1.67313	H	0.557873	-1.45859	-3.70623
H	2.156405	5.096235	-0.57067	C	1.723858	-0.30437	-2.33737

H	1.939071	0.619056	-2.90924	C	0.496012	-2.49556	0.477553
P	1.888105	0.048236	-0.5282	N	0.650847	-3.58069	0.047854
P	-1.55331	0.234538	-0.32161	H	-2.32346	-0.78033	3.315052
C	-2.9334	-0.81722	-0.8711	H	-3.43274	-2.26521	3.094431
C	-2.76963	-2.19827	-0.90724	H	-1.59882	-3.49742	2.030813
C	-4.12433	-0.26492	-1.33803	H	-0.07159	-0.82686	2.43704
C	-3.77847	-3.0094	-1.40162	C	0.968098	-2.62728	2.971256
H	-1.83464	-2.648	-0.54981	H	1.974665	-2.26812	2.705511
C	-5.13308	-1.0774	-1.82155	H	0.80407	-2.4395	4.046857
H	-4.26759	0.82213	-1.31125	H	0.942982	-3.71383	2.802164
C	-4.96049	-2.45224	-1.85497	H	2.534849	-1.00762	-2.59425
H	-3.6352	-4.09391	-1.42741	H	-1.93794	1.680601	-2.24701
H	-6.06654	-0.63175	-2.18056				
H	-5.75913	-3.09465	-2.23891			<b>I<sub>11</sub></b>	
C	-2.41887	1.592141	0.524285	C	-1.29779	1.021866	-1.99119
C	-2.05115	2.926186	0.349157	H	-0.4877	1.745779	-1.77364
C	-3.41981	1.29923	1.452154	C	-0.87259	0.098007	-3.11842
C	-2.66787	3.931487	1.074851	H	-1.73652	-0.52437	-3.41747
H	-1.27229	3.197881	-0.37099	H	-0.65186	0.734402	-3.99711
C	-4.03591	2.305481	2.17154	C	0.316273	-0.81823	-2.88648
H	-3.73601	0.258986	1.593939	H	0.066069	-1.60664	-2.14856
C	-3.66068	3.627096	1.988816	H	0.491741	-1.35896	-3.83437
H	-2.36998	4.972734	0.913139	C	1.612037	-0.13391	-2.4798
H	-4.82793	2.053945	2.883903	H	1.698576	0.851709	-2.97636
H	-4.14998	4.42328	2.558168	P	1.82257	0.111777	-0.65036
C	3.537034	-0.60423	-0.1441	P	-1.69161	0.165571	-0.41809
C	3.787909	-1.95492	-0.3963	C	-3.04889	-0.92376	-0.95641
C	4.511075	0.145343	0.5109	C	-2.8506	-2.30093	-0.96809
C	4.990383	-2.52606	-0.02448	C	-4.26375	-0.41158	-1.40751
H	3.015081	-2.58333	-0.85553	C	-3.84721	-3.14896	-1.4253
C	5.712109	-0.43445	0.883925	H	-1.89821	-2.71334	-0.61073
H	4.333684	1.201582	0.740034	C	-5.25918	-1.25982	-1.85718
C	5.958902	-1.76809	0.613639	H	-4.43858	0.671336	-1.39584
H	5.166938	-3.58675	-0.22838	C	-5.05099	-2.63072	-1.86831
H	6.467329	0.171919	1.394039	H	-3.67854	-4.23047	-1.42901
H	6.908359	-2.22411	0.909975	H	-6.21211	-0.84665	-2.20489
C	2.13959	1.845379	-0.43561	H	-5.84044	-3.30092	-2.22369
C	3.016028	2.533934	-1.27267	C	-2.58385	1.442743	0.517595
C	1.415942	2.567738	0.507837	C	-2.37134	2.807147	0.328643
C	3.151846	3.906492	-1.17422	C	-3.43679	1.040669	1.547425
H	3.617334	1.981723	-2.0051	C	-2.99978	3.739525	1.140453
C	1.546672	3.943184	0.60597	H	-1.70357	3.158559	-0.46612
H	0.721589	2.037367	1.174612	C	-4.06855	1.971899	2.349456
C	2.413199	4.614443	-0.23795	H	-3.60788	-0.03004	1.718101
H	3.845294	4.433549	-1.83695	C	-3.8513	3.327172	2.14955
H	0.959222	4.492391	1.349047	H	-2.82479	4.807411	0.972549
H	2.518672	5.701567	-0.16665	H	-4.74302	1.635139	3.143551
Ni	0.207713	-0.74209	0.568283	H	-4.3498	4.064796	2.785749
C	-2.44966	-1.80752	2.951813	C	3.397749	-0.72799	-0.31885
C	-1.45201	-2.46043	2.36687	C	3.531766	-2.06075	-0.71571
C	-0.0974	-1.92309	2.164043	C	4.393326	-0.1725	0.48465





