

Supplementary Information

Can the Solvent Enhance the Rate of Chemical Reactions through C-H/ π Interactions? Insights from Theory

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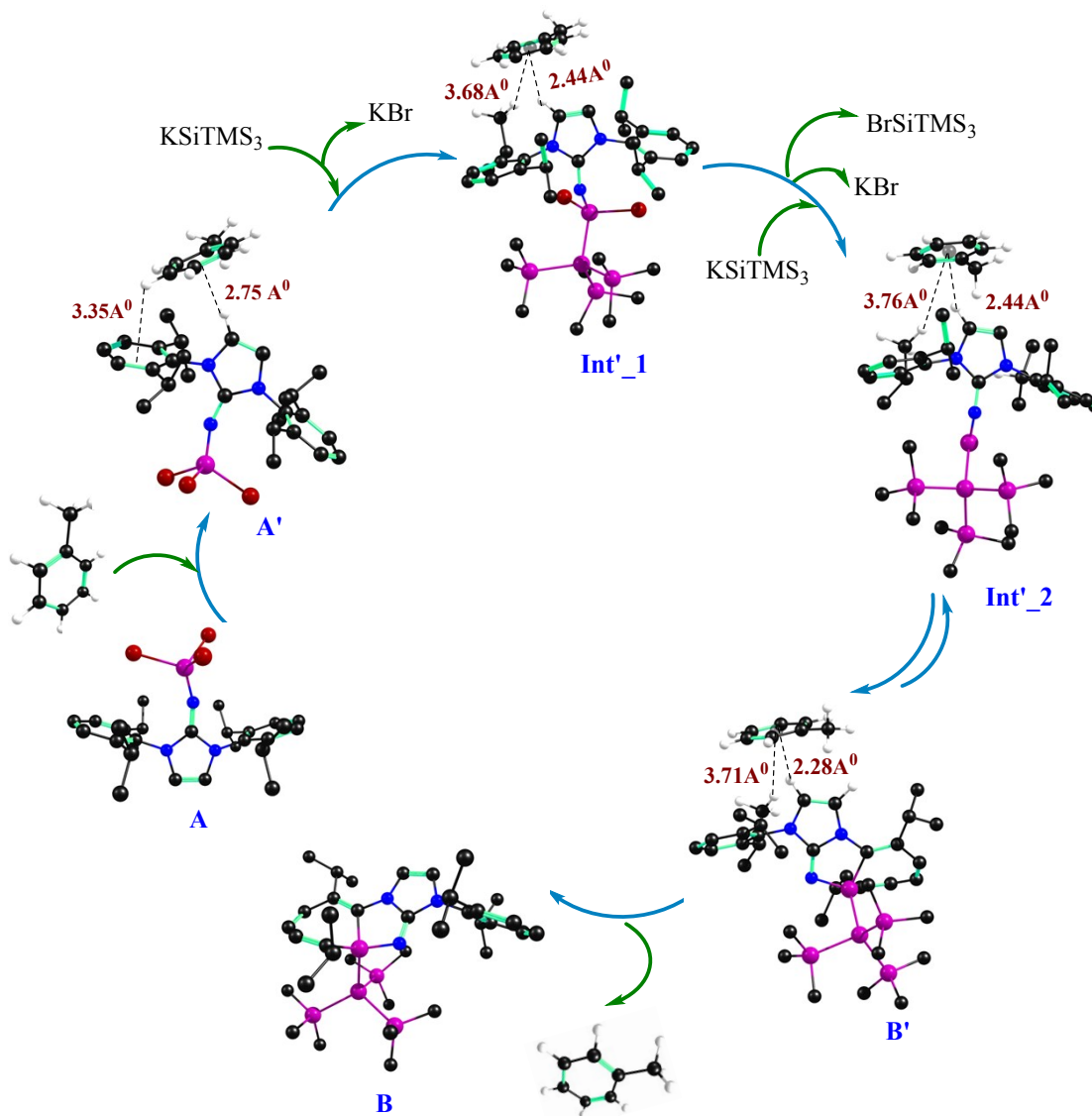
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Introduction

As discussed in the manuscript, in order to understand the orientation of toluene for the C-H/ π interactions with the reactant and intermediate complexes, the 3-D Figures for Scheme 1 b) are provided below in Scheme S1.



Scheme S1. The proposed mechanism for the formation of thesilepin complex in the presence of toluene.

Results and Discussion

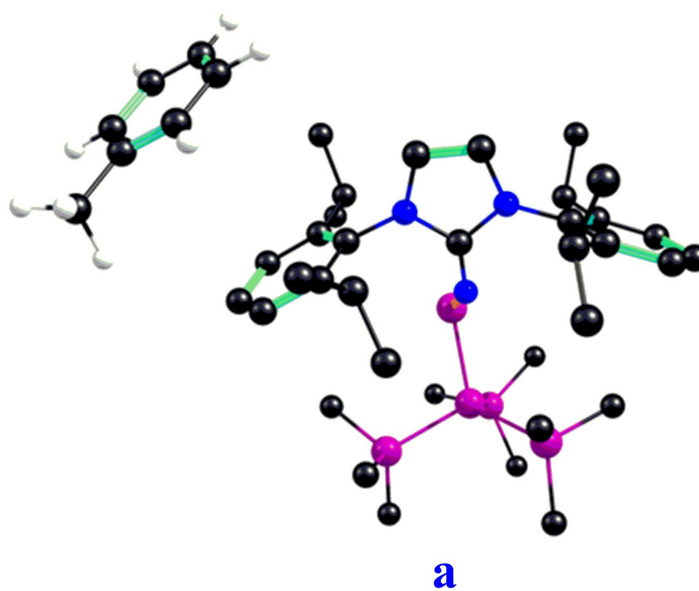
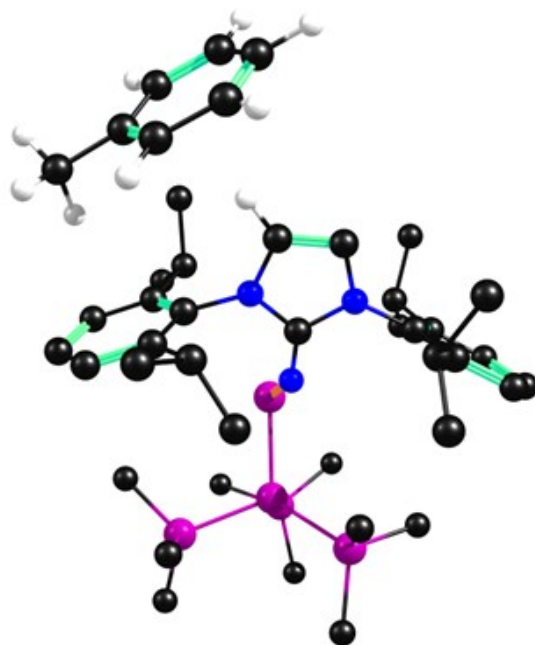
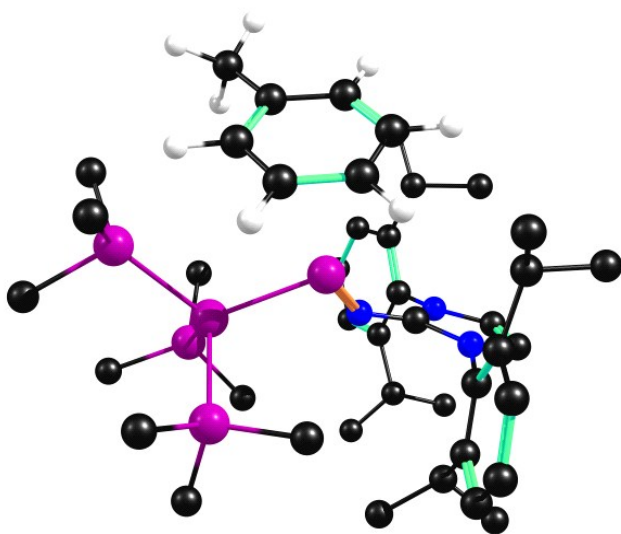


Fig. S1 The starting (*input*) geometry where toluene was added above the di-isopropyl phenyl (*dipp*) rings, for possible π - π stacking interactions. Hydrogen atoms (except in toluene) have been removed for the purpose of clarity.



b

Fig. S2 The final (output) geometry where toluene was added above the di-isopropyl phenyl (*dipp*) rings, for possible π - π stacking interactions. Hydrogen atoms (except in toluene) have been removed for the purpose of clarity.



c

Fig. S3 The starting (*input*) geometry where toluene was added at the silicon center, for the lone pair- π interactions. Hydrogen atoms (except in toluene) have been removed for the purpose of clarity.

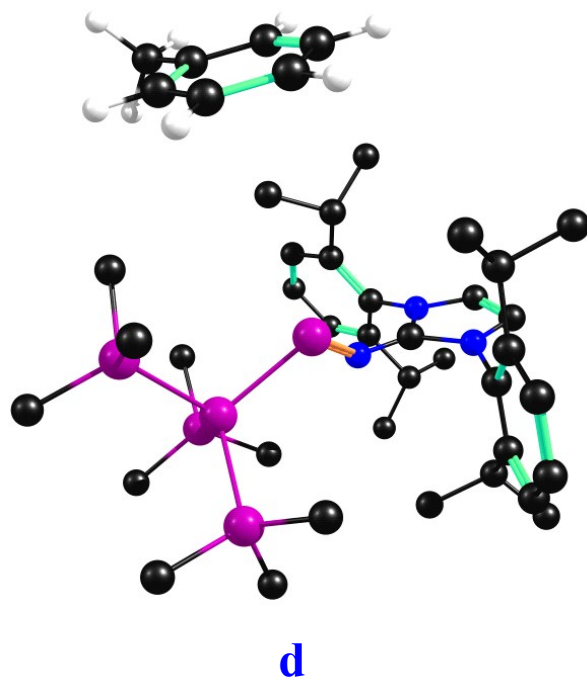


Fig. S4 The final (*output*) geometry where toluene was added at the silicon center, for lone pair- π interactions. Hydrogen atoms (except in toluene) have been removed for the purpose of clarity.

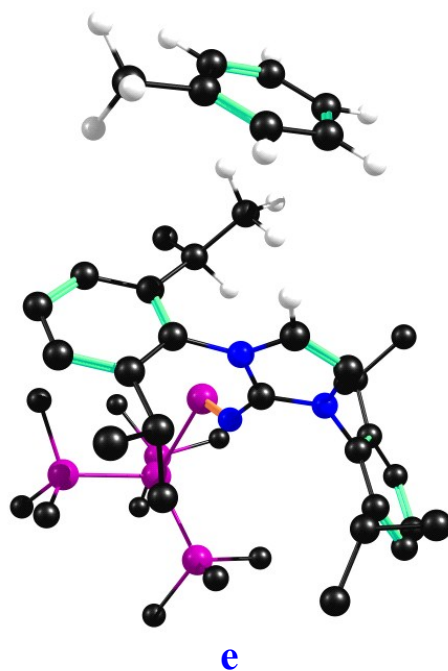
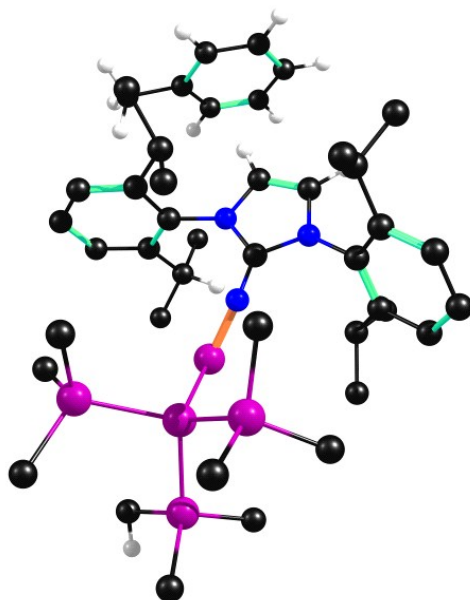


Fig. S5 The starting (input) geometry where toluene was added the C-H of the methyl group of *dipp*, for CH/π interactions. Hydrogen atoms (except in toluene) have been removed for the purpose of clarity.



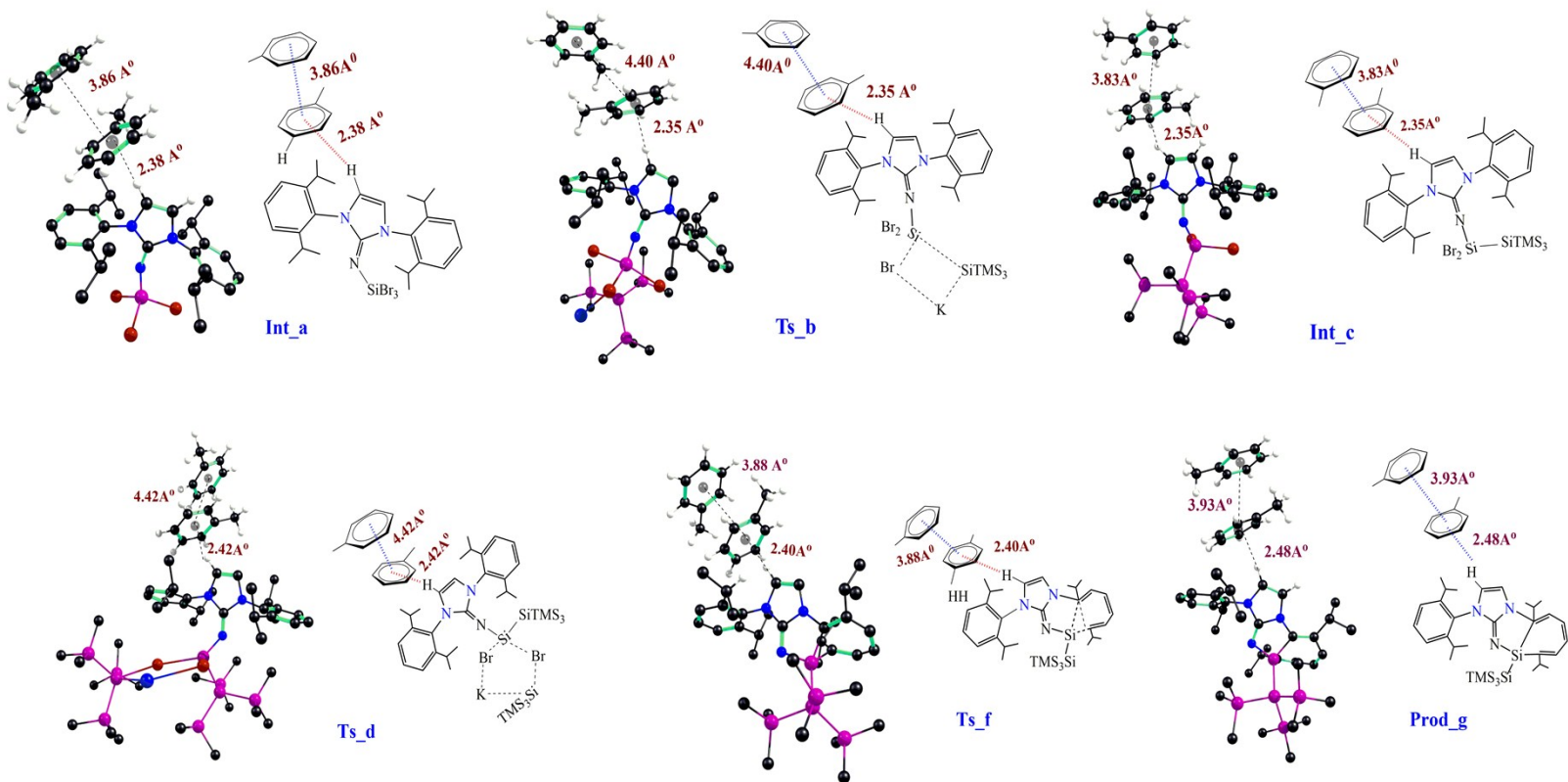
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Fig. S6 The final (output) geometry where toluene was added above the C-H of the methyl group of *dipp*, for CH/π interactions. Hydrogen atoms (except in toluene) have been removed for the purpose of clarity.

As discussed in manuscript the NBO analysis results are given in Table S1. Calculation suggest that (at B3-lyp/6-31g** level of theory) interaction energy higher in presence of toluene than in the absence of toluene (see Table S1 below).

Table S1 NBo results (second order perturbation energy E(2) in kcal/mol) for a) Ts'_2 and b) Ts_2.

Donor	Occupancy	Acceptor	Occupancy	a) E (2) in the presence of toluene	b) E(2) in the absence of toluene
LP (1) Si 25	1.51439	BD*(1) Br 26	0.61011	59.98	26.08
		-Si 46			
LP (4) Br 33	1.65152	LP* (2)Si 25	0.46303	130.30	139.87



As discussed in the manuscript to check the effect of solvent-solvent interaction we have performed quantum chemical calculations for the silepin formation complex in the presence of two toluene. Optimized geometry, as well as ChemDraw figures for the transition states, intermediates and product in the presence of two explicit toluene molecules, have provided below.

Fig. S7 The optimized geometries of the transition states, intermediates and product in the presence of two toluene molecules, where C-H/ π non-covalent interaction between solvent-substrate and π - π stacking noncovalent interaction between solvent-solvent have been shown. Hydrogen atoms (except for toluene) have been removed for the purpose of clarity.

To find the reason why energy barriers reduce in the presence of two toluene, we have performed NBO analysis at B3-lyp/6-31g**/D-2 level of theory for **Ts_d**. NBO results have summarized in Table S2.

Table S2 NBO results (second order perturbation energy E(2) in kcal/mol) for **Ts_d**.

Donor		Acceptor		E (2) in the presence of two toluene
Occupancy		Occupancy		
LP (1) Si 25	1.2439	BD*(1) Br 26 -Si 46	0.52361	60.98
LP (4) Br 33	1.65142	LP* (2)Si 25	0.50131	143.12

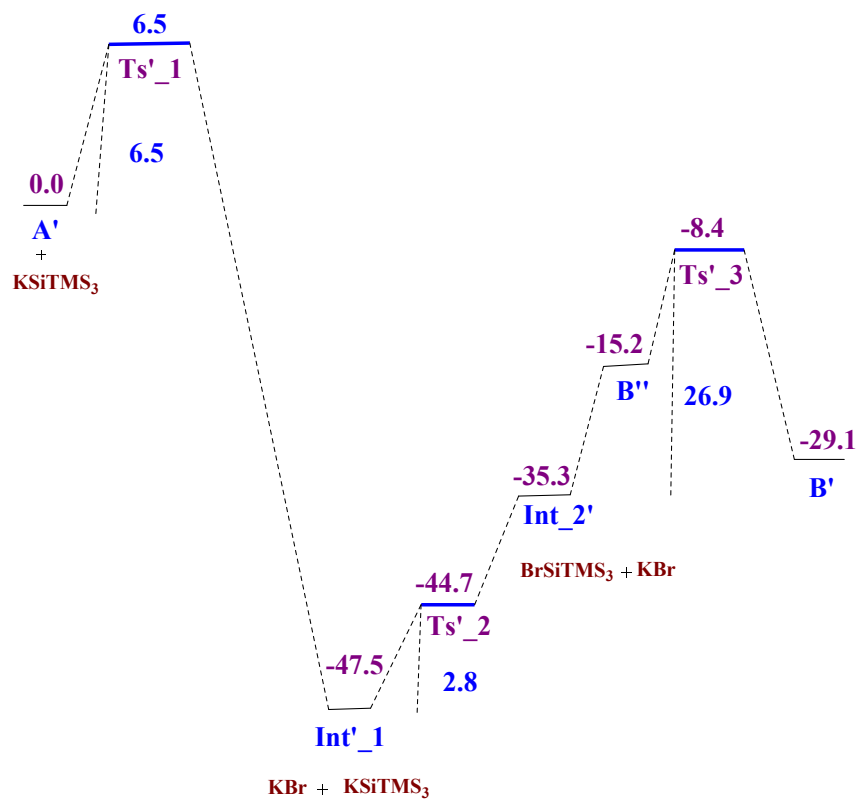


Fig. S8 The electronic energy profile (ΔE in kcal/mol) for the formation of the silepin complex **B'** in the presence of toluene at the TPSS-D3/def2-TZVP//B3-lyp-D3/TZVP level of theory.

