

Supporting Information

Charge Delocalization Characteristics of High Mobility Regioregular Polymers

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Full Calculation Details

All the work was done using density functional theory with the Gaussian09 software suite. The neutral and charged geometry optimizations were completed using the CAM-B3LYP functional with the 6-31g** basis set. The conductor-like polarizable continuum model and chlorobenzene solvent as implemented in the Gaussian 09 software package were used for solvent-based calculations. Excess charges were calculated using the natural population analysis in the NBO suite of calculations included in Gaussian09. The atom charges in the neutral species were subtracted from the charged and the differences were added up according to what atoms along the backbone were included in each unit, either CDT or PT/BT. The internal reorganization energies were completed using the following equation:

$$\lambda = \lambda_1 + \lambda_2 = (E_+^* - E_+) + (E^* - E)$$

where the lambda 1 is the difference in the charged species and lambda 2 is the difference in the neutral species.

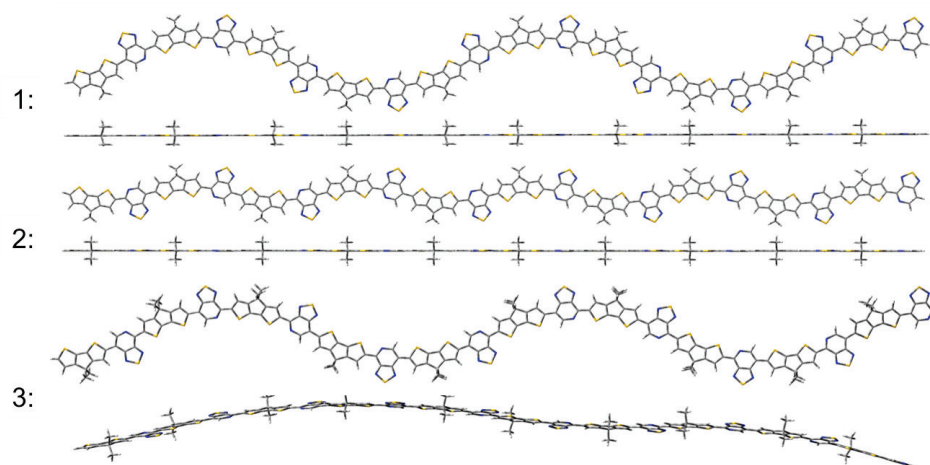


Figure S1. Geometry optimization in vacuum.

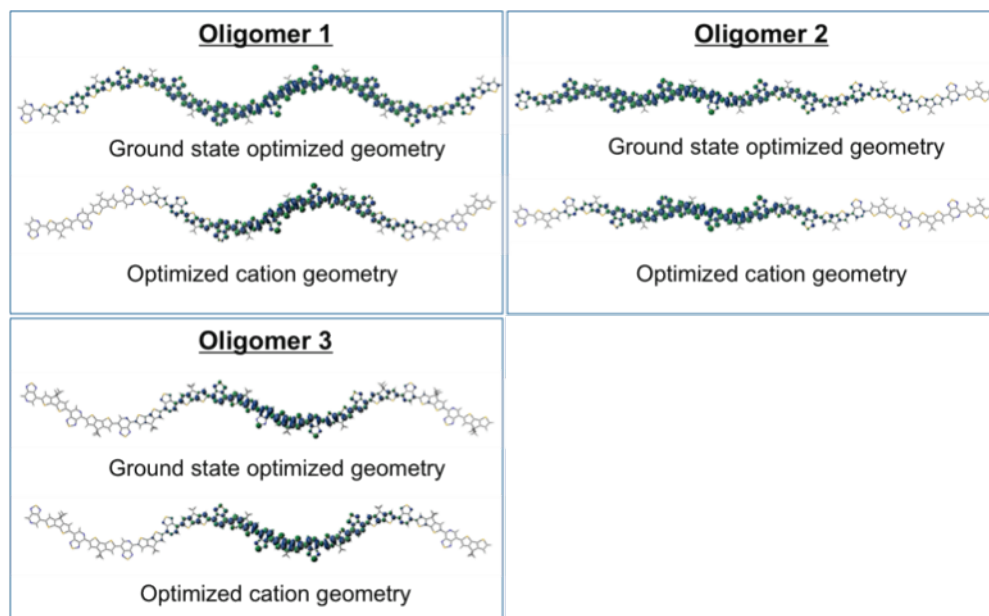


Figure S3. Cation spin density plots in vacuum.

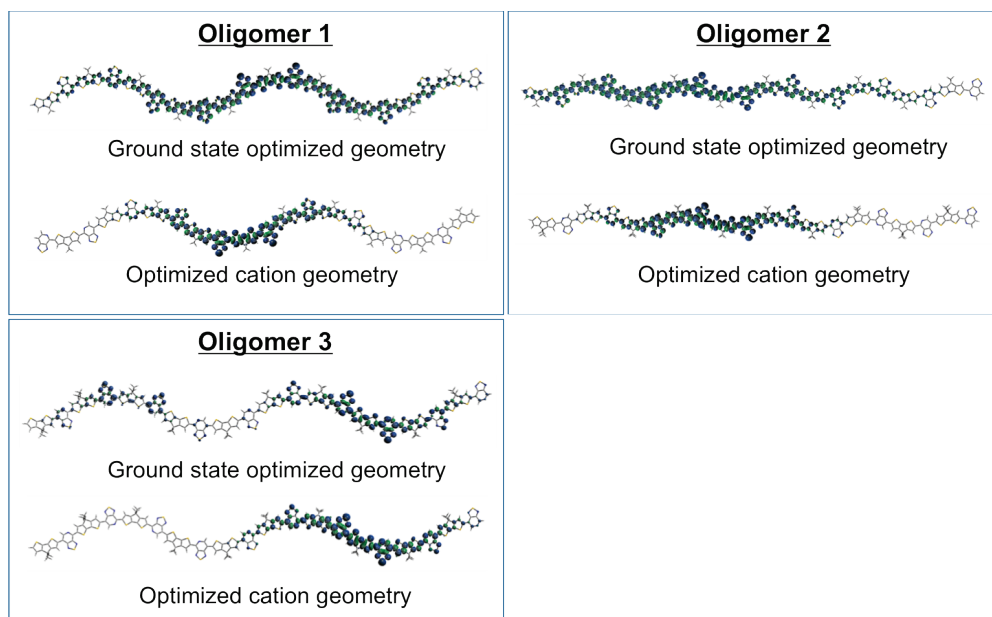


Figure S4. Anion spin density plots in vacuum.

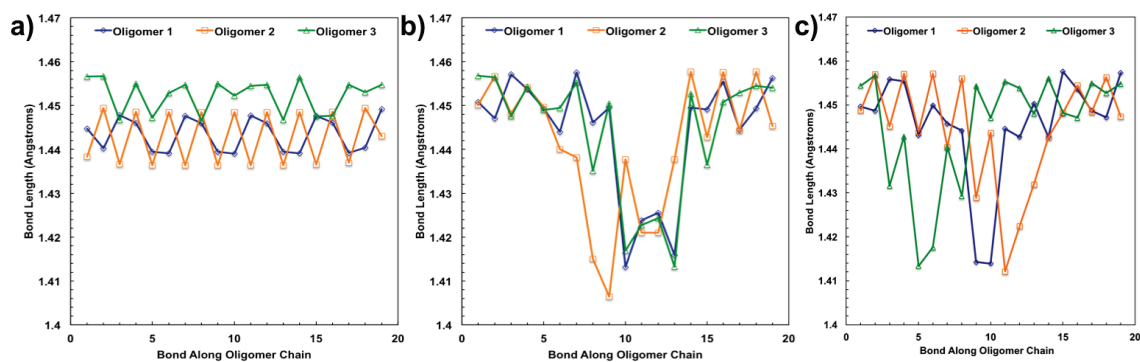


Figure S4. Bond lengths along the backbone for oligomers in vacuum for (a) the neutral species, (b) the cation species, and (c) the anion species.

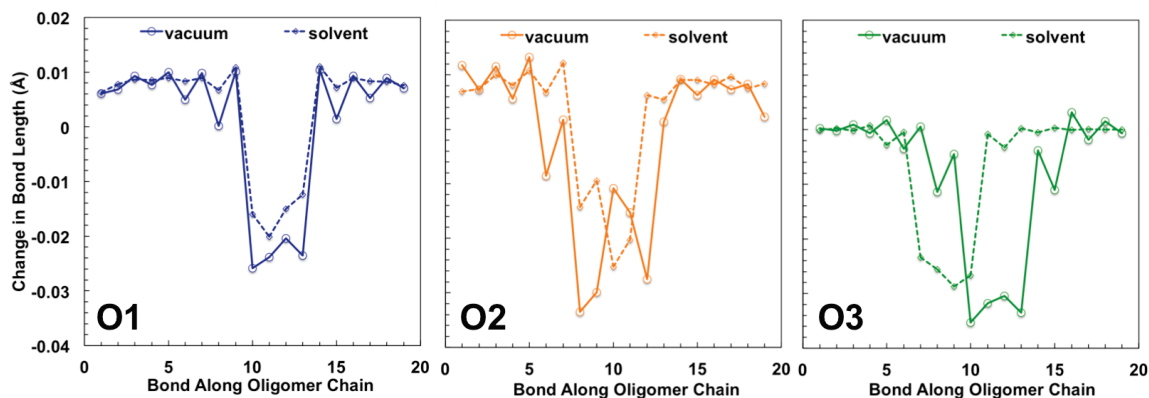


Figure S5. Bond lengths changes for oligomers in vacuum (cation species).

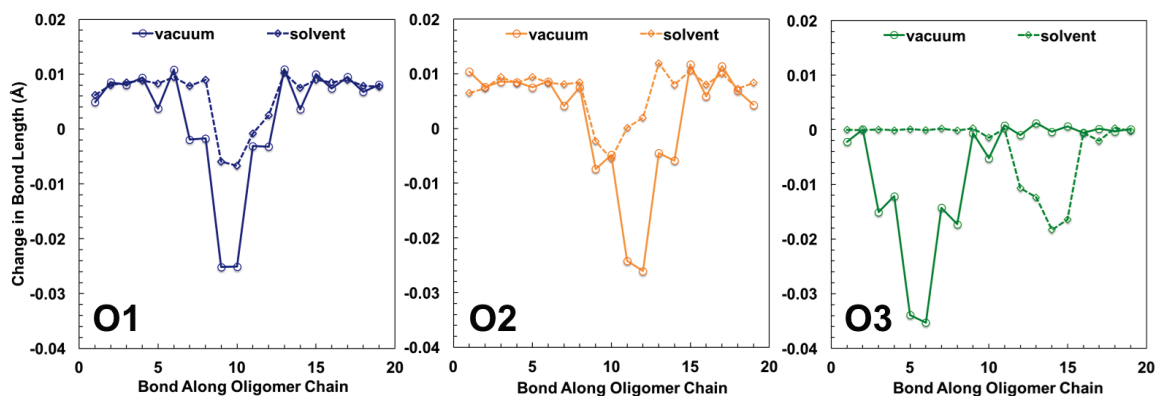


Figure S6. Bond lengths changes for oligomers in vacuum (cation species).

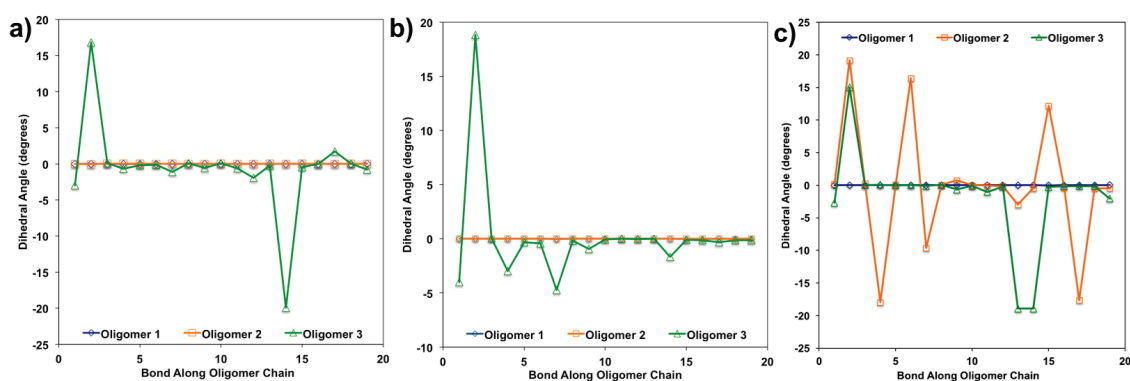


Figure S7. Bond dihedral plots for all oligomers in (a) the neutral geometry, (b) the optimized cation species geometry, and the (c) optimized anion species in vacuum.

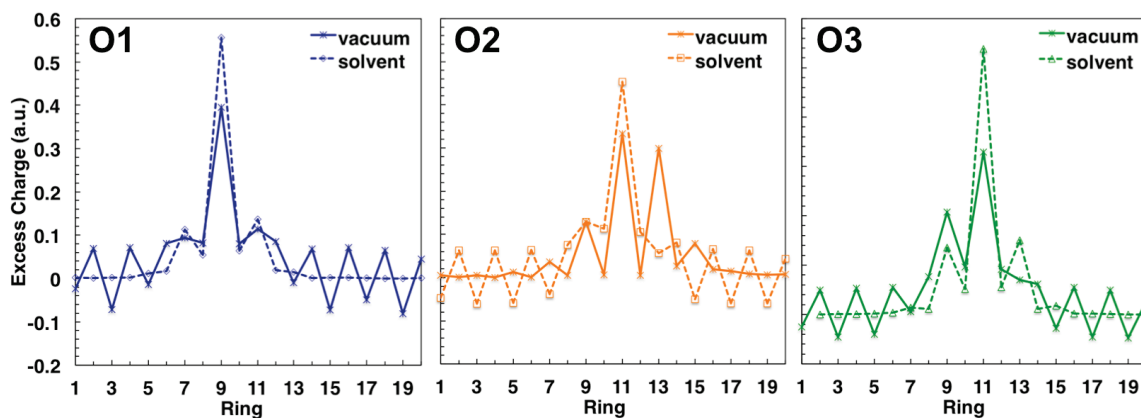


Figure S8. Excess charges of the cation species in vacuum and solvent.

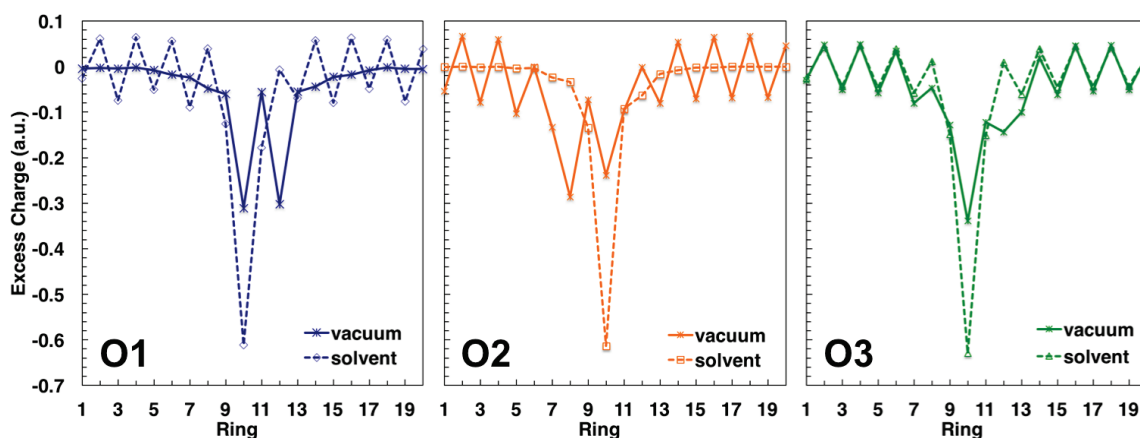


Figure S9. Excess charges of the cation species in vacuum and solvent.

Table S1. Absolute energies of the neutral optimized geometries.

Oligomer	Number of repeat units	Energy (hartrees)
1	1	-3948.182819
	2	-7895.182326
	4	-15789.18618
	5	-19736.1849
2	1	-3948.183182
	2	-7895.182542
	4	-15789.18127
	5	-19736.18062
3	5	-19575.78945

Table S2. Absolute energies of the cation species in neutral optimized geometries.

Oligomer	Number of repeat units	Energy (hartrees)
1	1	-3947.953786
	2	-7894.963822
	4	-15788.96959
	5	-19735.96946
2	1	-3947.957
	2	-7894.965
	4	-15788.96666
	5	-19735.96598
3	5	-19735.96005

Table S3. Absolute energies of the cation optimized geometries.

Oligomer	Number of repeat units	Energy (hartrees)
1	1	-3947.964391

	2	-7894.975136
	4	-15788.97964
	5	-19735.97863
2	1	-3947.965
	2	-7894.975
	4	-15788.97573
	5	-19735.975
3	5	-19735.96968

Table S4. Absolute energies of the neutral species in cation optimized geometries.