H	0.239486	-0.85577	2.18544	H	4.998856	-3.58246	-1.07249
C	1.831258	-2.14286	2.848531	H	6.217305	-0.5117	1.67285
H	2.608528	-1.73898	2.183174	H	6.639108	-2.69774	0.572792
H	1.891899	-1.61369	3.812235	C	2.194088	1.911579	-0.39911
H	2.050965	-3.2079	3.023612	C	3.172709	2.580523	-1.1331
H	2.490808	-0.67676	-2.79027	C	1.405867	2.645971	0.482127
H	-2.10853	1.673249	-2.2614	C	3.348557	3.945224	-0.99391
		<b>I<sub>12</sub></b>		H	3.815052	2.018861	-1.82297
C	-1.23699	1.162923	-1.92255	C	1.575953	4.014134	0.618297
H	-0.42525	1.873852	-1.67009	H	0.632196	2.126759	1.064367
C	-0.81624	0.291182	-3.09222	C	2.547003	4.665662	-0.12101
H	-1.68729	-0.30392	-3.42464	H	4.120885	4.457109	-1.57678
H	-0.58398	0.966625	-3.9382	H	0.938081	4.573509	1.310325
C	0.355582	-0.65605	-2.90033	H	2.683914	5.747014	-0.01898
H	0.084739	-1.47284	-2.20228	Ni	0.13173	-0.63952	0.352451
H	0.524138	-1.15307	-3.87331	C	-1.80943	-3.08259	2.771075
C	1.665	-0.02468	-2.45164	C	-0.83926	-2.25042	3.113765
H	1.7932	0.973238	-2.91367	C	0.341653	-1.87191	2.276473
P	1.844656	0.137368	-0.60801	C	0.2989	-2.49421	0.942551
P	-1.63594	0.232727	-0.3917	N	0.303762	-3.29256	0.079268
C	-3.06917	-0.74374	-0.95525	H	-1.81587	-3.59124	1.800427
C	-2.93634	-2.12185	-1.09522	H	-2.64108	-3.29029	3.448043
C	-4.28483	-0.14578	-1.28128	H	-0.85971	-1.75301	4.094253
C	-3.99964	-2.88564	-1.54886	H	0.301122	-0.7381	2.156474
H	-1.9809	-2.60149	-0.84485	C	1.671502	-2.18204	2.946691
C	-5.347	-0.91062	-1.72587	H	2.515121	-1.84884	2.322268
H	-4.40609	0.939281	-1.16977	H	1.735611	-1.66509	3.917278
C	-5.20585	-2.283	-1.85951	H	1.772776	-3.26392	3.122119
H	-3.88336	-3.9691	-1.655	H	2.512678	-0.63245	-2.81472
H	-6.29996	-0.43053	-1.97151	H	-2.10219	1.781593	-2.23422
H	-6.04815	-2.88843	-2.20979			<b>TS<sub>12-13</sub></b>	
C	-2.43329	1.494333	0.639564	C	-1.57257	0.732793	-1.97604
C	-2.24904	2.864023	0.466719	H	-0.76001	1.481906	-1.9073
C	-3.19513	1.059773	1.725743	C	-1.26192	-0.25635	-3.08173
C	-2.81835	3.769823	1.347875	H	-2.13935	-0.91009	-3.24205
H	-1.65017	3.241986	-0.36897	H	-1.1445	0.316963	-4.02137
C	-3.77191	1.964131	2.594441	C	-0.03689	-1.13093	-2.89
H	-3.3372	-0.01758	1.885656	H	-0.21856	-1.86847	-2.08275
C	-3.58425	3.325852	2.409937	H	0.088079	-1.72843	-3.81131
H	-2.66653	4.843097	1.192057	C	1.261239	-0.38872	-2.6112
H	-4.37685	1.602497	3.432085	H	1.298523	0.55141	-3.19471
H	-4.03767	4.043391	3.101006	P	1.573794	-0.01211	-0.81558
C	3.453245	-0.64843	-0.3045	P	-1.75268	-0.03777	-0.31832
C	3.692537	-1.88936	-0.90072	C	-3.194	-1.11098	-0.61667
C	4.370212	-0.17309	0.630965	C	-3.03874	-2.49022	-0.52491
C	4.828544	-2.61324	-0.59329	C	-4.43512	-0.5899	-0.97881
H	2.95663	-2.31111	-1.59841	C	-4.10691	-3.33172	-0.79455
C	5.503791	-0.90477	0.940946	H	-2.06633	-2.89854	-0.22131
H	4.196261	0.788506	1.126712	C	-5.49869	-1.43139	-1.2457
C	5.741401	-2.12226	0.32685	H	-4.57327	0.497292	-1.0386

