

Electronic Supplementary Information (ESI)

5-Aminotetrazole induces spin crossover in iron(III) pentadentate Schiff base complexes: experimental and theoretical investigations

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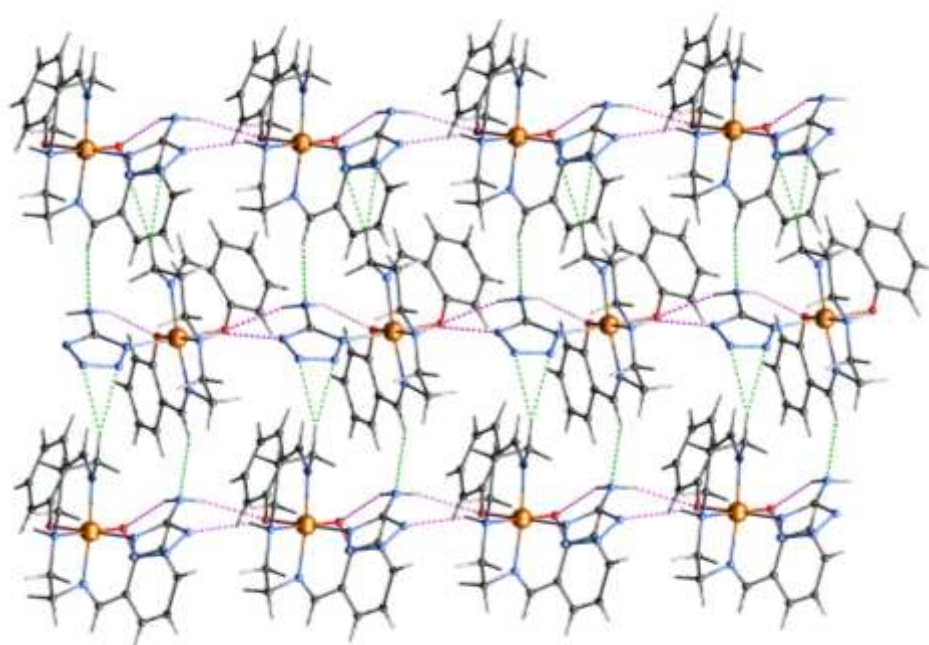


Figure S1. Part of the crystal structure of **2a** showing the N-H...O and N-H...N intermolecular hydrogen bonds (pink dashed lines) resulting in the formation of 1D supramolecular chains and C-H...N intermolecular non-covalent contacts (green dashed lines) connecting these chains into 2D layered structure. Parameters of the mentioned H-bonds can be found in Table 1.

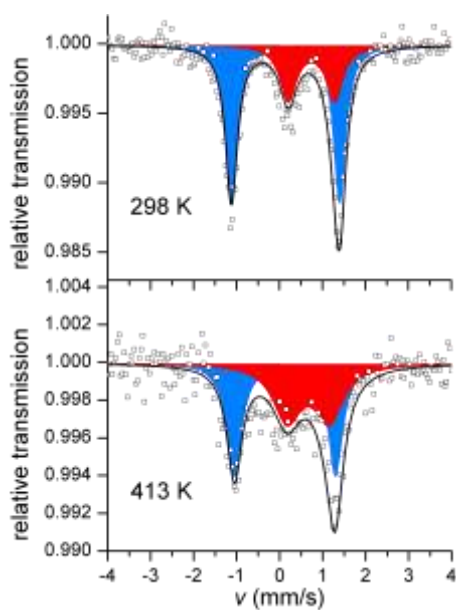


Figure S2. ^{57}Fe Mössbauer spectra for **2a** at $T = 298$ (top) and at $T = 413$ K (bottom), showing the iron(III) low-spin (LS) fractions (blue) and iron(III) high-spin (HS) fractions (red). The calculated parameters for data taken at 298 K: $\delta_{\text{LS}} = 0.14$ mm/s, $\Delta E_{\text{Q,LS}} = 2.52$ mm/s, $\delta_{\text{HS}} = 0.74$ mm/s, $\Delta E_{\text{Q,HS}} = 1.08$ mm/s, $A_{\text{LS}}:A_{\text{HS}} = 67:33$. The calculated parameters for data taken at 413 K: $\delta_{\text{LS}} = 0.12$ mm/s, $\Delta E_{\text{Q,LS}} = 2.35$ mm/s, $\delta_{\text{HS}} = 0.66$ mm/s, $\Delta E_{\text{Q,HS}} = 0.98$ mm/s, $A_{\text{LS}}:A_{\text{HS}} = 52:48$.