Oligomer	Number of repeat units	Energy (hartrees)
1	1	-3948.17272
	2	-7895.171445
	4	-15789.17518
	5	-19736.174
2	1	-3948.173615
	2	-7895.171585
	4	-15789.17016
	5	-19736.169
3	5	-19736.16348

Table S5. Absolute energies of the anion species in neutral optimized geometries.

Oligomer	Number of repeat units	Energy (hartrees)
1	1	-3948.25018
	2	-7895.255
	4	-15789.2523
	5	-19736.26187
2	1	-3948.249
	2	-7895.256
	4	-15789.2484
	5	-19736.24161
3	5	-19736.25301

Table S6. Absolute energies of the anion optimized geometries.

Oligomer	Number of repeat units	Energy (hartrees)
1	1	-3948.25401
	2	-7895.262
	4	-15789.25263
	5	-19736.26728
2	1	-3948.253
	2	-7895.263

	4	-15789.26351
	5	-19736.26346
3	5	-19736.26006

Table S7. Absolute energies of the neutral species in anion optimized geometries.

Oligomer	Number of repeat units	Energy (hartrees)
1	1	-3948.176193
	2	-7895.174265
	4	-15789.17778
	5	-19736.16137
2	1	-3948.176328
	2	-7895.174374
	4	-15789.17242
	5	-19736.17237
3	5	-19736.16603

Table S8. Intramolecular reorganization energies for cation species in vacuum.

Oligomer	n	λ_1 (eV)	λ_2 (eV)	λ (eV)
1	1	0.286	0.273	0.559
	2	0.305	0.294	0.599
	4	0.271	0.297	0.568
	5	0.248	0.294	0.542
2	1	0.216	0.258	0.474
	2	0.270	0.296	0.566
	4	0.226	0.300	0.545
	5	0.243	0.314	0.557
3	5	0.212	0.271	0.483

Table S9. Intramolecular reorganization energies for cation species in solvent.

Oligomer	n	λ_1 (eV)	λ_2 (eV)	λ (eV)
1	1	0.243	0.245	0.488
	2	0.264	0.222	0.486
	4	0.340	0.222	0.562
	5	0.330	0.221	0.551
2	1	0.216	0.250	0.466
	2	0.216	0.233	0.449
	4	0.216	0.212	0.428

	5	0.244	0.242	0.486
3	5	0.211	0.223	0.434

Table S10. Intramolecular reorganization energies for anion species in vacuum.

Oligomer	n	λ_1 (eV)	λ_2 (eV)	λ (eV)
1	1	0.103	0.179	0.285
	2	0.189	0.207	0.399
	4	0.009	0.217	0.227
	5	0.146	0.635	0.788
2	1	0.108	0.185	0.295
	2	0.189	0.221	0.413
	4	0.408	0.239	0.652
	5	0.590	0.223	0.819
3	5	0.190	0.240	0.434

Table S11. Intramolecular reorganization energies for anion species in solvent.

Oligomer	n	λ_1 (eV)	λ_2 (eV)	λ (eV)
1	1	0.135	0.480	0.615
	2	0.324	0.149	0.473
	4	0.435	0.214	0.649
	5	0.610	0.635	0.788
2	1	0.162	0.160	0.322
	2	0.162	0.133	0.295
	4	0.135	0.147	0.282
	5	0.590	0.223	0.819
3	5	0.154	0.154	0.308

First principle tight binding modeling of planar polymers

Methodology for images below: Occupied valence molecular orbitals of π -symmetry of oligomers consisting of 16 monomers were localized using combination of top-down and bottom-up approaches [1]. The Fock matrix is then projected onto these LMOs to get tight-binding Hamiltonian. The Hamiltonian of an infinite polymer is obtained by extrapolating the Hamiltonian of the oligomer, taking into account exponential decrease of its elements with spatial separation between LMOs, see Fig. S13.

[1] Z Li, H Li, B Suo, W Liu, **Localization of Molecular Orbitals: From Fragments to Molecule**, *Acc Chem Res* 47, 2758 (2014)

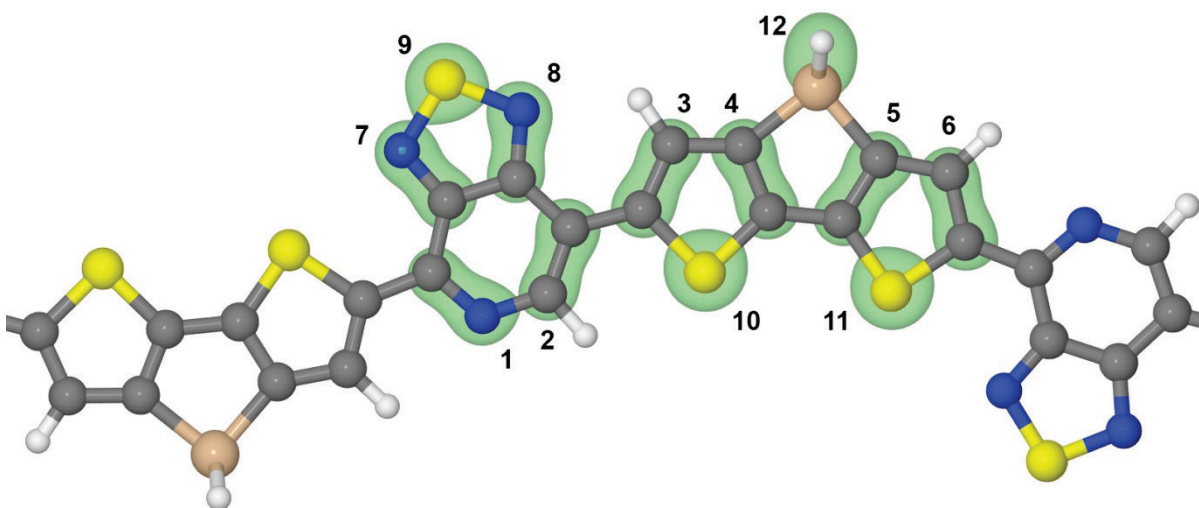


Figure S10. Localized molecular orbitals (LMO): there are 12 LMOs in the repeating unit. Shown here is the part of P1 (O2) polymer.

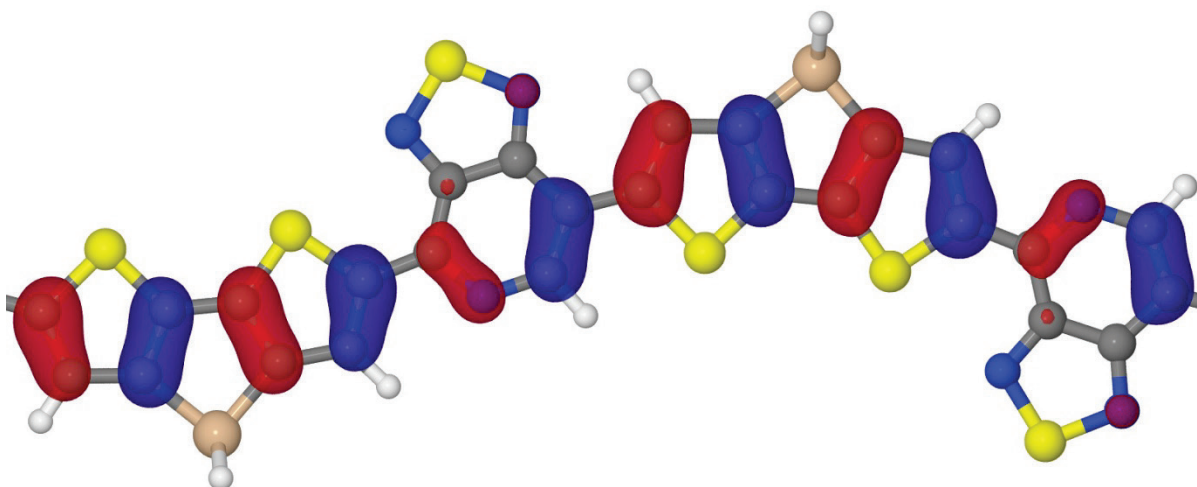


Figure S11. HOMO of the polymer P1 (central part of the long enough oligomer). It is composed primarily of LMOs 1-6 from Fig. S10.

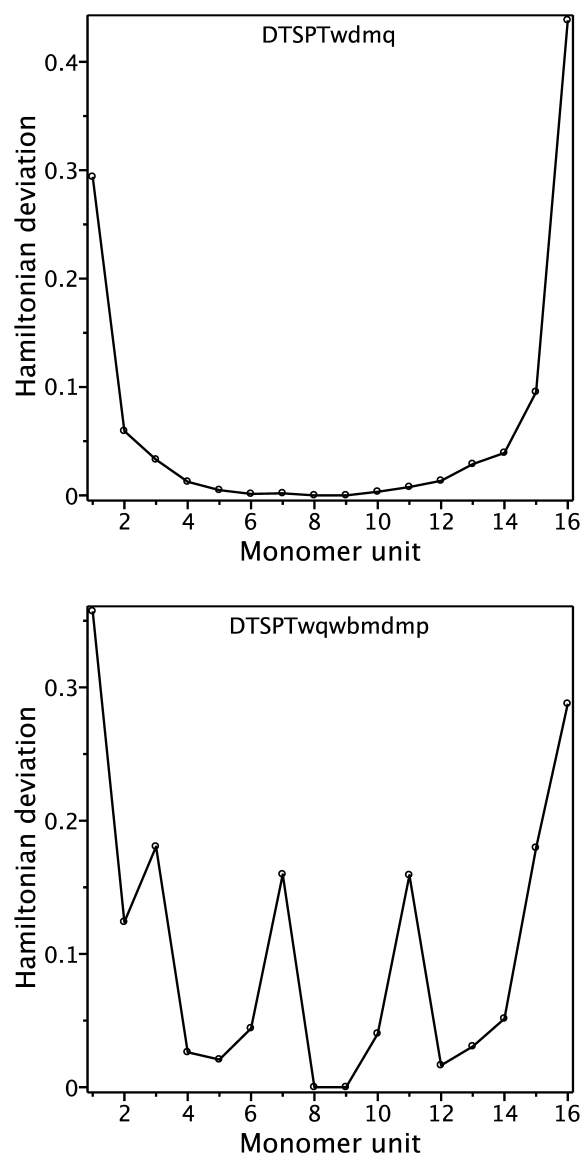


Figure S12. Intra-monomer tight-binding Hamiltonian deviations (Frobenius norm) across the oligomers P1 (left) and P2 (right). The same-order deviations are observed between different polymers (P1,P2,P3) – few tenths of eV, that is not enough to introduce a noticeable disorder in a tight-binding Hamiltonian with 1.2-1.4 eV inter-site couplings.

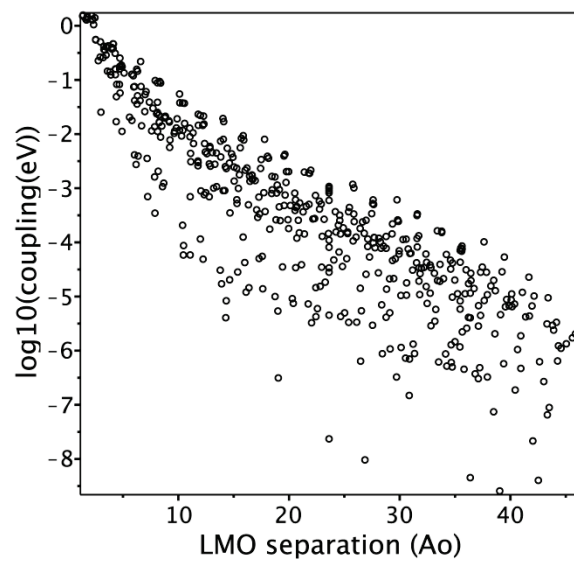


Figure S13. Exponential decrease of elements of tight-binding Hamiltonian with separation between LMOs.

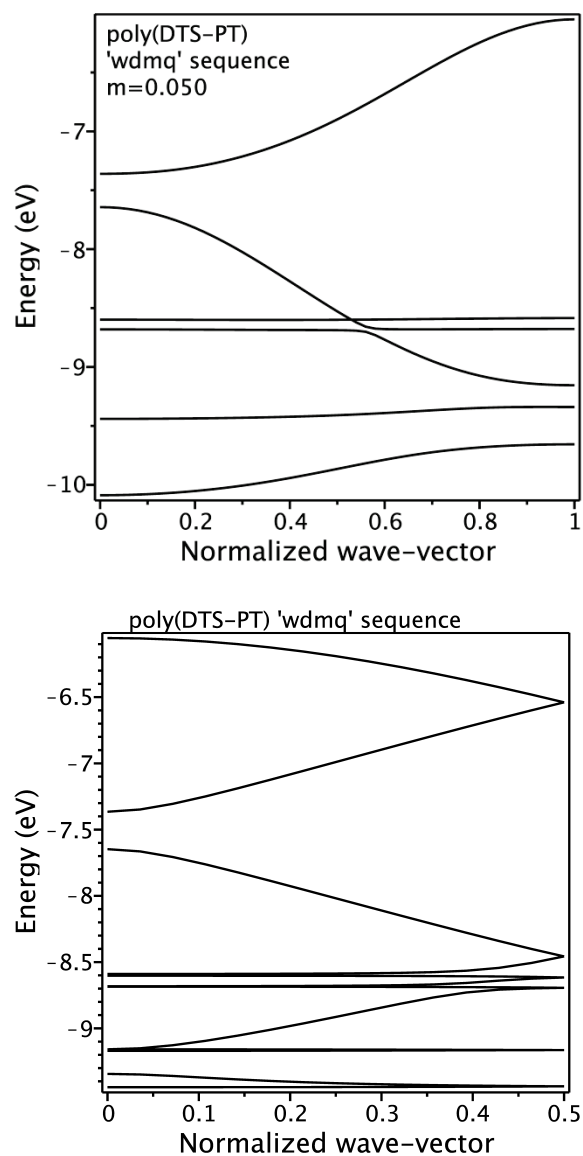


Figure S14. Electronic structure of the valence band of a planar P1 polymer: our simplified approach (π -bands only) vs. straightforward periodic boundary conditions calculations. Both approaches are numerically identical.

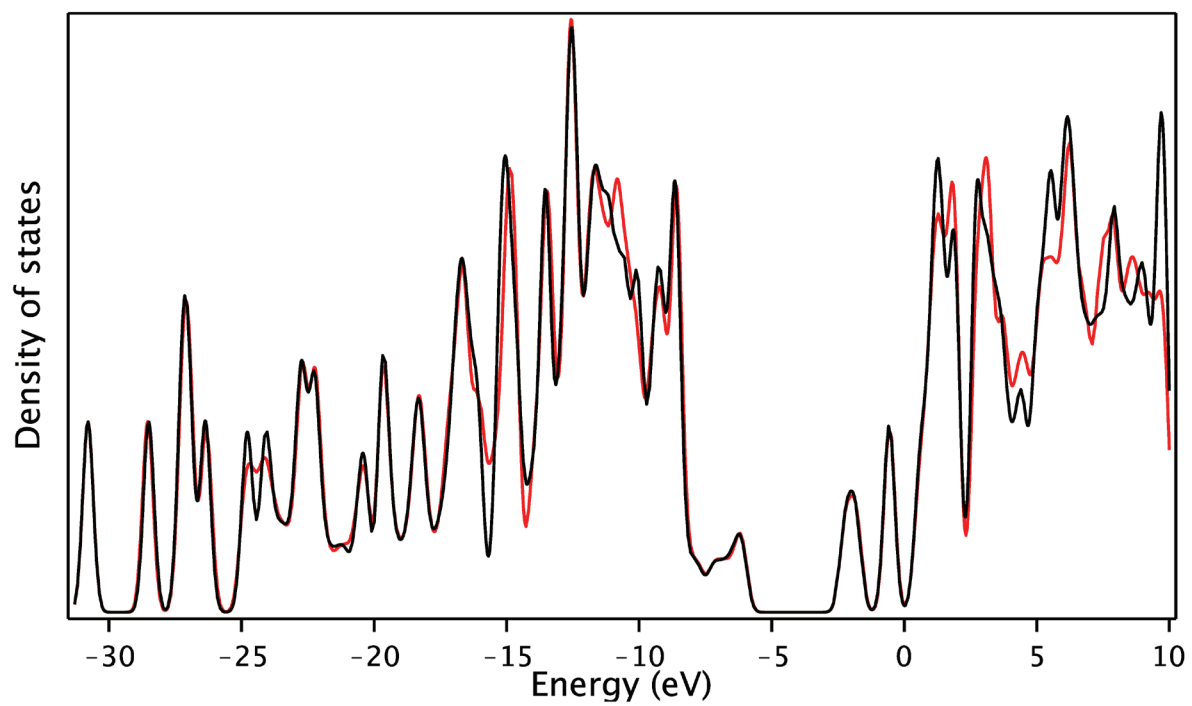


Figure S15. Comparison of electronic density of states: P1 (black) vs. P2 (red).