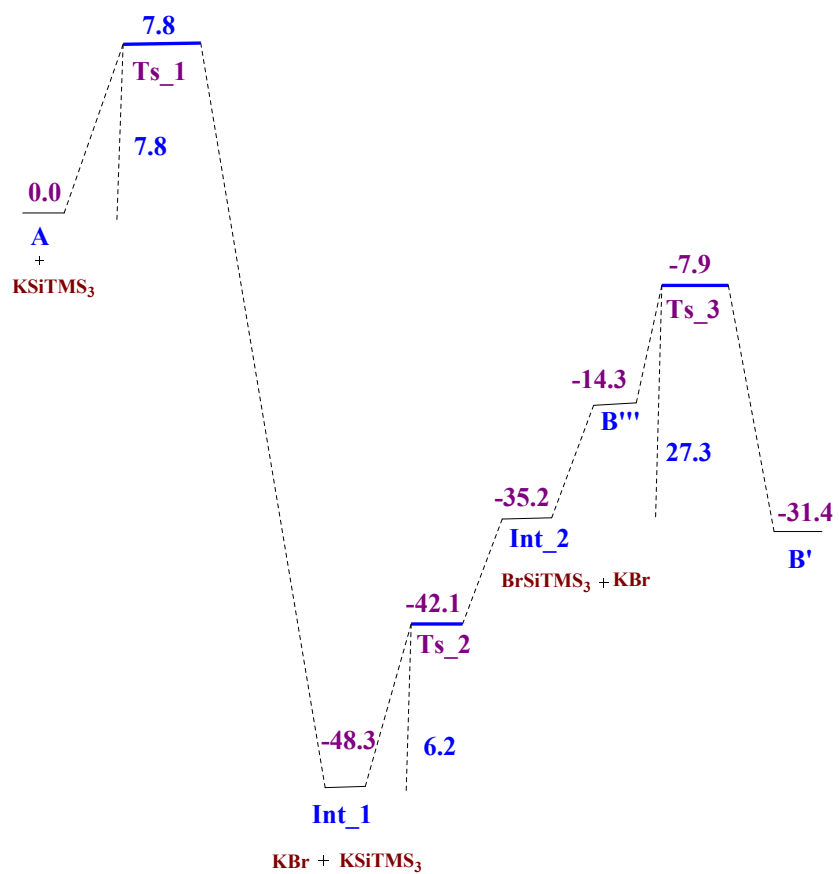


Fig. S9 The electronic energy profile (ΔE in kcal/mol) for the formation of the silepin complex **B'** in the absence of toluene at the TPSS-D3/def2-TZVP//B3-lyp-D3/TZVP level of theory.

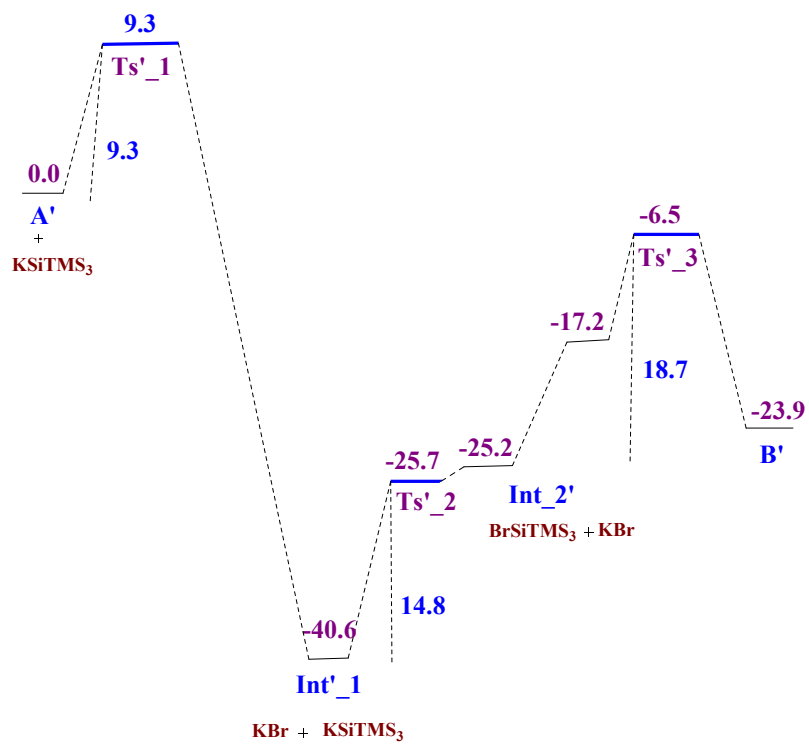


Fig. S10 The electronic energy profile (ΔE in kcal/mol) for the formation of silepin complex **B'** in the presence of toluene at the TPSS-D3/def2-TZVP//M06-2x/TZVP level of theory.

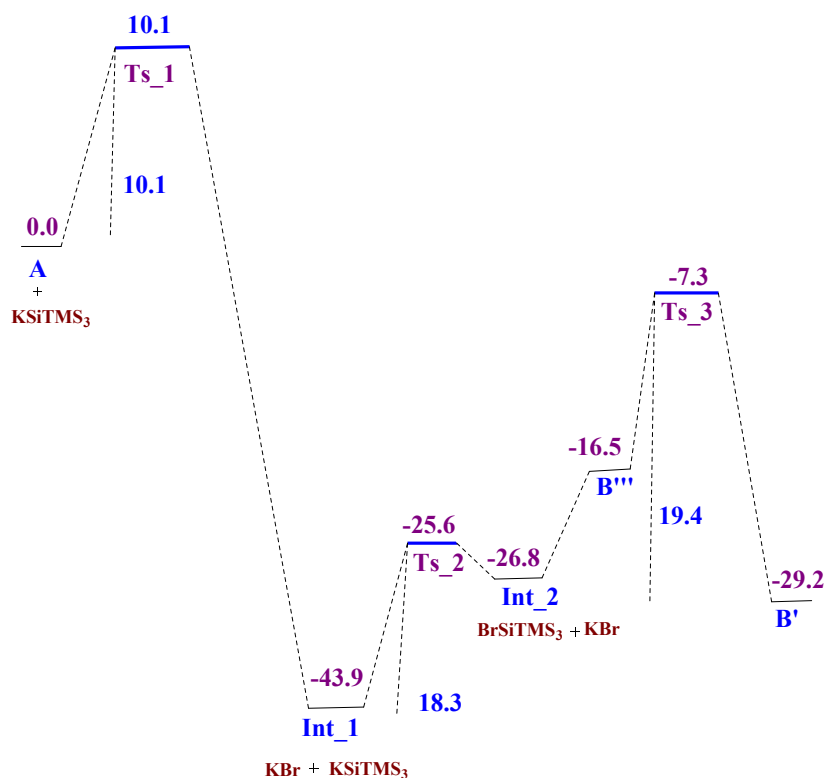


Fig. S11 The electronic energy profile (ΔE in kcal/mol) for the formation of silepin complex B' in the presence of toluene at the TPSS-D3/def2-TZVP//M06-2x/TZVP level of theory.

As discussed in manuscript, in order to further validate this result, we have employed *ab initio* molecular dynamics (AIMD) simulations at room temperature. We began by placing three toluene solvent molecules randomly around **Int_2**. We observed that after 6182 steps (corresponding to about 3.0 picoseconds (ps)), only one interaction remained. This structure possessed the same C-H/ π non-covalent interaction that had been found to be the most favourable (structure (i), discussed above) in the static DFT calculations. Moreover, once the interaction was formed, it remained for the duration of the AIMD simulation, up to 17,182 steps. The snapshots obtained from the simulations have been shown below in Fig. S12. These interesting results provide clear indication that the C-H/ π noncovalent interaction between solvent and substrate indeed predominates over other non-covalent interactions in this system.

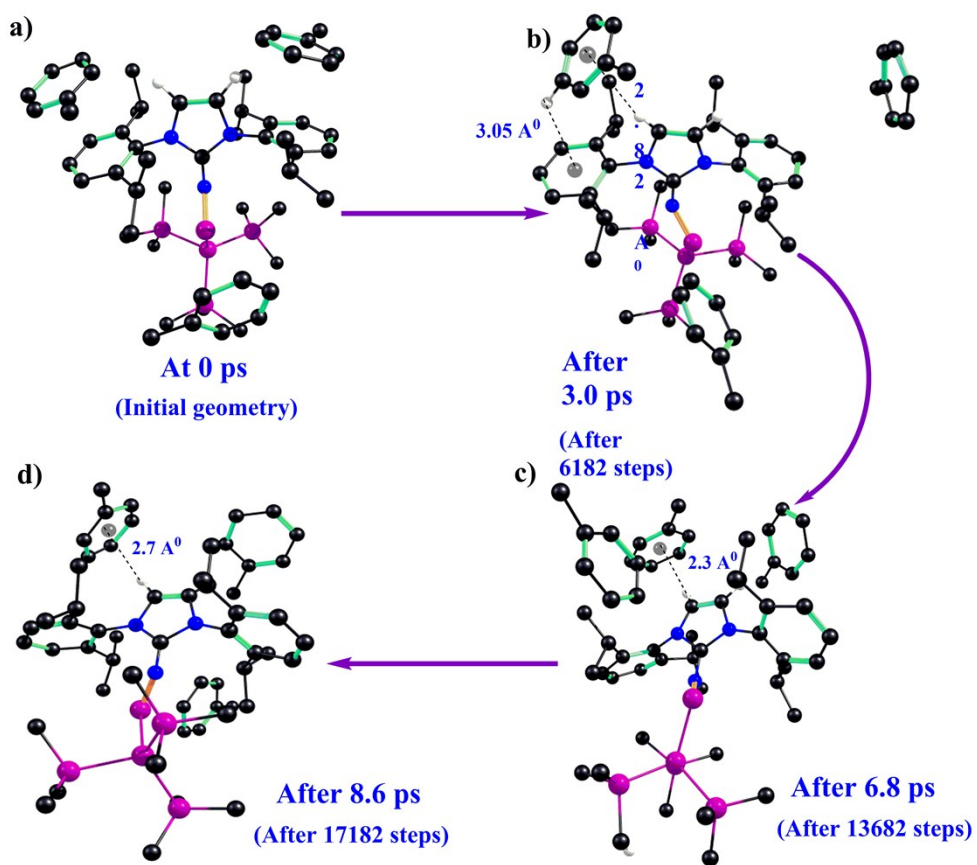


Fig. S12 The different snapshots for observed C-H/ π interactions in the room temperature *ab initio* molecular dynamics simulations. a) Initial geometry (starting point of simulation) at 0.0 ps, b) after 3.0 ps, when the bond distance for two different C-H/ π interactions, between the hydrogen atoms of C-H and the center of the π ring, are 2.82 Å and 3.05 Å, c) after 6.8 ps, when the bond distance for the C-H/ π interaction is 2.3 Å, and d) after 8.6 ps, when the bond distance for the C-H/ π interaction is 2.7 Å.

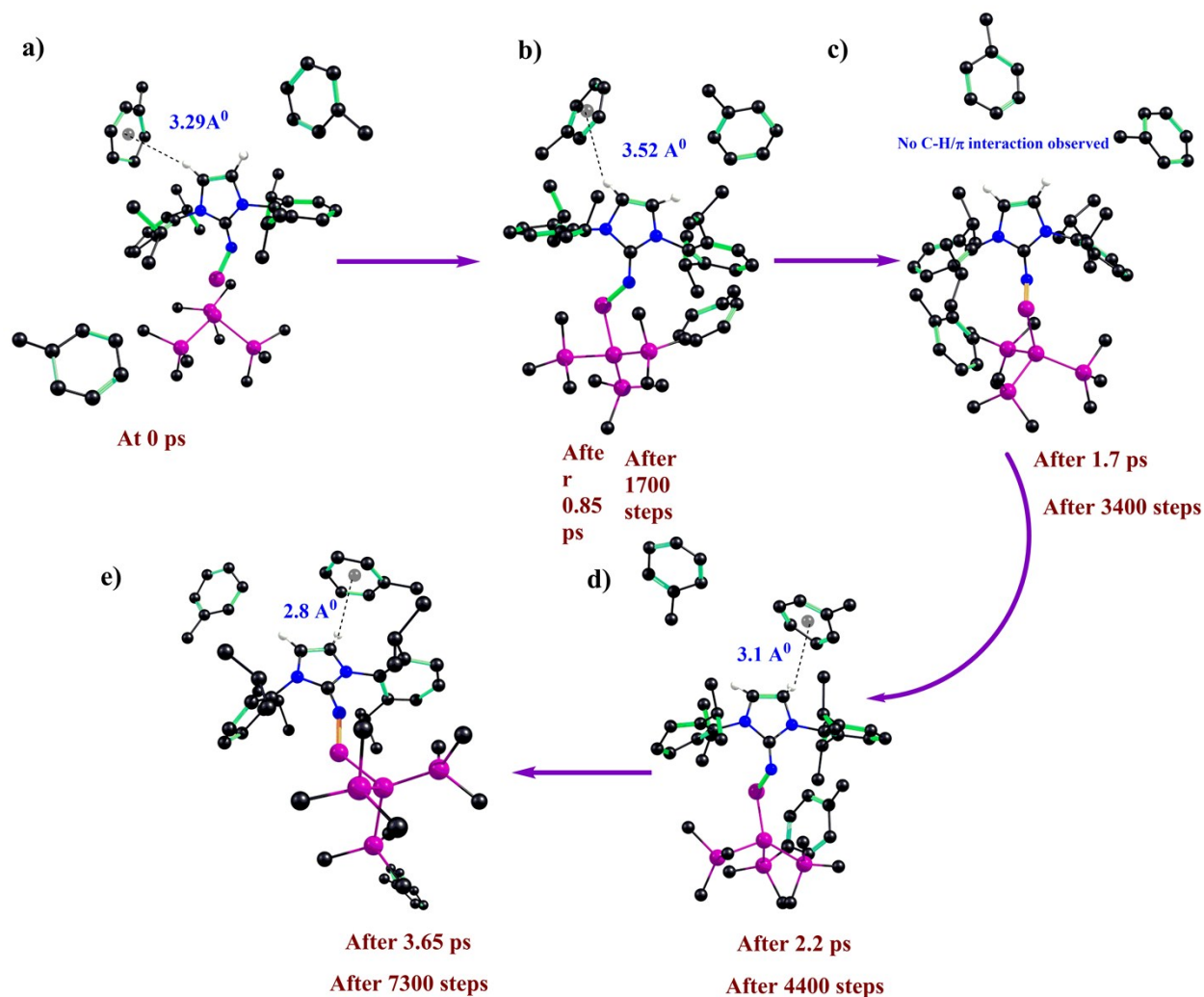


Fig. S13 The different snapshots for observed C-H/ π interactions in *ab initio* molecular dynamics simulations done at a temperature of 1000.0 K. a) Geometry at 0.0 ps, where the bond distance for C-H/ π interaction between the hydrogen atoms of C-H and the center of the π ring is 3.29 \AA b) after 0.85 ps, when the bond distance for C-H/ π interactions is 3.52 \AA c) after 1.7 ps, when C-H/ π interaction is not observed d) after 2.2 ps, when the bond distance for the C-H/ π interaction is 3.10 \AA , and e) after 3.65 ps, when the bond distance for the C-H/ π interaction is 2.8 \AA .

The free energy profiles for different cases. As discussed in the manuscript, shown below are the potential energy surfaces for the different cases where toluene is not involved in the CH/ π interaction, either in the reactant, transition state or the product.

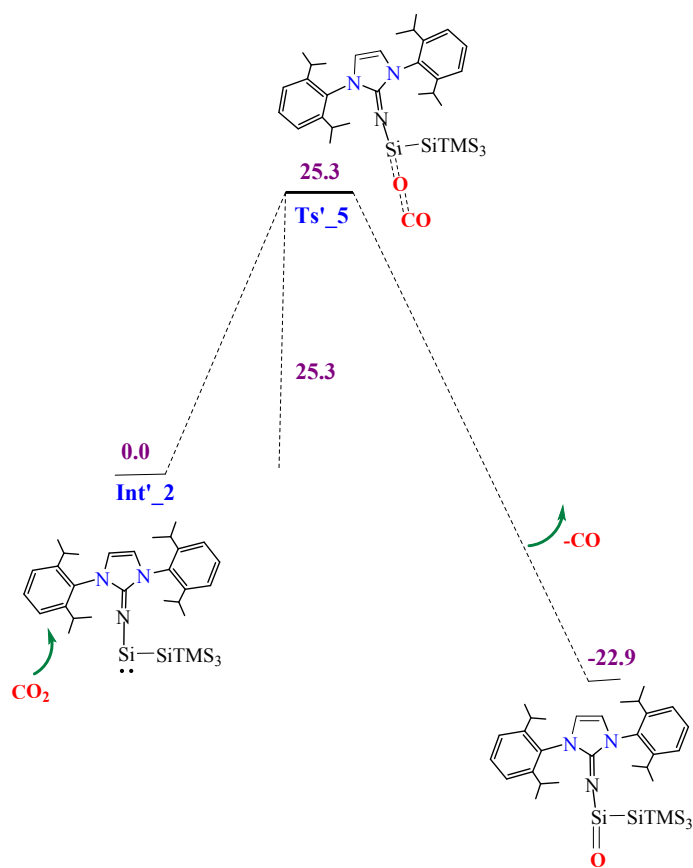


Fig. S14 The free energy profile for the slowest step of the CO₂ activation by the silepin complex without C-H/ π interaction.