Table S1. Cartesian coordinates of all the optimized structures for the low-spin (LS) and high-spin (HS) states:

Model A, B3LYP/def2-TZVP, LS				Model A, B3LYP/def2-TZVP, HS			
Fe	3.200400	5.571015	3.938523	Fe	3.293662	5.543875	4.175314
O	3.460806	4.586304	5.561361	O	3.212145	4.579186	5.867320
O	3.563209	7.229367	4.829211	O	3.775061	7.252115	5.069151
N	1.328660	5.926618	4.288223	N	1.227955	5.984554	4.405214
N	2.891803	6.674705	2.239394	N	2.824567	6.702478	2.256080
H	3.267184	7.567450	2.556669	H	3.165835	7.616984	2.546589
N	5.155727	5.469223	3.533358	N	5.319597	5.673874	3.473490
N	2.802972	3.889009	3.006549	N	2.997660	3.734434	3.153249
N	1.826540	3.752402	2.060286	N	2.143973	3.594241	2.093911
N	1.804323	2.527220	1.670634	N	2.156527	2.362127	1.718278
N	2.731531	1.795927	2.331252	N	2.990948	1.633550	2.492167
N	4.386109	2.344340	3.967356	N	4.441174	2.199113	4.314723
H	4.415672	2.904565	4.810431	H	4.356865	2.742280	5.163521
H	4.477073	1.351972	4.123524	H	4.521135	1.207002	4.479875
C	2.537409	4.052447	6.419733	C	2.201255	4.140219	6.569290
C	2.917772	3.464758	7.534745	C	2.442967	3.272550	7.656802
H	3.962679	3.195103	7.622326	H	3.471126	3.009697	7.871119
C	2.002878	3.064777	8.481893	C	1.410362	2.776525	8.425643
H	2.336302	2.464357	9.320297	H	1.635977	2.108529	9.248589
C	0.649940	3.424764	8.380254	C	0.080502	3.124734	8.159380
H	-0.062579	3.105526	9.128651	H	-0.724146	2.729989	8.764672
C	0.251707	4.194845	7.313849	C	-0.182071	3.981820	7.113584
H	-0.787219	4.491447	7.218651	H	-1.204817	4.270118	6.896531
C	1.160363	4.624158	6.322046	C	0.844709	4.504809	6.302553
C	0.655597	5.467433	5.280537	C	0.458243	5.425191	5.265324
H	-0.394062	5.756930	5.366773	H	-0.609116	5.667363	5.238337
C	0.757112	6.931363	3.396069	C	0.705074	6.963298	3.463517
H	0.957664	7.916320	3.831609	H	0.951744	7.961913	3.842834
H	-0.326192	6.815341	3.301928	H	-0.384515	6.898918	3.375356
C	1.426496	6.813311	2.036466	C	1.356488	6.750273	2.102474
H	1.092013	5.906539	1.538074	H	1.052177	5.786688	1.694537
H	1.199354	7.682597	1.411357	H	1.050095	7.543165	1.409744
C	3.596206	6.262083	1.000508	C	3.507884	6.295328	1.006344
H	3.389320	6.996093	0.212886	H	3.231797	6.987030	0.199678
H	3.159552	5.313791	0.690257	H	3.117072	5.312254	0.745155
C	5.108236	6.125054	1.169138	C	5.032303	6.247387	1.104334
H	5.548438	7.093143	1.432402	H	5.431608	7.242896	1.328180
H	5.517580	5.853289	0.192311	H	5.403913	5.982331	0.110458
C	5.569128	5.073822	2.190084	C	5.615432	5.242976	2.111693
H	5.143539	4.100523	1.952199	H	5.188862	4.254182	1.946181
H	6.659407	4.987345	2.148067	H	6.699557	5.177665	1.965627
C	6.047371	5.908387	4.350358	C	6.272252	6.169443	4.185910
H	7.098760	5.769199	4.085286	H	7.297888	6.069472	3.814421
C	5.787127	6.669224	5.539746	C	6.119370	6.915005	5.402497
C	4.549046	7.360957	5.680155	C	4.854967	7.478629	5.761165
C	4.423208	8.266238	6.755596	C	4.817917	8.336868	6.883980
H	3.490098	8.805851	6.853982	H	3.864141	8.772518	7.152581
C	5.446088	8.438504	7.665151	C	5.953271	8.593431	7.622846
H	5.308986	9.124281	8.493124	H	5.886786	9.242769	8.488163
C	6.656419	7.742852	7.535834	C	7.191399	8.032242	7.274202
H	7.451954	7.887402	8.254393	H	8.075070	8.245281	7.860409
C	6.821755	6.888664	6.467421	C	7.263268	7.218234	6.166215
H	7.762485	6.366223	6.331228	H	8.214383	6.791340	5.866155
C	3.326434	2.653448	3.146560	C	3.488090	2.499616	3.363350