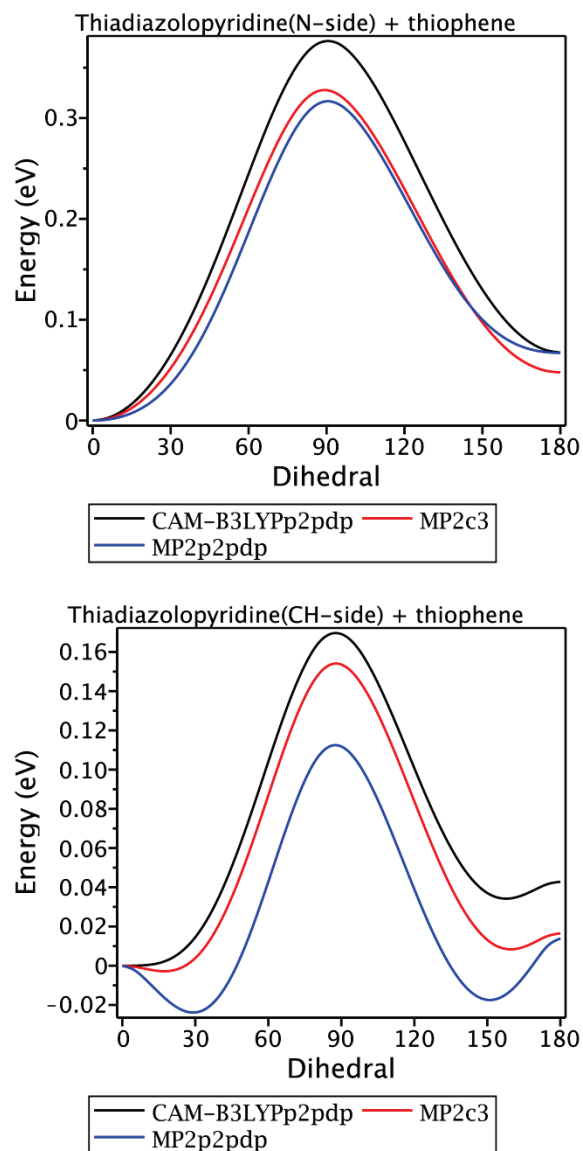


Figure S16. Potential energy surface for the two principal dihedrals determining geometry of the studied polymers. Zero dihedral corresponds to the trans orientation of sulfur atoms.

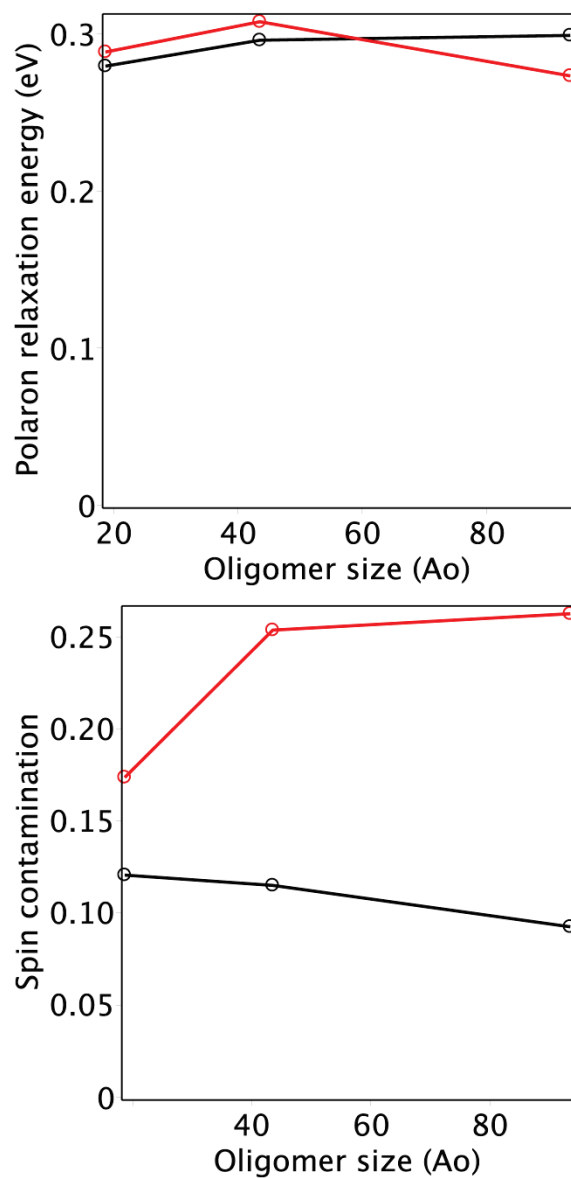


Figure S17. Convergence of polaron relaxation energy (λ_1 and λ_2) and spin contamination with oligomer size.

Tight-binding Hamiltonian for polymer P1 in indices of Fig.S10

i H[i,i,0](eV)

- 1 -11.53
- 2 -10.33
- 3 -9.85
- 4 -10.10
- 5 -10.09

6 -9.84
 7 -12.27
 8 -11.92
 9 -11.06
 10 -9.90
 11 -9.87
 12 -11.39

i j r H[i,j,r] distance(Ao)

7 9 0 -1.53 1.5
 4 5 0 -1.48 2.2
 8 9 0 -1.47 1.4
 1 2 0 -1.44 1.8
 5 6 0 -1.39 1.8
 3 4 0 -1.37 1.8
 2 3 0 -1.36 2.5
 7 8 0 -1.28 1.7
 6 1 1 1.27 2.3
 4 10 0 -1.26 1.8
 6 11 0 -1.26 1.8
 5 11 0 -1.25 1.8
 3 10 0 -1.24 1.8
 2 8 0 -1.23 2.3
 1 7 0 -1.02 2.4
 5 12 0 -0.54 2.6
 4 12 0 -0.53 2.6
 2 10 0 -0.49 3.0
 6 2 1 -0.45 4.2
 2 4 0 0.45 4.2
 1 9 0 0.41 3.7
 4 11 0 -0.41 3.3
 2 9 0 0.39 3.6
 4 6 0 0.39 4.1
 5 1 1 -0.37 4.2
 3 5 0 0.36 4.1
 6 7 1 0.35 3.3
 5 10 0 -0.34 3.4
 1 3 0 0.30 4.4
 11 1 1 0.28 3.5
 3 8 0 -0.26 3.0
 11 7 1 0.25 3.3
 6 9 1 -0.25 4.8
 2 7 0 -0.22 2.8
 6 3 1 0.21 6.7
 3 11 0 0.18 4.9
 6 8 1 0.17 4.8

6 10 0 0.17 5.0
 11 12 0 0.16 4.4
 5 7 1 -0.16 4.8
 2 5 0 -0.15 6.3
 10 12 0 0.15 4.4
 10 11 0 -0.14 3.7
 4 1 1 0.14 6.4
 3 12 0 -0.14 3.9
 11 2 1 -0.13 5.2
 3 6 0 -0.12 5.9
 3 9 0 0.12 4.4
 6 12 0 -0.12 4.0
 5 2 1 0.12 6.0
 2 6 0 0.09 8.0
 6 4 1 -0.09 8.4
 3 1 1 -0.09 8.2
 5 3 1 -0.08 8.5
 3 7 0 -0.08 4.5
 1 10 0 0.08 4.7
 2 11 0 -0.07 6.7
 5 9 1 0.07 6.1
 1 4 0 -0.07 6.0
 10 1 1 0.06 7.2
 4 8 0 0.06 4.8
 2 1 1 0.05 10.2
 6 10 1 0.05 7.1
 5 8 1 -0.05 6.4
 11 9 1 -0.05 4.5
 4 9 0 -0.04 6.1
 4 7 1 0.04 6.6
 11 3 1 0.04 7.5
 4 2 1 -0.04 8.2
 5 4 1 0.04 10.2
 6 5 1 0.04 10.4
 4 3 1 0.04 10.6
 4 7 0 0.03 6.3
 4 9 1 -0.03 7.8
 5 8 0 -0.03 7.0
 1 8 0 -0.02 3.1
 3 7 1 -0.02 8.2
 1 5 0 0.02 8.1
 2 2 1 -0.02 11.9
 4 8 1 0.02 8.3
 6 6 1 -0.02 12.1
 3 3 1 -0.02 12.3
 5 10 1 -0.02 8.9

10 2 1 -0.02 8.8
 7 10 0 -0.02 5.7
 6 8 0 0.02 8.9
 2 3 1 0.02 14.1
 3 2 1 0.02 10.0
 9 10 0 0.02 5.9
 3 9 1 0.02 9.2
 6 1 2 -0.02 14.2
 8 10 0 0.02 4.5
 5 9 0 0.02 8.3
 11 4 1 -0.02 9.3
 1 11 0 0.02 8.4
 6 11 1 0.02 10.6
 4 4 1 -0.01 12.4
 1 1 1 -0.01 11.9
 5 5 1 -0.01 12.3
 10 7 1 0.01 6.8
 5 7 0 -0.01 8.6
 8 11 0 -0.01 7.9
 3 8 1 -0.01 9.9
 10 3 1 0.01 11.1
 6 9 0 -0.01 10.2
 2 9 1 -0.01 10.5
 10 9 1 -0.01 7.7
 1 6 0 -0.01 9.7
 11 10 1 0.01 8.2
 11 8 1 0.01 5.0
 2 8 1 0.01 11.4
 2 7 1 0.01 9.7

Cartesian Coordinates for n=5 oligomers

Oligomer 1 in vacuum

Atom	X	Y	Z
C	-44.696956709606	-2.581357462190	-0.013726963434
C	-43.696661253613	-3.510346295510	-0.014797236089
C	-42.413902859125	-2.903341895538	-0.013223240763
C	-42.478007460725	-1.530986071638	-0.011005782860
S	-44.096780503628	-0.951529012158	-0.010788723025
H	-45.763603893925	-2.753265717450	-0.014487993224
H	-43.882717253998	-4.577605250131	-0.016627665616
C	-41.135777365807	-0.997539868416	-0.009527743727
C	-40.244302405666	-2.044859893649	-0.010835261997
S	-40.366012190854	0.533427820979	-0.006630053717
C	-38.905148690026	-1.611905417163	-0.009494828465
C	-38.783199973283	-0.236549143532	-0.007182332771
H	-38.052035119272	-2.278674778295	-0.010171400582
C	-40.969404466342	-3.383458853155	-0.013353045466
C	-40.646955782412	-4.196863559560	-1.276127012968
H	-39.588329049896	-4.471745453537	-1.297254995232
H	-41.234078959423	-5.119534201611	-1.299639318931
H	-40.871096709174	-3.624179509894	-2.178647130612

C	-40.648094676523	-4.200978885338	1.247051775791
H	-41.235205713147	-5.123741623762	1.267010452865
H	-39.589478575036	-4.475895956376	1.268256891038
H	-40.873085570846	-3.631256435809	2.151233391515
C	-37.541966983620	0.526392197255	-0.005388056808
C	-36.302602319417	-0.078290839408	-0.006113093142
C	-37.485793276020	1.958438189693	-0.002724544508
H	-36.233110800211	-1.160680963029	-0.008139582141
C	-36.216502880032	2.637115375139	-0.001031642789
C	-35.004398604905	1.858048082095	-0.002043124825
C	-33.678544785335	2.440033872497	-0.000471608884
C	-33.291833173954	3.764792657292	0.002160566684
S	-32.304763009128	1.349516657016	-0.002000823966
C	-31.891707739351	3.905606988495	0.002934487018
H	-34.010472256080	4.572894050544	0.003411087932
C	-31.235970659008	2.691012993167	0.000894073078
C	-29.816446545295	2.930064679493	0.001857020058
C	-29.595085272209	4.292721679238	0.004491750712
S	-28.367149384884	2.013263444210	0.000659400023
C	-28.226711063771	4.618662669879	0.005583889511
C	-27.426318999596	3.493970674933	0.003750556653
H	-27.813443339822	5.617843466259	0.007597237184
C	-30.906112668079	5.064362912774	0.005475372058
C	-25.983485322086	3.377544961229	0.004027919591
C	-25.092628330505	4.512043921514	0.006425603627
C	-24.123237327774	1.977720597669	0.002058129047
C	-23.667860537719	4.294296308227	0.006503691239
C	-23.150636156124	2.953803377433	0.004198510827
H	-23.831074865868	0.931306085976	0.000205535175
N	-38.519779784403	2.793742684570	-0.001546986797
N	-36.326668935069	3.961242057663	0.001368453001
N	-25.431992056003	5.795850270553	0.008684925111
N	-22.974516652826	5.429782803308	0.008838531990
N	-25.463642309738	2.171216457007	0.001968200744
N	-35.101423394914	0.547419074466	-0.004526059627
S	-37.916101522128	4.303841304493	0.001444787868
S	-24.050096892838	6.650994955358	0.010736864864
C	-31.052142174881	5.927051148097	1.268554338628
H	-32.031077308619	6.414447734538	1.289285051082
H	-30.951002383869	5.321063572342	2.171546832390
H	-30.286142579944	6.707496293750	1.290664563220
C	-31.051220849860	5.931831607232	-1.254431496024
H	-32.030127233190	6.419332790203	-1.274015331873
H	-30.285182448840	6.712328899764	-1.273030832305
H	-30.949449429234	5.329268922553	-2.159642226964
C	-21.727497146373	2.653341175990	0.004127857299
C	-20.663080193210	3.528496053870	0.005912848537
S	-21.172676447118	0.980735896425	0.001497194438
C	-19.416853554076	2.867539824411	0.005159296245
H	-20.806199766370	4.599729461416	0.007676795249
C	-19.535890474058	1.497522186206	0.002823052791
C	-17.954273931347	3.288270939051	0.006281946111
C	-18.220853615534	0.909746696162	0.002203643259
C	-17.286012776317	1.920855143416	0.004166915931
C	-17.599967854048	4.087685772117	1.269491052461
C	-17.599251193144	4.091931664227	-1.254029045244
S	-17.514046442711	-0.652214083101	-0.000183039099
C	-15.966970295945	1.433304425875	0.003728908447
H	-16.531192577748	4.319798564901	1.290617257764
H	-18.150376519903	5.032516002133	1.292321085603
H	-17.847066944724	3.524506932591	2.172013506552
H	-18.149624735356	5.036847952063	-1.273982461552
H	-16.530459215225	4.324088876771	-1.273780514411
H	-17.845860855435	3.531804866814	-2.158582478752
C	-15.902135493768	0.053369279749	0.001419548521
H	-15.087157154090	2.064250871565	0.005061032885
C	-14.693196315795	-0.759314889502	0.000329308031
C	-13.430451448106	-0.204782498657	0.001216493781
C	-14.695243887732	-2.192323078537	-0.001744363081
H	-13.317491631409	0.873959125256	0.002732962294

