

University of Groningen

Electrochemical and Photochemical Cyclization and Cycloreversion of Diarylethenes and Diarylethene-Capped Sexithiophene Wires

Staykov, Aleksandar; Areephong, Jetsuda; Browne, Wesley R.; Yoshizawa, Kazunari; Feringa, Bernard

Published in:
Acs Nano

DOI:
[10.1021/nn102806z](https://doi.org/10.1021/nn102806z)

IMPORTANT NOTE: You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.

Document Version
Publisher's PDF, also known as Version of record

Publication date:
2011

[Link to publication in University of Groningen/UMCG research database](#)

Citation for published version (APA):

Staykov, A., Areephong, J., Browne, W. R., Yoshizawa, K., & Feringa, B. (2011). Electrochemical and Photochemical Cyclization and Cycloreversion of Diarylethenes and Diarylethene-Capped Sexithiophene Wires. *Acs Nano*, 5(2), 1165-1178. <https://doi.org/10.1021/nn102806z>

Copyright

Other than for strictly personal use, it is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), unless the work is under an open content license (like Creative Commons).

Take-down policy

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Downloaded from the University of Groningen/UMCG research database (Pure): <http://www.rug.nl/research/portal>. For technical reasons the number of authors shown on this cover page is limited to 10 maximum.

Electrochemical and Photochemical Cyclization and Cycloreversion of Diarylethenes and Diarylethene-capped Sexithiophene Wires

Aleksandar Staykov,¹ Jetsuda Areephong,² Wesley Browne,^{*,2}
Ben Feringa,² and Kazunari Yoshizawa^{*,1}

¹) *Institute for Materials Chemistry and Engineering,
Kyushu University, Fukuoka 819-0395, Japan*

²) *Centre for Systems Chemistry, Stratingh Institute for Chemistry, University of
Groningen, Groningen 9747 AG, The Netherlands*

* To whom correspondence should be addressed.

E-mail: kazunari@ms.ifoc.kyushu-u.ac.jp

Tel: +81-92-802-2529

Fax: +81-92-802-2528

E-mail: w.r.browne@rug.nl

Tel: +31-503634428

Content:

1. Table S1	page S3
2. Table S2	page S5
3. Table S3	page S7
4. Table S4	page S11
5. Table S3	page S15

Table S1. Geometrical parameters at B3LYP/6-31G (d) level of theory for the closed-form isomer of 1,2-bis[5'-phenyl-2'-methylthien-3'-yl]cyclopentene. Units are in Å.

Energy: -1839.6887983321 Hartree.

C	-0.123973837	-0.000008113	0.278130107
C	-0.045785234	0.019792380	1.815527322
C	1.268901445	-0.277429192	2.292130718
C	2.261252061	-0.243802051	1.353983450
H	1.465466093	-0.460325865	3.343254132
C	-1.190132064	0.254226160	2.518404531
C	-1.449957767	0.123517976	4.006403402
C	-2.415147322	0.642511402	1.845228124
C	-2.828669476	0.802567990	4.198404108
C	-3.555091923	0.626791694	2.841191914
C	-2.413609055	0.994258718	0.528248271
C	-3.511953831	1.316415919	-0.328667329
C	-1.057939817	1.140747581	-0.187188690
C	-3.216208394	1.411694951	-1.658516257
H	-4.524329323	1.409422986	0.050550568
H	-0.667919718	0.579191705	4.624890074
H	-1.498153798	-0.938060301	4.291510811
H	-2.683150318	1.871757138	4.393281145
H	-3.393037108	0.387894454	5.039501724
H	-4.081563358	-0.339302676	2.812302240
H	-4.304678960	1.404480170	2.658845610
C	-0.505875635	2.556288538	0.110508545
H	-0.289685571	2.661641185	1.178247883
H	0.408896888	2.754915408	-0.451632040
H	-1.256835756	3.300145929	-0.168628726
C	-0.596615051	-1.407132094	-0.162005361
H	-1.617826794	-1.589966530	0.186891197
H	-0.575794791	-1.513721760	-1.248462759

