

**Theoretical Design New Macrocycles for Nucleophilic Fluorination with  
KF: Thiourea-Crown-ether is Predicted to Overcome the [2.2.2]-Cryptand**

Ellen V. Dalessandro and Josefredo R. Pliego Jr.\*

Departamento de Ciências Naturais, Universidade Federal de São João del-Rei  
36301-160, São João del-Rei, MG, Brazil.

## Supporting Information

Table S1 – Electronic energies and thermodynamic data from the steps of fluorination reactions studied with the promoters 18-crown-6 and [2,2,2]-cryptand and potassium fluoride salt.<sup>a</sup>

CATALYST	PROCESS	M06-2X <sup>b</sup>	$\Delta G_n^c$	$\Delta\Delta G_{\text{solv}}(\text{tol})^d$	$\Delta G_{\text{sol}}(\text{tol})^e$
18-crown-6	KF(g) + cat → KF-cat	-41.43	11.34	-4.88	-34.97
	KF-cat + EtOMs → TS	0.33	9.22	7.83	17.38
	KF-cat + EtOMs → TSsyn	4.09	7.80	8.36	20.25
	KF-cat + EtOMs → TSanti	8.66	8.40	5.21	22.27
	KF-cat + EtOMs → KOMs-cat + EtF	-36.88	0.97	6.29	-29.62
	KF-cat + EtOMs → KOMs-cat + C <sub>2</sub> H <sub>2</sub> +HF	-17.89	-10.51	5.52	-22.88
	KOMs(g) + cat → KOMs-cat	-47.85	13.56	4.19	-30.10
	2 KF-cat → (KF-cat) <sub>2</sub>	-39.96	11.37	15.59	-13.00
[2.2.2]-cryptand	KF(g) + cat → KF-cat	-45.65	11.37	-5.74	-40.02
	KF-cat + EtOMs → TS	-0.13	10.51	7.42	17.80
	KF-cat + EtOMs → TSsyn	9.65	9.63	6.68	25.96
	KF-cat + EtOMs → TSanti	8.95	9.25	6.08	24.28
	KF-cat + EtOMs → KOMs-cat + EtF	-37.77	2.64	6.15	-28.98
	KF-cat + EtOMs → KOMs-cat + C <sub>2</sub> H <sub>2</sub> +HF	-18.78	-8.84	5.38	-22.24
	KOMs(g) + cat → KOMs-cat	-52.96	15.26	3.19	-34.51
	2 KF-cat → (KF-cat) <sub>2</sub>	-37.77	13.63	15.83	-8.31

<sup>a</sup> Units in kcal mol<sup>-1</sup>, 1 mol L<sup>-1</sup> standard state, 298.15K. <sup>b</sup> Calculations at the M06-2X/ma-def2-TZVPP level. <sup>c</sup> Nuclear contribution from harmonic frequencies calculations. <sup>d</sup> Solvent effect calculated with the SMD model. <sup>e</sup> Free energy in solution.

Table S1 (continuation) – Electronic energies and thermodynamic data from the steps of fluorination reactions studied with the catoters PEG, PEGmet and PEGphen, and cesium fluoride salt.<sup>a</sup>