Model B, B3LYP/def2-TZVP+COSMO, LS				Model B, B3LYP/def2-TZVP+COSMO, HS			
Fe	3.207138	5.591310	3.922433	Fe	3.276579	5.665023	4.162119
O	3.463285	4.591812	5.544718	O	3.209618	4.702298	5.867257
O	3.555106	7.221000	4.838039	O	3.795408	7.335238	5.071293
N	1.329863	5.944446	4.272937	N	1.208946	6.053010	4.385331
N	2.890693	6.678217	2.224852	N	2.788175	6.716530	2.228511
H	3.260527	7.583264	2.511743	H	3.124950	7.653419	2.445411

N	5.156772	5.486101	3.511700	N	5.293892	5.710135	3.454712
N	2.799368	3.847085	3.015122	N	2.984136	3.712995	3.229151
N	1.797856	3.655035	2.121201	N	2.073601	3.451379	2.260349
N	1.761395	2.407903	1.800370	N	2.098743	2.187494	1.994449
N	2.717128	1.715962	2.466200	N	3.012739	1.558150	2.770704
N	4.420594	2.370681	4.011652	N	4.560792	2.347372	4.423477
H	4.492831	3.006477	4.798515	H	4.536440	2.995469	5.200430
H	4.527805	1.397672	4.258912	H	4.683667	1.389399	4.719155
C	2.537261	4.257719	6.401767	C	2.198192	4.193270	6.526512
C	2.911153	3.449633	7.505309	C	2.447244	3.284728	7.578393
H	3.951254	3.157611	7.583845	H	3.477449	3.033435	7.799424
C	1.993730	3.052117	8.454989	C	1.414424	2.727547	8.308929
H	2.322030	2.436512	9.284656	H	1.645095	2.030237	9.105908
C	0.646475	3.436258	8.363404	C	0.080478	3.053745	8.034523
H	-0.067948	3.123312	9.113354	H	-0.723480	2.615104	8.610623
C	0.254363	4.224126	7.303367	C	-0.189098	3.948100	7.018361
H	-0.779401	4.540098	7.215838	H	-1.214576	4.220790	6.795396
C	1.164696	4.647120	6.311053	C	0.837340	4.528392	6.247235
C	0.657561	5.500381	5.270527	C	0.437655	5.468755	5.227131
H	-0.386404	5.802985	5.365039	H	-0.631810	5.690723	5.192630
C	0.757061	6.950429	3.375779	C	0.672859	7.019669	3.432017
H	0.965470	7.934567	3.806101	H	0.925332	8.024095	3.787311
H	-0.326128	6.840258	3.290855	H	-0.415591	6.952942	3.358760
C	1.425512	6.824957	2.019243	C	1.317056	6.776189	2.074973
H	1.080506	5.928467	1.510942	H	0.993568	5.814403	1.679005
H	1.210157	7.695607	1.396001	H	1.025595	7.560930	1.371195
C	3.593609	6.270611	0.981277	C	3.461643	6.262726	0.986710
H	3.372215	7.004026	0.200014	H	3.163488	6.918192	0.161093
H	3.171470	5.316644	0.667875	H	3.086152	5.263913	0.765466
C	5.105090	6.155632	1.147307	C	4.984980	6.245577	1.072516
H	5.529090	7.127817	1.417051	H	5.363935	7.252123	1.275587
H	5.520100	5.892084	0.171484	H	5.357300	5.966327	0.083640
C	5.573759	5.104379	2.161274	C	5.586864	5.268267	2.091477
H	5.151892	4.131018	1.914430	H	5.171047	4.271828	1.941445
H	6.662943	5.024602	2.122103	H	6.669319	5.213609	1.943945
C	6.052249	5.924166	4.324450	C	6.260958	6.179816	4.163794
H	7.101607	5.802377	4.050281	H	7.280561	6.070167	3.785235
C	5.787497	6.663518	5.529958	C	6.126385	6.904186	5.401070
C	4.544094	7.336960	5.692236	C	4.884057	7.498414	5.778253
C	4.407999	8.213163	6.790340	C	4.869284	8.315365	6.930355
H	3.469530	8.741151	6.906316	H	3.931798	8.776898	7.215460
C	5.434446	8.379126	7.700687	C	6.013064	8.510107	7.681120
H	5.292979	9.045219	8.544126	H	5.965749	9.130901	8.568390
C	6.652969	7.702519	7.547310	C	7.231663	7.922248	7.311271
H	7.452172	7.842420	8.263418	H	8.122301	8.086372	7.903328
C	6.824457	6.874272	6.456095	C	7.279190	7.144893	6.172078
H	7.772177	6.371070	6.299181	H	8.216453	6.701575	5.854163
C	3.340331	2.626614	3.211037	C	3.538777	2.524039	3.521643