H	0.062592590	-2.160864024	0.276748200
S	-1.493586602	1.088843591	-2.009626238
S	1.656968461	0.186568560	-0.272903556
C	-4.143219756	1.707198016	-2.754148264
C	-3.791767877	1.461076229	-4.095030524
C	-5.420104863	2.246457728	-2.495279002
H	-2.816380163	1.043458766	-4.327501228
H	-5.709684266	2.476580810	-1.474675180
C	-4.681704580	1.732482449	-5.131981597
C	-6.308226604	2.512641097	-3.531875399
H	-4.385075686	1.531805373	-6.157896382
H	-7.285222150	2.931411098	-3.305666719
C	-5.944917657	2.257592481	-4.857434764
H	-6.637145428	2.473630469	-5.666473491
C	3.691617230	-0.485208251	1.561922685
C	4.171761258	-0.996185812	2.785858603
C	4.632359860	-0.212757325	0.550198182
H	3.473228326	-1.240180073	3.579889053
H	4.296791584	0.179133520	-0.405508692
C	5.530458381	-1.210801230	2.989014171
C	5.992950871	-0.431853680	0.754854377
H	5.873155572	-1.606959713	3.941279798
H	6.696054807	-0.212304338	-0.044077328
C	6.450911487	-0.929750090	1.974878909
H	7.511527286	-1.103379942	2.133915955

Table S2. Geometrical parameters at B3LYP/6-31G (d) level of theory for the open-form isomer of 1,2-bis[5'-phenyl-2'-methylthien-3'-yl]cyclopentene. Units are in Å.

Energy: -1839.7061207378 Hartree.

C	-0.599272878	-0.773138899	0.829720498
C	-0.415059589	-0.202933338	2.074842702
C	0.976287588	-0.024874714	2.386798892
C	1.842784686	-0.416698137	1.399290330
H	1.314347416	0.432174159	3.310861428
C	-1.482392749	0.143635449	3.031776136
C	-1.408460030	-0.378331054	4.461272437
C	-2.633648489	0.829771899	2.826389264
C	-2.531434752	0.384806271	5.193298559
C	-3.508766775	0.803103430	4.074646942
C	-3.108012557	1.527187719	1.618514272
C	-4.464266395	1.408506353	1.158144119
C	-2.370281413	2.400014409	0.840871104
C	-4.758402558	2.142096148	0.037744235
H	-5.187760917	0.753669981	1.632417010
H	-0.423243557	-0.224954719	4.918875117
H	-1.577844675	-1.466302157	4.467860970
H	-2.115521652	1.283581230	5.663581678
H	-3.008084409	-0.206179091	5.981709296
H	-4.320990321	0.068389152	3.956749746
H	-3.990774056	1.768483566	4.268379149
C	-0.952288713	2.857085242	1.006314396
H	-0.641166600	2.732099364	2.047119299
H	-0.257190741	2.275229296	0.388343135
H	-0.838408752	3.912638881	0.735530950
C	-1.871016288	-1.171099137	0.143029951
H	-2.666244719	-1.307585314	0.880723565
H	-2.212125984	-0.404179920	-0.563506644
H	-1.750310807	-2.108267442	-0.411683279