N	-12.255754481416	-0.878054943882	0.000367721209
C	-13.454432658452	-2.921518788094	-0.002685177516
N	-15.762118220789	-2.985009394916	-0.002997249405
C	-12.211729499004	-2.191928073586	-0.001511076856
N	-13.618019780458	-4.240049305737	-0.004613599412
S	-15.219891103784	-4.518439863881	-0.005167459626
C	-10.910703050762	-2.826133089071	-0.002295818046
C	-10.576563170477	-4.165412794116	-0.004174991875
S	-9.494816834671	-1.790763023551	-0.000674567514
C	-9.183323301092	-4.361418362542	-0.004339534124
H	-11.326603593008	-4.944488764710	-0.005353870891
C	-8.480235062320	-3.173355636618	-0.002584001240
C	-8.243712429537	-5.557883175886	-0.005978531706
C	-7.071338468613	-3.467776152121	-0.002893683073
C	-6.903474053984	-4.838020402376	-0.004840455261
C	-8.422855106456	-6.414768472861	-1.268746282970
C	-8.423053248687	-6.418391226628	1.254295477145
S	-5.587466091736	-2.608095178012	-0.001529885013
C	-5.548713614030	-5.217081438976	-0.005276782261
H	-9.420017830048	-6.863677413588	-1.289560277236
H	-8.297891976720	-5.813626739154	-2.171994997029
H	-7.687860001305	-7.224482241887	-1.290259308252
H	-9.420215121796	-6.867366839096	1.273659287652
H	-7.688053588407	-7.228156215949	1.273601151587
H	-8.298241309436	-5.819844931835	2.159287039174
C	-4.705298772195	-4.124350019798	-0.003657946867
H	-5.174519867424	-6.231556120440	-0.006700598502
C	-3.258871843448	-4.063634331524	-0.003472749088
C	-2.412155781317	-5.231272679176	-0.005076582560
N	-2.693404612139	-2.878073806884	-0.001743111932
C	-0.980125006439	-5.068118549136	-0.004745287187
N	-2.800369154248	-6.501202451234	-0.006910255384
C	-1.346639579699	-2.735791797129	-0.001447260728
C	-0.412034262237	-3.748360043821	-0.002828975406
N	-0.330678071536	-6.229286859706	-0.006350917654
S	-1.452137115098	-7.408454674864	-0.008100716288
H	-1.014790102585	-1.701298785406	0.000058468925
C	1.021413795081	-3.502114039141	-0.002382793935
C	2.052139831863	-4.416764469339	-0.003529444123
S	1.638809874148	-1.851585179849	-0.000097945870
C	3.322380540401	-3.803194682400	-0.002599500433
H	1.868753148078	-5.481856090940	-0.004981072350
C	3.254868618813	-2.429654888992	-0.000755132791
C	4.768234970905	-4.278398049266	-0.003124025549
C	4.590936524677	-1.891560247284	0.000075637023
C	5.487276022663	-2.936925582288	-0.001260471329
C	5.092762708351	-5.090932004544	-1.265964028867
C	5.092563802449	-5.094329355446	1.257575291209
S	5.355517690954	-0.357095838135	0.002199958605
C	6.823646558753	-2.498960754280	-0.000575295474
H	6.152113715597	-5.362856941824	-1.286673874913
H	4.507431412688	-6.014536769010	-1.288681572575
H	4.867189045646	-4.519210572966	-2.168751984905
H	4.507235413598	-6.017996053217	1.277711952536
H	6.151913215820	-5.366302788288	1.277723711551
H	4.866841288138	-4.525043272923	2.161863788088
C	6.939933826061	-1.122394050161	0.001271456874
H	7.679314095044	-3.162284582321	-0.001413688625
C	8.178233309951	-0.355132331134	0.002394601665
C	9.419581261157	-0.956004785042	0.001799913123
C	8.229180828619	1.076974880214	0.004203600317
H	9.492545750656	-2.038195864968	0.000466311669
N	10.618409393151	-0.326663904018	0.002733832344
C	9.496106100914	1.759755736524	0.005216169940
N	7.192363450392	1.908586729713	0.005125132007
C	10.710998169450	0.984693306364	0.004388470694
N	9.381401837914	3.083430700768	0.006868488630
S	7.790956028891	3.420920300832	0.007109696201
C	12.034488630273	1.570508196798	0.005282005473
C	12.417592295099	2.896630412605	0.006989324225

S	13.411441308213	0.483879842973	0.004108824463
C	13.817044838546	3.041373261438	0.007325950708
H	11.696681272895	3.702731467565	0.007911601179
C	14.476093078549	1.828306966894	0.005887026734
C	14.799875272225	4.202570212646	0.008879917891
C	15.894855401445	2.070884340863	0.006343973423
C	16.112794575741	3.434052659538	0.008063474901
C	14.652137538596	5.065714567946	1.271457187521
C	14.652411418307	5.068860400413	-1.251572825846
S	17.346271294608	1.157452254796	0.005377994170
C	17.480527603615	3.763269428008	0.008616564655
H	13.672139633898	5.550961883032	1.292043524873
H	14.754832905293	4.460585615334	2.174848856063
H	15.416380014823	5.847881091243	1.292877039242
H	13.672419731825	5.554161562663	-1.271159519088
H	15.416661448856	5.851074442864	-1.270876942788
H	14.755299156781	4.465986040247	-2.156448810335
C	18.283356019594	2.640394505497	0.007298440710
H	17.891581596604	4.763374224031	0.009901872856
C	19.726603251613	2.526763212335	0.007301003108
C	20.615524312231	3.662592484624	0.008785598616
N	20.248236431461	1.321283229509	0.005872637860
C	22.040613712462	3.447051560756	0.008663770070
N	20.274124072204	4.945902227456	0.010327768237
C	21.588881465562	1.129725109396	0.005772577016
C	22.559962200690	2.107371438482	0.007072129900
N	22.732187511756	4.583632289401	0.010130149083
S	21.654720139420	5.803113145403	0.011527552096
H	21.882583211068	0.083762259653	0.004517724150
C	23.983422948138	1.808766721566	0.006856157602
C	25.047023181672	2.684989701083	0.008004181281
S	24.539818715908	0.136705144951	0.004937216362
C	26.293897410607	2.025221726561	0.007335863297
H	24.902843805638	3.756096452451	0.009267089255
C	26.175980307030	0.655083270320	0.005694741300
C	27.756266031577	2.446956371373	0.007972832356
C	27.491342342709	0.068263057574	0.005115515923
C	28.425528830230	1.079949552673	0.006405588549
C	28.110277225492	3.247226390236	1.270724081948
C	28.110508978670	3.250232152328	-1.252803011548
S	28.198848875031	-1.493298533463	0.003348322863
C	29.744882959419	0.593054140947	0.005953074138
H	29.178906008774	3.480022838050	1.291534641638
H	27.559291530580	4.191728726012	1.293178386380
H	27.863707687970	2.684350582674	2.173580085246
H	27.559524022450	4.194783534110	-1.273110371352
H	29.179140712664	3.483081055280	-1.272860112324
H	27.864109623226	2.689507394279	-2.157042938684
C	29.810374243300	-0.786867676797	0.004313626338
H	30.624429134417	1.224381878031	0.006795595986
C	31.019479336128	-1.599354485388	0.003438914072
C	32.282260849487	-1.044926201101	0.004064570266
C	31.017278627984	-3.032361583119	0.001872788422
H	32.395293547264	0.033818422577	0.005231238403
N	33.456942478175	-1.718322974997	0.003364613515
C	32.257970530049	-3.761676628865	0.001107740776
N	29.950310699320	-3.824918866852	0.000979221975
C	33.500789179964	-3.032205251284	0.001936772046
N	32.094196085551	-5.080184666185	-0.000334558968
S	30.492321884189	-5.358413514763	-0.000674031875
C	34.801521934988	-3.666979548152	0.001286601673
C	35.134513524905	-5.006543018202	-0.000134822565
S	36.218353052839	-2.632881589938	0.002435481462
C	36.527506099874	-5.203778971170	-0.000314922423
H	34.383842097307	-5.784992466166	-0.000983257396
C	37.231780446415	-4.016396796641	0.000967875761
C	37.465727948143	-6.401240413255	-0.001574650509
C	38.640422863544	-4.312368812762	0.000678425839
C	38.806661823451	-5.682830415941	-0.000782860263
C	37.285567845231	-7.258387517498	-1.264022677697

C	37.285519195139	-7.261080678136	1.259034344264
S	40.125485530429	-3.454616538201	0.001625577944
C	40.160864770833	-6.063619456946	-0.001172100027
H	36.287914040868	-7.706211563532	-1.284602220151
H	37.411125501732	-6.657714710420	-2.167500949439
H	38.019671532781	-8.068914375135	-1.285290622336
H	36.287864293814	-7.708946935653	1.278620743206
H	38.019621446566	-8.071651697928	1.278600384822
H	37.411043540238	-6.662337167144	2.163796858205
C	41.005719443284	-4.972009317072	-0.000001156899
H	40.533685502853	-7.078585654163	-0.002251462342
C	42.452244388466	-4.913797929031	0.000066517714
C	43.296583589373	-6.083199364029	-0.001167047978
N	43.020112821310	-3.729385673055	0.001325462456
C	44.728910452833	-5.923012904589	-0.000995321707
N	42.905777048469	-7.352337401712	-0.002509622354
C	44.367217082778	-3.589906993211	0.001476167735
C	45.299707155960	-4.604411972629	0.000398971494
N	45.375954082309	-7.085528614485	-0.002221092962
S	44.252088721138	-8.262381774326	-0.003458136483
H	44.701239989798	-2.556107650813	0.002578803342
C	46.733742527164	-4.361466420318	0.000653978578
C	47.762041141443	-5.278810884643	-0.000264105529
S	47.355482808163	-2.712562376511	0.002332174323
C	49.033851512864	-4.668604496091	0.000360894276
H	47.575896693921	-6.343409625084	-0.001342478878
C	48.970088972473	-3.294888473387	0.001748259214
C	50.478255352774	-5.147966578001	-0.000119080418
C	50.307763309088	-2.760584616691	0.002290777585
C	51.201056071638	-3.808593063269	0.001233823490
C	50.800345523119	-5.961845106589	-1.262721381988
C	50.800337649277	-5.964395356830	1.260837885876
S	51.077028967137	-1.228412811504	0.003832679500
C	52.538666437688	-3.374671603265	0.001661154812
H	51.858903126459	-6.236847473942	-1.283416062941
H	50.212350451198	-6.883761107840	-1.285108405378
H	50.576361493861	-5.389771374740	-2.165681674547
H	50.212328441704	-6.886345422304	1.281364816263
H	51.858891366632	-6.239454051109	1.280975227329
H	50.576363635823	-5.394140902891	2.164950633699
C	52.659118911664	-1.998478867191	0.003035966419
H	53.392269438482	-4.040640042534	0.000980728268
C	53.899973053597	-1.235371259474	0.003781875947
C	55.139135731560	-1.840649815298	0.003204366260
C	53.956027646499	0.196563390629	0.005162715592
H	55.208367930928	-2.923065998738	0.002173680349
N	56.340174508012	-1.215432810215	0.003798480352
C	55.225369642306	0.874807797523	0.005810052373
N	52.922180229404	1.031891632595	0.005974453369
C	56.437364875055	0.095452500377	0.005050277565
N	55.115413307915	2.198930335075	0.007088846681
S	53.526223725129	2.542016358695	0.007429794552
C	57.763392936937	0.676284527726	0.005584215996
C	58.151918941694	2.000608643239	0.006831443349
S	59.135533745763	-0.416231148097	0.004523827457
C	59.552357601076	2.139370612541	0.006931344692
H	57.434446678096	2.809780604127	0.007612098876
C	60.205751837846	0.923652381314	0.005766825706
C	60.540230379307	3.296367062198	0.007995088845
C	61.626087034792	1.160084263230	0.005953178031
C	61.849764005179	2.522041112152	0.007233165261
C	60.396312436090	4.160588942163	1.270306111403
C	60.396243857349	4.162954059292	-1.252685515749
S	63.072755370638	0.239794647016	0.005044695409
C	63.219672961163	2.844410195554	0.007501513261
H	59.418421737433	4.650067683797	1.290804605836
H	60.496520462955	3.555391600075	2.173934366625
H	61.163886114256	4.939472641662	1.291290062897
H	59.418345717176	4.652457515845	-1.272219672272
H	61.163805875046	4.941886847438	-1.272246884495

H	60.496415892067	3.559453317139	-2.157451760066
C	64.015966362783	1.717929006919	0.006419632643
H	63.636440052666	3.842305224718	0.008433752625
C	65.461364899221	1.598147120851	0.006266751725
C	66.346585099937	2.741954397582	0.007319846979
N	65.971692493205	0.389169601564	0.005116239025
C	67.766774854274	2.517378522879	0.007065326974
N	66.014163224541	4.028381241018	0.008542989969
C	67.323222109046	0.195817678885	0.004896434340
C	68.258780055437	1.185291235539	0.005798004801
N	68.477664753221	3.643036095178	0.008103199580
S	67.407750254143	4.869683825710	0.009291627341
H	67.628701254219	-0.846097731394	0.003909138325
H	69.321669597475	0.982030741554	0.005575242909

Oligomer 1 in solvent

Atom	X	Y	Z
C	56.423331000000	3.156427000000	-0.194155000000
C	55.383702000000	4.054382000000	-0.191911000000
C	54.120418000000	3.407145000000	-0.157389000000
C	54.226601000000	2.025067000000	-0.134252000000
S	55.876294000000	1.494446000000	-0.154203000000
H	57.484807000000	3.360248000000	-0.216495000000
H	55.534968000000	5.127666000000	-0.213909000000
C	52.908390000000	1.450569000000	-0.101069000000
C	51.970485000000	2.475131000000	-0.102607000000
S	52.184011000000	-0.115967000000	-0.052209000000
C	50.648118000000	2.001730000000	-0.066251000000
C	50.559659000000	0.610721000000	-0.037414000000
H	49.775799000000	2.644060000000	-0.057075000000
C	52.655149000000	3.841968000000	-0.138462000000
C	52.280962000000	4.631994000000	-1.412383000000
H	51.212941000000	4.872321000000	-1.413744000000
H	52.839520000000	5.572398000000	-1.456411000000
H	52.505498000000	4.055356000000	-2.313889000000
C	52.326578000000	4.673642000000	1.121573000000
H	52.883056000000	5.616308000000	1.113342000000
H	51.258581000000	4.911621000000	1.155213000000
H	52.586809000000	4.128104000000	2.032793000000
C	49.351100000000	-0.188378000000	-0.003992000000
C	48.078311000000	0.387796000000	-0.043351000000
C	49.331409000000	-1.622787000000	0.073560000000
H	47.985736000000	1.467413000000	-0.110197000000
C	48.072116000000	-2.339125000000	0.110510000000
C	46.836324000000	-1.595055000000	0.069001000000
C	45.529841000000	-2.202308000000	0.105751000000
C	45.156811000000	-3.542132000000	0.184507000000
S	44.118535000000	-1.129888000000	0.047107000000
C	43.762597000000	-3.710895000000	0.197964000000
H	45.888870000000	-4.337557000000	0.228584000000
C	43.069281000000	-2.502308000000	0.129616000000
C	41.664839000000	-2.769012000000	0.149109000000
C	41.464846000000	-4.147715000000	0.229517000000
S	40.184158000000	-1.877587000000	0.099605000000
C	40.106760000000	-4.502031000000	0.251624000000
C	39.265568000000	-3.392721000000	0.188244000000
H	39.719024000000	-5.510287000000	0.310266000000
C	42.797678000000	-4.892859000000	0.270511000000
C	37.828076000000	-3.306071000000	0.183515000000
C	36.951129000000	-4.452604000000	0.246502000000
C	35.945005000000	-1.921894000000	0.104552000000
C	35.513526000000	-4.255846000000	0.233327000000
C	34.972569000000	-2.922485000000	0.158530000000
H	35.631125000000	-0.882151000000	0.046474000000
N	50.396170000000	-2.429639000000	0.119140000000
N	48.214338000000	-3.665237000000	0.183308000000
N	37.315474000000	-5.734768000000	0.318714000000
N	34.829268000000	-5.403142000000	0.296480000000
N	37.281082000000	-2.092229000000	0.115540000000

N	46.900070000000	-0.265503000000	-0.007503000000
S	49.828488000000	-3.970394000000	0.202203000000
S	35.932945000000	-6.620084000000	0.366342000000
C	42.966537000000	-5.683004000000	1.587830000000
H	43.957617000000	-6.145433000000	1.630290000000
H	42.853128000000	-5.029785000000	2.457287000000
H	42.217771000000	-6.478573000000	1.653632000000
C	42.958903000000	-5.835977000000	-0.942934000000
H	43.948020000000	-6.304322000000	-0.932894000000
H	42.206808000000	-6.630328000000	-0.909521000000
H	42.844247000000	-5.291864000000	-1.884371000000
C	33.554308000000	-2.638028000000	0.140831000000
C	32.481518000000	-3.524796000000	0.182424000000
S	32.975074000000	-0.954882000000	0.054830000000
C	31.231607000000	-2.880837000000	0.146063000000
H	32.633283000000	-4.594149000000	0.236700000000
C	31.333139000000	-1.495465000000	0.076909000000
C	29.766781000000	-3.317298000000	0.163158000000
C	30.021118000000	-0.925662000000	0.044323000000
C	29.081957000000	-1.952514000000	0.092685000000
C	29.413168000000	-4.064953000000	1.468227000000
C	29.420013000000	-4.189756000000	-1.064082000000
S	29.294185000000	0.639584000000	-0.039597000000
C	27.761186000000	-1.481311000000	0.062467000000
H	28.345880000000	-4.306662000000	1.492558000000
H	29.974739000000	-5.002051000000	1.533980000000
H	29.649725000000	-3.458631000000	2.346828000000
H	29.975473000000	-5.132274000000	-1.031303000000
H	28.351356000000	-4.426364000000	-1.074267000000
H	29.668138000000	-3.675681000000	-1.996660000000
C	27.672263000000	-0.090041000000	-0.009372000000
H	26.889039000000	-2.123035000000	0.090443000000
C	26.464068000000	0.706855000000	-0.056835000000
C	25.190990000000	0.129056000000	-0.028732000000
C	26.444823000000	2.141013000000	-0.138317000000
H	25.098961000000	-0.950911000000	0.033227000000
N	24.013291000000	0.781024000000	-0.072035000000
C	25.185668000000	2.856358000000	-0.185198000000
N	27.509461000000	2.947698000000	-0.179523000000
C	23.949664000000	2.111531000000	-0.149529000000
N	25.327749000000	4.182103000000	-0.261021000000
S	26.941785000000	4.488498000000	-0.271036000000
C	22.644571000000	2.718027000000	-0.194663000000
C	22.272701000000	4.058787000000	-0.274794000000
S	21.231841000000	1.646529000000	-0.146871000000
C	20.879576000000	4.228421000000	-0.297884000000
H	23.005618000000	4.853708000000	-0.313051000000
C	20.184546000000	3.019736000000	-0.235687000000
C	19.916204000000	5.411117000000	-0.376156000000
C	18.780786000000	3.287658000000	-0.265183000000
C	18.582839000000	4.666785000000	-0.345528000000
C	20.095047000000	6.202414000000	-1.691476000000
C	20.069182000000	6.352856000000	0.839455000000
S	17.298512000000	2.397895000000	-0.227755000000
C	17.225462000000	5.022723000000	-0.377157000000
H	21.086728000000	6.664150000000	-1.726335000000
H	19.987398000000	5.550158000000	-2.562379000000
H	19.347335000000	6.998566000000	-1.761748000000
H	21.058450000000	6.820935000000	0.836865000000
H	19.317549000000	7.147412000000	0.801496000000
H	19.947714000000	5.807771000000	1.779465000000
C	16.382733000000	3.914217000000	-0.321326000000
H	16.839293000000	6.031450000000	-0.437433000000
C	14.944886000000	3.830320000000	-0.327529000000
C	14.071167000000	4.978920000000	-0.394457000000
N	14.394876000000	2.617554000000	-0.266279000000
C	12.633162000000	4.785383000000	-0.392319000000
N	14.438869000000	6.260496000000	-0.461130000000
C	13.058428000000	2.449985000000	-0.265530000000
C	12.088610000000	3.453025000000	-0.324493000000