Model C, B3LYP/def2-TZVP+VDW, LS				Model C, B3LYP/def2-TZVP+VDW, HS			
Fe	3.210220	5.637238	3.941411	Fe	3.292722	5.681834	4.263387
O	3.492831	4.707016	5.583438	O	3.226891	4.799852	5.989870
O	3.594436	7.315595	4.772438	O	3.833891	7.428362	5.015467
N	1.349650	5.997368	4.303088	N	1.244013	6.127135	4.479282
N	2.894299	6.682993	2.218689	N	2.833001	6.729042	2.292250
H	3.293092	7.583044	2.482909	H	3.230163	7.644110	2.496921
N	5.152135	5.488404	3.528794	N	5.297496	5.651348	3.541185
N	2.779226	3.938378	3.087341	N	2.867002	3.849128	3.348505
N	1.765442	3.761121	2.189067	N	1.907056	3.640497	2.399027
N	1.730595	2.518935	1.858043	N	1.904516	2.388370	2.092514
N	2.686187	1.818110	2.514148	N	2.832992	1.715596	2.811166
N	4.405401	2.454521	4.057398	N	4.462234	2.424555	4.432274
H	4.464462	3.071848	4.858588	H	4.447887	3.027416	5.244532
H	4.504921	1.475588	4.277955	H	4.581138	1.450158	4.665290
C	2.559851	4.291088	6.393522	C	2.210279	4.176843	6.532177
C	2.944733	3.459702	7.472644	C	2.454979	3.200164	7.518485
H	3.997885	3.228263	7.569315	H	3.486114	3.008826	7.786881