S	-3.338293534	3.041915982	-0.463163853
S	0.933658475	-1.061230993	0.043798142
C	-6.029637942	2.232630401	-0.691227673
C	-6.072783480	2.516626573	-2.068052590
C	-7.248338755	2.030050477	-0.016718660
H	-5.144207289	2.658264218	-2.614503322
H	-7.240101334	1.841878182	1.052882488
C	-7.288522114	2.594364956	-2.744632104
C	-8.461228732	2.096628615	-0.697599283
H	-7.296627097	2.813565173	-3.809111698
H	-9.389765646	1.939227812	-0.155067502
C	-8.488899259	2.381478471	-2.064745078
H	-9.436377251	2.441591412	-2.592963513
C	3.309655050	-0.353674592	1.388527401
C	4.029708542	-0.407240310	2.596772955
C	4.034835283	-0.235047011	0.189286394
H	3.492254892	-0.532175312	3.532210813
H	3.500998260	-0.173237587	-0.755243621
C	5.420177123	-0.331281141	2.603777790
C	5.426855343	-0.171249192	0.198178275
H	5.954633449	-0.377580732	3.549049707
H	5.965240284	-0.078239687	-0.741337218
C	6.127198865	-0.214868576	1.404814199
H	7.212354800	-0.162821262	1.411271400

Table S3. Geometrical parameters at B3LYP/6-31G (d) level of theory for the open-open form isomer of the diarylethene-capped thiophene wire. Units are in Å.

Energy: -6614.1524294638 Hartree.

C	-1.710151443	2.369469561	-6.520297859
C	1.710151443	-2.369469561	6.520297859
C	-0.557204126	2.960336436	-6.028301887
C	0.557204126	-2.960336436	6.028301887
C	-0.194017769	2.518142913	-4.740963675
C	0.194017769	-2.518142913	4.740963675
C	-1.059234236	1.574499432	-4.210322486
C	1.059234236	-1.574499432	4.210322486
S	-2.355875164	1.231843256	-5.342719544
S	2.355875164	-1.231843256	5.342719544
H	0.005053082	3.700091117	-6.587406489
H	-0.005053082	-3.700091117	6.587406489
H	0.679623241	2.880522547	-4.210006711
H	-0.679623241	-2.880522547	4.210006711
C	-0.996579808	0.909113647	-2.935402585
C	0.996579808	-0.909113647	2.935402585
S	0.309530927	1.242421441	-1.806836646
S	-0.309530927	-1.242421441	1.806836646
C	-0.332750004	0.107150281	-0.629435255
C	0.332750004	-0.107150281	0.629435255
C	-1.489999583	-0.477102505	-1.113538610
C	1.489999583	0.477102505	1.113538610
C	-1.860052126	-0.029812436	-2.399513037
C	1.860052126	0.029812436	2.399513037
H	-2.058362253	-1.211409743	-0.552798740
H	2.058362253	1.211409743	0.552798740
H	-2.740306589	-0.386979162	-2.923331668
H	2.740306589	0.386979162	2.923331668
C	-2.347369951	2.583457385	-7.787788678

C	2.347369951	-2.583457385	7.787788678
C	-3.503303335	2.004525383	-8.252098909
C	3.503303335	-2.004525383	8.252098909
C	-3.887062008	2.402745831	-9.558610626
C	3.887062008	-2.402745831	9.558610626
C	-3.108064681	3.629473653	-10.065919783
C	3.108064681	-3.629473653	10.065919783
S	-1.593963890	3.693303477	-8.964945720
S	1.593963890	-3.693303477	8.964945720
H	-4.065325584	1.271050052	-7.683633691
H	4.065325584	-1.271050052	7.683633691
C	-4.855879905	1.894577035	-10.379385202
C	4.855879905	-1.894577035	10.379385202
C	-5.841281257	0.813541167	-10.066165789
C	5.841281257	-0.813541167	10.066165789
C	-6.846834798	0.804832417	-11.274394239
C	6.846834798	-0.804832417	11.274394239
C	-6.308668383	1.857860170	-12.310287992
C	6.308668383	-1.857860170	12.310287992
C	-5.029370149	2.370022463	-11.726495561
C	5.029370149	-2.370022463	11.726495561
C	-4.109724205	3.185484457	-12.322564088
C	4.109724205	-3.185484457	12.322564088
C	-4.145120983	3.825219601	-13.593502223
C	4.145120983	-3.825219601	13.593502223
C	-3.158657314	4.750724497	-13.803828162
C	3.158657314	-4.750724497	13.803828162
S	-2.063523926	4.933126764	-12.411158150
S	2.063523926	-4.933126764	12.411158150
C	-2.791648991	3.429051554	-11.569417401
C	2.791648991	-3.429051554	11.569417401
H	-4.909066882	3.596088475	-14.327321068
H	4.909066882	-3.596088475	14.327321068