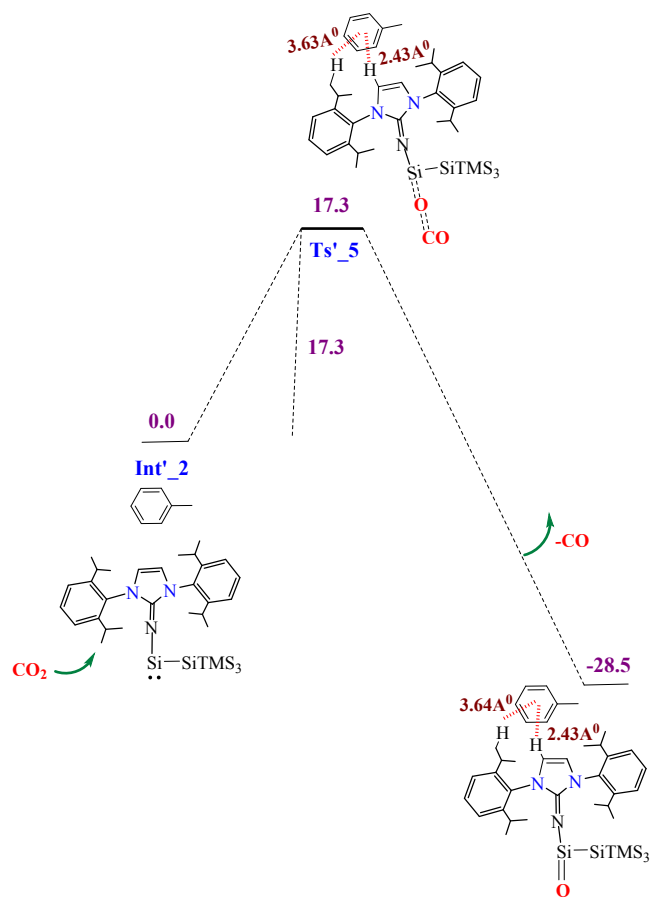


Fig. S15 The free energy profile for the case where toluene is not involved in C-H/ π interaction with the substrate (**Int'_2**) for the slowest step of the CO₂ activation process by the silepin complex.

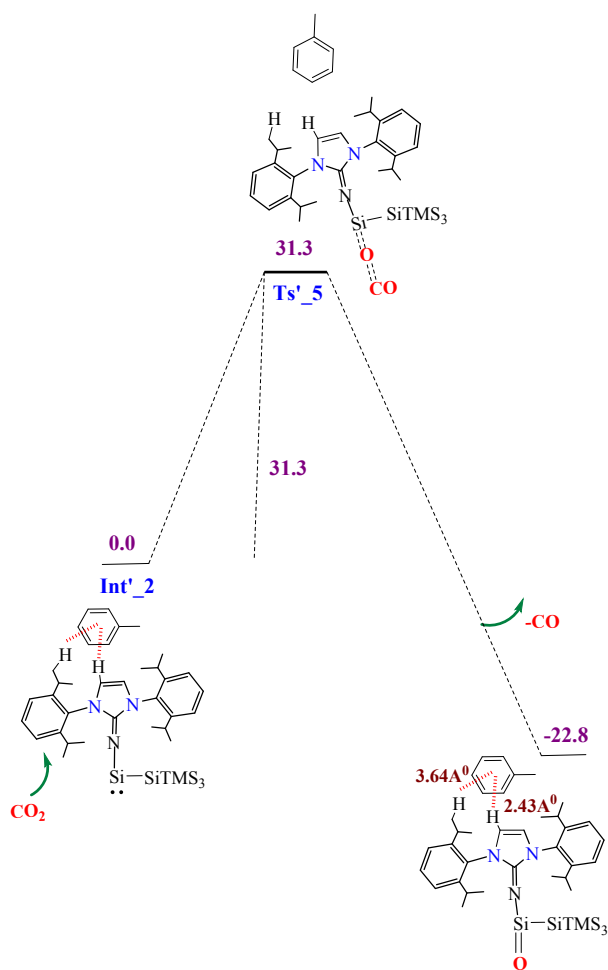


Fig. S16 The free energy profile for the case where toluene is not involved in C-H/ π interaction with the transitionstate (Ts'_5) for the slowest step of the CO₂ activation process by the silepin complex.

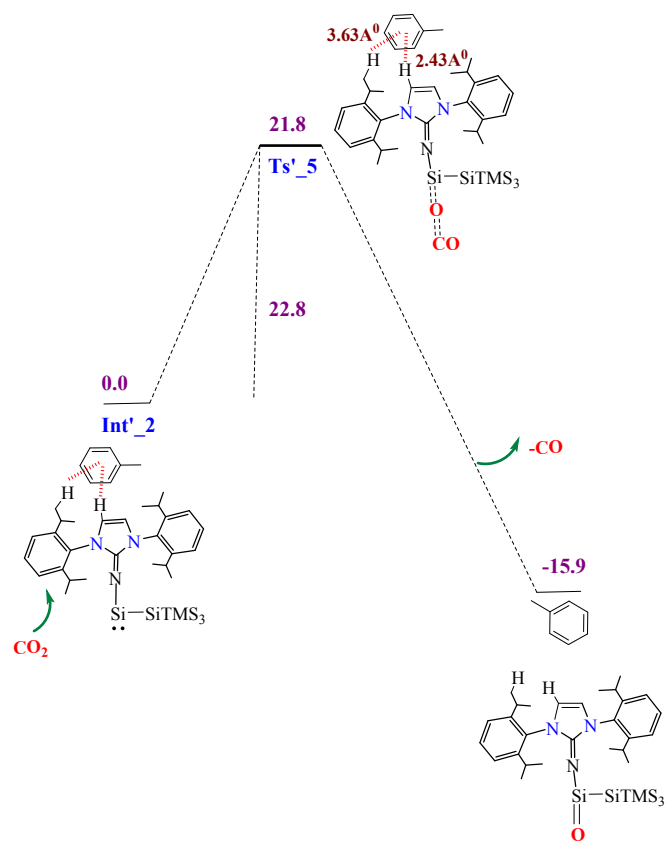


Fig. S17 The free energy profile for the case where toluene is not involved in C-H/ π interaction with the product (IV) for the slowest step of the CO₂ activation process by the silepin complex.

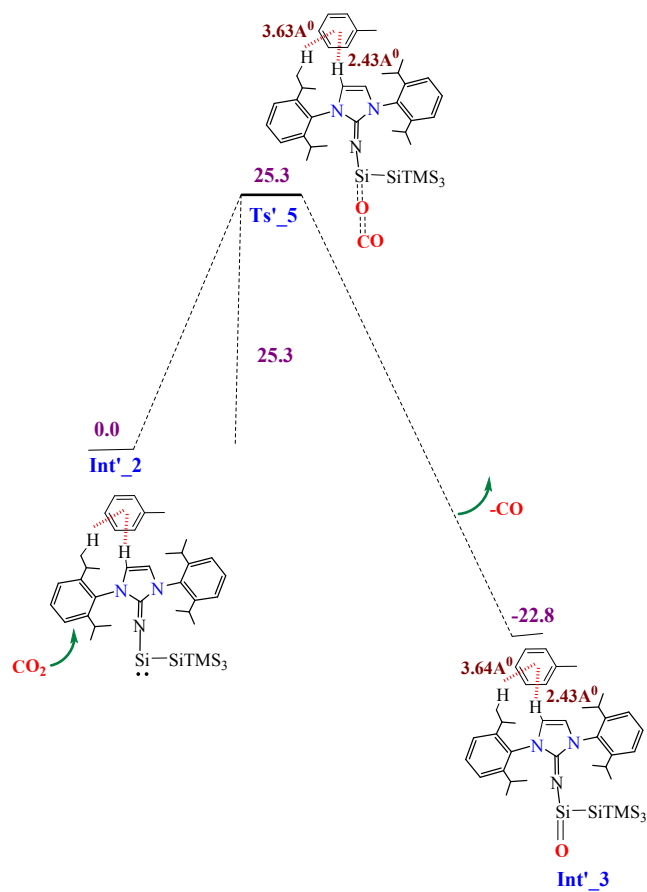


Fig. S18 The free energy profile for the case where toluene is involved in C-H/ π interaction with the substrate (**Int'_2**), transition state (**Ts'_5**) and product (**Int'_3**) for the slowest step of the CO_2 activation process by the silepin complex.

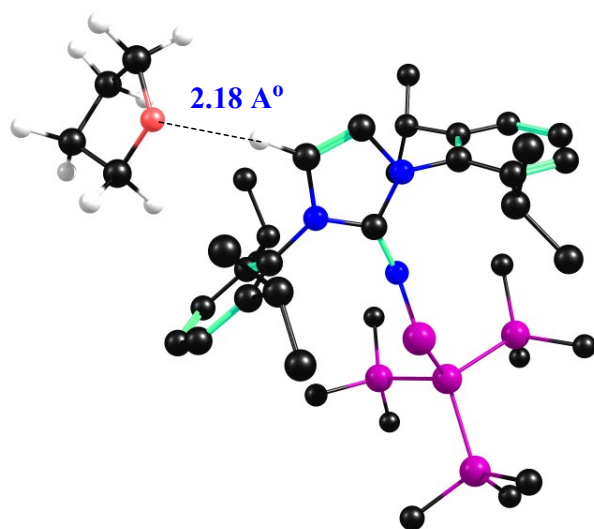


Fig. S19 The optimized geometry of a structure that demonstrates the presence of C-H/O interactions between a silylene molecule and an explicit tetrahydrofuran (THF) solvent molecule.

XYZ coordinates of all the stationary points obtained after full optimization at the TPSS-D3/def2-TZVP level of theory.

A

C	10.082536	13.076027	12.027611	C	10.735605	14.823016	16.994218
C	9.697576	11.925344	12.734787	C	9.820899	15.975064	17.450352
C	9.655526	10.645362	12.155292	Toluene			
C	9.988681	10.544248	10.800538	C	-0.039135	-0.000012	0.105997
C	10.364079	11.669216	10.068972	C	0.044611	-0.000017	1.506246
C	10.416524	12.919666	10.677471	C	1.280276	0.000004	2.152374
N	9.349779	12.064998	14.124970	C	2.462607	-0.000001	1.407596
C	10.274534	12.015027	15.152083	C	2.394324	-0.000000	0.014383
N	9.545836	12.273709	16.298230	C	1.153400	0.000001	-0.627404
C	8.206508	12.499332	15.972869	H	-0.870031	-0.000030	2.095557
C	8.086129	12.370196	14.630906	H	1.321395	0.000020	3.238541
C	10.119432	12.413503	17.610816	H	3.426272	-0.000003	1.909906
C	10.098232	11.306783	18.475898	H	3.306353	0.000007	-0.576831
C	10.607481	11.490697	19.765233	H	1.110647	0.000013	-1.714508
C	11.134168	12.718318	20.158379	C	-1.383261	-0.000000	-0.584583
C	11.175490	13.784956	19.265062	H	-1.269678	-0.000019	-1.672274
C	10.671608	13.655197	17.966577	H	-1.970254	-0.882649	-0.303404
N	11.542133	11.822986	15.010629	H	-1.970210	0.882688	-0.303428
Si	12.952097	11.122850	15.413409	A_Tol			
Br	12.869015	8.876077	15.219139	C	11.032025	13.409927	18.164412
Br	14.544524	11.857615	14.017796	C	10.641778	12.167330	17.636063
C	9.541888	9.960987	18.036186	C	10.796108	10.951699	18.326153
C	10.447502	8.791575	18.459851	C	11.332028	11.013911	19.616131

C	11.709523	12.231852	20.176261	C	9.556447	15.265618	11.846825
C	11.569503	13.415181	19.456370	H	8.033279	12.741750	16.812072
N	10.052031	12.140671	16.322815	H	7.697458	12.516739	14.067937
C	10.730500	11.845443	15.154833	H	11.472199	10.100174	20.184023
N	9.783796	11.959729	14.154610	H	12.130354	12.256684	21.177756
C	8.559878	12.355537	14.693217	H	11.889105	14.352445	19.901067
C	8.723718	12.466152	16.031811	H	10.617719	9.706626	16.614150
C	10.073889	11.749053	12.760783	H	8.292522	10.167133	17.394667
C	10.372241	12.866032	11.967056	H	8.619790	9.279231	18.896659
C	10.621604	12.640799	10.607303	H	8.616350	8.425734	17.338313
C	10.589710	11.354185	10.080404	H	12.284633	8.633793	18.173753
C	10.329154	10.259721	10.904763	H	10.999358	7.549690	17.614487
C	10.072427	10.430966	12.268054	H	10.942470	8.199560	19.257263
C	10.489308	14.264892	12.552260	H	10.139277	14.551945	16.600780
C	11.956717	14.736275	12.510109	H	12.482725	14.050072	15.919482
C	9.802471	9.249355	13.190656	H	13.090118	15.042625	17.253581
C	8.287380	9.028016	13.380578	H	12.175325	15.799804	15.929596
N	11.969725	11.550293	14.967703	H	10.421646	16.782443	17.514285
Si	13.443089	10.962529	15.301444	H	11.390187	16.190945	18.866787
Br	14.296223	11.443848	17.325945	H	9.671414	15.763285	18.760607
C	10.400189	9.627031	17.686144	H	10.336677	9.260646	10.480455
C	8.887692	9.362936	17.837507	H	10.786661	11.197359	9.023116
C	10.938701	14.685765	17.338238	H	10.858266	13.481011	9.960048
C	12.253484	14.906650	16.559597	H	10.231065	9.498926	14.168463
Br	13.481970	8.715756	15.125460	H	7.815304	8.781773	12.422473
Br	14.919907	11.762279	13.813915	H	7.798569	9.919074	13.785038
C	11.209734	8.436256	18.221180	H	8.110046	8.198783	14.074726
C	10.583410	15.924600	18.175734	H	10.014134	7.560145	11.810397
C	10.478386	7.951546	12.722627	H	10.376222	7.186294	13.499262

H	11.544976	8.104440	12.534256	C	4.093823	21.310751	9.230794
H	10.190115	14.221719	13.604202	N	5.442800	18.082390	10.464255
H	12.308029	14.824281	11.475798	C	5.660603	17.706754	11.777184
H	12.606639	14.028597	13.032837	N	5.677501	16.325741	11.753745
H	12.052632	15.717926	12.987560	C	5.443653	15.867580	10.453499
H	9.819513	15.377151	10.789065	C	5.304251	16.951381	9.657395
H	9.636237	16.251654	12.317627	C	5.806759	15.489528	12.916624
H	8.512482	14.939364	11.903943	C	7.097223	15.193525	13.392969
C	17.115610	6.798053	15.628547	C	7.189852	14.333972	14.490806
C	17.571973	5.482243	15.561457	C	6.044731	13.813253	15.092025
C	18.902058	5.182150	15.867795	C	4.782019	14.155944	14.620292
C	19.767026	6.210875	16.241030	C	4.634835	15.010307	13.520997
C	19.304149	7.527700	16.306819	C	8.331431	15.797901	12.735831
C	17.974262	7.843235	16.002102	C	9.511703	15.955553	13.705840
H	16.888716	4.688555	15.269712	C	3.251864	15.419531	13.037042
H	19.258640	4.157009	15.816419	C	2.436359	14.201606	12.564593
H	20.803930	5.990551	16.482114	N	5.785823	18.515434	12.772639
H	19.985992	8.323408	16.600171	Si	6.233690	19.042083	14.239058
C	17.469473	9.264544	16.068370	Br	8.402111	19.660620	14.262035
H	16.078794	7.023273	15.389624	C	7.929106	19.510973	10.187693
H	16.607867	9.348386	16.739072	C	9.006171	20.541557	10.557830
H	18.247346	9.946516	16.424346	C	2.841472	19.242911	10.053319
H	17.136315	9.612064	15.083941	C	1.626782	19.705209	9.235193
A'				C	8.430518	18.593923	9.054413
C	4.121185	20.007679	9.739448	C	2.525689	19.339700	11.562816
C	5.382613	19.446922	10.007253	Br	5.028718	20.857594	14.775262
C	6.589091	20.147704	9.837693	Br	5.984118	17.615420	15.960324
C	6.505803	21.449466	9.331056	C	2.502950	16.210868	14.126226
C	5.273978	22.019417	9.018621	C	8.757765	14.985696	11.495248

H	5.405012	14.813787	10.232203	H	3.017904	18.186314	9.816060
H	5.135544	17.037413	8.596415	H	2.300409	20.377425	11.832704
H	8.164884	14.079878	14.893388	H	3.369478	19.015959	12.176948
H	6.140389	13.150549	15.947933	H	1.654207	18.721546	11.807123
H	3.897646	13.767074	15.117661	H	1.304185	20.709431	9.531343
H	8.057074	16.803925	12.396313	H	0.786396	19.025724	9.411262
H	7.954631	14.930562	10.753909	H	1.836087	19.715548	8.161406
H	9.030233	13.964046	11.783540	H	3.657088	19.406875	6.678719
H	9.626497	15.453831	11.019159	C	2.184897	17.105129	6.482063
H	9.209899	16.483521	14.615124	H	1.641235	17.996912	6.155537
H	10.306038	16.534310	13.223384	H	1.927899	16.931675	7.534943
H	9.934313	14.984706	13.988788	H	1.821113	16.247110	5.908465
H	3.374869	16.085274	12.177383	C	3.676148	17.280270	6.320831
H	3.076582	17.091669	14.430174	C	4.504253	16.180332	6.055539
H	2.331394	15.593509	15.014859	C	5.887827	16.331803	5.946145
H	1.529505	16.542756	13.749050	C	6.470454	17.590494	6.105146
H	1.460952	14.524451	12.184104	C	5.658745	18.694346	6.371080
H	2.262822	13.498134	13.386541	C	4.275642	18.538476	6.470334
H	2.959316	13.666080	11.765044	H	4.059153	15.195223	5.933061
H	7.412777	22.025966	9.181697	H	6.510847	15.465928	5.738593
H	5.232458	23.030265	8.621653	H	7.547154	17.708339	6.028385
H	3.142066	21.780053	9.003043	H	6.099351	19.676998	6.514520
H	7.768670	18.890177	11.075815	Ts'_1			
H	8.615106	19.176887	8.144635	C	4.181222	20.017418	9.717688
H	7.704706	17.812986	8.815392	C	5.428462	19.437188	10.013581
H	9.369740	18.111302	9.348769	C	6.647067	20.121698	9.866355
H	9.322221	21.127945	9.687454	C	6.592470	21.425667	9.362489
H	9.888689	20.022081	10.944896	C	5.376398	22.014971	9.028089
H	8.650593	21.227758	11.332054	C	4.183018	21.321218	9.212004

N	5.454544	18.075700	10.480412	Si	4.067013	23.373209	16.717276
C	5.687918	17.702262	11.798680	C	5.497889	24.581736	16.285211
N	5.597991	16.317845	11.787491	Si	2.708509	20.001738	16.861970
C	5.303506	15.865388	10.500766	C	1.260231	20.952330	17.657570
C	5.217796	16.948448	9.694157	K	7.679340	22.327991	16.062266
C	5.767595	15.480538	12.944864	Si	5.422236	20.925168	19.186950
C	7.074403	15.188019	13.376285	C	4.064693	21.156479	20.501529
C	7.208960	14.324801	14.466932	C	2.227300	19.686951	15.053980
C	6.088721	13.787720	15.099731	C	2.706755	18.330683	17.768979
C	4.809332	14.127067	14.673227	C	6.782680	22.201191	19.621574
C	4.620695	14.996061	13.591866	C	6.192896	19.219406	19.517263
C	8.284388	15.793792	12.677126	C	2.847428	23.606160	15.277489
C	9.498882	15.948060	13.604071	C	3.272375	24.165809	18.255434
C	3.220970	15.409667	13.163680	H	5.197806	14.814781	10.287000
C	2.501469	14.263243	12.426598	H	5.029931	17.030211	8.636002
N	5.954721	18.474244	12.782184	H	8.198583	14.074851	14.835289
Si	6.202901	19.351912	14.129492	H	6.217064	13.116747	15.944973
Br	8.497002	19.701284	14.331329	H	3.944681	13.728746	15.196589
C	7.971179	19.465700	10.237967	H	7.999589	16.801694	12.355856
C	9.065711	20.480989	10.598200	H	7.831904	14.934415	10.708945
C	2.883041	19.271999	10.001978	H	8.944102	13.961457	11.692757
C	1.679266	19.788135	9.200417	H	9.514270	15.452341	10.911237
C	8.459835	18.517457	9.125543	H	9.228005	16.474610	14.524018
C	2.569503	19.324676	11.511759	H	10.276363	16.527427	13.094902
Br	5.543915	21.465505	13.337360	H	9.931960	14.977038	13.870812
Br	5.864261	17.833625	15.821961	H	3.319154	16.246324	12.464531
C	2.388603	15.905190	14.360500	H	2.925698	16.677457	14.915870
C	8.663016	14.985013	11.419238	H	2.154156	15.087830	15.051342
Si	4.779956	21.121953	16.930248	H	1.441433	16.327414	14.007305