CATALYST	PROCESS	M06-2X <sup>b</sup>	$\Delta G_g^c$	$\Delta\Delta G_{\text{solv}}(\text{tol})^d$	$\Delta\Delta G_{\text{solv}}(\text{acet})^e$	$\Delta G_{\text{sol}}(\text{tol})^f$	$\Delta G_{\text{sol}}(\text{acet})^g$
PEG	CsF(g) + cat → CsF-cat	-50.94	13.31	-0.89	-4.25	-38.52	-41.88
	CsF-cat + EtOMs → TS	10.82	9.26	4.86	7.80	24.32	27.88
	CsF-cat + EtOMs → TSsyn	20.39	5.36	5.25	9.59	32.08	35.34
	CsF-cat + EtOMs → TSanti	19.39	7.42	5.40	6.88	30.50	33.69
	CsF-cat + EtOMs → CsOMs-cat + EtF	-19.79	0.68	2.93	5.71	-16.18	-13.40
	CsF-cat + EtOMs → CsOMs-cat + C <sub>2</sub> H <sub>2</sub> +HF	-0.80	-10.80	2.16	2.85	-9.44	-8.75
	2 CsF-cat → (CsF-cat) <sub>2</sub>	-25.12	14.40	5.56	11.81	-5.16	1.09
PEGmet	CsF(g) + cat → CsF-cat	-44.35	9.73	-0.75	-4.06	-35.37	-38.68
	CsF-cat + EtOMs → TS	9.55	10.95	3.69	6.78	24.19	27.28
	CsF-cat + EtOMs → TSsyn	21.51	7.52	4.79	8.56	33.82	37.59
	CsF-cat + EtOMs → TSanti	17.45	8.49	3.79	6.78	29.73	32.72
	CsF-cat + EtOMs → CsOMs-cat + EtF	-20.79	0.70	2.68	4.95	-17.41	-15.14
	CsF-cat + EtOMs → CsOMs-cat + C <sub>2</sub> H <sub>2</sub> +HF	-1.80	-10.78	1.91	2.09	-10.67	-10.49
	2 CsF-cat → (CsF-cat) <sub>2</sub>	-25.38	13.09	21.38	10.77	-7.37	-1.52
PEGphen	CsF(g) + cat → CsF-cat	-46.21	9.75	5.85	-4.73	-37.35	-41.19
	CsF-cat + EtOMs → TS	10.28	9.37	5.50	10.57	25.14	30.21
	CsF-cat + EtOMs → TSsyn	21.75	7.56	5.69	10.40	35.00	39.71
	CsF-cat + EtOMs → TSanti	17.79	9.80	5.65	10.35	33.24	37.94
	CsF-cat + EtOMs → CsOMs-cat + EtF	-18.24	3.41	3.26	6.24	-11.57	-8.59
	CsF-cat + EtOMs → CsOMs-cat + C <sub>2</sub> H <sub>2</sub> +HF	0.75	-8.07	2.49	3.38	-4.83	-3.94
	2 CsF-cat → (CsF-cat) <sub>2</sub>	-30.88	16.77	8.99	17.11	-5.12	3.00

<sup>a</sup> Units in kcal mol<sup>-1</sup>, 1 mol L<sup>-1</sup> standard state, 298.15K. <sup>b</sup> Calculations at the M06-2X/ma-def2-TZVPP level. <sup>c</sup> Nuclear contribution from harmonic frequencies calculations. <sup>d</sup> Toluene solvent effect calculated with the SMD model. <sup>e</sup> Acetonitrile solvent effect calculated with the SMD model. <sup>f,g</sup> Free energy in solution (toluene e acetonitrile).

Table S1 (continuation) – Electronic energies and thermodynamic data from the steps of fluorination reactions studied with the catoters PEG, PEGmet and PEGphen, and potassium fluoride salt.<sup>a</sup>