C	-2.959777997	5.570713669	-15.001713023
C	2.959777997	-5.570713669	15.001713023
C	-2.593105525	7.134625115	-17.317284173
C	2.593105525	-7.134625115	17.317284173
C	-1.725287019	6.193891465	-15.265218533
C	1.725287019	-6.193891465	15.265218533
C	-4.010941877	5.758058980	-15.922415917
C	4.010941877	-5.758058980	15.922415917
C	-3.827031973	6.527703398	-17.065917300
C	3.827031973	-6.527703398	17.065917300
C	-1.545351313	6.964911208	-16.411234111
C	1.545351313	-6.964911208	16.411234111
H	-0.896186957	6.055182977	-14.577783596
H	0.896186957	-6.055182977	14.577783596
H	-4.982290371	5.314629223	-15.728099220
H	4.982290371	-5.314629223	15.728099220
H	-4.652051827	6.661760955	-17.759975493
H	4.652051827	-6.661760955	17.759975493
H	-0.582038355	7.431652819	-16.597041233
H	0.582038355	-7.431652819	16.597041233
H	-2.452797455	7.738230416	-18.209565708
H	2.452797455	-7.738230416	18.209565708
C	-3.955671044	4.892611425	-9.772471128
C	3.955671044	-4.892611425	9.772471128
H	-4.201678776	4.921889521	-8.708137282
H	4.201678776	-4.921889521	8.708137282
H	-3.411364263	5.802574377	-10.032212249
H	3.411364263	-5.802574377	10.032212249
H	-4.888525665	4.869706715	-10.344250492
H	4.888525665	-4.869706715	10.344250492
C	-1.850717852	2.230646408	-11.852654399
C	1.850717852	-2.230646408	11.852654399
H	-2.267679009	1.308740116	-11.435827914

H	2.267679009	-1.308740116	11.435827914
H	-1.743365329	2.105253313	-12.932967293
H	1.743365329	-2.105253313	12.932967293
H	-0.862511487	2.392906574	-11.418126592
H	0.862511487	-2.392906574	11.418126592
F	-6.507907004	1.021220895	-8.893253472
F	6.507907004	-1.021220895	8.893253472
F	-5.246328310	-0.414022248	-9.957755900
F	5.246328310	0.414022248	9.957755900
F	-6.902660491	-0.420966840	-11.838776048
F	6.902660491	0.420966840	11.838776048
F	-8.084882461	1.143639074	-10.852990745
F	8.084882461	-1.143639074	10.852990745
F	-6.141375791	1.277321397	-13.534375202
F	6.141375791	-1.277321397	13.534375202
F	-7.235304377	2.850273672	-12.479150238
F	7.235304377	-2.850273672	12.479150238

Table S4. Geometrical parameters at B3LYP/6-31G (d) level of theory for the closed-closed form isomer of the diarylethene-capped thiophene wire. Units are in Å.

Energy: -6614.1902448279 Hartree.