H	1.503482	14.582942	12.106166	H	2.147126	20.629648	14.501878
H	2.387600	13.394062	13.084323	H	5.101957	25.603910	16.223278
H	3.061571	13.946183	11.540339	H	2.399314	23.598823	18.593691
H	7.510478	21.989623	9.234145	H	2.949709	25.192191	18.030915
H	5.356765	23.027881	8.634397	H	5.465023	18.418575	19.345495
H	3.242550	21.803780	8.966249	H	5.939219	24.361631	15.302212
H	7.790782	18.867930	11.137093	H	7.042072	19.031757	18.849633
H	8.657190	19.077752	8.204061	H	6.291100	24.605321	17.047126
H	7.719881	17.745166	8.901609	H	3.277158	20.403056	20.385311
H	9.389417	18.023950	9.432514	H	6.544876	19.143639	20.555339
H	9.402255	21.045377	9.720768	H	2.622053	24.672591	15.140532
H	9.933814	19.951626	11.004582	H	3.269492	23.221001	14.342800
H	8.713696	21.186501	11.356986	H	3.593039	22.142039	20.429662
H	3.034608	18.220378	9.729209	H	7.720667	21.998531	19.083934
H	2.377523	20.356441	11.822829	H	4.485076	21.050087	21.511604
H	3.403719	18.955911	12.112123	H	1.902094	23.082774	15.454107
H	1.683037	18.723373	11.742023	H	6.472012	23.228929	19.394679
H	1.383624	20.792466	9.523656	H	7.022987	22.158321	20.692326
H	0.821816	19.126663	9.362657	H	3.680049	19.406129	6.669603
H	1.884156	19.820701	8.125980	C	2.167784	17.134654	6.441104
H	1.730374	17.844552	17.635779	H	1.651884	18.023291	6.064659
H	0.341715	20.352717	17.584154	H	1.873722	17.005203	7.490612
H	2.867520	18.467514	18.844707	H	1.806719	16.262658	5.887259
H	1.451046	21.147231	18.718842	C	3.666468	17.277739	6.321881
H	3.478088	17.651876	17.395338	C	4.479589	16.159989	6.086557
H	1.268794	19.156778	14.974492	C	5.868468	16.283688	6.014069
H	1.068623	21.915022	17.171638	C	6.471139	17.531609	6.181524
H	3.982713	24.211876	19.089653	C	5.674630	18.652779	6.419898
H	2.989199	19.081795	14.550849	C	4.286668	18.524754	6.481442

H	4.018698	15.182841	5.958812	C	0.088609	16.918382	11.201850
H	6.479680	15.404330	5.829440	C	0.869094	18.042361	10.950791
H	7.551571	17.627749	6.133612	C	2.250468	17.924901	10.814030
H	6.130565	19.627071	6.573044	C	2.884325	16.684932	10.943595
Int'_1				N	2.806394	13.387231	9.257564
C	4.254551	15.509118	15.738737	Si	3.614285	13.189893	7.820220
C	4.450870	14.128614	15.891646	Si	2.427047	13.759301	5.887202
C	3.337955	13.331340	16.186788	Si	0.552586	12.319410	5.765313
C	2.063503	13.889766	16.310837	C	-0.359996	12.630481	4.133542
C	1.880826	15.262644	16.142139	C	-0.180465	14.427751	11.620170
C	2.984109	16.072064	15.857321	C	-0.655660	14.417969	13.086678
C	5.820107	13.522902	15.700508	C	4.393429	16.543273	10.825513
C	2.927384	13.836984	12.768092	C	5.065515	16.666750	12.208463
C	3.351003	12.559954	12.674252	C	7.245315	11.444308	10.156726
N	3.363508	12.218214	11.319018	C	-1.372112	14.315071	10.654388
C	2.963868	13.299444	10.543913	C	5.012634	17.537957	9.833247
N	2.689847	14.296390	11.473251	Br	5.577661	14.403670	7.941066
C	3.663301	10.890936	10.850560	C	0.610765	10.535032	11.978671
C	2.592740	10.052269	10.480595	Si	3.807229	13.427722	3.986084
C	2.910359	8.747938	10.093744	C	5.591264	13.971810	4.277249
C	4.230479	8.298346	10.094786	Si	1.777191	16.028097	6.055565
C	5.263267	9.149843	10.467591	C	3.308121	17.125966	5.874318
C	5.002770	10.472914	10.844026	C	3.807723	11.616949	3.441658
C	1.149882	10.542789	10.531479	C	3.091966	14.459905	2.564371
C	0.200042	9.745180	9.626227	C	0.954491	16.347412	7.719545
C	6.143687	11.402408	11.231665	C	0.538178	16.484809	4.695799
C	6.731901	11.000068	12.598980	C	1.037912	10.493529	5.807587
C	2.071033	15.571126	11.215570	C	-0.610660	12.672116	7.212992
C	0.673483	15.654198	11.334397	Br	4.422946	11.071822	7.380629

H	-1.240998	13.514002	13.289825	H	4.596990	15.537372	10.443713
H	0.192582	14.440545	13.777340	H	-0.069492	12.607311	8.162460
H	7.530580	11.692007	12.888997	H	3.051864	18.175244	6.070591
H	5.967344	11.009672	13.382903	H	-0.682289	13.672034	4.033461
H	-1.287803	15.289489	13.292651	H	-0.006047	15.825241	7.787221
H	7.155207	9.990065	12.554093	H	2.842330	18.809074	10.599364
H	2.767363	14.471254	13.623708	H	1.575986	15.999498	8.549058
H	3.638925	11.851532	13.431728	H	3.723167	17.063490	4.861578
H	-1.036382	14.345195	9.615284	H	-1.251040	11.991481	4.075554
H	0.444244	13.542661	11.469995	H	2.120140	8.070210	9.788119
H	-1.897606	13.367593	10.818188	H	0.574621	9.684170	8.601444
H	8.007349	12.179677	10.437332	H	1.147222	11.577999	10.170845
H	5.738172	12.415425	11.322574	H	4.093923	16.825791	6.575495
H	6.288462	8.791232	10.449355	H	4.969697	18.566721	10.208934
H	-0.989298	17.021520	11.291105	H	0.766228	17.419054	7.859411
H	0.315735	17.559011	4.750418	H	6.065809	17.286603	9.672264
H	7.739567	10.471623	10.053772	H	0.130197	9.875383	5.809331
H	4.690868	15.910945	12.904152	H	4.504137	17.499112	8.866017
H	0.919191	16.268977	3.692779	H	0.048382	8.726166	10.000388
H	-0.405920	15.943183	4.823890	H	1.205565	11.170631	12.640078
H	-2.092348	15.125842	10.808716	H	1.627287	10.250331	6.695987
H	-1.041770	13.676709	7.140206	H	1.636326	10.218323	4.933416
H	-1.435795	11.948890	7.235723	H	-0.778456	10.235814	9.602383
H	6.832510	11.727393	9.185334	H	0.619263	9.515401	12.380863
H	0.397378	19.016093	10.846297	H	3.159486	15.533999	2.771457
H	4.873080	17.654541	12.644115	H	2.039542	14.218063	2.377045
H	4.452116	7.278153	9.792623	H	-0.422315	10.901066	11.996098
H	6.149474	16.537049	12.113235	H	5.647037	15.007929	4.626792
H	0.278400	12.393193	3.274476	H	6.079304	13.342490	5.028017

H	2.813801	11.298674	3.107219	C	10.986134	13.349677	13.423076
H	3.653507	14.261293	1.641919	C	11.218458	12.162657	12.737125
H	4.121903	10.957159	4.256983	C	10.253356	11.157538	12.721987
H	6.155257	13.892787	3.338175	C	9.043816	11.309436	13.407069
H	4.502785	11.483808	2.602230	C	9.541618	14.853850	14.869982
H	5.105096	16.147295	15.511253	C	9.798700	16.090420	13.991362
H	6.577267	14.058721	16.283456	C	7.986256	10.216770	13.424740
H	6.119490	13.577474	14.646432	C	8.036791	9.309630	12.188206
H	5.836689	12.470725	15.998734	N	6.097592	13.467694	13.270730
H	3.469015	12.258725	16.313848	Si	4.720406	13.364724	12.265147
H	1.213435	13.249955	16.531340	Br	1.850557	13.285772	12.399249
H	0.890017	15.699094	16.229090	K	1.784505	10.222751	11.621308
H	2.853254	17.142313	15.721918	C	5.536663	16.258359	15.510613
Ts'_2				C	6.392241	16.357851	16.793841
C	4.313347	15.374577	15.731731	C	10.386989	14.912354	16.158336
C	4.436294	13.972401	15.831832	C	2.867328	11.083982	17.574292
C	3.357258	13.131534	16.150828	C	8.086495	9.372652	14.712091
C	2.105822	13.729020	16.333553	Br	4.875111	10.965865	11.486563
C	1.944870	15.102335	16.198252	Si	5.264610	14.460050	10.198965
C	3.036737	15.916591	15.901905	Si	3.590541	14.127746	8.563251
C	3.529569	11.624062	16.294522	C	2.150857	15.338600	8.764510
C	3.013271	10.882610	15.048033	Si	7.359598	13.831070	9.308253
N	5.737501	13.387168	15.688114	C	8.679385	13.878530	10.652040
C	6.506482	12.961796	16.775515	C	7.920947	15.003244	7.922378
C	7.691273	12.534815	16.294887	C	7.270582	12.077145	8.596953
N	7.660983	12.673422	14.907952	Si	5.243456	16.759846	10.705064
C	6.434760	13.201171	14.488973	C	3.648881	17.181607	11.639344
C	8.843799	12.513860	14.104243	C	6.744912	17.193499	11.774154
C	9.788380	13.554321	14.117424	C	5.314267	17.850948	9.153734

C	5.194888	17.678392	15.039376	H	-0.057624	11.646096	15.468566
Si	-0.814212	13.017943	12.106794	H	-1.639610	11.277102	16.181702
Si	-1.846562	11.653251	13.717942	H	-1.926339	9.551405	12.299208
C	-1.119905	11.909203	15.449406	H	-2.174881	9.182574	14.013036
Si	-1.586439	12.268024	10.011433	H	-0.548114	9.506749	13.423983
C	-0.691188	10.695461	9.402569	H	-0.581639	15.492322	14.666916
C	-1.319592	13.574123	8.669012	H	-2.289389	15.043466	14.825623
C	-3.431524	11.814038	10.020606	H	-1.847789	16.706515	14.394382
Si	-1.605882	15.206992	12.407772	H	-4.080990	14.767172	12.274476
C	-3.381123	15.446745	11.775388	H	-3.451455	15.263913	10.696736
C	-0.493748	16.444834	11.507070	H	-3.714509	16.476738	11.963052
C	-1.581830	15.651027	14.250285	H	-0.833407	17.471766	11.696890
C	-1.600491	9.804830	13.314455	H	-0.500033	16.281330	10.423912
C	-3.717115	11.949599	13.863043	H	0.541897	16.356677	11.852073
C	4.308157	14.410838	6.829313	H	10.173373	15.834150	16.711475
C	2.852286	12.383573	8.616599	H	10.171734	14.062170	16.812255
H	-1.868111	14.496813	8.889018	H	3.087733	10.016603	17.688143
H	-1.665804	13.199354	7.696734	H	3.237242	11.607759	18.462171
H	-0.260325	13.831012	8.578581	H	11.456622	14.896685	15.918281
H	-0.779903	9.863460	10.114154	H	1.777964	11.196428	17.542900
H	0.367952	10.885538	9.188784	H	8.559928	12.144900	16.798782
H	-1.144610	10.355842	8.462343	H	6.128695	13.014045	17.782801
H	-3.628946	10.952418	10.668762	H	9.209201	16.047312	13.073050
H	-3.758388	11.552062	9.004735	H	8.488594	14.876778	15.164172
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H	6.813327	16.278531	16.433406	H	2.156146	19.656146	11.857280
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H	4.806234	17.332341	17.531628	H	5.901896	18.911598	13.736289
H	6.264345	18.343312	17.554465	H	3.027542	20.761613	12.935546
H	8.004392	16.240443	19.257595	H	3.446529	18.412386	9.417636
H	8.550071	17.276263	17.921842	H	4.505780	17.655690	8.213031
H	8.744955	15.517995	17.815005	H	5.407895	17.862700	15.066968
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H	6.445802	9.905517	17.971395	H	5.031174	19.597884	15.124037
H	7.849697	10.739677	17.284127	H	3.058995	16.805427	8.781166
H	7.064529	9.434475	16.375154	H	2.228356	17.557972	15.609836
H	4.155170	10.094355	16.830341	H	2.024052	19.314312	15.413177
H	4.813799	9.842732	15.207328	Ts_2			
H	3.898393	11.318592	15.567248	C	1.218478	2.799379	3.040799
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C	-1.082707	2.432157	3.747247	Si	1.149798	1.068118	-2.514719
C	-0.046620	3.289923	3.382187	Si	-0.825912	1.306863	-3.781583
C	0.644107	-0.970032	3.710004	C	-1.972266	2.659847	-3.119620
C	-0.273800	-1.868101	2.868099	Si	2.728401	-0.071562	-3.849605
N	2.664116	0.824990	2.732348	C	4.022002	-0.904985	-2.764924
C	3.648099	0.512372	3.676366	C	3.610198	1.148781	-5.007682
C	4.511495	-0.350152	3.104634	C	1.908129	-1.407470	-4.916006
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C	5.912883	-1.015736	0.276397	C	1.952853	4.410601	-3.418363
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C	6.178279	-3.205493	-0.734224	Si	-4.697315	-0.194121	0.314464
C	5.023065	-3.656297	-0.097884	Si	-5.520503	-1.870937	1.738736
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C	3.063757	-3.327159	1.500980	C	-5.675193	1.222157	-2.747160
C	2.472410	-4.616488	0.913712	C	-7.780626	-0.555742	-1.390803
N	2.182973	0.073761	0.472613	Si	-5.107112	1.882543	1.325397
Si	0.757516	-0.028665	-0.419483	C	-6.899157	2.474976	1.116422
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C	1.756335	-1.475253	-5.357943	Si	3.246358	-0.236759	1.287431
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C	-2.823255	0.094343	-2.255838	C	-5.449004	-1.019671	-0.035728
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C	-2.098035	0.381866	0.253584	C	4.674269	-0.440429	2.518828

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H	4.990219	-1.106228	2.157165	H	3.071877	-8.809597	-2.077585
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H	3.424426	-1.621578	2.807065	H	4.643651	-9.046034	-2.871771
H	6.820105	-2.845011	1.700972	H	5.194656	-6.324919	3.076306
H	6.414774	-4.573325	1.681170	H	6.589476	-7.329224	2.636800
H	6.534750	-3.703062	3.219448	H	6.273904	-6.954680	4.341909

H	2.780222	-7.606003	4.664791	C	6.982755	8.648936	10.083408
H	3.938842	-8.241430	5.849555	N	5.559941	9.939848	6.901149
H	2.800635	-9.336194	5.041260	C	5.244535	11.274120	6.721202
H	6.497513	-10.416828	3.125158	N	4.967116	11.394636	5.369902
H	5.156872	-11.127256	4.039913	C	5.125364	10.155449	4.741706
H	6.318735	-10.065317	4.855652	C	5.489446	9.259887	5.684839
H	0.475285	-10.091590	0.096765	C	4.430079	12.572740	4.732330
H	0.443403	-11.876685	0.004731	C	3.055677	12.845919	4.895364
H	1.557667	-10.941088	-1.013157	C	2.544014	13.967164	4.235741
H	4.103480	-12.353839	0.020304	C	3.364098	14.771559	3.447027
H	3.076900	-13.453676	0.958944	C	4.716266	14.478384	3.310357
H	4.381590	-12.555198	1.758572	C	5.284957	13.374568	3.957462
H	0.854361	-10.618731	3.271298	C	2.154887	11.941450	5.730692
H	2.271363	-11.537402	3.806813	C	0.900816	12.651694	6.263254
H	0.960565	-12.357481	2.938157	C	6.763085	13.053421	3.794367
H	-1.164646	0.321906	0.582091	C	7.643824	14.313912	3.773795
H	-2.907635	0.298889	2.568582	N	5.177884	12.173313	7.666363
H	-2.298165	-0.271745	4.135553	Si	5.740250	13.715474	7.895845
H	-2.278307	-1.342895	2.724390	Si	4.972523	14.756857	9.821278
H	-0.003712	0.142523	4.713020	Si	3.848180	16.635080	8.916982
H	2.287827	0.843910	4.102656	C	2.805619	16.110404	7.429459
H	2.869147	1.280104	1.723317	C	3.203564	8.650831	7.961039
H	1.124525	1.023764	-0.033352	C	2.086562	9.253129	8.830949
Ts'_6				C	8.119538	10.010443	8.247344
C	6.911378	9.314526	8.855993	C	9.150055	10.460665	9.291878
C	5.677161	9.291513	8.183259	C	2.833704	7.237145	7.474109
C	4.538442	8.644937	8.692277	C	8.788746	9.107748	7.189007
C	4.665881	7.984598	9.920273	O	8.176424	13.364344	8.385617
C	5.873830	7.986999	10.608540	C	8.399158	14.144199	7.488449

O	9.128690	14.779361	6.810829	H	2.593242	10.095892	4.614560
O	6.576212	14.557525	6.844862	H	0.193494	12.877015	5.457032
C	7.001201	12.220623	2.515883	H	1.151157	13.586437	6.771669
C	1.731495	10.688215	4.933724	H	0.388112	12.000227	6.978136
Si	3.536850	13.260650	10.948277	H	7.914707	8.648691	10.638912
C	1.965946	13.041671	9.918196	H	5.952884	7.477289	11.565155
Si	6.775779	15.446582	11.191885	H	3.804732	7.475334	10.344510
C	8.143111	16.356009	10.258532	H	7.755508	10.910889	7.742398
C	4.382874	11.590037	11.178549	H	8.089990	8.829938	6.395295
C	3.057845	13.956910	12.644160	H	9.161336	8.186431	7.651929
C	6.070067	16.635159	12.488987	H	9.636376	9.630021	6.731002
C	7.524355	13.944788	12.063302	H	9.913110	11.078270	8.808991
C	2.702869	17.397481	10.218778	H	9.654376	9.604975	9.755250
C	5.109028	17.918062	8.340901	H	8.682863	11.059695	10.078944
H	4.956244	10.038507	3.685578	H	3.301576	9.283885	7.075142
H	5.706186	8.206562	5.617485	H	1.890768	7.262101	6.916420
H	5.345841	15.123675	2.706013	H	2.710988	6.551209	8.320290
H	2.945085	15.639737	2.945190	H	3.611543	6.833947	6.818251
H	1.494742	14.220864	4.342898	H	1.153951	9.313205	8.258457
H	7.064633	12.451439	4.658604	H	2.353705	10.259133	9.162456
H	6.706926	12.794240	1.629298	H	1.896437	8.640331	9.719016
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H	8.063416	11.967806	2.423009	H	2.038108	15.385265	7.717995
H	7.490250	14.892382	2.855369	H	3.420714	15.655129	6.644844
H	8.699132	14.022913	3.806521	H	2.203968	18.286437	9.811026
H	7.432952	14.940121	4.641840	H	3.253579	17.700665	11.116291
H	2.735845	11.613264	6.600924	H	1.925526	16.688208	10.527038
H	1.165242	10.981797	4.042629	H	5.830549	17.460222	7.654432
H	1.091356	10.048077	5.551431	H	5.661461	18.349028	9.183435