N	11.951979000000	5.934367000000	-0.458044000000
S	13.058742000000	7.148905000000	-0.517063000000
H	12.741798000000	1.410859000000	-0.211861000000
C	10.669719000000	3.172246000000	-0.317732000000
C	9.599913000000	4.062628000000	-0.361733000000
S	10.084604000000	1.490493000000	-0.244043000000
C	8.347959000000	3.422608000000	-0.336522000000
H	9.755322000000	5.131738000000	-0.409716000000
C	8.444527000000	2.036445000000	-0.273720000000
C	6.884896000000	3.864202000000	-0.360477000000
C	7.130342000000	1.471002000000	-0.251759000000
C	6.195168000000	2.501503000000	-0.300690000000
C	6.541750000000	4.618960000000	-1.664258000000
C	6.533509000000	4.732042000000	0.868723000000
S	6.396857000000	-0.092060000000	-0.182149000000
C	4.872547000000	2.035202000000	-0.281726000000
H	5.475354000000	4.863908000000	-1.694223000000
H	7.106453000000	5.554689000000	-1.722132000000
H	6.782094000000	4.016000000000	-2.544140000000
H	7.092324000000	5.672809000000	0.843846000000
H	5.465608000000	4.972208000000	0.873485000000
H	6.774136000000	4.212702000000	1.800346000000
C	4.777977000000	0.643950000000	-0.217749000000
H	4.003137000000	2.680442000000	-0.313186000000
C	3.566238000000	-0.148090000000	-0.179540000000
C	2.296033000000	0.436405000000	-0.194556000000
C	3.540109000000	-1.583202000000	-0.120838000000
H	2.209209000000	1.517745000000	-0.236481000000
N	1.115238000000	-0.210318000000	-0.160224000000
C	2.277463000000	-2.293009000000	-0.083641000000
N	4.600825000000	-2.395629000000	-0.093440000000
C	1.045105000000	-1.541641000000	-0.105433000000
N	2.413048000000	-3.620455000000	-0.028761000000
S	4.025570000000	-3.934880000000	-0.025276000000
C	-0.263122000000	-2.141770000000	-0.068201000000
C	-0.642877000000	-3.481728000000	-0.015378000000
S	-1.669409000000	-1.060954000000	-0.087587000000
C	-2.036953000000	-3.643375000000	0.009593000000
H	0.085316000000	-4.281708000000	0.003193000000
C	-2.724562000000	-2.429255000000	-0.023381000000
C	-3.007762000000	-4.821276000000	0.066308000000
C	-4.129789000000	-2.688673000000	0.007478000000
C	-4.336413000000	-4.067881000000	0.058596000000
C	-2.828477000000	-5.642852000000	1.362881000000
C	-2.866452000000	-5.736732000000	-1.170638000000
S	-5.606043000000	-1.788443000000	-0.000259000000
C	-5.696019000000	-4.415457000000	0.090761000000
H	-1.840244000000	-6.112789000000	1.382539000000
H	-2.926907000000	-5.009326000000	2.248583000000
H	-3.582006000000	-6.434602000000	1.419259000000
H	-1.880253000000	-6.211082000000	-1.183089000000
H	-3.623072000000	-6.527107000000	-1.146939000000
H	-2.988637000000	-5.170056000000	-2.097701000000
C	-6.531444000000	-3.300333000000	0.065293000000
H	-6.088660000000	-5.422681000000	0.131283000000
C	-7.968544000000	-3.206184000000	0.085469000000
C	-8.850645000000	-4.349423000000	0.129184000000
N	-8.509454000000	-1.988058000000	0.061614000000
C	-10.287022000000	-4.144740000000	0.147787000000
N	-8.492552000000	-5.635164000000	0.156025000000
C	-9.844432000000	-1.810174000000	0.079152000000
C	-10.821517000000	-2.806864000000	0.123328000000
N	-10.976714000000	-5.289767000000	0.188951000000
S	-9.879189000000	-6.514020000000	0.201876000000
H	-10.153309000000	-0.767636000000	0.054557000000
C	-12.238006000000	-2.514790000000	0.143485000000
C	-13.314957000000	-3.397525000000	0.155511000000
S	-12.809222000000	-0.826787000000	0.157128000000
C	-14.561561000000	-2.746839000000	0.173537000000
H	-13.168341000000	-4.468962000000	0.151514000000

C	-14.453530000000	-1.360084000000	0.176746000000
C	-16.028157000000	-3.176958000000	0.192114000000
C	-15.762815000000	-0.783343000000	0.196474000000
C	-16.706459000000	-1.807206000000	0.205905000000
C	-16.364760000000	-3.989471000000	1.462487000000
C	-16.399626000000	-3.982446000000	-1.072968000000
S	-16.482942000000	0.787232000000	0.222319000000
C	-18.024972000000	-1.329535000000	0.231330000000
H	-17.433635000000	-4.223103000000	1.494105000000
H	-15.811039000000	-4.933542000000	1.469021000000
H	-16.106684000000	-3.432169000000	2.367108000000
H	-15.845783000000	-4.926062000000	-1.100236000000
H	-17.468882000000	-4.216546000000	-1.076052000000
H	-16.167230000000	-3.419811000000	-1.981239000000
C	-18.107708000000	0.063853000000	0.241092000000
H	-18.899752000000	-1.968078000000	0.247052000000
C	-19.312735000000	0.866760000000	0.259635000000
C	-20.587534000000	0.293884000000	0.216036000000
C	-19.327017000000	2.301716000000	0.325674000000
H	-20.682929000000	-0.785901000000	0.155909000000
N	-21.763046000000	0.950756000000	0.239561000000
C	-20.583798000000	3.022374000000	0.349878000000
N	-18.259716000000	3.104670000000	0.371043000000
C	-21.822239000000	2.282016000000	0.306427000000
N	-20.437403000000	4.348290000000	0.413229000000
S	-18.822370000000	4.648540000000	0.438959000000
C	-23.125565000000	2.893490000000	0.330566000000
C	-23.494116000000	4.235705000000	0.401265000000
S	-24.540838000000	1.826360000000	0.265291000000
C	-24.886930000000	4.409902000000	0.403404000000
H	-22.759172000000	5.028318000000	0.447884000000
C	-25.584724000000	3.203191000000	0.333959000000
C	-25.847814000000	5.595691000000	0.464511000000
C	-26.987893000000	3.475421000000	0.341151000000
C	-27.182906000000	4.855305000000	0.415399000000
C	-25.673547000000	6.534387000000	-0.750575000000
C	-25.686596000000	6.389367000000	1.780718000000
S	-28.471920000000	2.589859000000	0.282220000000
C	-28.539603000000	5.215204000000	0.425482000000
H	-24.682798000000	6.999048000000	-0.734034000000
H	-25.782796000000	5.987851000000	-1.691245000000
H	-26.422893000000	7.331617000000	-0.725489000000
H	-24.694515000000	6.848989000000	1.829227000000
H	-26.433481000000	7.187315000000	1.838258000000
H	-25.808629000000	5.739223000000	2.651300000000
C	-29.384551000000	4.108984000000	0.358724000000
H	-28.923738000000	6.225159000000	0.477801000000
C	-30.822537000000	4.028811000000	0.342106000000
C	-31.694531000000	5.179368000000	0.396711000000
N	-31.374321000000	2.817428000000	0.270787000000
C	-33.132757000000	4.989220000000	0.371540000000
N	-31.324942000000	6.459977000000	0.470990000000
C	-32.710981000000	2.653038000000	0.248577000000
C	-33.679198000000	3.658262000000	0.293178000000
N	-33.812222000000	6.139736000000	0.427895000000
S	-32.703673000000	7.351536000000	0.506159000000
H	-33.029069000000	1.614685000000	0.189029000000
C	-35.098489000000	3.380445000000	0.263262000000
C	-36.167209000000	4.272422000000	0.298962000000
S	-35.685137000000	1.700427000000	0.167552000000
C	-37.419841000000	3.634753000000	0.250822000000
H	-36.010632000000	5.340835000000	0.357523000000
C	-37.324441000000	2.249085000000	0.178280000000
C	-38.882512000000	4.078508000000	0.257481000000
C	-38.639026000000	1.685968000000	0.133448000000
C	-39.573416000000	2.717385000000	0.177460000000
C	-39.215025000000	4.956252000000	-0.969967000000
C	-39.242920000000	4.824264000000	1.561802000000
S	-39.372850000000	0.124710000000	0.038359000000
C	-40.896164000000	2.252775000000	0.135053000000

H	-40.282380000000	5.198170000000	-0.988006000000
H	-38.655258000000	5.895924000000	-0.929857000000
H	-38.961895000000	4.443743000000	-1.902059000000
H	-38.677067000000	5.758236000000	1.634791000000
H	-40.309098000000	5.071482000000	1.578004000000
H	-39.016756000000	4.214266000000	2.440589000000
C	-40.991187000000	0.862246000000	0.058162000000
H	-41.765318000000	2.898745000000	0.157635000000
C	-42.203139000000	0.071602000000	-0.001001000000
C	-43.473270000000	0.655303000000	0.023502000000
C	-42.228921000000	-1.361974000000	-0.091465000000
H	-43.560946000000	1.735153000000	0.092366000000
N	-44.653942000000	0.008705000000	-0.031245000000
C	-43.491078000000	-2.070798000000	-0.150326000000
N	-41.167966000000	-2.173635000000	-0.131200000000
C	-44.723320000000	-1.320266000000	-0.117705000000
N	-43.354846000000	-3.396923000000	-0.233425000000
S	-41.742582000000	-3.710702000000	-0.235537000000
C	-46.032094000000	-1.920517000000	-0.175418000000
C	-46.409369000000	-3.258175000000	-0.267370000000
S	-47.439191000000	-0.842411000000	-0.129730000000
C	-47.804207000000	-3.420538000000	-0.301290000000
H	-45.680324000000	-4.056602000000	-0.306228000000
C	-48.492335000000	-2.209466000000	-0.235396000000
C	-48.772764000000	-4.597970000000	-0.394786000000
C	-49.898877000000	-2.470453000000	-0.277137000000
C	-50.102437000000	-3.846958000000	-0.369070000000
C	-48.633215000000	-5.548332000000	0.815790000000
C	-48.587452000000	-5.381475000000	-1.713879000000
S	-51.375414000000	-1.572911000000	-0.244186000000
C	-51.463168000000	-4.194161000000	-0.413992000000
H	-47.646085000000	-6.020895000000	0.817657000000
H	-48.759421000000	-5.008826000000	1.758385000000
H	-49.388019000000	-6.339253000000	0.766855000000
H	-47.597537000000	-5.847291000000	-1.744369000000
H	-49.337943000000	-6.173973000000	-1.794806000000
H	-48.685818000000	-4.723149000000	-2.581302000000
C	-52.297452000000	-3.081996000000	-0.356442000000
H	-51.855106000000	-5.200114000000	-0.484988000000
C	-53.739868000000	-2.988829000000	-0.373848000000
C	-54.609579000000	-4.144797000000	-0.460948000000
N	-54.276445000000	-1.775210000000	-0.305018000000
C	-56.042732000000	-3.939125000000	-0.469712000000
N	-54.251120000000	-5.428997000000	-0.537242000000
C	-55.629146000000	-1.606890000000	-0.315124000000
C	-56.555803000000	-2.617930000000	-0.393443000000
N	-56.744690000000	-5.078276000000	-0.553071000000
S	-55.644313000000	-6.299421000000	-0.614183000000
H	-55.959422000000	-0.573279000000	-0.254569000000
H	-57.621495000000	-2.425089000000	-0.397402000000

Oligomer 2 in vacuum

Atom	X	Y	Z
C	-0.569466642024	-59.398983875201	-0.102798912355
C	-1.245397605741	-58.310174014385	0.368368338328
C	-0.425352751795	-57.152701278859	0.393318059574
C	0.848925873039	-57.397629764816	-0.059808123151
S	1.075200084471	-59.037692591476	-0.524573735526
H	-0.940057528754	-60.405860054531	-0.230524859278
H	-2.282191223760	-58.348460304579	0.679859466695
C	1.612636967649	-56.174755278596	-0.001691856878
C	0.803036775245	-55.172285138290	0.490042477452
S	3.200208581428	-55.641227520972	-0.364345824231
C	1.468422377480	-53.935629202836	0.581915649115
C	2.778840129240	-54.018647067240	0.156597301245
H	1.038063384323	-53.009506943544	0.937978220534
C	-0.593125258976	-55.694953614136	0.796090942772
C	-0.931950158643	-55.558614502672	2.288552377041
H	-0.974474469996	-54.504521954658	2.577263932606

H	-1.906423112501	-56.006318352928	2.504362862911
H	-0.181283325466	-56.054237485702	2.907940859004
C	-1.658490010124	-54.993252996137	-0.060323620439
H	-2.644838780250	-55.431723230485	0.117073560693
H	-1.712735839701	-53.930047999427	0.190525485542
H	-1.428452743265	-55.083730134430	-1.124128868901
C	3.801633296645	-52.999088013779	0.085693338429
C	3.589744262746	-51.628769444333	0.481149697679
C	4.675737400401	-50.690745388499	0.371223703419
C	5.950976715147	-51.115321310409	-0.125339857468
C	7.100941218957	-50.231213528863	-0.267862521882
C	8.353228849082	-50.577834937008	-0.736938588095
S	7.037085884510	-48.526749877809	0.160148815172
C	9.250646449223	-49.494984321638	-0.754296244401
H	8.606303754981	-51.581200975580	-1.055122004030
C	8.677814804729	-48.328602250254	-0.298326788518
C	9.659226711914	-47.276378879106	-0.348743649603
C	10.841950058000	-47.795080825804	-0.837581936103
S	9.759810201928	-45.605290746464	0.020597972157
C	11.862042126882	-46.830804663966	-0.921006136800
C	11.438153444426	-45.588296572357	-0.492648756535
H	12.869997601685	-47.003383745951	-1.273040536191
C	10.703840736684	-49.278062018885	-1.150274204142
C	12.156139347812	-44.336122093299	-0.413898462459
C	13.536060340507	-44.182411092535	-0.802448002567
C	12.109532892090	-42.072920984287	0.142899390622
C	14.158342552604	-42.890023918723	-0.684471869192
C	13.414041677273	-41.771358166399	-0.186863689378
H	11.460041802692	-41.294867489202	0.529512951877
N	2.473061245707	-51.088715987770	0.956460095287
N	4.345118838033	-49.466324104666	0.768259227544
N	14.350510116341	-45.117969610164	-1.277790609392
N	15.428424781967	-42.888759666713	-1.075703581510
N	11.510785328921	-43.282628188549	0.037521505435
S	2.788178207558	-49.518412058098	1.237103706260
S	15.785849840515	-44.403583137700	-1.549027380430
C	10.930510395133	-49.563703934835	-2.642790938283
H	10.753809719014	-50.620411855180	-2.863526596126
H	10.258961484126	-48.966158273809	-3.263061992809
H	11.960440309539	-49.328535608731	-2.925842884500
C	11.654962618136	-50.126725844490	-0.292537183623
H	11.490059026369	-51.192605697911	-0.474983427795
H	12.696618262821	-49.900675834559	-0.537554035915
H	11.502552412559	-49.932631652274	0.771358264485
C	6.000267492686	-52.451209239049	-0.462452332329
H	6.921489994808	-52.873547857474	-0.849315284922
N	4.987741406027	-53.345195502195	-0.364533471140
C	13.967326252523	-40.431618152413	-0.036171118632
C	13.304654959735	-39.315263875180	0.436353594331
S	15.630721123893	-40.046556930734	-0.457421010915
C	14.115733540903	-38.166625888262	0.461507411760
H	12.269166205645	-39.334186099196	0.751643061571
C	15.392583015055	-38.413133179653	0.008055494022
C	13.944847638971	-36.709167460123	0.864068034751
C	16.152176511618	-37.191460681892	0.066709427752
C	15.341313123224	-36.187505383169	0.558051861931
C	13.605603295782	-36.572008722314	2.356289789988
C	12.880032932564	-36.008068509742	0.006597992604
S	17.740201434119	-36.656270205159	-0.295218893689
C	16.005567746939	-34.951518257427	0.649587402142
H	13.563444764948	-35.517754864745	2.644294093597
H	12.630812716317	-37.019017487920	2.572040007929
H	14.355689494721	-37.067608508427	2.976392112051
H	11.893443047050	-36.445902853742	0.184145098742
H	12.826117103206	-34.944671481787	0.256507779204
H	13.110170624163	-36.099551669023	-1.057095010710
C	17.316931234805	-35.034251562226	0.224809399925
H	15.574730556057	-34.025363639605	1.004922439311
C	18.338327279356	-34.013716477789	0.154391547931
C	18.124847909872	-32.643559494755	0.549221081724