C	2.023129	2.970298	8.370267	C	1.422190	2.510372	8.120540
H	2.357879	2.334807	9.181747	H	1.649902	1.758422	8.866750
C	0.659993	3.283052	8.250282	C	0.089350	2.770119	7.781450
H	-0.058441	2.892231	8.957951	H	-0.715291	2.224636	8.255424
C	0.257804	4.099034	7.219374	C	-0.178478	3.733349	6.832865
H	-0.789858	4.359413	7.114307	H	-1.205846	3.949470	6.561119
C	1.172734	4.616036	6.277150	C	0.848916	4.447731	6.187635
C	0.667250	5.497908	5.267316	C	0.456246	5.446831	5.225665
H	-0.386090	5.774035	5.350034	H	-0.621057	5.622989	5.145196
C	0.801677	7.016330	3.418553	C	0.754478	7.121457	3.542408
H	1.079358	7.991065	3.832977	H	1.079815	8.103905	3.900567
H	-0.288741	6.961826	3.358211	H	-0.338680	7.124129	3.476761
C	1.427738	6.836173	2.044727	C	1.364723	6.838006	2.171303
H	1.066671	5.912922	1.597909	H	1.007336	5.872987	1.813846
H	1.196417	7.681347	1.389528	H	1.075508	7.616629	1.456164
C	3.568446	6.193378	0.993071	C	3.463751	6.171045	1.075723
H	3.345881	6.876956	0.165770	H	3.190839	6.784693	0.207501
H	3.127338	5.227065	0.754284	H	3.033193	5.181231	0.928475
C	5.082159	6.064125	1.147934	C	4.987138	6.073904	1.147702
H	5.521374	7.039948	1.382376	H	5.423613	7.066885	1.302364
H	5.484243	5.762639	0.177296	H	5.330735	5.730677	0.168125
C	5.546548	5.043987	2.197624	C	5.549964	5.116009	2.210088
H	5.101707	4.070711	2.000786	H	5.074933	4.140131	2.124397
H	6.634490	4.938410	2.144521	H	6.626473	4.989573	2.049644
C	6.048652	5.920103	4.342153	C	6.275311	6.146525	4.217384
H	7.098673	5.755028	4.087235	H	7.293944	5.976680	3.852263
C	5.789352	6.694405	5.524298	C	6.155350	6.967869	5.389154
C	4.565831	7.416019	5.645061	C	4.921624	7.619691	5.708103
C	4.434371	8.306163	6.729802	C	4.922432	8.526711	6.790737
H	3.509461	8.861869	6.813170	H	3.989721	9.021998	7.027030
C	5.438338	8.439797	7.667521	C	6.063589	8.754821	7.529943
H	5.296320	9.113616	8.504335	H	6.025760	9.444282	8.365340
C	6.634754	7.718325	7.555490	C	7.271780	8.112157	7.218772
H	7.415349	7.831858	8.295668	H	8.161305	8.303086	7.803732
C	6.806072	6.875708	6.477775	C	7.307798	7.244916	6.150003
H	7.736174	6.330519	6.358619	H	8.237016	6.753448	5.881924
C	3.311959	2.712194	3.264802	C	3.402630	2.637905	3.573402

Model D, B3LYP/def2-TZVP+VDW+COSMO, LS				Model D, B3LYP/def2-TZVP+VDW+COSMO, HS			
Fe	3.217879	5.661852	3.927917	Fe	3.277177	5.781319	4.211975
O	3.497049	4.724399	5.575446	O	3.226889	4.895095	5.953743
O	3.592048	7.317458	4.774823	O	3.844103	7.481867	5.009651
N	1.352383	6.019893	4.291116	N	1.221668	6.165183	4.432337
N	2.893441	6.687082	2.206503	N	2.793459	6.740916	2.246187
H	3.289693	7.597290	2.436985	H	3.167782	7.678152	2.386301
N	5.154036	5.506143	3.509572	N	5.277567	5.691699	3.501529
N	2.778312	3.903983	3.105754	N	2.884849	3.823953	3.377560
N	1.743807	3.674393	2.260127	N	1.902120	3.513533	2.499231
N	1.694447	2.412912	2.003189	N	1.897817	2.234379	2.318069
N	2.673929	1.750514	2.667084	N	2.862890	1.645049	3.065397
N	4.434431	2.485356	4.116772	N	4.534900	2.536206	4.545250
H	4.535493	3.174538	4.854465	H	4.572448	3.254174	5.257641
H	4.550278	1.531605	4.426040	H	4.666713	1.608762	4.922310
C	2.559556	4.296806	6.375235	C	2.223497	4.236312	6.486801
C	2.937010	3.436605	7.435536	C	2.491008	3.244090	7.451475
H	3.986562	3.184124	7.523116	H	3.526154	3.053691	7.706392
C	2.010451	2.939588	8.327874	C	1.470590	2.530560	8.052459
H	2.339258	2.282944	9.125147	H	1.714528	1.769182	8.784081
C	0.651218	3.274011	8.217311	C	0.131611	2.781927	7.729668
H	-0.071043	2.882152	8.921283	H	-0.663279	2.223342	8.205981
C	0.256140	4.115274	7.199491	C	-0.156841	3.757219	6.795543
H	-0.787592	4.393565	7.102249	H	-1.188483	3.968968	6.537372
C	1.175291	4.635683	6.263841	C	0.857832	4.491062	6.152180
C	0.669170	5.532530	5.259009	C	0.443080	5.488369	5.191810
H	-0.378791	5.821416	5.350456	H	-0.634333	5.656586	5.120851
C	0.803519	7.040800	3.402439	C	0.707343	7.138979	3.479432
H	1.089924	8.014154	3.810778	H	1.018849	8.133154	3.813322