H	4.603506	18.738146	7.814304	C	5.129683	6.359581	3.555080
H	2.214340	12.694320	8.910480	H	8.201403	7.726620	3.097327
H	1.417022	13.985721	9.823661	H	8.655822	6.425406	5.149602
H	1.293584	12.305791	10.377944	H	6.847196	5.079791	6.203847
H	4.713233	11.190320	10.214806	H	4.584772	5.041344	5.167882
H	3.692993	10.867321	11.633413	C'			
H	5.262134	11.671125	11.826885	C	5.225927	5.603068	4.943259
H	2.609121	14.953530	12.563053	C	5.080060	6.389729	3.791114
H	3.930024	14.032836	13.303705	C	6.221957	7.005416	3.262058
H	2.327992	13.296142	13.130440	C	7.468526	6.858580	3.873790
H	8.745859	15.668871	9.658771	C	7.595953	6.086998	5.029483
H	8.809048	16.839823	10.985551	C	6.468766	5.455422	5.561218
H	7.749313	17.130312	9.593088	C	3.720515	6.605080	3.171137
H	5.701069	17.555332	12.021068	C	5.530904	9.140338	5.902705
H	6.853595	16.914651	13.205553	N	5.571048	9.883575	7.083126
H	5.241889	16.188658	13.049847	C	5.204733	11.196072	6.836564
H	7.877669	13.211983	11.330055	N	4.927632	11.234531	5.479773
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H	8.378992	14.250465	12.681024	C	5.709808	9.313775	8.398607
H	4.133670	6.348578	3.117750	C	6.953031	9.384854	9.051159
C	5.868125	7.903154	1.686150	C	7.041446	8.808804	10.322553
H	6.039564	7.279008	0.800075	C	5.942062	8.180725	10.905321
H	6.527979	8.772550	1.607507	C	4.727566	8.118913	10.230445
H	4.829743	8.248327	1.645000	C	4.582078	8.693007	8.962259
C	6.138341	7.122465	2.950699	C	8.159802	10.013919	8.371994
C	7.408747	7.129582	3.542625	C	8.857215	8.978705	7.463611
C	7.666527	6.396647	4.701847	C	3.246215	8.625460	8.235588
C	6.652387	5.641750	5.294941	C	2.916066	7.175832	7.832827
C	5.382284	5.623487	4.714186	N	5.084776	12.147459	7.716070

Si	5.895696	13.497570	8.202694	C	7.816321	14.212996	7.363297
O	6.551704	14.552133	6.958940	O	8.861913	14.633040	6.937246
C	4.383807	12.369582	4.776244	O	7.632477	13.299292	8.366100
C	3.009305	12.648067	4.925568	H	4.984910	9.795653	3.864066
C	2.492560	13.727994	4.204716	H	5.784976	8.093525	5.889746
C	3.308000	14.490487	3.370552	H	5.286354	14.803053	2.602161
C	4.660292	14.193068	3.246007	H	2.885074	15.328128	2.822311
C	5.232584	13.126879	3.951554	H	1.442471	13.983403	4.299263
C	2.115738	11.787055	5.812044	H	7.016287	12.213446	4.669050
C	1.718351	10.478565	5.094443	H	6.645053	12.482228	1.637445
C	6.710164	12.797378	3.793512	H	6.368339	11.000159	2.567567
C	6.942669	11.930423	2.536566	H	8.004031	11.673891	2.446340
C	0.847918	12.511538	6.289460	H	7.443725	14.598820	2.790575
C	7.596447	14.053783	3.729059	H	8.650525	13.761655	3.773733
Si	4.947262	14.730471	9.920659	H	7.394062	14.725721	4.564616
Si	6.681656	15.413155	11.377104	H	2.696656	11.525835	6.704565
C	7.237827	13.945460	12.433803	H	1.147741	10.703667	4.186301
Si	3.969231	16.575608	8.811401	H	1.090922	9.864730	5.750792
C	5.312981	17.807152	8.313206	H	2.593230	9.886005	4.812440
Si	3.378538	13.343071	11.002489	H	0.143911	12.676254	5.465618
C	2.802752	14.144371	12.619195	H	1.081256	13.479888	6.740630
C	3.074383	15.992018	7.251780	H	0.338657	11.899433	7.040675
C	2.729040	17.431325	9.959228	H	7.980804	8.850535	10.864428
C	2.110944	9.247969	9.066089	H	6.033945	7.741259	11.894989
C	9.162016	10.628718	9.358657	H	3.875912	7.631102	10.696983
C	1.888266	13.111495	9.863582	H	7.794992	10.824935	7.734965
C	4.158115	11.664848	11.377585	H	8.172033	8.578378	6.710233
C	8.180956	16.091612	10.450841	H	9.235529	8.139542	8.059046
C	6.002782	16.769733	12.512540	H	9.703468	9.442585	6.944549

H	9.914758	11.199025	8.806262	H	8.905266	16.487883	11.174988
H	9.682821	9.858785	9.939717	H	7.912495	16.901488	9.764828
H	8.665655	11.315969	10.049262	H	5.736382	17.666570	11.940586
H	3.329492	9.207464	7.313811	H	6.759672	17.057476	13.253854
H	1.978664	7.142890	7.266257	H	5.108346	16.439669	13.053150
H	2.802723	6.540146	8.718466	H	7.566615	13.110288	11.804896
H	3.710415	6.753334	7.209683	H	6.429356	13.585658	13.080262
H	1.177122	9.239674	8.492668	H	8.078942	14.236975	13.076086
H	2.344891	10.282307	9.328018	H	4.354015	5.106503	5.363113
H	1.940289	8.691186	9.994156	H	3.108033	5.699824	3.227944
H	2.615786	16.845715	6.735426	H	3.802846	6.904495	2.122083
H	2.281385	15.275814	7.489262	H	3.179979	7.399356	3.702778
H	3.762952	15.506653	6.551335	H	6.133154	7.613331	2.364086
H	2.308145	18.319777	9.470832	H	8.338522	7.353472	3.450778
H	3.202785	17.752688	10.894082	H	8.562761	5.978672	5.512039
H	1.898812	16.763383	10.216893	H	6.556847	4.849781	6.459107
H	6.063193	17.324493	7.676969	Ts_5			
H	5.822832	18.224345	9.188675	C	-2.460375	2.524866	-1.585085
H	4.871805	18.640400	7.750526	C	-2.190514	2.547606	-0.202244
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H	1.373569	14.061888	9.681678	C	-4.513509	2.283493	0.327369
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H	4.539797	11.198789	10.463265	C	-3.796647	2.399901	-1.976121
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H	4.994183	11.759811	12.078852	C	0.153726	1.789151	0.302910
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H	3.629801	14.247251	13.331202	C	1.031846	3.850957	0.754734
H	2.027256	13.527672	13.092205	C	-0.285134	4.020222	0.510541
H	8.677088	15.307399	9.870516	C	2.639107	1.929600	0.575307

C	3.343972	2.049699	-0.636846	C	2.752061	0.033979	3.891053
C	4.640903	1.526162	-0.684364	C	2.903115	1.925400	-3.141489
C	5.196777	0.897003	0.425280	C	0.024964	-6.228676	-0.237070
C	4.472220	0.786363	1.610170	C	2.525496	-4.720084	0.727881
C	3.177245	1.306023	1.716253	C	-2.656440	-3.952502	-2.548753
C	2.745013	2.746856	-1.850863	C	-3.342366	-3.623518	0.435446
C	3.352073	4.153707	-2.023813	H	-0.895800	4.907502	0.509340
C	2.403398	1.253390	3.026421	H	1.802359	4.561332	1.003873
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N	0.019069	0.518846	0.071639	H	-5.314437	2.173253	1.051793
Si	0.222463	-0.889734	0.971204	H	-5.845549	2.192485	-1.356831
O	-1.392964	-0.958940	2.201047	H	-4.046238	2.373938	-3.031599
C	-1.345564	-1.267981	3.393240	H	-1.819008	2.093733	2.367103
O	-0.558544	-1.425849	4.280386	H	-4.042193	4.169992	2.755488
C	-2.865259	2.402477	2.259861	H	-2.353937	4.537172	2.358158
C	-3.009165	3.817669	2.857868	H	-2.753925	3.806687	3.923296
C	-1.341094	2.629592	-2.614397	H	-4.771377	1.742755	3.114453
C	-0.939235	4.097352	-2.871373	H	-3.350278	1.321190	4.074978
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Si	-0.087343	-2.742914	-0.497352	H	-1.788930	4.658083	-3.277247
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C	-3.069578	-1.142893	-1.354768	H	-0.603599	4.593310	-1.956867
Si	1.238609	-2.348550	-2.396268	H	-2.447003	2.511965	-4.500382
C	0.406173	-1.024233	-3.458111	H	-2.042010	0.928825	-3.805984
Si	0.632496	-4.670119	0.654151	H	-0.787168	1.910303	-4.578345
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C	8.719057	12.720602	13.099829	H	5.259813	11.695374	13.023911
N	7.308319	15.140579	10.947138	H	3.858889	12.253628	10.699595
Si	7.410813	16.706484	11.520826	H	8.031696	14.473809	16.516743
C	5.899365	14.742434	14.816987	H	10.163573	13.292776	16.133358
C	6.080374	16.092685	15.530188	H	10.624871	12.216276	13.964350
C	8.990307	12.073167	11.747974	H	5.450908	14.957684	13.841667
C	10.481955	12.043052	11.381115	H	5.353721	13.602375	16.597506
C	3.872846	16.253657	10.406927	H	4.757165	12.885505	15.090742
C	3.831353	17.782472	10.267985	H	3.973377	14.333768	15.751781
C	6.341896	12.375253	8.186014	H	6.473680	15.967253	16.546004
C	7.830537	12.728994	7.996756	H	5.109153	16.592352	15.609359
Si	9.185695	17.895348	10.609692	H	6.742338	16.742729	14.954071
Si	8.405232	20.101324	10.293093	H	8.486354	12.685445	10.992572
C	7.355184	20.182181	8.718703	H	8.871821	10.002566	12.424965
O	6.432475	17.349799	12.542245	H	8.576892	10.216018	10.686195
Si	10.808456	17.764273	12.320991	H	7.320659	10.651563	11.857582
C	10.269113	18.835776	13.782537	H	11.038003	11.334644	12.005401
Si	9.800361	16.810816	8.609599	H	10.940388	13.030042	11.488460
C	11.000138	17.898729	7.625204	H	10.596097	11.725634	10.339377
C	10.973346	15.976681	12.911688	H	3.538503	16.997161	7.774993
C	12.487302	18.361344	11.679505	H	4.276472	15.806432	5.744942
C	10.647068	15.169557	9.014053	H	5.528943	13.687180	5.920673
C	8.254326	16.491255	7.571466	H	4.584943	16.035566	11.209916
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Si	4.928300	14.733172	9.818840	H	1.421484	14.211521	4.348425
Si	3.807843	16.620041	8.926301	H	7.015291	12.511106	4.640314
C	2.807031	16.114759	7.403889	H	6.641422	12.869474	1.614527
C	3.175905	8.636878	7.915607	H	6.395601	11.351710	2.494044
C	2.064863	9.260395	8.778602	H	8.016702	12.063260	2.395794
C	8.088501	10.022566	8.206594	H	7.404096	14.965573	2.847604
C	9.109317	10.486391	9.254858	H	8.624038	14.111265	3.797993
C	2.793856	7.216406	7.458564	H	7.344289	15.008279	4.634204
C	8.772729	9.115842	7.160879	H	2.694188	11.590707	6.573439
O	8.131163	13.374476	8.342927	H	1.107753	10.986178	4.018485
C	8.342938	14.172184	7.458773	H	1.051136	10.031583	5.514657
O	9.061736	14.826735	6.788888	H	2.544452	10.099859	4.564985
O	6.510201	14.577255	6.832331	H	0.138149	12.853713	5.460242
C	6.950203	12.294427	2.495233	H	1.100348	13.557267	6.774513
C	1.683013	10.683302	4.900593	H	0.348743	11.964610	6.971909
Si	3.483718	13.230581	10.924720	H	7.883217	8.669261	10.600300
C	1.923308	13.023567	9.876848	H	5.925925	7.489844	11.525774
Si	6.725346	15.407392	11.204858	H	3.781353	7.471226	10.299498
C	8.099365	16.322794	10.287814	H	7.722620	10.916965	7.692480
C	4.326795	11.557404	11.147096	H	8.080585	8.826222	6.364580
C	2.990282	13.912376	12.621994	H	9.151075	8.202772	7.634886
C	6.010483	16.583829	12.507819	H	9.618052	9.641287	6.702807
C	7.466896	13.896817	12.067039	H	9.870449	11.107183	8.773186
C	2.627574	17.344213	10.218602	H	9.617290	9.637195	9.725909
C	5.068081	17.926913	8.405434	H	8.632720	11.086069	10.035603
H	4.906430	10.066561	3.640105	H	3.273765	9.253285	7.017860
H	5.670161	8.220462	5.555634	H	1.850236	7.237670	6.902218
H	5.260365	15.178423	2.720882	H	2.666515	6.549105	8.318643
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H	1.129945	9.313525	8.209342	H	8.318022	14.195753	12.692806
H	2.337619	10.270941	9.090514	C			
H	1.877011	8.664944	9.678866				
H	2.294513	16.987912	6.978796	C	1.524290	-2.123056	2.871167
H	2.047638	15.367554	7.654876	C	0.406249	-2.620183	2.177896
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H	3.155775	17.629648	11.135391	C	0.218326	-2.297109	4.914430
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H	5.803445	17.492632	7.718423	N	0.492268	-2.818388	0.753098
H	5.603546	18.339327	9.267916	C	0.230616	-1.838885	-0.191685
H	4.564761	18.756769	7.892282	N	0.164398	-2.520870	-1.397979
H	2.182718	12.682739	8.869759	C	0.393507	-3.883866	-1.188103
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H	1.242893	12.286685	10.322775	C	-0.255708	-1.938652	-2.650075
H	4.668511	11.168003	10.183113	C	-1.635251	-1.722286	-2.849331
H	3.632041	10.829612	11.585965	C	-2.028895	-1.194459	-4.082261
H	5.198480	11.631665	11.806414	C	-1.090835	-0.899810	-5.069385
H	2.544394	14.910571	12.545683	C	0.263085	-1.117152	-4.840254
H	3.856124	13.980112	13.290676	C	0.714661	-1.636723	-3.620587
H	2.254325	13.248610	13.094803	C	-2.661856	-2.074008	-1.777440
H	8.697424	15.641461	9.676807	C	-3.968433	-1.274366	-1.895493
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H	7.711303	17.111511	9.636074	C	3.089858	-0.799844	-4.018772
H	5.638507	17.505590	12.045296	N	0.025812	-0.576878	0.036893
H	6.789990	16.861888	13.229273	Si	0.745015	0.888237	-0.198226
H	5.182469	16.129117	13.062292	Si	-0.436728	2.767080	0.469441
H	7.824162	13.169928	11.329745	Si	-1.346548	3.683705	-1.511921
H	6.733985	13.398170	12.711035	C	-2.062906	2.312416	-2.595880

C	-2.014858	-3.458157	2.043148	H	2.045900	-4.077947	-3.443146
C	-3.235062	-2.542377	2.245685	H	3.678446	-3.444896	-3.720793
C	2.823152	-1.814950	2.142928	H	3.096922	-0.884424	-5.111612
C	3.659375	-0.724223	2.826480	H	4.120425	-0.923812	-3.671728
C	-2.344291	-4.914387	2.422241	H	2.757733	0.202196	-3.742935
C	3.656168	-3.102015	1.963634	H	-2.217783	-1.826660	-0.806221
O	2.437045	0.944021	0.268770	H	-3.417837	-3.868006	-2.757506
C	2.772365	1.186810	-1.037054	H	-3.714009	-3.819605	-1.007258
O	3.872342	1.386909	-1.485130	H	-2.095587	-4.194363	-1.620671
O	1.582485	1.162782	-1.717098	H	-4.547716	-1.576570	-2.775450
C	2.614154	-3.270926	-3.914086	H	-3.780156	-0.199648	-1.961669
C	-2.985734	-3.583745	-1.791494	H	-4.589227	-1.458597	-1.013190
Si	-2.090030	2.040822	1.986658	H	2.238052	-1.577707	4.826254
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Si	1.116944	4.245611	1.467403	H	-1.791600	-3.028994	4.723992
C	2.643223	4.512820	0.387655	H	2.562645	-1.443334	1.147457
C	-1.340290	0.835481	3.230710	H	3.101393	-3.863970	1.407113
C	-2.824194	3.522371	2.909265	H	3.929575	-3.521265	2.938832
C	0.267112	5.917819	1.734136	H	4.577342	-2.881168	1.412870
C	1.671245	3.551818	3.137654	H	4.488569	-0.437521	2.173008
C	-2.725117	4.901542	-1.060184	H	4.083407	-1.074200	3.774886
C	-0.010940	4.592956	-2.492010	H	3.061294	0.170674	3.019685
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H	-1.419414	-0.486491	-6.019228	H	-1.487499	-5.572252	2.242685
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H	-3.131391	5.370529	-1.965754	C	2.341598	-0.778722	1.233309
H	-2.356213	5.697457	-0.403337	C	2.004205	-1.538336	0.123900
H	-3.549980	4.396835	-0.543948	H	1.664599	-1.037856	-0.779872
H	0.830295	3.927290	-2.714784	C	2.088119	-2.941529	0.139189
H	0.373703	5.461195	-1.945067	H	1.893249	-3.190706	-1.992854
H	-0.424211	4.951614	-3.443859	C	1.679814	-3.735780	-1.068941
H	-3.049806	0.355284	0.422640	H	2.179416	-4.707441	-1.095925
H	-3.969369	1.865318	0.332579	H	0.597186	-3.918081	-1.038222
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H	-3.641593	3.195436	3.565439	H	2.907756	-4.549846	3.810486
H	3.238191	3.598141	0.301543	C	2.792350	-1.457790	2.410138
H	3.278121	5.285760	0.841246	B	3.159449	-0.689899	3.597932
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H	-0.643430	5.823799	2.335844	H	6.204087	0.676682	6.813411
H	2.122917	2.561105	3.014347	H	6.881190	-0.299922	4.554716
H	0.833107	3.459360	3.837370	C	5.912809	-0.808021	4.558655
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D				H	5.629438	-1.013610	3.519515
H	2.425680	1.131403	0.236434	C	4.212698	1.434062	7.140674