N	19.525268564641	-34.359088656143	-0.295014980680
C	19.210132530091	-31.704653451542	0.439514872864
N	17.007467468449	-32.104234580200	1.023707137280
C	20.536844680957	-33.464533875567	-0.392618337595
C	20.486019644601	-32.128261263155	-0.056130079550
N	18.878241329166	-30.480353308898	0.835902632398
S	17.321127668527	-30.533514819342	1.303923434950
H	21.458806515980	-33.886139853105	-0.778509805990
C	21.635049039413	-31.243277429283	-0.198448328521
C	22.887589252146	-31.588664231642	-0.668068161411
S	21.570057999580	-29.539101709880	0.230691139387
C	23.784170994017	-30.505236900887	-0.684792759971
H	23.141285485779	-32.591590295091	-0.987138041078
C	23.210551313817	-29.339536954935	-0.227861434477
C	25.237111657259	-30.286927424705	-1.080946877558
C	24.191125216093	-28.286569115595	-0.277807617726
C	25.374135110391	-28.804057532415	-0.767265155175
C	25.463662961804	-30.571361121037	-2.573712275580
C	26.189076130875	-31.135442561628	-0.223997875169
S	24.290527042549	-26.615640906902	0.092632001948
C	26.393477413019	-27.838951482991	-0.850275220058
H	25.287742686033	-31.628055385474	-2.795132031004
H	24.791510758025	-29.973916445870	-3.193425822834
H	26.493345334524	-30.335192288312	-2.856826463704
H	26.024961096445	-32.201321770023	-0.407151232087
H	27.230498990680	-30.908409653779	-0.469088546076
H	26.036751323097	-30.942206726403	0.840065424124
C	25.968714755904	-26.597064033273	-0.420994502241
H	27.401485269891	-28.010508948512	-1.202656165150
C	26.685774850389	-25.344367477487	-0.341627416402
C	28.065476562848	-25.189371059628	-0.730376403511
N	26.039703966753	-24.291667477192	0.110589094767
C	28.686740850977	-23.896548437354	-0.611869091487
N	28.880582181583	-26.124040227879	-1.206360693980
C	26.637504689372	-23.081542483533	0.216546140581
C	27.941655259119	-22.778728359746	-0.113519646490
N	29.956746267625	-23.894073994386	-1.003351532221
S	30.315292798296	-25.408359590855	-1.477504744504
H	25.987546938625	-22.304279778784	0.603959461495
C	28.493867361729	-21.438600957414	0.037565524503
C	27.830010125203	-20.322663962253	0.509430478281
S	30.157419445257	-21.052460307788	-0.382080174126
C	28.640342410126	-19.173522439198	0.535452181663
H	26.794177054062	-20.342213164469	0.823549985957
C	29.917802138280	-19.419231804679	0.083275877177
C	28.468143017413	-17.716147979485	0.937774166736
C	30.676554054323	-18.197074562855	0.142587869816
C	29.864576600748	-17.193613229812	0.633083605501
C	28.127367653119	-17.579116510742	2.429660297518
C	27.403719738079	-17.015759932071	0.079235638667
S	32.264589671716	-17.660911222072	-0.217835717019
C	30.527961627050	-15.957188049169	0.725170087154
H	28.084289460389	-16.524872136208	2.717560330369
H	27.152640294878	-18.026703889268	2.644491624079
H	28.877153912900	-18.074221029876	3.050520611762
H	26.417227829439	-17.454187258733	0.255860630102
H	27.348909452719	-15.952381991118	0.329030161345
H	27.634935484226	-17.107161637471	-0.984230625701
C	31.839775902210	-16.039125077546	0.301645864919
H	30.096194856599	-15.031275992013	1.080009957615
C	32.860613603978	-15.017963438801	0.232043228887
C	32.645963544501	-13.647878662808	0.626462739609
N	34.048170540134	-15.362709782617	-0.216205878618
C	33.730749444815	-12.708311692220	0.517446298542
N	31.527866562103	-13.109168890240	1.099961920956
C	35.059295574933	-14.467571039725	-0.313069870974
C	35.007303202657	-13.131218346450	0.022922892383
N	33.397778724456	-11.484148079324	0.913353717934
S	31.840331309570	-11.538207969199	1.380159426602
H	35.981921760726	-14.888749158772	-0.697834597443

C	36.155858456871	-12.245534144360	-0.118833825160
C	37.408493938622	-12.589946776224	-0.588908470692
S	36.090184954241	-10.541782817937	0.311884982590
C	38.304639110283	-11.506152575902	-0.604616406458
H	37.662533905027	-13.592419847603	-0.909125407087
C	37.730594837321	-10.341118951957	-0.146515028980
C	39.757426474800	-11.286883914510	-1.000774271905
C	38.710725379877	-9.287686250241	-0.195665545089
C	39.893873721837	-9.804252206050	-0.685757123801
C	39.983872652302	-11.569856912931	-2.493832370526
C	40.709864031928	-12.135790568052	-0.144740261982
S	38.809528937453	-7.617039768535	0.176252079981
C	40.912819385095	-8.838670135706	-0.768056087601
H	39.808341729642	-12.626418574737	-2.716194226658
H	39.311388494729	-10.972113510282	-3.112897312644
H	41.013418309560	-11.333017035407	-2.776883299440
H	40.546159448350	-13.201568978686	-0.328845379749
H	41.751157915888	-11.908104774862	-0.389773208351
H	40.557612793362	-11.943589844686	0.919520964617
C	40.487625313991	-7.597333259769	-0.337629052966
H	41.920837394781	-9.009511640859	-1.120751626043
C	41.204244568608	-6.344431827894	-0.257354523911
C	42.583830759676	-6.188673760647	-0.646206114668
N	40.557892421050	-5.292304847866	0.195779976415
C	43.204674090362	-4.895735204770	-0.526809357288
N	43.399176830702	-7.122699525551	-1.123047081358
C	41.155299517865	-4.082048868938	0.302563011505
C	42.459296032752	-3.778541509712	-0.027482947156
N	44.474612434790	-4.892529969621	-0.918504800595
S	44.833599315386	-6.406323008181	-1.393874971099
H	40.505135221167	-3.305295338988	0.690651450039
C	43.011121607460	-2.438359400636	0.124502531445
C	42.347095683289	-1.322994015799	0.597490274364
S	44.674402721606	-2.051368481046	-0.295450483626
C	43.157071492084	-0.173608185145	0.624076187721
H	41.311390162560	-1.343120046384	0.911998477975
C	44.434428417652	-0.418578445637	0.171211943281
C	42.984606310654	1.283423816370	1.027553731338
C	45.192839926870	0.803756025578	0.231134476484
C	44.380769676636	1.806605618966	0.722698073255
C	42.644381084740	1.419257293780	2.519675019897
C	41.919640212133	1.984138363287	0.169955382801
S	46.780576594057	1.340637911188	-0.129532726089
C	45.043845452418	3.043167227174	0.815435046839
H	42.601127034463	2.473277100610	2.808370531335
H	41.669861906747	0.971242816283	2.734564129693
H	43.394551324125	0.923903777121	3.139872657140
H	40.933343492211	1.545298457351	0.346648222654
H	41.864627169173	3.047316129477	0.420554945557
H	42.150460642209	1.893589026691	-0.893669745115
C	46.355499174435	2.961914188738	0.391307260047
H	44.611965117289	3.968698475347	1.171131486992
C	47.376066104852	3.983391342639	0.322010036241
C	47.161286709068	5.353133508149	0.717505097034
N	48.563486272890	3.639236093706	-0.127033934976
C	48.245857134259	6.292990871163	0.608794896044
N	46.043245092814	5.891279208221	1.191784521560
C	49.574384440910	4.534653038055	-0.223692787380
C	49.522315777235	5.870707579862	0.113481200715
N	47.912780002912	7.516803381527	1.005701626328
S	46.355509650598	7.462099953136	1.473004773539
H	50.496858690320	4.114002631319	-0.609392724074
C	50.670697588851	6.756662688229	-0.027915115887
C	51.923657702408	6.412437725762	-0.497262346212
S	50.604333417725	8.460576263717	0.402076374991
C	52.819441861342	7.496520688252	-0.513149766671
H	52.178209014308	5.409865353205	-0.816764486318
C	52.244832395965	8.661590435504	-0.055848410328
C	54.272340328033	7.716064065195	-0.908741615712
C	53.224680103264	9.715306218538	-0.105008168603

C	54.408181518596	9.198878275801	-0.594339479277
C	54.499561108904	7.432482836402	-2.401565355213
C	55.224652387911	6.867849970137	-0.051883781137
S	53.322853859095	11.386163032612	0.266207721422
C	55.426900115415	10.164733496904	-0.676640670675
H	54.324473422319	6.375762725235	-2.623529558676
H	53.827166671216	8.029730713476	-3.021205870473
H	55.529158136737	7.669532713588	-2.684254032072
H	55.061375688055	5.801933206991	-0.235577194540
H	56.265986950819	7.095760872534	-0.296535501867
H	55.071845740264	7.060491006890	1.012218254509
C	55.001156655349	11.406117883961	-0.246966765327
H	56.435122798403	9.994035451980	-1.028818399684
C	55.717410990234	12.659291808083	-0.166934348275
C	57.097087509309	12.815264934844	-0.555309621800
N	55.070592146537	13.711408117071	0.285498246523
C	57.717522267605	14.108430603547	-0.436188919645
N	57.912880156797	11.881268939032	-1.031466040323
C	55.667601772859	14.921895749829	0.392034108275
C	56.971654142091	15.225640436508	0.062399556343
N	58.987612274826	14.111827760694	-0.827400421087
S	59.347204616585	12.597960153204	-1.302018597653
H	55.017055098090	15.698620477201	0.779529069897
C	57.523062378255	16.566013049580	0.214080187972
C	56.858570396004	17.681346473765	0.686482421448
S	59.186363090868	16.953417009371	-0.205492544080
C	57.668167792526	18.830998469244	0.712911129313
H	55.822778974532	17.661018977019	1.000704824498
C	58.945736027903	18.586284866153	0.260516474826
C	57.495164797754	20.288118237674	1.115837144625
C	59.703781211754	19.808906386698	0.320251691952
C	58.891258205679	20.811602683070	0.811212436906
C	57.154472574746	20.424380563532	2.607812027125
C	56.430253265120	20.988248876663	0.257695674161
S	61.291476366677	20.346263884365	-0.040092330280
C	59.553904913032	22.048488664970	0.903755680645
H	57.110884523183	21.478489456188	2.896129505437
H	56.180001304923	19.976199188046	2.822586095327
H	57.904597482485	19.929434307046	3.228390118162
H	55.444012003841	20.549228705511	0.434270451257
H	56.374911084419	22.051504552432	0.507890078229
H	56.661401085329	20.897377145637	-0.805831207014
C	60.865648915973	21.967530232728	0.480081482605
H	59.121614872314	22.973995846340	1.259009428150
C	61.885950301751	22.989472523275	0.410783031380
C	61.670422267731	24.359195799216	0.805791165416
N	63.073574854123	22.645673013590	-0.037719559439
C	62.754613581773	25.299475284089	0.697109246906
N	60.551975845855	24.896989666236	1.279581775154
C	64.084217319505	23.541562541031	-0.134324209152
C	64.031428917353	24.877638325185	0.202325340718
N	62.420840734211	26.523269556448	1.093559729234
S	60.863527454798	26.468025543967	1.560399911787
H	65.007023375146	23.121161047411	-0.519480436139
C	65.179534232930	25.764224496668	0.060964217879
C	66.432472810168	25.420669539620	-0.408498234413
S	65.112517423418	27.467968426343	0.491351581050
C	67.327922341255	26.505358967856	-0.424079655377
H	66.687468056524	24.418315237269	-0.728364206740
C	66.752799856841	27.669708507329	0.033498110570
C	68.780742602529	26.725744831050	-0.819669911053
C	67.732571852755	28.724436872987	-0.015406457003
C	68.915719845916	28.208532326551	-0.504778913751
C	69.008011996715	26.442599387870	-2.312568288922
C	69.733448385183	25.877629564051	0.036846658736
S	67.829706118098	30.394994416345	0.356312003596
C	69.934123979240	29.175823746247	-0.586625086226
H	68.833465360977	25.385838743502	-2.534858297203
H	68.335274921901	27.039703208505	-2.931981065610
H	70.037468318287	26.680283713975	-2.595257576911

H	69.570724551659	24.811667326418	-0.147184531297
H	70.774673532309	26.106156423294	-0.207720465937
H	69.580548796636	26.069873049434	1.101010394401
C	69.507285812798	30.415596793628	-0.156716737644
H	70.942603550619	29.006384873859	-0.938757301690
C	70.223286882083	31.672819944821	-0.075499614857
C	71.608178812693	31.817909238219	-0.468204860182
N	69.570293896707	32.717734316081	0.377342681056
C	72.229797318937	33.109219926860	-0.349669801927
N	72.420889342301	30.881088060495	-0.944365901826
C	70.177930885503	33.935636605489	0.482547885453
C	71.470716439131	34.201658375502	0.147350017107
N	73.502332172456	33.118654564329	-0.740302474607
S	73.855788745542	31.601856613231	-1.214110787040
H	69.539962992187	34.724650394421	0.869224905687
H	71.908202237035	35.186178765046	0.248977386033

Oligomer 2 in solvent

Atom	X	Y	Z
C	-58.946250551995	-0.708406842536	-1.399067769438
C	-58.480436615358	-1.943175967567	-1.749648809172
C	-57.064540309819	-1.961298775764	-1.853018595394
C	-56.497822805818	-0.739519035547	-1.577830541232
S	-57.673457252709	0.455494281835	-1.187954764226
H	-59.971690114610	-0.402372084348	-1.248690949726
H	-59.130259191705	-2.792324706454	-1.922930402666
C	-55.064863310791	-0.848567398366	-1.704914026544
C	-54.749133139240	-2.143051378484	-2.060012262770
S	-53.685128590356	0.157282988097	-1.539922529828
C	-53.362917330626	-2.343169529144	-2.206671379165
C	-52.641490153868	-1.193292937587	-1.959266006563
H	-52.886419268992	-3.275003468083	-2.479017262478
C	-56.002254190653	-2.996273401040	-2.193063553986
C	-56.173122181080	-3.529826325842	-3.624095615546
H	-55.358517959548	-4.214432387589	-3.876044083449
H	-57.115496083811	-4.076631897885	-3.717916140278
H	-56.174363380267	-2.713777177204	-4.350347541042
C	-56.004735430086	-4.157571337247	-1.186713469336
H	-56.944956533914	-4.712772173675	-1.246563496095
H	-55.187856294513	-4.851735756500	-1.402609283519
H	-55.884882550247	-3.792080553640	-0.164244011096
C	-51.214232842391	-0.959110884898	-1.995557758277
C	-50.249347776636	-1.979762728193	-2.320275314197
C	-48.852537515889	-1.643061391790	-2.345158122042
C	-48.430110018458	-0.308532503750	-2.043836165007
C	-47.040689037176	0.131192565081	-2.068476448716
C	-46.594615181785	1.435216473262	-2.129254830697
S	-45.696627283443	-0.996794481600	-1.959658666701
C	-45.190345470420	1.533949440562	-2.068103469996
H	-47.264374411440	2.280099140482	-2.230308570115
C	-44.577344188915	0.305160134964	-1.968434382584
C	-43.150663403784	0.497450280408	-1.936398475359
C	-42.883032497517	1.849347220358	-2.009773823626
S	-41.732464842896	-0.461920444081	-1.824377399255
C	-41.504736558498	2.132375456055	-1.974455653451
C	-40.740359384342	0.987445775395	-1.875330409730
H	-41.062890509270	3.118432196524	-2.017878797576
C	-44.167411150140	2.659481193318	-2.106645290988
C	-39.303856750701	0.826242274135	-1.812748019707
C	-38.378815368053	1.931453186439	-1.831779034438
C	-37.489959544111	-0.632099723247	-1.666464619149
C	-36.967459580664	1.665994224969	-1.781328366809
C	-36.492617704577	0.317174575760	-1.708514378981
H	-37.224902228298	-1.679629788158	-1.567317675326
N	-50.489025379404	-3.253329056533	-2.615463355744
N	-48.075243136101	-2.675704187921	-2.659376502976
N	-38.668728111017	3.227174345374	-1.893025868003
N	-36.229914517936	2.772680765500	-1.805779068560
N	-38.824108920338	-0.396478067397	-1.728353302423