C	-5.456479033	6.339164871	-1.735001233
C	5.456479033	-6.339164871	1.735001233
S	-6.745051722	7.131261583	-0.839753649
S	6.745051722	-7.131261583	0.839753649
C	-7.222684443	8.088258268	-2.215497348
C	7.222684443	-8.088258268	2.215497348
C	-6.435079703	7.790310438	-3.313411277
C	6.435079703	-7.790310438	3.313411277
C	-5.426607050	6.811229501	-3.024268124
C	5.426607050	-6.811229501	3.024268124
H	-4.699943401	6.483913692	-3.757706745
H	4.699943401	-6.483913692	3.757706745
C	-4.615623723	5.345869856	-1.105306202
C	4.615623723	-5.345869856	1.105306202
C	-4.476779972	5.048838891	0.235308143
C	4.476779972	-5.048838891	-0.235308143
C	-3.547006995	4.015455518	0.497992021
C	3.547006995	-4.015455518	-0.497992021
C	-2.953280262	3.498199611	-0.637075115
C	2.953280262	-3.498199611	0.637075115
S	-3.583659862	4.300691115	-2.068146345
S	3.583659862	-4.300691115	2.068146345
H	-5.014281333	5.579066589	1.014453386
H	5.014281333	-5.579066589	-1.014453386
H	-3.301042805	3.674666143	1.498042221
H	3.301042805	-3.674666143	-1.498042221
C	-1.962751337	2.456134769	-0.751670312
C	1.962751337	-2.456134769	0.751670312
S	-1.568397554	1.435557189	0.624134631

S	1.568397554	-1.435557189	-0.624134631
C	-0.377476335	0.533832087	-0.303333194
C	0.377476335	-0.533832087	0.303333194
C	-0.324572465	1.012535590	-1.598880182
C	0.324572465	-1.012535590	1.598880182
C	-1.208970184	2.086306602	-1.848944405
C	1.208970184	-2.086306602	1.848944405
H	-1.280479642	2.588624720	-2.807817054
H	1.280479642	-2.588624720	2.807817054
H	-0.342328456	-0.603852634	2.350623880
H	0.342328456	0.603852634	-2.350623880
C	-6.545965293	8.454089931	-4.619489044
C	6.545965293	-8.454089931	4.619489044
C	-7.648533204	8.726654954	-5.364145555
C	7.648533204	-8.726654954	5.364145555
C	-7.309816343	9.602378180	-6.548069726
C	7.309816343	-9.602378180	6.548069726
C	-5.761600204	9.773824465	-6.529043032
C	5.761600204	-9.773824465	6.529043032
C	-5.290398800	8.971367247	-5.280140261
C	5.290398800	-8.971367247	5.280140261
C	-9.034419160	8.271269928	-5.193539921
C	9.034419160	-8.271269928	5.193539921
C	-10.164667321	9.145405834	-5.343924536
C	10.164667321	-9.145405834	5.343924536
C	-11.377989402	8.531061524	-5.176848390
C	11.377989402	-8.531061524	5.176848390
S	-11.135942020	6.821712748	-4.860197521
S	11.135942020	-6.821712748	4.860197521
C	-9.402958996	6.962651294	-4.933843756
C	9.402958996	-6.962651294	4.933843756
H	-10.061156124	10.205341649	-5.537594439
H	10.061156124	-10.205341649	5.537594439

C	-8.327862333	9.090343329	-2.072734196
C	8.327862333	-9.090343329	2.072734196
H	-8.336114954	9.530917945	-1.070478524
H	8.336114954	-9.530917945	1.070478524
H	-8.204243277	9.899074502	-2.798291592
H	8.204243277	-9.899074502	2.798291592
H	-9.312255106	8.639571185	-2.249279182
H	9.312255106	-8.639571185	2.249279182
C	-8.550021455	5.739966255	-4.774484632
C	8.550021455	-5.739966255	4.774484632
H	-7.609060453	5.857422918	-5.319562076
H	7.609060453	-5.857422918	5.319562076
H	-8.297573322	5.552333092	-3.723511627
H	8.297573322	-5.552333092	3.723511627
H	-9.057251534	4.849923653	-5.160524563
H	9.057251534	-4.849923653	5.160524563
F	-7.911950600	10.829786854	-6.449315489
F	7.911950600	-10.829786854	6.449315489
F	-7.719165247	9.057596656	-7.723202076
F	7.719165247	-9.057596656	7.723202076
F	-5.420481193	11.075536504	-6.411253589
F	5.420481193	-11.075536504	6.411253589
F	-5.212651829	9.281924880	-7.660430781
F	5.212651829	-9.281924880	7.660430781
F	-4.474361358	7.942189607	-5.673012854
F	4.474361358	-7.942189607	5.673012854
F	-4.558467015	9.757836309	-4.449222715
F	4.558467015	-9.757836309	4.449222715
C	-12.721406424	9.120192049	-5.247510674
C	12.721406424	-9.120192049	5.247510674
C	-15.282421278	10.287509454	-5.390388967
C	15.282421278	-10.287509454	5.390388967
C	-13.806259804	8.567610810	-4.544207127