H	3.733457	2.294201	9.059398	C	10.425134	-3.612149	2.038436
C	4.587329	2.189223	8.384435	C	11.309412	-3.459143	3.134703
H	4.921569	3.199720	8.113479	C	12.683173	-3.393378	2.897033
H	5.410741	1.701023	8.912804	C	13.205653	-3.484081	1.603920
C	2.892440	1.470424	6.659825	C	12.315141	-3.614907	0.525644
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C	2.523878	0.804500	5.500890	C	10.785426	-3.305712	4.545742
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Ts_a				H	3.133301	-1.276932	1.686416
C	6.476482	-0.979646	1.626419	H	4.259152	-3.541013	1.466862
C	5.247191	-1.631202	1.474336	H	6.244246	-5.633761	2.972944
C	5.209824	-3.027911	1.592537	H	6.934212	-5.815625	1.352746
C	6.345716	-3.781829	1.856910	H	5.195187	-5.564749	1.555066
C	7.606569	-3.110742	2.002139	H	12.712038	-3.676255	-0.485505
C	7.653210	-1.677835	1.872658	H	10.572221	-3.829898	-1.408035
B	8.926338	-3.758381	2.254508	H	9.419050	-4.731831	-0.413050
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C	6.178626	-5.282025	1.937168	H	15.059338	-4.469625	1.154361
C	3.996812	-0.860812	1.158193	H	13.360269	-3.259957	3.738152
C	8.930359	-0.883156	2.028492	H	11.152075	-2.373157	4.987604

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C 3.869712 -0.001783 -1.120536
C 3.207750 -1.205750 -0.849665
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H -1.259490 -0.017024 -3.346742
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H -4.862546 -0.002813 1.205041
H -2.084389 0.885454 2.901674
H -2.080056 -0.883959 2.900465
H -3.610395 -0.002608 2.983090
H 3.717578 -2.148503 -1.037091
H 1.911721 -3.371849 -0.049589
H 0.636415 -2.532688 0.846371
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H 1.847922 3.390192 -0.326185
H 0.299169 2.634424 -0.737150
H 0.868082 2.629310 0.933746
Ts_b
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C -1.852744 -0.006218 -1.190943
C -3.180894 -0.014937 -1.602576
C -4.242040 -0.031848 -0.691933
C -3.944846 -0.042922 0.679032
B -0.097432 -0.006046 0.592287
O 0.249558 -0.010834 2.139499
C 1.462483 -0.000146 2.326911
O 2.510339 0.011835 2.791955

C	-0.801029	0.007795	-2.275880	H	5.444907	-0.870095	-2.416255
C	-5.666505	-0.022579	-1.169254	H	3.695109	2.168504	-1.184543
C	-2.451907	-0.047150	2.654653	H	1.862623	3.402669	-0.342891
C	1.291231	0.007435	-0.104584	H	0.313721	2.640287	-0.743500
C	1.927743	1.243181	-0.402026	H	0.899139	2.626252	0.919966
C	3.201990	1.224501	-0.962740	F			
C	3.864615	0.021319	-1.246375	C	5.483015	-2.184897	4.983032
C	3.219227	-1.188193	-0.957203	C	5.050276	-0.892169	4.427238
C	1.943313	-1.219999	-0.397796	C	6.005167	-0.103010	3.639911
C	1.217105	2.548267	-0.127893	C	7.236366	-0.645776	3.353435
C	1.241252	-2.533411	-0.143213	C	7.620318	-1.908951	3.849995
C	5.254826	0.031236	-1.826638	C	6.729938	-2.658914	4.652832
H	-1.283212	0.008664	-3.255916	B	3.495697	-1.002867	3.745424
H	-0.161290	0.893367	-2.215226	C	2.777174	-1.660841	2.591945
H	-0.147511	-0.868020	-2.222894	C	1.339481	-1.615532	2.554706
H	-3.399307	-0.011405	-2.667496	C	0.666588	-2.235911	1.507255
H	-5.729834	-0.229455	-2.240554	C	1.340169	-2.899221	0.473519
H	-6.267007	-0.758596	-0.624781	C	2.737706	-2.934772	0.510164
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H	-4.763552	-0.061604	1.394587	C	0.504520	-0.930960	3.611457
H	-1.912680	0.839941	3.003471	C	4.967171	-2.414136	1.466516
H	-1.891405	-0.928281	2.984507	C	0.573363	-3.543489	-0.648836
H	-3.424992	-0.063866	3.150167	C	5.625762	1.271255	3.183106
H	3.724105	-2.126962	-1.174749	C	8.959970	-2.471041	3.511724
H	1.945491	-3.368631	-0.151101	C	4.557116	-2.952276	5.877003
H	0.719208	-2.541577	0.822159	O	2.947700	-0.201549	4.786665
H	0.484914	-2.723271	-0.915155	C	4.167889	-0.044380	5.394701
H	5.998902	0.064189	-1.020249	O	4.416116	0.581043	6.379065
H	5.413704	0.910355	-2.457868	H	5.277941	-3.054759	0.638098

H	5.405948	-1.424452	1.303444	O	3.767997	-0.620013	-1.418180
H	5.393550	-2.826727	2.384925	C	4.645863	1.908870	1.277902
H	3.275244	-3.444608	-0.285882	C	0.179566	1.893027	3.580288
H	1.227004	-4.137941	-1.291922	C	0.643468	-0.523587	-0.819122
H	-0.221254	-4.187980	-0.257036	O	3.718248	1.664458	-1.664095
H	0.089305	-2.775476	-1.265162	B	3.034011	2.592723	-0.967164
H	-0.420649	-2.205509	1.495205	C	2.833498	4.070733	-0.882849
H	0.715066	0.142409	3.655150	C	3.944907	4.868289	-1.324515
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H	-0.556699	-1.062955	3.388469	C	2.677339	6.882395	-0.761248
H	7.051641	-3.624955	5.031534	C	1.599983	6.088907	-0.355811
H	4.978525	-3.925229	6.132783	C	1.655447	4.698095	-0.402681
H	4.373762	-2.396070	6.805149	C	5.213355	4.258360	-1.871975
H	3.581858	-3.111429	5.398455	C	0.453584	3.905749	0.034401
H	9.665948	-1.691577	3.218691	C	2.595008	8.383869	-0.718266
H	8.843170	-3.156740	2.659130	H	-0.454730	4.298272	-0.433613
H	9.364470	-3.058911	4.340444	H	0.538322	2.849626	-0.231322
H	7.939623	-0.083303	2.745946	H	0.320277	3.980036	1.118648
H	6.300099	1.626065	2.402055	H	0.690822	6.567502	0.001012
H	4.596011	1.308479	2.809023	H	1.743228	8.721386	-0.122530
H	5.686006	1.968104	4.030202	H	3.513382	8.814334	-0.306101
Ts_c				H	2.479420	8.781522	-1.734647
C	1.222845	0.342681	0.264939	H	4.678734	6.859441	-1.559340
C	2.561039	0.837648	0.165794	H	5.661712	3.545433	-1.170995
C	3.170125	1.584304	1.227054	H	5.949626	5.038896	-2.073926
C	2.354821	1.940146	2.307565	H	5.020943	3.720440	-2.806899
C	1.032737	1.509954	2.405468	H	2.790151	2.523474	3.114234
C	0.490614	0.704220	1.380563	H	4.806637	2.991842	1.308551
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H -0.331270 1.014756 3.988366
H -0.599418 2.596789 3.260268
H 0.768438 2.366574 4.368547
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H 1.130956 -1.504794 -0.825698

G

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C -1.385415 1.410100 -1.319533
C -2.287975 2.043157 -0.449119
C -1.791422 2.954039 0.486275
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H 3.234120 6.285739 -2.922281
C 2.425763 5.841915 -1.005542
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H 3.588869 6.765903 0.551208
H 3.594385 7.637437 -0.994497
H 2.163137 7.692882 0.052661
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O 1.207014 5.275554 2.147982
C 1.397945 5.093491 1.037640

D'

H 1.248491 0.154478 3.468971
C 0.354316 -0.254972 3.011586
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Cl	0.452736	-2.070998	5.017911	B	-3.175180	2.851185	3.834573
C	-1.402677	-1.921811	3.004056	H	-2.055275	2.508738	1.700055
Cl	-2.175825	-3.324407	3.685988	C	-4.587268	4.847863	5.419068
C	-1.943038	-1.344667	1.853248	H	-5.388584	4.102599	5.346596
H	-2.832203	-1.781266	1.411383	H	-4.992663	5.736231	5.908328
H	-1.755744	0.203778	0.380686	C	-3.367009	4.186480	3.271502
C	-1.333697	-0.229829	1.281926	H	-2.758514	3.224967	0.239905
C	-0.185544	0.314775	1.860680	C	-2.179349	3.444843	1.143783
H	0.298953	1.179051	1.417451	H	-1.188657	3.786921	0.827445
C	-2.010567	0.241198	6.259338	H	-3.806551	4.429159	6.065635
H	-1.229611	0.089548	7.000038	C	-4.046568	5.183184	4.052240
C	-1.992060	1.384858	5.481008	C	-4.194340	6.447454	3.511639
C	-0.888227	2.400475	5.613493	H	-4.701518	7.215735	4.090453
H	-1.262739	3.427401	5.523423	C	-3.703836	6.767742	2.229133
H	-0.148736	2.253112	4.816679	C	-3.887490	8.156465	1.686687
H	-0.374511	2.304079	6.572626	H	-4.952553	8.414498	1.655078
H	-3.218863	-1.652504	8.037176	H	-3.402200	8.887481	2.344315
H	-3.757985	-2.677461	6.688201	H	-3.470563	8.256194	0.682133
H	-2.022505	-2.421285	6.992860	C	-3.050169	5.783158	1.476987
C	-3.014526	-0.734813	6.114774	H	-2.674485	6.032227	0.487436
C	-3.009324	-1.946779	7.001034	C	-2.871204	4.495888	1.969825
C	-4.008758	-0.560438	5.141397				
H	-4.769255	-1.326898	5.016600	Ts_a'			
C	-4.041815	0.566747	4.332389	C	5.911316	0.080267	3.982522
H	-4.780296	0.162677	2.364329	C	5.092268	-1.022747	4.322217
H	-6.051011	0.317429	3.584835	C	5.601921	-2.063834	5.145601
C	-5.087001	0.717345	3.259832	C	6.910440	-1.967582	5.608505
H	-5.225663	1.764409	2.963576	C	7.737071	-0.881622	5.276974
C	-3.040293	1.569797	4.519468	C	7.222283	0.127821	4.458600

B	3.655685	-1.085330	3.814734	H	0.756951	-5.779717	1.014883
O	2.796259	0.128880	4.785511	H	-0.536508	-4.614941	0.658474
C	3.333601	0.654931	5.713785	H	-0.450814	-2.872883	2.271947
O	3.816509	1.177157	6.615278	H	0.685009	0.114827	3.541114
C	4.746810	-3.257314	5.502472	H	0.609560	-1.064200	4.857047
C	9.141672	-0.799879	5.816784	H	-0.596252	-1.105495	3.565143
C	5.389403	1.182031	3.088412	H	7.302573	-2.757241	6.246079
C	2.742197	-1.829967	2.907436	H	5.224444	-3.863233	6.276206
C	1.305988	-1.876625	2.965774	H	3.759421	-2.953785	5.869152
C	0.633970	-2.837153	2.219855	H	4.582957	-3.897764	4.626821
C	1.298063	-3.742703	1.383657	H	9.750618	-0.099735	5.238750
C	2.689036	-3.636004	1.258877	H	9.625364	-1.781706	5.809139
C	3.422570	-2.705986	1.980775	H	9.125361	-0.452433	6.857722
C	0.541647	-4.782862	0.609538	H	7.857046	0.967018	4.181572
C	0.459855	-0.928735	3.780767	H	6.062322	1.346388	2.240766
C	4.908846	-2.631582	1.715783	H	4.400616	0.940544	2.678173
Cl	-0.415551	-1.464499	-0.895929	H	5.310660	2.132901	3.628540
C	1.088241	-0.638535	-0.601543	H	2.265517	2.073409	1.067651
C	1.088466	0.498231	0.208484	H	4.397440	1.272905	0.038709
C	2.277485	1.184827	0.443697	H	4.395496	-0.763695	-1.376534
C	3.468905	0.736777	-0.129049	H	0.153700	0.837491	0.642063
C	3.475583	-0.402792	-0.929506	E'			
C	2.286834	-1.093909	-1.166968	C	-0.904604	-0.953755	1.488850
Cl	2.325315	-2.515342	-2.172345	C	0.118848	-0.861307	0.479457
H	5.144013	-3.181341	0.801162	C	-0.096637	-1.541494	-0.777497
H	5.247029	-1.599408	1.591176	C	-1.230425	-2.325583	-0.945265
H	5.493918	-3.072766	2.529621	C	-2.183595	-2.478741	0.067241
H	3.208842	-4.283284	0.557575	C	-2.007169	-1.765204	1.259737
H	0.855544	-4.785194	-0.439204	B	1.464897	-0.241112	0.626828

O	1.661471	0.584325	2.134438	H	-4.251036	-2.979668	0.393317
C	2.738115	1.005173	2.450121	H	-2.771747	-1.834857	2.028900
O	3.746237	1.423595	2.801341	H	-0.708505	0.862979	2.655419
C	0.849490	-1.435116	-1.950934	H	-0.082189	-0.581399	3.462389
C	-3.369580	-3.380692	-0.114702	H	-1.826455	-0.336820	3.316379
C	-0.872111	-0.208316	2.801544	H	5.749008	-1.875351	-0.345454
C	2.838469	-0.132519	-0.043468	H	4.268206	-3.049614	1.090516
C	3.204791	1.037175	-0.756387	H	2.862301	-2.230987	1.787648
C	4.478399	1.119189	-1.314653	H	2.713216	-3.075789	0.245585
C	5.406939	0.077845	-1.182918	H	7.235851	1.158636	-1.554911
C	5.032012	-1.066484	-0.469200	H	6.709635	0.136666	-2.893440
C	3.765306	-1.194784	0.102254	H	7.438422	-0.605712	-1.457326
C	2.209770	2.157110	-0.949339	H	4.758194	2.018377	-1.859774
C	3.385226	-2.452714	0.849070	H	2.706678	3.090170	-1.225495
C	6.777358	0.194512	-1.800239	H	1.500625	1.905516	-1.746131
Cl	-4.526931	-0.321700	-1.586651	H	1.616849	2.345358	-0.045550
C	-3.348071	0.871309	-1.122019	H	-2.384363	2.787766	1.514440
C	-3.328550	1.406031	0.172775	H	-0.737532	3.572606	-0.169512
C	-2.383368	2.376299	0.510718	H	-2.443691	0.879608	-3.066515
C	-1.461103	2.809717	-0.438988	H	-0.769592	2.612526	-2.476082
C	-1.478079	2.273099	-1.727408		Ts_b'		
C	-2.417007	1.302933	-2.068243	C	-2.774011	0.370244	0.607578
Cl	-4.472653	0.887704	1.379137	C	-1.600219	0.301104	-0.221675
H	0.390036	-1.883689	-2.834505	C	-1.777295	0.121776	-1.640799
H	1.095492	-0.395386	-2.183474	C	-3.055602	-0.059608	-2.154268
H	1.792914	-1.958391	-1.762811	C	-4.190024	-0.071923	-1.334589
H	-1.383804	-2.828308	-1.896773	C	-4.023214	0.168680	0.035447
H	-3.599304	-3.529894	-1.172536	B	-0.194715	0.273766	0.291267
H	-3.153701	-4.363886	0.324953	O	0.004870	0.462988	1.857894

C	1.176659	0.288660	2.175897	H	-4.903724	0.216437	0.670490
O	2.165284	0.172190	2.744830	H	-2.166276	1.576007	2.301370
C	-0.630897	0.136219	-2.624922	H	-2.276983	-0.153562	2.654609
C	-5.553914	-0.336554	-1.904663	H	-3.750120	0.805226	2.462577
C	-2.733967	0.665335	2.087794	H	3.336661	-2.622887	-0.865061
C	1.241402	-0.007871	-0.236881	H	1.276331	-3.443519	-0.014074
C	2.132534	1.062307	-0.524852	H	0.150092	-2.350379	0.806145
C	3.433114	0.771110	-0.925643	H	0.016223	-2.604276	-0.932978
C	3.882896	-0.549838	-1.059730	H	6.013348	-0.249939	-0.929576
C	2.994510	-1.594407	-0.774360	H	5.416369	-0.540342	-2.563717
C	1.681686	-1.352030	-0.373479	H	5.536485	-1.892242	-1.421556
C	1.657915	2.492717	-0.438769	H	4.115559	1.591041	-1.139754
C	0.734610	-2.499635	-0.110128	H	2.497956	3.190789	-0.412856
C	5.291617	-0.831267	-1.513353	H	1.038957	2.740870	-1.308853
Cl	-5.237068	3.202007	-2.388095	H	1.040292	2.673243	0.449454
C	-3.823604	3.648141	-1.476435	H	-2.774130	4.245399	1.700705
C	-3.868412	3.769428	-0.081433	H	-0.657965	4.711211	0.489994
C	-2.723526	4.148509	0.621526	H	-2.611492	3.799337	-3.239521
C	-1.539436	4.405764	-0.064988	H	-0.577702	4.488763	-1.997514
C	-1.494019	4.280400	-1.454345	F'			
C	-2.632236	3.898506	-2.159579	C	-0.902651	-1.237302	1.260617
Cl	-5.336956	3.461888	0.802955	C	0.126894	-0.795356	0.363768
H	-1.020534	0.147679	-3.645535	C	0.099904	-1.254343	-0.987420
H	0.006241	1.014834	-2.493641	C	-0.889698	-2.139750	-1.396605
H	0.007437	-0.747393	-2.521749	C	-1.867335	-2.614251	-0.513656
H	-3.177710	-0.189715	-3.226780	C	-1.857396	-2.141105	0.802459
H	-5.594675	-0.098198	-2.970560	B	1.233642	0.071485	0.908932
H	-5.800171	-1.400510	-1.788089	O	1.291248	0.791332	2.131265
H	-6.320500	0.238259	-1.377506	C	2.630022	1.071234	1.982387