S	-49.051724183638	-3.955087987817	-2.897452886426
S	-37.257685631415	4.031335710409	-1.884407014332
C	-44.328155252288	3.610752772788	-0.910486619714
H	-45.290726718111	4.127297840349	-0.959839622963
H	-44.277515179775	3.065994211559	0.035038366770
H	-43.538155342283	4.366733980174	-0.915723758201
C	-44.242614253841	3.443430868741	-3.426291015037
H	-45.204344465524	3.956817016644	-3.511342923093
H	-43.452016574840	4.197681896806	-3.467112878871
H	-44.129496705845	2.778815815443	-4.285837584889
C	-49.457742913052	0.550570996795	-1.722843061733
H	-49.229155886873	1.572557290788	-1.438816575656
N	-50.780373473246	0.250515415563	-1.711281719778
C	-35.082135509050	-0.048536576628	-1.683476539732
C	-34.552151585274	-1.290174675288	-1.967354891993
S	-33.826187457219	1.087108257541	-1.211352993762
C	-33.155186834876	-1.339797116058	-1.789220753576
H	-35.156955231652	-2.121625298148	-2.307243885895
C	-32.631541543782	-0.134939241171	-1.376829257387
C	-32.063598955842	-2.385725036522	-1.961700181996
C	-31.203597412927	-0.267287932609	-1.247649885676
C	-30.845711086228	-1.559190560788	-1.575492490426
C	-31.975966454649	-2.873862965489	-3.416315950929
C	-32.264835493646	-3.576290153663	-1.010932233090
S	-29.863167729662	0.708122233490	-0.804881038716
C	-29.459638157068	-1.781244572570	-1.471924164843
H	-31.137982496114	-3.566129399953	-3.535779890020
H	-32.891979066872	-3.400192544502	-3.698613629194
H	-31.832897455617	-2.037596514525	-4.104440431881
H	-33.184997576304	-4.112083693169	-1.259741935094
H	-31.431032188249	-4.278350522722	-1.097542567985
H	-32.329335369891	-3.244417865711	0.027836143405
C	-28.780193441958	-0.650747097120	-1.065430604500
H	-28.953848865116	-2.714078762754	-1.680389460070
C	-27.366392592547	-0.440101677938	-0.841410033781
C	-26.371581021957	-1.468112308336	-1.015360532554
N	-26.975605905964	0.756291876420	-0.456141036768
C	-24.988193731472	-1.151465472600	-0.789090577012
N	-26.570105476600	-2.731976334645	-1.375894451215
C	-25.668523699708	1.037257926755	-0.230582415466
C	-24.609360732990	0.170266929723	-0.389186155670
N	-24.179728934780	-2.189249498930	-0.985799261464
S	-25.113664699742	-3.449165799034	-1.418306442241
H	-25.483049804145	2.049952172564	0.111775904236
C	-23.231937554622	0.590251028031	-0.165107232923
C	-22.774459527396	1.889504683318	-0.083652711420
S	-21.926691588720	-0.560214979391	0.089582001496
C	-21.396853675743	1.965692457369	0.200021318466
H	-23.414821837545	2.748443260098	-0.240271906004
C	-20.812756617150	0.725055998659	0.325121301683
C	-20.375841029494	3.078228505270	0.384438340431
C	-19.407193196941	0.896652943874	0.587261036125
C	-19.125431002842	2.247062761439	0.630485192613
C	-20.714980211641	3.961022538591	1.595772844149
C	-20.243505685836	3.937874504551	-0.882453379299
S	-18.026220741324	-0.084864008867	0.860763613808
C	-17.767588648562	2.510554440209	0.889787419663
H	-21.656370931386	4.491903603937	1.429684004398
H	-20.812605515718	3.362155729006	2.504161578609
H	-19.930499311864	4.705651200827	1.756222183170
H	-21.178390171107	4.468472156610	-1.083120601374
H	-19.452480234601	4.682203834417	-0.756792652317
H	-20.002643260866	3.322658314035	-1.752403085209
C	-17.031658433277	1.352583995799	1.039467449450
H	-17.320331715862	3.492067415348	0.966990676556
C	-15.621575606274	1.172099584686	1.308997177377
C	-14.696883615008	2.266778693880	1.464416686512
N	-15.165265954173	-0.058263975939	1.410558299892
C	-13.316047677645	1.984434313092	1.744261358203
N	-14.961584836331	3.566593304644	1.380131923629

C	-13.856295694040	-0.310843245949	1.660029227317
C	-12.869341617468	0.629021282492	1.861117354977
N	-12.575637895111	3.083030366474	1.863611690476
S	-13.564496644225	4.354340776135	1.635135757531
H	-13.602071464958	-1.365343980974	1.687922774758
C	-11.496014623174	0.249335129800	2.167268709111
C	-11.066560253687	-0.978964208718	2.625901253314
S	-10.143933226010	1.346394498782	1.924480896045
C	-9.665847968072	-1.049878424671	2.763081245717
H	-11.747653163294	-1.785507375772	2.867117521829
C	-9.040357141166	0.125977832264	2.414015291946
C	-8.659533469604	-2.093589771742	3.225462950531
C	-7.621984224982	-0.024811685295	2.608682950085
C	-7.370117444493	-1.299444249210	3.073861985173
C	-8.670780405887	-3.332362506361	2.316138995013
C	-8.903572433973	-2.502028914788	4.686720705071
S	-6.198364199027	0.913317943158	2.416834506701
C	-5.999017084271	-1.538557470058	3.285055107208
H	-7.890638073041	-4.035512437690	2.620461476623
H	-9.633751585112	-3.846149688127	2.382592477974
H	-8.498547516511	-3.056803653157	1.273181601251
H	-9.870524170991	-3.002835874975	4.786743899769
H	-8.127518763640	-3.194871484616	5.023420304947
H	-8.896925004663	-1.630710954475	5.345585530348
C	-5.225116891302	-0.438117758838	2.976647731343
H	-5.568962236406	-2.462824731209	3.646025816452
C	-3.792079678025	-0.252188009521	3.049824808603
C	-2.877242443171	-1.278373943292	3.482032182856
N	-3.304994944713	0.918279463552	2.696063119670
C	-1.470809136310	-0.987686492135	3.535237545472
N	-3.172915345710	-2.518698809257	3.857258104989
C	-1.974137217047	1.174238975084	2.736136496379
C	-0.989783766379	0.306527954679	3.156059058580
N	-0.742798296134	-2.020754122919	3.950049280032
S	-1.772566042432	-3.246246587870	4.241130093305
H	-1.699773337191	2.164896101608	2.389013027741
C	0.412815897122	0.699576394171	3.199686386012
C	0.903690282458	1.988440669331	3.162594034520
S	1.718388969045	-0.477111894522	3.248688680827
C	2.311535151372	2.035224065856	3.151296725721
H	0.262460287306	2.860942127890	3.158800098432
C	2.883345165149	0.783185795125	3.187630622434
C	3.371376834323	3.126168379810	3.126288661568
C	4.316421863535	0.926037441279	3.193269376094
C	4.628597674874	2.269842404984	3.153531884323
C	3.277293511932	4.031793639217	4.364341086238
C	3.286637081173	3.966228345889	1.842329105650
S	5.704097266561	-0.083450355383	3.222547547803
C	6.016090451351	2.505035789794	3.144597266912
H	2.331681985910	4.581042387005	4.364980895343
H	3.336693990402	3.446990608694	5.285109036171
H	4.091829063600	4.761248275297	4.365871731780
H	2.341244369658	4.514537138399	1.806638756634
H	4.101419826745	4.694704395753	1.808619809015
H	3.352343836638	3.334397435254	0.953620586496
C	6.743425342228	1.332587448924	3.179054917964
H	6.489884881273	3.476608594303	3.114860284489
C	8.175160698290	1.123432304168	3.184583044432
C	9.133958737675	2.198281703561	3.130679040297
N	8.618096823833	-0.115014109971	3.234244928807
C	10.536862860301	1.888752663936	3.153657883013
N	8.883837881572	3.501710885934	3.057518228324
C	9.945444891380	-0.393708793346	3.240779725445
C	10.970906467338	0.526113106294	3.225062208462
N	11.308128681897	2.970991004766	3.096880242551
S	10.319280815284	4.260382313499	3.019554252236
H	10.179526404885	-1.453162664921	3.251240942577
C	12.369852014103	0.121061000312	3.277521058128
C	12.855357155854	-1.106228477206	3.679769884970
S	13.671862316756	1.180485519466	2.754867439888

C	14.255185732732	-1.206629282319	3.552284622438
H	12.217113108942	-1.891184485194	4.066057196567
C	14.824999240713	-0.053940476735	3.059862794130
C	15.311247839481	-2.263476224539	3.841626997928
C	16.251420025400	-0.233467340703	2.985877183850
C	16.563143326106	-1.502883387317	3.428554484195
C	15.103899026439	-3.519390671013	2.980718781100
C	15.342332240330	-2.636111924154	5.332159840048
S	17.629972130195	0.666696009020	2.503435234944
C	17.944876600131	-1.768594667428	3.384105552125
H	15.915375605140	-4.233428769454	3.146108112743
H	14.162560462767	-4.010728799999	3.241970560714
H	15.077906136860	-3.267786095248	1.917994849542
H	14.404146989269	-3.114833002493	5.626096244980
H	16.156955872918	-3.337333339277	5.532885067055
H	15.487998103019	-1.751171291847	5.955859697085
C	18.666602457504	-0.693528636207	2.906246290688
H	18.418620976324	-2.693860561282	3.682313007272
C	20.090791323472	-0.538988179310	2.703032159479
C	21.053443847060	-1.570606873340	2.996137981141
N	20.522342586691	0.607273597570	2.220965534410
C	22.449628917132	-1.310754884096	2.775742023329
N	20.812926745057	-2.789865953526	3.467656242334
C	21.841204742739	0.833680509854	2.003008193290
C	22.872448322146	-0.041616116414	2.264969493084
N	23.225418400711	-2.345138935818	3.088111737641
S	22.248469275592	-3.535420042451	3.612850876032
H	22.062159241443	1.805510003670	1.574224573314
C	24.264930988017	0.321794546753	2.035126569212
C	24.760206877879	1.597453002571	1.858652752147
S	25.540091346599	-0.880404270549	1.894948425148
C	26.143594982152	1.613017587139	1.593233582782
H	24.142060174410	2.483178444059	1.935807584364
C	26.693906194787	0.350881647389	1.576578447737
C	27.198969632717	2.679250959271	1.340777946947
C	28.107604133225	0.462744873400	1.325774808682
C	28.428313720583	1.797253165920	1.180621670806
C	27.336755581778	3.629381914320	2.540665858751
C	26.904095595286	3.475490263329	0.059902725959
S	29.463533623811	-0.574773151991	1.151900370161
C	29.796315762299	2.002025622596	0.921229266892
H	26.414045568446	4.198250412297	2.684785945025
H	27.547494628369	3.076048196578	3.458672228229
H	28.149792579686	4.340943230208	2.372504077057
H	25.977647729036	4.045990221100	0.169316764949
H	27.713630950230	4.181417361181	-0.144892792126
H	26.800188793481	2.811417397071	-0.801233423022
C	30.500534516378	0.816042121807	0.873703199764
H	30.272390054364	2.961465847630	0.772220656333
C	31.908138817972	0.575946612397	0.640021921840
C	32.860710074786	1.626765804003	0.383403443194
N	32.333033584222	-0.669635903489	0.658575791003
C	34.241795144586	1.287182268137	0.178327490100
N	32.622986860447	2.932334734758	0.307634380949
C	33.637026985261	-0.977339249724	0.448528408581
C	34.659536466030	-0.081698164681	0.224392668211
N	35.009449816343	2.349863164852	-0.047150749673
S	34.042927495708	3.657614085815	-0.000611389173
H	33.852211095127	-2.040761996403	0.458213968312
C	36.040039532762	-0.516764843775	0.054423730210
C	36.564934392859	-1.741641907283	0.412098241837
S	37.254259952618	0.495604244755	-0.714655870905
C	37.921585367367	-1.877787592147	0.056451570215
H	35.987593510378	-2.499905614988	0.926274190810
C	38.421123261995	-0.754420133154	-0.563313350007
C	38.992922616444	-2.948078433014	0.205338385633
C	39.812333740393	-0.968737850579	-0.865854704359
C	40.171169328788	-2.230478161405	-0.437184351876
C	38.623708230901	-4.228616873848	-0.559855533952
C	39.264670418545	-3.269650096631	1.683308276946

S	41.107583392311	-0.115025069126	-1.598967549692
C	41.521393296953	-2.529133623843	-0.701005309316
H	39.438061182654	-4.955867338269	-0.500811048791
H	37.729427751504	-4.686369110368	-0.128143144015
H	38.427487832566	-4.015430897233	-1.613119112010
H	38.378565277260	-3.712451135908	2.146510410629
H	40.086301704636	-3.985548141955	1.772786195936
H	39.530662219659	-2.368210728190	2.240050142511
C	42.172411567340	-1.486006140093	-1.327875848414
H	42.021895849106	-3.455515192941	-0.454268784807
C	43.546273413073	-1.369972675861	-1.767024758910
C	44.521339906719	-2.420438810106	-1.616093951145
N	43.916486294249	-0.243297789973	-2.337780953909
C	45.867472300503	-2.198670887031	-2.067873011755
N	44.334933531274	-3.626337115244	-1.089021410244
C	45.186096539024	-0.053165188978	-2.774437243689
C	46.227445923586	-0.948515409498	-2.666098740711
N	46.661183651943	-3.247294319193	-1.868169696676
S	45.757872796459	-4.405207012798	-1.168187729716
H	45.354334175908	0.904869881773	-3.255145145651
C	47.570711628797	-0.622765008383	-3.128327919586
C	48.062172839509	0.638612402512	-3.394002756858
S	48.771060266536	-1.859368795521	-3.475627087934
C	49.380446997924	0.616122235001	-3.891188597649
H	47.489307636022	1.540431202880	-3.217614357902
C	49.885244825759	-0.660500137626	-3.993917508296
C	50.405417523475	1.651798904409	-4.328976277557
C	51.237708453711	-0.588685649803	-4.484538597924
C	51.564879240071	0.735504566786	-4.691275390423
C	50.774721524235	2.601769071254	-3.178756259694
C	49.914633487510	2.452181342546	-5.545572777458
S	52.514750876322	-1.664734227422	-4.879049009441
C	52.875345275355	0.900349190958	-5.180074806997
H	49.907523169171	3.198061681512	-2.881766367978
H	51.125857505765	2.045762791114	-2.306462609651
H	51.566025179078	3.288512579803	-3.491597425379
H	49.033517510219	3.044163317511	-5.282989263733
H	50.693150527727	3.138641219348	-5.889483400596
H	49.650220116748	1.788873656188	-6.372295241942
C	53.527366687895	-0.304632984411	-5.337160388775
H	53.346433253686	1.845307956858	-5.413652241024
C	54.870548718799	-0.588883203705	-5.804695824177
C	55.798100182944	0.442849601612	-6.209122605818
N	55.244468536623	-1.847360036350	-5.856344901158
C	57.107769312854	0.059673059372	-6.657243007300
N	55.597204126511	1.757007454373	-6.224500181341
C	56.495064419985	-2.192447810351	-6.285896159840
C	57.455579200171	-1.316344295852	-6.691465776640
N	57.868663076073	1.097814167063	-7.002012631966
S	56.971557298284	2.435413665531	-6.767228727059
H	56.694965298207	-3.259469906836	-6.287405562314
H	58.432806443093	-1.641837490942	-7.023398647545