C	-5.33463	-2.80516	-1.15463	H	2.113866	-0.99195	-2.97011
H	-3.97735	-4.41601	-0.7152	H	-2.48737	1.298542	-2.23966
H	-6.47086	-1.01215	-1.52483				
H	-6.17803	-3.4714	-1.36285				
C	-2.50457	1.304259	0.648697	C	-1.62974	0.871679	-2.00913
C	-2.35203	2.653982	0.338715	H	-0.94334	1.738623	-1.93314
C	-3.16864	0.969702	1.830692	C	-1.12612	-0.09808	-3.06328
C	-2.83696	3.6346	1.189703	H	-1.88958	-0.87988	-3.23041
H	-1.83691	2.958652	-0.57843	H	-1.05291	0.455409	-4.01895
C	-3.66069	1.947236	2.67267	C	0.208932	-0.76541	-2.78405
H	-3.30086	-0.08886	2.089521	H	0.098608	-1.52302	-1.98153
C	-3.49114	3.287447	2.357678	H	0.491364	-1.34111	-3.68299
H	-2.70818	4.689575	0.92557	C	1.323859	0.208696	-2.42856
H	-4.18536	1.660969	3.589841	H	1.108041	1.209767	-2.84662
H	-3.87536	4.063882	3.026241	P	1.586247	0.406494	-0.60729
C	3.288086	-0.5747	-0.6024	P	-1.75975	0.13897	-0.33528
C	3.595419	-1.90461	-0.9007	C	-2.95112	-1.19752	-0.64611
C	4.24868	0.184373	0.067498	C	-2.50992	-2.51598	-0.59611
C	4.821051	-2.44767	-0.56429	C	-4.2719	-0.9373	-1.00536
H	2.842305	-2.53909	-1.38645	C	-3.3753	-3.55564	-0.89702
C	5.473328	-0.36351	0.410614	H	-1.4684	-2.73122	-0.32329
H	4.03502	1.227471	0.328961	C	-5.1353	-1.97688	-1.29755
C	5.767534	-1.67923	0.096261	H	-4.63459	0.097686	-1.04341
H	5.039054	-3.49112	-0.81546	C	-4.68721	-3.28779	-1.24365
H	6.213336	0.253606	0.930753	H	-3.01369	-4.5876	-0.85638
H	6.735567	-2.10983	0.368705	H	-6.17342	-1.7627	-1.57247
C	1.796758	1.801816	-0.82505	H	-5.37289	-4.10908	-1.47514
C	2.623671	2.467836	-1.7288	C	-2.75635	1.36287	0.555668
C	1.086425	2.555817	0.103265	C	-2.73939	2.720022	0.243243
C	2.725626	3.847041	-1.7079	C	-3.48907	0.945187	1.666741
H	3.210662	1.892828	-2.45609	C	-3.44867	3.629781	1.010951
C	1.178465	3.938343	0.120893	H	-2.16493	3.084518	-0.61589
H	0.433582	2.035256	0.816657	C	-4.20013	1.853359	2.426988
C	1.99843	4.585651	-0.7859	H	-3.50859	-0.11987	1.929476
H	3.380345	4.356483	-2.42226	C	-4.18265	3.200301	2.101362
H	0.598255	4.51185	0.852014	H	-3.43103	4.691783	0.744718
H	2.075898	5.677482	-0.7769	H	-4.77891	1.504318	3.288139
Ni	0.070416	-0.80412	0.43898	H	-4.74597	3.919449	2.7035
C	0.056289	-0.04218	2.839833	C	3.231391	-0.32591	-0.37979
C	1.350063	-0.26587	2.579877	C	3.547591	-1.52266	-1.02048
C	1.90123	-1.66759	2.391018	C	4.113837	0.170761	0.577829
C	0.928403	-2.26932	1.474404	C	4.716832	-2.19847	-0.7198
N	0.011116	-2.87951	1.042791	H	2.847399	-1.96513	-1.73982
H	-0.65875	-0.86419	2.970151	C	5.286175	-0.50301	0.872105
H	-0.33831	0.968888	2.98192	H	3.875364	1.103303	1.10319
H	2.058328	0.569491	2.49937	C	5.591235	-1.6899	0.225004
H	2.8687	-1.60066	1.859332	H	4.942483	-3.14087	-1.22826
C	2.085697	-2.44323	3.682948	H	5.973158	-0.09399	1.620307
H	2.498502	-3.44517	3.492709	H	6.516158	-2.22403	0.462744
H	2.777757	-1.90412	4.348267	C	1.907363	2.188537	-0.46305
H	1.1279	-2.55813	4.212164	C	2.950586	2.817418	-1.1384

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C	1.042599	2.959914	0.307199
C	3.122106	4.186239	-1.0443
H	3.647841	2.219676	-1.73854
C	1.211345	4.332282	0.397723
H	0.226656	2.463807	0.851988
C	2.251109	4.945347	-0.27793
H	3.948445	4.670278	-1.57518
H	0.523733	4.925293	1.009089
H	2.389899	6.028774	-0.20516
Ni	0.052917	-0.34115	0.663134
C	-0.51276	-1.21175	2.280579
C	0.89089	-1.14502	2.204758
C	1.721544	-2.38062	1.942828
C	1.220424	-3.09703	0.772179
N	0.831109	-3.66926	-0.15585
H	-1.03305	-2.16696	2.108475
H	-1.0491	-0.53027	2.954411
H	1.42172	-0.41034	2.829708
H	2.751812	-2.06958	1.674151
C	1.794331	-3.31247	3.143662
H	2.413919	-4.20142	2.946298
H	2.228883	-2.77013	3.996898
H	0.786969	-3.64511	3.43665
H	2.279507	-0.09358	-2.89114
H	-2.60781	1.282439	-2.32523

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