H	-0.286155	6.992789	3.351635	H	-0.383997	7.121052	3.422425
C	1.427266	6.852346	2.031279	C	1.321199	6.835806	2.117280
H	1.052592	5.940218	1.574679	H	0.966005	5.866927	1.769591
H	1.209030	7.699693	1.378309	H	1.035923	7.600101	1.389627
C	3.562500	6.194542	0.977110	C	3.427184	6.160686	1.037761
H	3.326356	6.874511	0.153313	H	3.130633	6.747744	0.161899
H	3.132198	5.222355	0.742025	H	3.021568	5.156845	0.917131
C	5.075877	6.082979	1.125321	C	4.950689	6.103743	1.102436
H	5.502921	7.062984	1.359270	H	5.359984	7.107732	1.251348
H	5.479525	5.782903	0.155781	H	5.300964	5.761881	0.125600
C	5.548630	5.067232	2.172530	C	5.535029	5.162613	2.164844
H	5.104756	4.093234	1.973697	H	5.074159	4.178867	2.081817
H	6.635336	4.966380	2.120268	H	6.611490	5.054100	2.004798
C	6.056029	5.937381	4.316026	C	6.262291	6.153205	4.189071
H	7.103960	5.786897	4.051319	H	7.277784	5.982434	3.822515
C	5.793334	6.695156	5.512232	C	6.146902	6.935759	5.393801
C	4.565637	7.402420	5.651835	C	4.930916	7.606458	5.730345
C	4.424216	8.266436	6.756044	C	4.937775	8.455383	6.857215
H	3.494687	8.813123	6.854860	H	4.018429	8.969408	7.108948
C	5.431111	8.392577	7.695475	C	6.076763	8.615231	7.623822
H	5.285059	9.048704	8.545825	H	6.045926	9.263080	8.492188
C	6.634425	7.686134	7.562711	C	7.269676	7.956117	7.292952
H	7.418132	7.793633	8.301204	H	8.157516	8.092613	7.896072
C	6.811521	6.866332	6.464714	C	7.296866	7.142761	6.178105
H	7.747693	6.336287	6.328024	H	8.215886	6.642674	5.892958
C	3.325842	2.694188	3.343669	C	3.450887	2.651555	3.709617