Oligomer 3 in vacuum

Atom	X	Y	Z
C	-10.785492477085	104.241744501127	36.270205588576
C	-10.740165361576	103.041536651048	36.918974812228
C	-11.117411111626	101.968849892563	36.069586439653
C	-11.437224918926	102.386246217781	34.800635402559
S	-11.286501625899	104.088657355088	34.614128584073
H	-10.554810849998	105.220321299194	36.665733670442
H	-10.449478904308	102.943049784482	37.957967825208
C	-11.796277287054	101.235633371225	34.003939282825
C	-11.703052408742	100.109161585451	34.787265481395
S	-12.335047792739	100.896834855010	32.412129928025
C	-12.061796464519	98.937407733559	34.091947436787
C	-12.418582342028	99.180593956120	32.782045996650
H	-12.079758353743	97.945790465397	34.527338592852
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N	-11.319296867377	76.000523086783	27.406818894590
N	-8.805894360301	64.397016082858	28.966940882134
N	-7.901384967883	50.905752283779	28.674071021510
N	-6.015453739212	39.788420438439	27.902719994711
N	-0.087516426409	29.410062077554	28.517323546865
N	4.888742594869	21.014449829741	28.167129519741
N	5.769669571114	10.581010452253	23.926077827889
N	5.647633805773	-2.047147697248	19.041111532635

Oligomer 3 in solvent

Atom	X	Y	Z
C	-56.711741840215	-3.828897809193	1.076408161232
C	-55.851833254789	-4.876139642241	1.242436791790
C	-54.495420146889	-4.462920651064	1.161810160279
C	-54.365735319271	-3.113620848797	0.936773989215
S	-55.887974620609	-2.319670633636	0.818565468857
H	-57.792096640140	-3.845401096715	1.088896752843
H	-56.185446193576	-5.892420347080	1.414059555042
C	-52.960977643231	-2.786119345973	0.869565374470
C	-52.225358501100	-3.931496502009	1.052447448573
S	-51.974131800564	-1.401221006247	0.629891843483
C	-50.831896797705	-3.704923849996	1.002466060795
C	-50.516030542199	-2.382584537641	0.781929163983
H	-50.070377415215	-4.462929662405	1.119731635386
C	-53.133547234911	-5.135193723139	1.260197523264
C	-52.941902881740	-6.183674419558	0.153182622409
H	-51.932860318351	-6.603167538961	0.194425001414
H	-53.654546102593	-7.003907628883	0.276709081258
H	-53.091619575482	-5.743346049009	-0.835320952344
C	-52.916698351404	-5.772335925347	2.641625601025
H	-53.625476749370	-6.589702300311	2.801184769074
H	-51.905603518248	-6.181743015605	2.718842280817
H	-53.052586717881	-5.037993594434	3.438948722554
C	-49.201404664823	-1.767946173782	0.673225281523
C	-49.017706606844	-0.410223445376	0.520144466791
C	-47.979907743778	-2.520531499049	0.715498119851
H	-49.885360029898	0.242915645558	0.483289891115
C	-46.721944087736	-1.835147235728	0.598041579194
C	-46.692396306499	-0.405957301411	0.437950740930
C	-45.466797383509	0.365566060819	0.309242680008
C	-45.415838766915	1.737580162867	0.159385399467
S	-43.857544524315	-0.340956014380	0.323684252103
C	-44.101331221000	2.222158870935	0.056682586418
H	-46.319226565678	2.332424382570	0.129820451453
C	-43.161433362201	1.214282619078	0.129053519612
C	-41.850188154185	1.796466167831	0.015415727146
C	-41.974567698139	3.158895632714	-0.126905940791
S	-40.212467866458	1.279473989225	0.007196103128
C	-40.730358057421	3.814452521667	-0.247515573936
C	-39.664239438520	2.942601128833	-0.196561620256
H	-40.593611816898	4.879680405906	-0.368127462834
C	-43.436817771959	3.580290028808	-0.115535970642
C	-38.242302123382	3.238481767176	-0.291472202045
C	-37.725897772543	4.572116643676	-0.424919773874
C	-36.305366593383	4.782478952280	-0.515565880987
C	-35.416184381242	3.649856935656	-0.470927400053
N	-47.834916466935	-3.836831852449	0.855336356157
N	-45.669644737441	-2.643558718082	0.652206747489
N	-38.417475783575	5.708166610844	-0.479754126441
N	-35.966850593053	6.061997155339	-0.635739718852

S	-46.239331058797	-4.152632772086	0.837517542400
S	-37.344427115503	6.920261134706	-0.632915308263
C	-43.745517237175	4.513924846461	1.065427510782
H	-44.813945951134	4.743694316156	1.100115189184
H	-43.460644306671	4.055149466015	2.015020775397
H	-43.199909638618	5.455643894147	0.959895829251
C	-43.842444070732	4.244007643012	-1.440877313406
H	-44.911599325439	4.473165432520	-1.440709340707
H	-43.295371268677	5.180299602194	-1.581296925349
H	-43.630238489313	3.590070828745	-2.289811762942
C	-37.273025832341	2.259816410902	-0.263163466829
H	-37.565839309193	1.218206495833	-0.166914449142
C	-33.974304619474	3.759356539501	-0.557393994481
C	-33.171735268296	4.873922527992	-0.689159142865
S	-33.037008702345	2.275727176901	-0.493214562979
C	-31.804830463334	4.539326705974	-0.739230351714
H	-33.578035002892	5.874336973759	-0.745257033424
C	-31.586494969050	3.180127944131	-0.645313727677
C	-30.494746551854	5.300814248104	-0.873521603196
C	-30.170398801560	2.932776173092	-0.707165053900
C	-29.513291939547	4.139057128040	-0.839233335989
C	-30.276014357000	6.261363423457	0.306086984174
C	-30.420274250143	6.064922517019	-2.204975605425
S	-29.105009699998	1.588174462470	-0.665663389738
C	-28.114859802782	3.989705943606	-0.909686024053
H	-29.296610311637	6.741511003393	0.230052843429
H	-31.038254297854	7.045270977665	0.305193334054
H	-30.327292006919	5.731871034886	1.260191992039
H	-31.185933827637	6.844738819306	-2.239866710682
H	-29.443816526747	6.544364494882	-2.315552597984
H	-30.573030738615	5.393846670333	-3.053284937013
C	-27.729616089883	2.667224004665	-0.829785755733
H	-27.399378013566	4.793730366165	-1.014055690618
C	-26.407843008670	2.075906818298	-0.865064145389
C	-25.195791740069	2.844344115488	-0.988298191813
C	-25.119799539317	0.133145143283	-0.805463334226
C	-23.933334813730	2.159611415329	-1.034492105010
N	-25.081042535339	4.166320471051	-1.070134466795
C	-23.886971441853	0.730703319567	-0.953460365503
H	-25.181310084875	-0.944106570059	-0.692818042117
N	-22.898349414709	2.987314176205	-1.149826328972
S	-23.496473202877	4.499176351918	-1.192767513107
C	-22.658295385536	-0.049427446224	-1.023151392396
C	-22.560932927817	-1.404144193044	-1.267213995073
S	-21.074527045973	0.661789052532	-0.744760771867
C	-21.234186184162	-1.873835401152	-1.212585594851
H	-23.420213959380	-2.023144405599	-1.493027376142
C	-20.329795226772	-0.873415230023	-0.934181576619
C	-20.535642417468	-3.211546161011	-1.405114401169
C	-19.003472097858	-1.434398621980	-0.923360196245
C	-19.090998530148	-2.785579616766	-1.189352444766
C	-20.755805399192	-3.764246041330	-2.822010701610
C	-20.984883689815	-4.239658884094	-0.354907931488
S	-17.390419719473	-0.903858272546	-0.673844272646
C	-17.834703628029	-3.420597728804	-1.195323311555
H	-21.812779209970	-3.993917079616	-2.982795070369
H	-20.440804395544	-3.042728721842	-3.579337511885
H	-20.184168348459	-4.685411208342	-2.964645428637
H	-22.045479666658	-4.474754925683	-0.479798907054
H	-20.417604286691	-5.168103360429	-0.463384764243
H	-20.833172500077	-3.859592913360	0.657953155956
C	-16.804951873654	-2.540062187633	-0.933698702731
H	-17.661061963432	-4.471474380330	-1.381519440310
C	-15.377613979039	-2.767801834924	-0.853651967890
C	-14.766317154099	-4.058737596800	-1.047391344969
C	-13.335975105603	-4.185901295252	-0.958174937766
N	-15.383099313908	-5.204871200283	-1.315458103341
C	-13.257012829606	-1.869407313524	-0.504178285977
C	-12.533504817766	-3.028966407260	-0.675155660517
N	-12.916765899077	-5.432177405579	-1.164814565791

S	-14.233958273617	-6.344593982206	-1.443099852517
H	-12.737268275385	-0.944284703320	-0.271344265531
C	-11.081859955472	-3.076097531464	-0.580787246140
C	-10.256498802933	-4.178889490990	-0.555728009840
S	-10.149990929914	-1.583024145950	-0.477108115525
C	-8.891925244960	-3.834235671531	-0.446990024827
H	-10.644178718248	-5.185906288038	-0.616613472830
C	-8.685109627395	-2.475704594213	-0.393453778557
C	-7.573760556391	-4.590944874822	-0.376928842328
C	-7.271232204132	-2.222434117803	-0.288556800325
C	-6.602605206284	-3.423919189279	-0.276575367803
C	-7.330776075804	-5.418054297547	-1.649060421431
C	-7.505190811887	-5.490943068487	0.866784963735
S	-6.209535982142	-0.876735091224	-0.177932095230
C	-5.202575580627	-3.273146501277	-0.177975793098
H	-6.346661690590	-5.893331594765	-1.612784165611
H	-8.083931877584	-6.205347173570	-1.741905653275
H	-7.377240310104	-4.789770039322	-2.541524345963
H	-8.261656550374	-6.278413760811	0.809431706351
H	-6.524086876237	-5.968298155655	0.938865917445
H	-7.675905883607	-4.914866796141	1.779126097816
C	-4.813606373434	-1.952749462783	-0.117463234316
H	-4.486739006646	-4.082450405229	-0.150965277928
C	-3.468192216162	-1.406579810995	-0.021890132271
C	-3.202898622333	-0.054358408937	-0.064082761603
C	-2.299219488304	-2.226640918372	0.122506657822
H	-4.026173370129	0.645582564060	-0.178468525058
C	-1.005819288633	-1.605583490402	0.207928669398
N	-2.235607876744	-3.554705054548	0.194169853521
C	-0.889294478531	-0.172819017076	0.151105529158
N	-0.008277224229	-2.472353771823	0.339550443918
S	-0.667345477209	-3.956193390258	0.353973254396
C	0.376762446439	0.536376338297	0.229627921998
C	0.510716568395	1.910321160774	0.178016125321
S	1.936487427389	-0.256511301574	0.397310458348
C	1.848457710644	2.327359163150	0.271191982405
H	-0.352252365922	2.554955526364	0.075072944194
C	2.723689785965	1.267119343914	0.392521463145
C	2.592091938152	3.655012947071	0.270769519464
C	4.064891271556	1.782660882781	0.477423245046
C	4.022820976745	3.155937082213	0.410434724844
C	2.182137597225	4.532353402229	1.463975559870
C	2.386529251259	4.416336828030	-1.048116393534
S	5.665383473957	1.179533446770	0.635649435415
C	5.301762769887	3.749209457165	0.484351051680
H	1.130589651900	4.820466786442	1.381515345926
H	2.320972184152	4.001692749590	2.408682152387
H	2.782778218559	5.445691145462	1.489815339267
H	1.336946336376	4.699702973400	-1.164677125359
H	2.987198666122	5.329974831906	-1.059173580079
H	2.675174996556	3.803678559804	-1.905260225137
C	6.310982992618	2.818754383074	0.602300704651
H	5.501585647385	4.810938421444	0.454032242398
C	7.747248247584	3.041276940833	0.684631699370
C	8.327519178177	4.340421606936	0.877608586629
C	8.667464321615	2.021626606627	0.582170981583
C	9.757582971622	4.479503892824	0.951343974552
N	7.690263377048	5.501530430996	1.009278759280
H	8.322630074408	1.004325173403	0.420028672704
C	10.591692307507	3.310176096417	0.831014008737
N	10.157830907106	5.733362417345	1.134114040037
S	8.822000759948	6.653017033999	1.205994056743
C	12.037520815248	3.349964321968	0.888867735391
C	12.894936811208	4.417838879230	1.059736971712
S	12.904956321898	1.832029971614	0.714342675097
C	14.245622886518	4.021278548495	1.049974397200
H	12.536857918568	5.430690737961	1.182867928960
C	14.398843482403	2.661165669034	0.872815217126
C	15.594169545484	4.713560702026	1.182230301413
C	15.804475129278	2.352234136032	0.873002605095

C	16.520037877549	3.513653158409	1.048601410933
C	15.749752383945	5.395043842314	2.550781067567
C	15.821210865429	5.728832761846	0.051079910335
S	16.815775298488	0.972785801187	0.713229563576
C	17.915678758379	3.303197099384	1.058861047472
H	16.753468296578	5.816247857277	2.654586355158
H	15.028323096440	6.210067465984	2.655200437532
H	15.587967228818	4.684929135673	3.364961129144
H	15.097137323582	6.545147213851	0.121128950753
H	16.824093451923	6.159008592384	0.120148573972
H	15.715112251068	5.256979407041	-0.928410128339
C	18.252704020776	1.977472193985	0.891855456982
H	18.664141391219	4.073273321766	1.180474882587
C	19.578071661091	1.377279354394	0.853756454213
C	19.782018245772	0.015311214161	0.790011634552
C	20.787530464431	2.149305032802	0.878185841566
H	18.924057597923	-0.651363214445	0.777269048921
C	22.056386846656	1.476359006812	0.830942591164
N	20.911764502843	3.473566523523	0.940958893112
C	22.107794295848	0.040840504568	0.758266041696
N	23.096543329194	2.301712962789	0.859722352837
S	22.503016363717	3.810471001803	0.940211186206
C	23.345755563209	-0.719853296733	0.702772760631
C	23.415634976420	-2.097982784915	0.640657481340
S	24.944155548872	0.008659568280	0.703784481763
C	24.737762486720	-2.569606491880	0.593836379940
H	22.520567509713	-2.705774367047	0.631240502662
C	25.663495610700	-1.546166112811	0.620307565873
C	25.420256248992	-3.927403866144	0.521184099435
C	26.985193234449	-2.112661974677	0.569029833442
C	26.876753350572	-3.487272666992	0.511068881559
C	25.048099520126	-4.678825190988	-0.766682129103
C	25.097408080467	-4.787385302195	1.753298350061
S	28.611887732401	-1.565866187873	0.557896394231
C	28.129488886557	-4.127905043847	0.455853605337
H	23.981709143336	-4.920333407779	-0.772368942337
H	25.270339520460	-4.077961484806	-1.651481911463
H	25.607801061735	-5.615543893250	-0.836054716089
H	24.030666879488	-5.025558991740	1.782599888400
H	25.653319623963	-5.728291125727	1.717862161520
H	25.359808645200	-4.266576549443	2.676997040181
C	29.174622227108	-3.227232464281	0.472939667785
H	28.289474287825	-5.196041495861	0.404889421184
C	30.604682069468	-3.452621910220	0.429404643284
C	31.203191041565	-4.761414913980	0.359941899519
C	32.635944403013	-4.883312912959	0.312674571961
N	30.571750203875	-5.930422154223	0.328876056798
C	32.741085906316	-2.525747539226	0.413557718739
C	33.453034908201	-3.702570803949	0.337497123986
N	33.041875851531	-6.149241378331	0.245793753885
S	31.711101505473	-7.083612149028	0.245699151727
H	33.273002219647	-1.579311858623	0.450275729257
C	34.907216526681	-3.742224847389	0.285237105512
C	35.740780454656	-4.837680078495	0.348763158401
S	35.829250443586	-2.248991281139	0.124804474455
C	37.105734955250	-4.485474154210	0.276569221005
H	35.358401857444	-5.844126027869	0.442406458749
C	37.303433085596	-3.129647780614	0.155768713997
C	38.430592333943	-5.233141254707	0.296210421113
C	38.716221501065	-2.864469566159	0.085509825076
C	39.394807103045	-4.063472839692	0.164551816361
C	38.548135100459	-6.200501107472	-0.892156633645
C	38.633578407393	-5.986364937744	1.620266563924
S	39.759638898687	-1.510619081569	-0.065029827121
C	40.791968142906	-3.900506583147	0.104144658279
H	39.533300205429	-6.674731283452	-0.901946686768
H	37.793732767334	-6.988468982116	-0.817822279136
H	38.407925545959	-5.677511397194	-1.840918937100
H	37.883417182054	-6.774346329232	1.729757679850
H	39.621707032405	-6.453915106854	1.645185013535

H	38.550660071296	-5.310326498366	2.474340384599
C	41.156178160023	-2.575488322340	-0.021333180982
H	41.521825471961	-4.697285221963	0.147404882717
C	42.468462674536	-1.971600541017	-0.115866401569
C	43.694904264539	-2.727974314434	-0.098159200572
C	43.726594523228	-0.018895400931	-0.320973876973
C	44.949425952295	-2.031863458950	-0.180344477689
N	43.829804126247	-4.047410043126	-0.009305750047
C	44.973194910309	-0.603953882429	-0.284912352667
H	43.645577206403	1.056292498843	-0.442129249289
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