CATALYST	PROCESS	M06-2X <sup>b</sup>	$\Delta G_g^c$	$\Delta\Delta G_{solv}(tol)^d$	$\Delta\Delta G_{solv}(acet)^e$	$\Delta G_{sol}(tol)^f$	$\Delta G_{sol}(acet)^g$
PEG	KF(g) + cat → KF-cat	-57.50	12.57	-2.01	-5.43	-46.94	-50.36
	KF-cat + EtOMs → TS	7.50	11.96	4.86	8.86	24.32	28.32
	KF-cat + EtOMs → TSsyn	17.26	9.57	5.25	9.16	32.08	35.99
	KF-cat + EtOMs → TSanti	15.82	9.28	5.40	9.46	30.50	34.56
	KF-cat + EtOMs → KOMs-cat + EtF	-22.04	2.53	3.09	5.65	-16.42	-13.86
	KF-cat + EtOMs → KOMs-cat + C <sub>2</sub> H <sub>2</sub> +HF	-3.05	-8.95	2.32	2.79	-9.68	-9.21
	KOMs(g) + cat → KOMs-cat	-49.07	16.35	3.86	7.08	-28.86	-25.64
	2 KF-cat → (KF-cat) <sub>2</sub>	-33.05	14.34	8.10	15.62	-10.61	-3.09
PEGmet	KF(g) + cat → KF-cat	-51.97	10.45	-2.33	-6.23	-43.85	-47.75
	KF-cat + EtOMs → TS	8.24	11.1	5.12	9.16	24.46	28.50
	KF-cat + EtOMs → TSsyn	20.32	6.62	5.62	9.61	32.56	36.55
	KF-cat + EtOMs → TSanti	15.92	8.30	5.00	8.95	29.22	33.17
	KF-cat + EtOMs → KOMs-cat + EtF	-22.16	2.14	3.29	5.94	-16.73	-14.08
	KF-cat + EtOMs → KOMs-cat + C <sub>2</sub> H <sub>2</sub> +HF	-3.17	-9.34	2.52	3.08	-9.99	-9.43
	KOMs(g) + cat → KOMs-cat	-43.67	13.84	3.74	6.57	-26.09	-23.26
	2 KF-cat → (KF-cat) <sub>2</sub>	-29.69	14.38	9.17	18.00	-6.14	2.69
PEGphen	KF(g) + cat → KF-cat	-54.19	11.76	-2.00	-6.23	-44.43	-48.66
	KF-cat + EtOMs → TS	9.41	9.68	5.92	11.16	25.01	30.25
	KF-cat + EtOMs → TSsyn	18.40	7.73	6.46	11.96	32.59	38.09
	KF-cat + EtOMs → TSanti	14.59	8.60	5.85	10.69	29.04	33.88
	KF-cat + EtOMs → KOMs-cat + EtF	-15.57	-0.68	3.78	7.38	-12.47	-8.87
	KF-cat + EtOMs → KOMs-cat + C <sub>2</sub> H <sub>2</sub> +HF	3.42	-12.16	3.01	4.52	-5.73	-4.22
	KOMs(g) + cat → KOMs-cat	-39.29	12.33	4.56	8.01	-22.40	-18.95
	2 KF-cat → (KF-cat) <sub>2</sub>	-28.12	13.43	11.16	22.07	-3.53	7.38

<sup>a</sup> Units in kcal mol<sup>-1</sup>, 1 mol L<sup>-1</sup> standard state, 298.15K. <sup>b</sup> Calculations at the M06-2X/ma-def2-TZVPP level. <sup>c</sup> Nuclear contribution from harmonic frequencies calculations. <sup>d</sup> Toluene solvent effect calculated with the SMD model. <sup>e</sup> Acetonitrile solvent effect calculated with the SMD model. <sup>f,g</sup> Free energy in solution (toluene e acetonitrile).

Table S1 (continuation) – Electronic energies and thermodynamic data from the steps of fluorination reactions studied with the catoters TCE and TCEbut, and potassium fluoride salt.<sup>a</sup>

CATALYST	PROCESS	M06-2X <sup>b</sup>	$\Delta G_g^c$	$\Delta\Delta G_{\text{solv}}(\text{tol})^d$	$\Delta G_{\text{sol}}(\text{tol})^e$
TCE	KF(g) + cat → KF-cat	-72.31	14.43	2.95	-54.93
	KF-cat + EtOMs → TS	12.41	10.57	3.23	26.21
	KF-cat + EtOMs → TSsyn	21.21	8.92	3.76	33.89
	KF-cat + EtOMs → TSanti	19.12	6.27	3.47	28.86
	KF-cat + EtOMs → KOMs-cat + EtF	-24.44	-0.14	1.84	-22.74
	KF-cat + EtOMs → KOMs-cat + C <sub>2</sub> H <sub>2</sub> + HF	-5.45	-11.62	1.07	-16.00
	KOMs(g) + cat → KOMs-cat	-66.29	15.54	7.57	-43.18
	2 KF-cat → (KF-cat) <sub>2</sub>	-30.62	17.43	8.29	-4.90
TCEbut	KF(g) + cat → KF-cat	-74.21	17.37	3.91	-52.93
	KF-cat + EtOMs → TS	12.54	9.17	2.82	24.54
	KF-cat + EtOMs → TSanti	21.77	4.25	2.43	28.45
	KF-cat + EtOMs → KOMs-cat + EtF	-23.78	0.17	1.09	-22.52
	KF-cat + EtOMs → KOMs-cat + C <sub>2</sub> H <sub>2</sub> + HF	-4.79	-11.31	0.32	-15.78
	KOMs(g) + cat → KOMs-cat	-67.53	18.79	7.78	-40.96
	2 KF-cat → (KF-cat) <sub>2</sub>	-5.03	13.16	6.55	14.68