Model E, B3LYP/def2-TZVP+VDW+COSMO+DKH2, LS				Model E, B3LYP/def2-TZVP+VDW+COSMO+DKH2, HS			
Fe	3.214299	5.666057	3.910526	Fe	3.282129	5.760743	4.221050
O	3.511172	4.740114	5.548612	O	3.237540	4.856133	5.944546
O	3.583700	7.319577	4.745393	O	3.829510	7.455223	5.023018
N	1.382285	6.016458	4.283302	N	1.240114	6.156528	4.439238
N	2.903605	6.686636	2.203750	N	2.811526	6.741770	2.255175
H	3.303533	7.596475	2.430875	H	3.194961	7.674229	2.401216
N	5.136822	5.506241	3.507425	N	5.278491	5.680301	3.517193
N	2.769539	3.926457	3.109556	N	2.873735	3.816928	3.366599
N	1.712496	3.694039	2.293169	N	1.877686	3.519526	2.500140
N	1.643185	2.430811	2.060522	N	1.854741	2.241641	2.320011
N	2.630513	1.769054	2.711505	N	2.819833	1.640500	3.056368
N	4.435793	2.505948	4.098846	N	4.520541	2.510456	4.513672
H	4.561568	3.202245	4.825677	H	4.572323	3.225458	5.228198
H	4.543659	1.555632	4.421321	H	4.641802	1.581112	4.889647
C	2.584161	4.308630	6.354610	C	2.226393	4.204778	6.473060
C	2.973229	3.458121	7.409443	C	2.484902	3.209095	7.427345
H	4.022908	3.206532	7.492789	H	3.516887	2.995654	7.674670
C	2.059583	2.955991	8.303164	C	1.462912	2.511436	8.032419
H	2.392384	2.300006	9.098864	H	1.697722	1.742535	8.758680
C	0.702873	3.282695	8.201221	C	0.130306	2.787473	7.724260
H	-0.011654	2.883292	8.908254	H	-0.669340	2.240606	8.205517
C	0.302459	4.120987	7.189928	C	-0.143653	3.768434	6.800070
H	-0.743071	4.393034	7.102520	H	-1.174021	3.997843	6.554373
C	1.208741	4.645877	6.254781	C	0.870490	4.486690	6.152706
C	0.701915	5.539581	5.255777	C	0.460726	5.492537	5.205039
H	-0.342335	5.838786	5.352839	H	-0.614408	5.680224	5.149623
C	0.839643	7.053689	3.413285	C	0.737862	7.147188	3.500169
H	1.161700	8.015559	3.822167	H	1.070187	8.131341	3.843701
H	-0.251300	7.030334	3.381651	H	-0.353789	7.148349	3.448379
C	1.439361	6.854588	2.036690	C	1.341235	6.848661	2.133249
H	1.059614	5.933758	1.602598	H	0.977681	5.883701	1.783428
H	1.214924	7.693811	1.375831	H	1.056708	7.619047	1.411756
C	3.565917	6.184549	0.976869	C	3.441538	6.157122	1.049322
H	3.330166	6.859191	0.148767	H	3.153321	6.745917	0.171743
H	3.132563	5.211724	0.750309	H	3.028159	5.156630	0.927859
C	5.077261	6.068977	1.125059	C	4.963553	6.086792	1.118350
H	5.507400	7.048525	1.355322	H	5.380994	7.087720	1.265289
H	5.480659	5.761483	0.157884	H	5.312852	5.738534	0.143480
C	5.539890	5.057380	2.178389	C	5.538463	5.145183	2.184625

H	5.091602	4.084852	1.983442	H	5.072123	4.164233	2.103726
H	6.626311	4.950899	2.133788	H	6.614898	5.030911	2.028461
C	6.032659	5.925360	4.323360	C	6.258115	6.157874	4.198243
H	7.082423	5.763999	4.072875	H	7.274887	5.990876	3.833302
C	5.758966	6.681473	5.513863	C	6.137502	6.953066	5.389634
C	4.540582	7.390703	5.640504	C	4.917762	7.595788	5.736992
C	4.384841	8.247668	6.738397	C	4.914108	8.446175	6.855413
H	3.459994	8.803773	6.824216	H	3.984544	8.935002	7.118616
C	5.373443	8.371264	7.690467	C	6.054816	8.646316	7.600890
H	5.221929	9.029224	8.537912	H	6.020433	9.301556	8.463097
C	6.569520	7.659589	7.575805	C	7.256593	8.019694	7.257858
H	7.339763	7.757393	8.329276	H	8.148690	8.185369	7.846704
C	6.752347	6.839591	6.484134	C	7.284346	7.194724	6.157479
H	7.686551	6.303031	6.365973	H	8.211962	6.713394	5.869729
C	3.308286	2.716841	3.355209	C	3.426997	2.639487	3.693391