O	3.331092	1.676550	2.733364	H	-1.130567	0.303138	2.761379
C	1.102247	-0.780741	-2.006821	H	-0.094577	-1.028727	3.264751
C	-2.898150	-3.612148	-0.964029	H	-1.850043	-1.259936	3.183478
C	-0.998005	-0.781491	2.696751	H	4.962958	-2.174988	-0.373551
C	2.891966	0.387918	0.609452	H	3.966954	-2.738065	1.695173
C	3.184376	1.323847	-0.481837	H	3.824550	-1.319475	2.756198
C	4.039257	0.929015	-1.483258	H	2.379132	-2.014471	2.016998
C	4.682356	-0.327865	-1.453545	H	6.543051	-0.106998	-2.446944
C	4.453114	-1.216018	-0.380074	H	5.197183	-0.446099	-3.527465
C	3.625695	-0.884445	0.669101	H	5.888101	-1.757959	-2.522992
C	2.563626	2.685544	-0.469023	H	4.234541	1.600708	-2.314108
C	3.440788	-1.794496	1.844750	H	2.651429	3.169451	-1.442817
C	5.623488	-0.699776	-2.551224	H	1.507055	2.641805	-0.184712
Cl	-4.159698	-0.282198	-1.673554	H	3.069595	3.314638	0.275191
C	-3.049212	0.882014	-1.013390	H	-2.318552	2.537962	1.864471
C	-3.122543	1.271132	0.331285	H	-0.622920	3.564318	0.377365
C	-2.241972	2.233930	0.826188	H	-2.030125	1.124337	-2.884439
C	-1.286433	2.799697	-0.014890	H	-0.463127	2.839744	-2.012641
C	-1.201947	2.399777	-1.349763				
C	-2.080632	1.441059	-1.848354	Ts_c'			
Cl	-4.302101	0.577643	1.406288	C	1.210716	0.360269	0.237730
H	0.849486	-1.157729	-3.000572	C	2.518709	0.842007	0.175883
H	1.136588	0.311643	-2.060050	C	3.065467	1.519345	1.264224
H	2.107297	-1.139811	-1.762463	C	2.302061	1.723214	2.414859
H	-0.909505	-2.465416	-2.433890	C	0.994382	1.243478	2.482014
H	-3.068433	-3.548597	-2.042101	C	0.447039	0.557026	1.397855
H	-2.554841	-4.630317	-0.738362	Cl	-1.182547	-0.038994	1.514209
H	-3.847398	-3.461321	-0.442073	Cl	0.553192	-0.471937	-1.139699
H	-2.628185	-2.477912	1.491040	C	0.754187	-3.229848	1.863926
				C	1.368017	-2.460776	2.843257

C	2.696029	-1.969647	2.593242	H	-0.336351	-2.688873	4.125712
C	3.335268	-2.258501	1.359654	H	0.423219	-1.093070	4.222599
C	2.663667	-3.024674	0.412027	H	6.342247	-3.931756	4.024577
C	1.378058	-3.522221	0.642361	H	3.623977	-3.553847	4.994738
C	4.713843	-1.753339	1.035317	H	4.968983	-3.725311	6.117277
B	3.284554	-1.155780	3.696030	H	3.841552	-2.373314	6.306545
O	2.930280	-0.443662	4.788070	H	9.308169	-2.421155	2.674197
C	4.183000	-0.032259	5.348145	H	8.143439	-2.813111	1.411004
C	5.212365	-0.762086	4.549588	H	8.369186	-3.935743	2.767197
C	5.273877	-2.192372	4.667938	H	7.972390	-0.201588	2.651858
C	6.284582	-2.848714	3.960504	H	6.893325	1.866745	3.091721
C	7.252350	-2.150917	3.236872	H	5.209613	1.877333	3.656841
C	7.208243	-0.740701	3.205544	H	6.523568	1.867931	4.828644
C	6.224788	-0.022301	3.860180	H	4.081171	1.896856	1.200268
C	0.621537	-2.165810	4.120876	H	0.390556	1.401222	3.368983
C	0.654572	-4.318734	-0.407508	H	3.097563	0.684031	-0.727353
C	4.365525	-2.992349	5.575471	H	2.708479	2.268677	3.261032
C	8.331462	-2.880086	2.490455	G'			
C	6.211482	1.481488	3.851889	H	-3.157559	0.504347	-1.411253
O	4.247835	0.773527	6.220036	C	-2.324851	0.541735	-2.121452
H	4.759105	-1.393805	0.003438	H	-1.657543	1.359798	-1.837516
H	5.017282	-0.934557	1.690536	H	-1.768248	-0.398166	-2.019463
H	5.445128	-2.562756	1.132257	C	-2.821408	0.701058	-3.536257
H	3.149273	-3.226740	-0.539613	C	-3.915464	-0.050284	-3.991319
H	1.336719	-4.668980	-1.186027	H	-4.413670	-0.736132	-3.309663
H	0.142028	-5.178600	0.035326	C	-4.374931	0.048362	-5.300289
H	-0.111751	-3.693105	-0.882604	C	-5.541555	-0.783225	-5.773903
H	-0.249298	-3.604681	2.050745	H	-6.349509	-0.148215	-6.156996
H	1.184833	-2.477882	5.007272	H	-5.238600	-1.455297	-6.586305

H	-5.940727	-1.395826	-4.962172	N	12.148678	10.729738	15.032896
Cl	-0.275379	-1.746854	-4.482769	N	10.201311	11.875338	14.168364
C	-0.893868	-1.506239	-6.092876	N	10.418128	11.805845	16.360389
C	-2.003281	-2.223474	-6.558232	C	11.036647	11.383294	15.175720
Cl	-2.818753	-3.381617	-5.544222	C	9.274031	12.551671	16.067455
C	-2.477457	-2.009147	-7.853380	C	9.132657	12.577486	14.729098
H	-3.339460	-2.568534	-8.201311	C	11.022287	11.853467	17.665106
C	-1.848906	-1.080317	-8.680231	C	10.793283	10.806775	18.577742
H	-2.232268	-0.911877	-9.680912	C	11.325622	10.957721	19.863337
H	-0.255220	0.365132	-8.852335	C	12.041143	12.097810	20.222004
C	-0.744610	-0.365104	-8.216002	C	12.255802	13.112390	19.296247
H	0.584541	-0.022225	-6.547105	C	11.759383	13.006308	17.992983
C	-0.267735	-0.577022	-6.924702	C	9.801837	9.671198	18.359481
C	-3.716785	0.934759	-6.190782	C	8.358239	10.147608	18.621531
C	-2.615740	1.701920	-5.752445	C	10.087989	8.506438	19.316238
C	-1.914505	2.666697	-6.677680	C	12.027155	14.109539	16.979365
H	-0.829438	2.615593	-6.544200	C	13.533908	14.340725	16.765440
H	-2.137906	2.456485	-7.729331	C	11.307399	15.412472	17.373947
H	-2.227357	3.696832	-6.466935	C	10.463417	11.833672	12.753563
C	-2.188556	1.569853	-4.428287	C	10.054579	10.715243	11.999062
H	-1.333882	2.151539	-4.088981	C	10.345511	10.740637	10.628667
B	-4.189548	1.036807	-7.624849	C	11.008313	11.815208	10.042113
O	-4.595050	1.121448	-8.777154	C	11.365586	12.919610	10.804745
a				C	11.089644	12.957773	12.174667
Si	12.742020	9.296395	15.751194	C	9.326242	9.516623	12.616108
Si	15.153545	9.353890	15.233981	C	8.037878	9.897465	13.386592
Si	16.055636	10.416057	17.170573	C	8.943669	8.468313	11.558994
Si	16.289612	7.276545	15.121428	C	11.415613	14.205280	12.982532
Si	15.604896	10.535458	13.249666	C	12.636482	14.984592	12.467103

C	10.218198	15.180982	12.996165	H	10.053126	9.907026	10.001713
C	17.019671	11.986518	16.730348	H	11.236901	11.790881	8.980123
C	14.626439	10.886471	18.307555	H	11.862618	13.761630	10.333400
C	17.201376	9.370185	18.266282	H	10.024033	9.053669	13.326328
C	16.080515	6.224231	13.555892	H	7.442380	10.612409	12.806677
C	16.473777	6.184512	16.666015	H	8.241510	10.327240	14.368864
C	18.172264	7.532385	15.023937	H	7.426226	9.000404	13.533528
C	14.684680	9.692549	11.817869	H	8.208388	8.890877	10.864087
C	17.448015	10.580668	12.792743	H	8.476851	7.601140	12.037791
C	14.968910	12.312852	13.354180	H	9.799122	8.111381	10.977178
H	8.676029	12.986430	16.849544	H	11.621004	13.887657	14.010351
H	8.347712	12.985513	14.117956	H	12.396453	15.501382	11.529757
H	11.195952	10.165310	20.592421	H	13.503973	14.343442	12.301950
H	12.454818	12.182385	21.223272	H	12.903080	15.748638	13.205360
H	12.842891	13.982893	19.576784	H	9.993894	15.499629	11.971669
H	9.876488	9.372790	17.306799	H	10.473770	16.069016	13.585646
H	8.073356	10.957900	17.943464	H	9.316304	14.738275	13.420204
H	8.252694	10.509765	19.650582	H	17.844537	11.770604	16.042731
H	7.652867	9.321036	18.474757	H	17.444158	12.424494	17.643599
H	11.109290	8.139112	19.180865	H	16.380754	12.741243	16.260145
H	9.406053	7.681444	19.094695	H	14.108707	9.996638	18.683400
H	9.944185	8.782129	20.367596	H	17.505383	9.999383	19.116072
H	11.616767	13.792222	16.016566	H	18.111342	9.024510	17.766573
H	14.018153	13.428967	16.405992	H	15.070530	5.816786	13.453669
H	14.033684	14.654995	17.688751	H	16.777899	5.376666	13.612366
H	13.684836	15.123670	16.013720	H	16.310243	6.785283	12.643891
H	11.476273	16.184418	16.614358	H	15.524507	6.121419	17.210197
H	11.672992	15.792335	18.334675	H	17.013333	6.696172	17.470101
H	10.228502	15.247311	17.461200	H	17.041145	5.280039	16.403892

H	18.470704	7.915462	14.042034	Si	15.359690	9.891155	15.320106
H	18.673259	6.564363	15.170135	Si	16.472227	10.933299	17.128438
H	18.554487	8.226341	15.779578	Si	15.962852	7.612173	15.274793
H	13.598054	9.760567	11.948545	Si	15.769527	10.982444	13.278172
H	14.954141	8.633176	11.739256	N	12.352491	11.181154	15.311389
H	14.942136	10.174256	10.864361	N	10.345516	12.039576	14.309994
H	17.794349	9.599415	12.447537	N	10.495035	12.190519	16.502059
H	18.073273	10.875481	13.643273	C	11.185016	11.738597	15.379019
H	17.615369	11.302823	11.981949	C	9.279244	12.764969	16.117054
H	15.074474	12.814498	12.382819	C	9.182208	12.659034	14.773257
H	15.516454	12.906390	14.093264	C	11.052183	12.242000	17.826961
H	13.909550	12.311297	13.631127	C	10.858710	11.151121	18.694175
H	10.422038	6.012704	14.876076	C	11.424772	11.239030	19.971199
C	12.831713	5.239822	13.801997	C	12.149723	12.362927	20.359527
H	11.960356	4.710774	13.411375	C	12.320155	13.429838	19.481413
H	13.664599	4.529738	13.854021	C	11.771274	13.394128	18.194501
H	13.102430	6.012828	13.070451	C	10.012687	9.955649	18.282257
C	12.550214	5.850258	15.154707	C	8.539733	10.189897	18.681336
C	13.596804	6.110244	16.048722	C	10.521805	8.624106	18.851275
C	13.359642	6.705549	17.284499	C	11.993105	14.539726	17.216639
C	12.062052	7.050826	17.661643	C	13.395119	14.431061	16.585680
C	11.009211	6.798402	16.785527	C	11.777916	15.919944	17.859948
C	11.254700	6.205746	15.546050	C	10.720482	11.882726	12.931557
H	14.613660	5.857461	15.767670	C	10.735942	10.591480	12.373822
H	14.188646	6.899883	17.958390	C	11.101066	10.473579	11.028767
H	11.872514	7.512750	18.626485	C	11.436578	11.595042	10.274722
H	9.991213	7.056111	17.065412	C	11.416706	12.860018	10.853669
b				C	11.065795	13.033582	12.197317
Si	13.008463	9.731182	15.904221	C	10.323133	9.367784	13.177560

C	8.836812	9.040006	12.928582	H	13.539227	15.212668	15.831198
C	11.211220	8.145740	12.898844	H	11.862951	16.702071	17.097350
C	11.025471	14.430338	12.805084	H	12.528726	16.127923	18.629756
C	12.304489	15.241915	12.533205	H	10.786989	15.993593	18.320754
C	9.789454	15.201587	12.296708	H	11.126588	9.491438	10.566309
C	16.911868	12.735114	16.736642	H	11.720550	11.480602	9.231979
C	15.335575	10.913371	18.644934	H	11.685445	13.726862	10.256526
C	18.097179	10.070705	17.591435	H	10.434565	9.606630	14.238914
C	14.914044	6.682939	13.995888	H	8.666797	8.794704	11.873753
C	15.586210	6.835192	16.965150	H	8.196412	9.890107	13.188433
C	17.786751	7.308872	14.854478	H	8.531484	8.180100	13.536075
C	14.899649	10.081165	11.856672	H	11.054093	7.747913	11.889571
C	17.616618	11.096856	12.857589	H	10.978945	7.351151	13.613309
C	15.034637	12.721918	13.352195	H	12.270744	8.396647	13.005274
H	8.604834	13.186521	16.843803	H	10.931480	14.324563	13.890509
H	8.396490	12.950940	14.096833	H	12.441564	15.430312	11.462711
H	11.303677	10.415832	20.667865	H	13.190281	14.723127	12.905743
H	12.589832	12.404767	21.352358	H	12.235431	16.213936	13.034240
H	12.895499	14.295807	19.795755	H	9.854255	15.356764	11.213768
H	10.059596	9.879603	17.189748	H	9.727929	16.182970	12.779877
H	8.144592	11.105979	18.231445	H	8.861560	14.658186	12.501820
H	8.447439	10.277951	19.770173	H	17.621792	12.799395	15.903816
H	7.918804	9.349487	18.350401	H	17.377014	13.205698	17.613392
H	11.561640	8.449561	18.559262	H	16.027091	13.320122	16.469558
H	9.918036	7.804634	18.450426	H	15.072732	9.887339	18.928722
H	10.443617	8.590682	19.944101	H	14.399870	11.448917	18.446034
H	11.259283	14.440200	16.409688	H	15.818493	11.390388	19.508227
H	13.529699	13.456784	16.107075	H	17.939229	9.027436	17.886598
H	14.166650	14.549922	17.355105	H	18.570593	10.592054	18.434564

H	18.802120	10.079025	16.751743	C	10.137577	5.099355	15.071106
H	13.849193	6.759708	14.241331	H	13.368053	4.076510	15.210356
H	15.179385	5.617571	13.986892	H	12.996781	4.518989	17.610895
H	15.059034	7.075632	12.983531	H	10.787392	5.339847	18.404722
H	14.526898	6.966059	17.215633	H	8.954493	5.713465	16.762755
H	16.181844	7.287836	17.766037	c			
H	15.799473	5.757837	16.950755	Si	13.012684	9.454171	15.678420
H	18.035449	7.704468	13.862662	Si	15.359395	9.772571	15.149171
H	18.002132	6.231865	14.851262	Si	16.414611	10.692792	17.066239
H	18.452541	7.786290	15.581080	Si	16.159339	7.551095	14.891524
H	13.819082	10.038568	12.027345	Si	15.767912	11.015516	13.178035
H	15.268121	9.057490	11.727700	N	12.273835	10.913924	15.138119
H	15.065123	10.620697	10.914379	N	10.157471	11.577751	14.195549
H	18.065751	10.101590	12.761511	N	10.377587	11.779812	16.385261
H	18.170927	11.638414	13.632485	C	11.063627	11.369245	15.237359
H	17.760676	11.626522	11.906008	C	9.101639	12.237534	16.040327
H	15.087365	13.205654	12.367959	C	8.962840	12.100424	14.697426
H	15.550748	13.360483	14.076242	C	11.025855	11.972531	17.652506
H	13.983167	12.648833	13.650018	C	11.040838	10.916830	18.588322
H	9.333125	5.269892	14.358492	C	11.743267	11.125773	19.783352
C	11.618008	4.382598	13.140120	C	12.403079	12.330211	20.030616
H	10.719096	4.584003	12.549975	C	12.354657	13.363367	19.096866
H	11.918129	3.343300	12.962215	C	11.658370	13.210697	17.889426
H	12.423404	5.023339	12.761932	C	10.276955	9.626236	18.334012
C	11.375668	4.636371	14.609316	C	8.832032	9.755545	18.854100
C	12.396350	4.428795	15.547906	C	10.960295	8.386129	18.921849
C	12.187801	4.678096	16.902990	C	11.621466	14.344425	16.874280
C	10.948108	5.139829	17.349288	C	12.985756	14.517937	16.188253
C	9.922969	5.350393	16.428084	C	11.135804	15.661186	17.500785

C	10.511427	11.447352	12.809762	H	8.260797	8.841151	18.633465
C	10.607471	10.157199	12.247464	H	11.994048	8.297937	18.557394
C	10.986652	10.062155	10.901859	H	10.415371	7.481774	18.613625
C	11.253726	11.203923	10.146455	H	10.971949	8.402843	20.022197
C	11.144327	12.467154	10.723845	H	10.894778	14.074794	16.093771
C	10.780007	12.619180	12.069496	H	13.306200	13.582118	15.710344
C	10.250434	8.912722	13.045318	H	13.756935	14.817082	16.913671
C	8.766514	8.558567	12.833682	H	12.928726	15.296886	15.412377
C	11.156449	7.715701	12.732897	H	11.047019	16.437243	16.725626
C	10.648289	14.011938	12.671607	H	11.839159	16.031756	18.261651
C	11.854200	14.914959	12.370042	H	10.152686	15.539508	17.979273
C	9.343686	14.680421	12.197710	H	11.076879	9.079338	10.436828
C	15.597381	9.998279	18.646506	H	11.551767	11.106818	9.100272
C	18.279447	10.280863	17.104530	H	11.357779	13.353396	10.123037
C	16.224085	12.588792	17.110108	H	10.386874	9.145484	14.111569
C	14.975687	6.560628	13.764557	H	8.570573	8.317361	11.777366
C	16.226214	6.649919	16.575063	H	8.111273	9.395318	13.117915
C	17.901179	7.498248	14.110245	H	8.488354	7.684570	13.442201
C	15.105289	10.046120	11.672508	H	10.995050	7.328405	11.715353
C	17.625607	11.373714	12.912229	H	10.948899	6.895665	13.435411
C	14.821201	12.662774	13.257685	H	12.218466	7.982566	12.832760
H	8.413405	12.612115	16.788053	H	10.589893	13.902174	13.764646
H	8.120506	12.308899	14.049741	H	11.936549	15.140265	11.296123
H	11.789159	10.329137	20.526980	H	12.793620	14.450432	12.695811
H	12.959416	12.462537	20.960947	H	11.742161	15.873891	12.898195
H	12.873436	14.301643	19.303118	H	9.358624	14.827253	11.106785
H	10.231728	9.484159	17.242647	H	9.220669	15.665724	12.672532
H	8.309365	10.603783	18.389349	H	8.461362	14.070966	12.440448
H	8.824470	9.909380	19.944414	H	14.542152	10.305995	18.703237