C	13.806259804	-8.567610810	4.544207127
C	-12.948425417	10.267847853	-6.029510611
C	12.948425417	-10.267847853	6.029510611
C	-14.213178380	10.846870636	-6.093868125
C	14.213178380	-10.846870636	6.093868125
C	-15.072999112	9.143314783	-4.618865523
C	15.072999112	-9.143314783	4.618865523
H	-13.652200124	7.691487262	-3.919721399
H	13.652200124	-7.691487262	3.919721399
H	-12.131520893	10.692207793	-6.605567115
H	12.131520893	-10.692207793	6.605567115
H	-14.366507454	11.731484325	-6.706097611
H	14.366507454	-11.731484325	6.706097611
H	-15.896324819	8.700215253	-4.065147290
H	15.896324819	-8.700215253	4.065147290
H	-16.269801591	10.737157450	-5.446397450
H	16.269801591	-10.737157450	5.446397450

Table S5. Geometrical parameters at B3LYP/6-31G (d) level of theory for the open-closed form isomer of the diarylethene-capped thiophene wire. Units are in Å.

Energy: -6614.1743959202 Hartree.

C	1.459474132	-3.053388879	-2.636651181
C	4.531374908	-3.860005348	-16.576628087
C	1.190500655	-4.307661462	-3.160555483
C	4.830805856	-2.622536622	-16.042886242
C	1.473646019	-4.425142344	-4.536031143
C	4.543037671	-2.510459523	-14.663047575
C	1.968143233	-3.262351877	-5.105136734
C	4.017232871	-3.661269645	-14.107718918
S	2.083607181	-1.994479147	-3.896626378
S	3.867440907	-4.910635119	-15.335907786
H	0.791754799	-5.118557132	-2.560981503
H	5.257546869	-1.815643960	-16.629268668
H	1.317946729	-5.337410206	-5.101731163
H	4.725640359	-1.608225549	-14.089085262
C	2.361909041	-3.018924857	-6.468101894
C	3.616459012	-3.912848936	-12.745887108
S	2.292239899	-4.297918551	-7.673150264
S	3.677983679	-2.635956141	-11.539780087
C	2.891527409	-3.230633156	-8.934120207
C	3.079282994	-3.707303053	-10.280439003
C	3.122931149	-1.967874668	-8.417774567
C	2.852003180	-4.968359890	-10.799575382
C	2.827542575	-1.850210075	-7.042900298
C	3.151771292	-5.083232923	-12.175200403
H	3.496253526	-1.145510148	-9.018471316
H	2.479795886	-5.793239332	-10.201203216
H	2.950564148	-0.928213774	-6.484617978
H	3.033123550	-6.004843701	-12.734906397
C	1.298669119	-2.598325936	-1.285371965