H	16.111737	10.379472	19.543599	H	9.915949	16.165586	21.670160
H	15.634283	8.899684	18.668718	H	11.082070	14.814167	21.780329
H	18.783005	10.663615	16.204408	C	9.032143	14.204854	21.572146
H	18.449078	9.195312	17.151271	C	8.459453	14.381358	20.312370
H	18.753640	10.740199	17.986930	C	7.505717	13.490061	19.830893
H	16.669021	13.063573	16.223492	C	7.109859	12.404842	20.607159
H	16.718701	12.997934	18.005863	C	7.677832	12.216462	21.863707
H	15.161135	12.862845	17.148587	C	8.631107	13.111172	22.339736
H	13.970334	6.509270	14.209494	H	8.767850	15.235991	19.699591
H	15.344485	5.531482	13.627209	H	7.063555	13.647258	18.842293
H	14.882416	7.027379	12.772892	H	6.354209	11.707289	20.234108
H	15.241405	6.666605	17.065558	H	7.371716	11.366958	22.481918
H	16.952511	7.119454	17.254595	d			
H	16.522161	5.598192	16.432586	Si	13.202959	9.397147	15.865415
H	17.886967	7.919507	13.094112	Si	15.451952	9.801441	15.081518
H	18.260989	6.458797	14.044336	Si	16.652163	10.754650	16.873838
H	18.622816	8.076034	14.706071	Si	16.282361	7.621706	14.729338
H	14.024125	9.869739	11.776480	Si	15.620944	11.066769	13.108241
H	15.606825	9.073514	11.562094	N	12.381685	10.836470	15.534606
H	15.267240	10.622347	10.747364	N	10.209663	11.564891	14.796796
H	18.208589	10.443298	12.853553	N	10.690592	11.852987	16.929513
H	18.028145	11.971858	13.743448	C	11.212234	11.351704	15.739286
H	17.779571	11.938232	11.978227	C	9.400806	12.351814	16.713473
H	14.887231	13.192843	12.294346	C	9.104516	12.169126	15.409481
H	15.214813	13.319821	14.046307	C	11.458481	11.965251	18.139562
H	13.765770	12.451884	13.482497	C	11.579423	10.838817	18.973891
H	9.075258	12.961264	23.330323	C	12.389178	10.963825	20.108833
C	10.071017	15.151816	22.077477	C	13.042404	12.159825	20.394876
H	10.043656	15.220594	23.178479	C	12.882406	13.266558	19.565601

C	12.082403	13.196234	18.420143	H	8.209660	12.393397	14.854223
C	10.806856	9.559800	18.682549	H	12.518239	10.115023	20.772358
C	9.361635	9.686025	19.207381	H	13.676731	12.230865	21.274454
C	11.477663	8.298025	19.241872	H	13.386756	14.195368	19.812737
C	11.898519	14.399942	17.503896	H	10.758459	9.444418	17.593498
C	12.912342	14.377755	16.341846	H	8.847195	10.539122	18.756870
C	11.978703	15.741542	18.249824	H	9.360358	9.823412	20.295149
C	10.410220	11.385991	13.384837	H	8.792307	8.779153	18.974252
C	10.447464	10.076716	12.868143	H	12.513559	8.218220	18.897990
C	10.703761	9.928202	11.501836	H	10.936151	7.412325	18.893554
C	10.895672	11.039060	10.682642	H	11.465210	8.282954	20.337816
C	10.827493	12.322076	11.214419	H	10.895051	14.327574	17.068680
C	10.592379	12.526782	12.579586	H	12.903455	13.421826	15.812872
C	10.145259	8.875977	13.753649	H	13.925922	14.543111	16.722970
C	8.618562	8.680255	13.867487	H	12.685209	15.175790	15.627050
C	10.831834	7.583929	13.289111	H	11.672133	16.552961	17.581226
C	10.488599	13.941902	13.134698	H	13.000620	15.958080	18.580150
C	11.618157	14.869544	12.654879	H	11.327721	15.754186	19.129620
C	9.118177	14.552948	12.771708	H	10.753073	8.933471	11.070060
C	16.001084	10.076426	18.520288	H	11.098406	10.901209	9.623872
C	18.508295	10.383080	16.755973	H	10.972154	13.179873	10.564033
C	16.425811	12.633435	16.909721	H	10.525127	9.094657	14.757122
C	15.038029	6.613482	13.711222	H	8.183922	8.464839	12.884342
C	16.511981	6.722095	16.383931	H	8.135576	9.577979	14.266773
C	17.937739	7.619620	13.804228	H	8.391726	7.842330	14.536376
C	14.916688	10.075976	11.652796	H	10.414117	7.215439	12.345373
C	17.413260	11.541234	12.704376	H	10.690617	6.802159	14.042358
C	14.594143	12.643473	13.267521	H	11.908256	7.733463	13.154929
H	8.821248	12.775027	17.516477	H	10.552462	13.884774	14.225937

H	11.579182	15.024883	11.571272	H	17.459594	12.119547	11.771589
H	12.599879	14.465192	12.909200	H	14.594542	13.197417	12.319753
H	11.513698	15.850442	13.131995	H	14.975062	13.304678	14.053229
H	9.025604	14.661232	11.684933	H	13.561287	12.381817	13.520551
H	9.010742	15.544563	13.225711	H	7.276076	11.863085	20.435709
H	8.290928	13.924951	13.116449	C	9.349614	13.536062	21.028145
H	14.950514	10.352954	18.667712	H	8.946662	13.091957	21.943900
H	16.576561	10.490204	19.359486	H	9.825471	14.487665	21.283033
H	16.072082	8.984200	18.566310	H	10.132230	12.866276	20.651481
H	18.926975	10.761963	15.816357	C	8.269194	13.723307	19.991136
H	18.705234	9.305951	16.799104	C	8.242204	14.855898	19.166241
H	19.048610	10.858782	17.585628	C	7.272903	15.002408	18.171654
H	16.802301	13.108526	15.996693	C	6.304644	14.014699	17.985507
H	16.960621	13.067160	17.765259	C	6.309808	12.886412	18.809211
H	15.365259	12.883730	17.010421	C	7.280340	12.746301	19.801655
H	14.082069	6.528077	14.242057	H	8.991851	15.631313	19.301005
H	15.416966	5.598601	13.531096	H	7.277696	15.887334	17.540864
H	14.839005	7.078302	12.739015	H	5.551482	14.124112	17.210205
H	15.570371	6.696995	16.945259	H	5.558024	12.112809	18.677255
H	17.263644	7.212738	17.012800	e			
H	16.835642	5.685740	16.218694	Si	13.202959	9.397147	15.865415
H	17.828451	8.050660	12.802131	Si	15.451952	9.801441	15.081518
H	18.315102	6.594514	13.690918	Si	16.652163	10.754650	16.873838
H	18.695887	8.204003	14.337574	Si	16.282361	7.621706	14.729338
H	13.874174	9.794964	11.841264	Si	15.620944	11.066769	13.108241
H	15.489403	9.159774	11.467429	N	12.381685	10.836470	15.534606
H	14.940640	10.678855	10.735023	N	10.209663	11.564891	14.796796
H	18.046755	10.654947	12.586448	N	10.690592	11.852987	16.929513
H	17.846172	12.155728	13.502913	C	11.212234	11.351704	15.739286

C	9.400806	12.351814	16.713473	C	15.038029	6.613482	13.711222
C	9.104516	12.169126	15.409481	C	16.511981	6.722095	16.383931
C	11.458481	11.965251	18.139562	C	17.937739	7.619620	13.804228
C	11.579423	10.838817	18.973891	C	14.916688	10.075976	11.652796
C	12.389178	10.963825	20.108833	C	17.413260	11.541234	12.704376
C	13.042404	12.159825	20.394876	C	14.594143	12.643473	13.267521
C	12.882406	13.266558	19.565601	H	8.821248	12.775027	17.516477
C	12.082403	13.196234	18.420143	H	8.209660	12.393397	14.854223
C	10.806856	9.559800	18.682549	H	12.518239	10.115023	20.772358
C	9.265653	9.626532	18.699480	H	13.676731	12.230865	21.274454
C	11.477663	8.298025	19.241872	H	13.386756	14.195368	19.812737
C	11.898519	14.399942	17.503896	H	10.758459	9.444418	17.593498
C	12.912342	14.377755	16.341846	H	8.895867	10.453315	18.087050
C	11.978703	15.741542	18.249824	H	8.900289	9.771156	19.723056
C	10.410220	11.385991	13.384837	H	8.840802	8.694151	18.310807
C	10.447464	10.076716	12.868143	H	12.513559	8.218220	18.897990
C	10.703761	9.928202	11.501836	H	10.936151	7.412325	18.893554
C	10.895672	11.039060	10.682642	H	11.465210	8.282954	20.337816
C	10.827493	12.322076	11.214419	H	10.895051	14.327574	17.068680
C	10.592379	12.526782	12.579586	H	12.903455	13.421826	15.812872
C	10.145259	8.875977	13.753649	H	13.925922	14.543111	16.722970
C	8.618562	8.680255	13.867487	H	12.685209	15.175790	15.627050
C	10.831834	7.583929	13.289111	H	11.672133	16.552961	17.581226
C	10.488599	13.941902	13.134698	H	13.000620	15.958080	18.580150
C	11.618157	14.869544	12.654879	H	11.327721	15.754186	19.129620
C	9.118177	14.552948	12.771708	H	10.753073	8.933471	11.070060
C	16.001084	10.076426	18.520288	H	11.098406	10.901209	9.623872
C	18.508295	10.383080	16.755973	H	10.972154	13.179873	10.564033
C	16.425811	12.633435	16.909721	H	10.525127	9.094657	14.757122

H	8.183922	8.464839	12.884342	H	18.315102	6.594514	13.690918
H	8.135576	9.577979	14.266773	H	18.695887	8.204003	14.337574
H	8.391726	7.842330	14.536376	H	13.874174	9.794964	11.841264
H	10.414117	7.215439	12.345373	H	15.489403	9.159774	11.467429
H	10.690617	6.802159	14.042358	H	14.940640	10.678855	10.735023
H	11.908256	7.733463	13.154929	H	18.046755	10.654947	12.586448
H	10.552462	13.884774	14.225937	H	17.846172	12.155728	13.502913
H	11.579182	15.024883	11.571272	H	17.459594	12.119547	11.771589
H	12.599879	14.465192	12.909200	H	14.594542	13.197417	12.319753
H	11.513698	15.850442	13.131995	H	14.975062	13.304678	14.053229
H	9.025604	14.661232	11.684933	H	13.561287	12.381817	13.520551
H	9.010742	15.544563	13.225711	H	8.132003	9.439949	22.320501
H	8.290928	13.924951	13.116449	C	8.593294	12.127979	22.215176
H	14.950514	10.352954	18.667712	H	8.362918	11.822290	23.240694
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H	19.048610	10.858782	17.585628	C	6.698381	11.011682	19.086977
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H	15.365259	12.883730	17.010421	C	7.732034	9.886282	21.413350
H	14.082069	6.528077	14.242057	H	7.407448	12.886838	19.865922
H	15.416966	5.598601	13.531096	H	6.297110	11.460527	18.182248
H	14.839005	7.078302	12.739015	H	6.103572	9.006433	18.553822
H	15.570371	6.696995	16.945259	H	7.022128	8.007160	20.640764
H	17.263644	7.212738	17.012800	Int_a			
H	16.835642	5.685740	16.218694	C	4.156797	19.957216	9.726710
H	17.828451	8.050660	12.802131	C	5.414982	19.415576	10.044630

C	6.619284	20.125548	9.895023	Br	5.990276	17.648203	16.030337
C	6.536812	21.417108	9.362850	C	2.539965	16.284888	14.209755
C	5.309038	21.968125	9.004103	C	8.765994	14.968595	11.599725
C	4.131037	21.250150	9.193231	H	5.413302	14.788231	10.341158
N	5.471853	18.059199	10.525804	H	5.178433	16.988540	8.669735
C	5.666684	17.701507	11.847518	H	8.166418	14.091067	14.990480
N	5.675039	16.320245	11.843818	H	6.144270	13.172133	16.057646
C	5.456270	15.844830	10.547235	H	3.900031	13.786149	15.230683
C	5.334685	16.917414	9.733761	H	8.053411	16.797557	12.469394
C	5.804146	15.494402	13.013920	H	7.969379	14.904135	10.852072
C	7.095616	15.198967	13.487880	H	9.035419	13.950870	11.904148
C	7.190594	14.344866	14.589785	H	9.639666	15.429459	11.125297
C	6.046826	13.829566	15.197883	H	9.193844	16.508557	14.702197
C	4.783125	14.170855	14.727700	H	10.297293	16.554418	13.315891
C	4.633475	15.017438	13.622709	H	9.932904	15.009481	14.093929
C	8.329846	15.797953	12.825709	H	3.364555	16.045850	12.249439
C	9.504543	15.974458	13.799573	H	3.133456	17.171428	14.451795
C	3.248273	15.426246	13.144123	H	2.387602	15.716196	15.133836
C	2.398054	14.203901	12.752348	H	1.560555	16.610954	13.842793
N	5.777769	18.524130	12.834097	H	1.421809	14.528324	12.375400
Si	6.230772	19.060969	14.295675	H	2.224867	13.547812	13.612680
Br	8.400060	19.680811	14.312719	H	2.891731	13.615041	11.971737
C	7.956467	19.508692	10.289712	H	7.441580	22.000778	9.228870
C	9.025697	20.555925	10.634914	H	5.268788	22.971099	8.587203
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C	2.509236	19.300634	11.508059	H	7.763131	17.757258	8.980592
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Si	6.146497	19.351699	14.114619	H	6.343503	13.067791	15.861429
Br	8.441468	19.702655	14.264197	H	4.012050	13.684965	15.332701
C	7.666108	19.289825	9.986448	H	7.795813	16.810109	12.187903
C	8.863071	20.184364	10.339227	H	7.453325	14.980697	10.525913
C	2.583118	19.451610	10.297283	H	8.649661	13.979718	11.374126
C	1.347942	20.071598	9.627661	H	9.151506	15.483914	10.572874
C	7.962537	18.448139	8.728028	H	9.227692	16.434891	14.215051
C	2.405601	19.467578	11.829147	H	10.131491	16.504652	12.691124
Br	5.461116	21.467037	13.343521	H	9.850588	14.943829	13.470868
Br	5.841148	17.826980	15.811457	H	3.136226	16.274163	12.747766
C	2.362957	15.817276	14.689879	H	2.936074	16.561846	15.247060
C	8.350077	15.010533	11.151696	H	2.184772	14.959016	15.347302
Si	4.810946	21.122448	16.962738	H	1.389238	16.249301	14.434684
Si	4.044141	23.350897	16.711468	H	1.310333	14.609489	12.448688
C	5.430859	24.564672	16.166770	H	2.279849	13.381913	13.289153
Si	2.762723	19.963485	17.088404	H	2.820097	14.019025	11.725579
C	1.355730	20.921148	17.946730	H	7.292363	21.893415	9.166213
K	7.662943	22.354062	15.982220	H	5.165868	23.098649	8.836107
Si	5.584677	21.009309	19.183667	H	3.014762	21.995657	9.316721
C	4.303167	21.262630	20.568735	H	7.530464	18.603058	10.826533
C	2.148082	19.563343	15.339519	H	8.142588	19.100814	7.866555
C	2.865008	18.330032	18.056623	H	7.126256	17.785804	8.484741
C	6.948261	22.314395	19.512412	H	8.854473	17.831271	8.885557
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H	9.727035	19.558044	10.586277	H	3.124706	23.071263	14.392973
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H	7.212287	19.133117	18.798780	H	5.126720	20.064953	5.167971
H	6.250537	24.638541	16.897145	H	6.527725	19.174093	5.786805
H	3.523666	20.493404	20.526531	H	5.546135	20.163296	6.887632
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C	0.641563	16.516218	4.629152	H	4.852030	17.660176	12.572760
C	0.964259	10.510047	5.784373	H	4.558881	7.298677	9.882578
C	-0.607752	12.718825	7.229912	H	6.121534	16.555076	12.000727
Br	4.386096	11.031062	7.373005	H	0.209987	12.455431	3.275751
H	-1.257274	13.436312	13.196085	H	4.532304	15.556762	10.366079
H	0.189239	14.338688	13.690997	H	-0.051940	12.650996	8.170601
H	7.549089	11.903975	12.838837	H	3.185028	18.133995	6.031966
H	6.000008	11.211591	13.361767	H	-0.715469	13.740952	4.066593
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H	7.214692	10.178133	12.591224	H	2.775191	18.824208	10.593348
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H	0.395639	13.534835	11.346172	H	2.211552	8.047056	9.867987
H	-1.952007	13.376257	10.729986	H	0.665609	9.657323	8.607670
H	8.020959	12.272381	10.350063	H	1.187104	11.556654	10.181025
H	5.753785	12.504928	11.227542	H	4.183555	16.754442	6.545009
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H	7.805320	10.534751	10.085696	H	0.042877	9.914077	5.824967
H	4.686960	15.913908	12.823155	H	4.392701	17.531396	8.804206
H	1.026051	16.277454	3.632767	H	0.131065	8.690803	9.997694
H	-0.323867	16.012120	4.750249	H	1.230054	11.154020	12.651212
H	-2.164363	15.130073	10.814848	H	1.584161	10.252513	6.647574
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H	-1.442234	12.007064	7.268718	H	-0.710432	10.189400	9.588554
H	6.864175	11.700177	9.131284	H	0.660351	9.493020	12.389939

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H	2.104603	14.205363	2.336346
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H	5.713104	14.855243	4.621873
H	6.064724	13.177665	5.051476
H	2.749132	11.259387	3.080917
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H	4.028678	10.867565	4.247197
H	6.192721	13.701365	3.356436
H	4.450590	11.377924	2.597610
H	5.087895	16.230451	15.390108
H	6.242861	14.174834	16.499216
H	5.817387	13.375950	14.981437
H	5.338697	12.649534	16.526583
H	2.932601	12.691722	16.508247
H	0.803259	13.935706	16.354428
H	0.800979	16.333894	15.686991
H	2.960190	17.476103	15.213086
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H	0.551180	16.078830	18.490854
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Br	1.845495	13.240906	12.389714	C	-0.398870	16.477903	11.829679
K	1.812861	10.276637	11.221899	C	-1.153250	15.402397	14.593542
C	4.770160	15.827588	15.605584	C	-1.662531	9.696531	12.817066
C	5.804001	16.124125	16.711867	C	-3.650916	11.789101	13.834413
C	10.113124	15.212477	16.316185	C	4.370717	14.475453	6.835049
C	4.095254	9.958104	17.088197	C	2.859434	12.505807	8.629882
C	8.381979	9.550698	14.486575	H	-2.031476	14.949145	9.138068
Br	4.943385	10.957662	11.452057	H	-1.850393	13.831134	7.772979
Si	5.279589	14.535562	10.237893	H	-0.424081	14.370064	8.682824
Si	3.634325	14.235576	8.566722	H	-0.933563	10.196289	9.703370
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Si	7.400076	14.005279	9.344150	H	-1.340507	10.894670	8.135847
C	8.709034	14.157586	10.690714	H	-3.722079	11.250046	10.539037
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C	7.390825	12.235148	8.668725	H	-4.111957	12.976376	10.478869
Si	5.205703	16.801762	10.885514	H	-3.791416	12.757430	14.329069
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Si	-0.810019	13.034194	12.082139	H	-1.347791	10.635798	15.835267
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H	-3.483485	15.521963	11.294579	H	12.343427	12.617164	12.279092
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H	-0.665594	17.491621	12.157092	H	0.724143	13.936222	17.088183
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Si	3.982952	13.693759	4.112886	H	-0.627208	15.353699	4.725006
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C	11.766421	12.710688	12.872937	C	15.346028	13.775530	13.752754
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