C	1.561254120	-1.344883479	-0.789362618
C	1.327502723	-1.192371929	0.602652032
C	0.517173482	-2.356909297	1.201350201
S	0.730694016	-3.743837862	-0.039563189
H	1.955882031	-0.540206245	-1.399994336
C	1.652633130	-0.164423837	1.442156000
C	2.253726243	1.166220662	1.108601997
C	1.808912530	2.068847465	2.294792389
C	1.682361079	1.092263597	3.499891913
C	1.405071308	-0.236272304	2.862022356
C	1.023788997	-1.399044565	3.466475869
C	0.637134140	-1.646673941	4.814206673
C	0.118213141	-2.890988275	5.048835638
S	0.033685635	-3.901725569	3.584794379
C	1.065221833	-2.678561319	2.614607352
H	0.734440545	-0.892072423	5.585674300
C	-0.365745168	-3.414457990	6.329260026
C	-1.275618387	-4.402563158	8.806684302
C	-0.497621223	-4.798211561	6.551036211
C	-0.711693408	-2.535416220	7.375814271
C	-1.157942599	-3.025283152	8.598365381
C	-0.945317238	-5.284730259	7.777208308
H	-0.225755435	-5.496180205	5.764717690
H	-0.649485178	-1.462879537	7.221391649
H	-1.422749701	-2.329806849	9.389937907
H	-1.032109482	-6.357031861	7.928513357
H	-1.626679276	-4.782690040	9.761939347
C	-0.977205672	-1.947812917	1.195849083
H	-1.269314314	-1.662500770	0.182128941
H	-1.613018494	-2.771290103	1.526423164
H	-1.141939043	-1.092223336	1.857990864
C	2.525508212	-3.197086670	2.611361010
H	3.184898297	-2.480264600	2.112424478

H	2.864831203	-3.321294359	3.642748155
H	2.602572818	-4.157438967	2.098124955
F	1.847577142	1.677642011	-0.086404585
F	3.623553545	1.129432211	1.082121076
F	2.661308055	3.084379893	2.530931690
F	0.581753606	2.578648079	2.013038744
F	2.861954370	1.093847007	4.194635482
F	0.715671874	1.500057622	4.371584360
C	4.699660810	-4.328753294	-17.933312603
S	5.226976566	-3.238303914	-19.207945058
C	5.197747633	-4.498501997	-20.411205474
C	4.802145055	-5.698351310	-19.848284619
C	4.506543363	-5.586809238	-18.449289119
H	4.175554468	-6.430252318	-17.854395406
C	4.626847828	-6.957058366	-20.580721657
C	5.427739014	-7.561424469	-21.496406520
C	4.772404640	-8.812716857	-22.041020218
C	3.319680192	-8.776046402	-21.504046443
C	3.393609172	-7.789642330	-20.314139892
C	6.801798069	-7.232317283	-21.900585687
C	7.231217680	-7.188916832	-23.270738610
C	8.560349358	-6.896623512	-23.434835884
S	9.320941798	-6.701798135	-21.865144299
C	7.833962910	-6.993716376	-21.009919245
H	6.554075543	-7.340003423	-24.101472130
C	5.531767084	-4.173265337	-21.835467520
H	5.227001876	-3.153253575	-22.091197179
H	5.016697579	-4.861297702	-22.512073598
H	6.606726591	-4.263195814	-22.034694259
C	7.825957611	-7.008943768	-19.510601601
H	7.027022795	-7.658347689	-19.141126326
H	7.657026324	-6.008909911	-19.092316882
H	8.775916355	-7.380767938	-19.113294291

F	4.778113814	-8.864121900	-23.405242249
F	5.403677767	-9.936080926	-21.598295129
F	2.499012609	-8.262464918	-22.452892047
F	2.868298751	-9.994230363	-21.146251140
F	3.524314519	-8.495541082	-19.143184821
F	2.260910055	-7.052765316	-20.207309221
C	9.323483016	-6.765278784	-24.682829327
C	10.757343164	-6.529258028	-27.097778818
C	10.476671284	-5.964675061	-24.761879633
C	8.905395772	-7.448205148	-25.840090980
C	9.610969293	-7.324898725	-27.034113954
C	11.187271071	-5.852338973	-25.955367882
H	10.809379972	-5.411946236	-23.887142193
H	8.034694740	-8.095361655	-25.793204603
H	9.270806440	-7.862792978	-27.914898967
H	12.074842219	-5.226576585	-25.993682829
H	11.311457082	-6.440838511	-28.028042267