<sup>a</sup> Units in kcal mol<sup>-1</sup>, 1 mol L<sup>-1</sup> standard state, 298.15K. <sup>b</sup> Calculations at the M06-2X/ma-def2-TZVPP level. <sup>c</sup> Nuclear contribution from harmonic frequencies calculations. <sup>d</sup> Solvent effect calculated with the SMD model. <sup>e</sup> Free energy in solution.

## Coordinates of the optimized structures obtained at PBE/ma-def2-SVP level of theory

### C2H5OMs

O	0.15655742880324	-0.13756911913876	1.22268928277232
S	-1.21591839803663	-1.08795177491060	1.21659226241529
O	-0.98715040445893	-2.27507695439453	2.06817896615301
O	-1.67792858219800	-1.26817347566971	-0.17679172303905
C	-2.27284072298576	0.08721923003659	2.06772440856033
H	-1.83929780288689	0.29135460194216	3.06235199208443
H	-3.25710124252414	-0.40783411774644	2.15797919826333
H	-2.34304808590411	1.00163979219688	1.45332979284407
C	1.33239378381551	-0.73370848089702	0.60566760796324
C	2.46808573896419	0.26011740104082	0.74337821417442
H	1.10581021429657	-0.95201012113144	-0.45983911999030
H	1.56194351959061	-1.69046983346339	1.12196591313708
H	2.22922033716670	1.21452669654485	0.23470300474118
H	3.38383032064807	-0.15805901950777	0.28022783415703
H	2.68572389570957	0.47377517509836	1.80788236576363

### KF

F	-4.03790550122702	0.70353095616225	-0.29250484027565
K	-1.81186449877298	0.68750904383775	-0.47872515972435

### CsF

F	-4.10384851194105	0.70987818977961	-0.32680025769467
Cs	-1.62596148805895	0.65275181022039	-0.26771974230533

### C2H5F

F	0.14174435200525	-0.21292123328063	1.18684952173446
C	1.30327554436429	-0.70499755712419	0.56568078863047
C	2.45980452411323	0.24981203446645	0.77372987013957
H	1.06550398935224	-0.83768899101545	-0.51233427842652
H	1.50943862366831	-1.70593326857985	1.00321290244750
H	2.23838274608040	1.24590490222269	0.34165049539105
H	3.36828015742119	-0.14643044700334	0.27589743396961
H	2.68472006299508	0.37622456031433	1.85102326611386

### KOMs

O	0.18191245358366	0.32544337208520	1.41137374339820
S	-0.94134163661995	-0.69230632942493	1.31852788057918
O	-0.60064469890922	-1.95395696849603	2.09104116737106
O	-1.27116252882669	-1.00907175293321	-0.12880940670352
C	-2.40619925150558	0.03621283051075	2.07185594999285
H	-2.16105390988284	0.27974911076467	3.12110588639390
H	-3.22109419325500	-0.70828105910042	2.01632878338331
H	-2.66061152759231	0.94777494278112	1.50208671781921
K	1.40941529300794	-1.83499414618715	0.12107927776581

### CsOMs

O	0.20593796275367	0.21625261873394	1.91080060397803
S	-0.90270062767918	-0.78834258144598	1.65336541398667
O	-0.82630268706634	-1.96172782783729	2.61290128752488
O	-0.90930382718751	-1.25077611799009	0.20791239949107
C	-2.47011641519273	0.05235770399389	1.95925426879411
H	-2.47867465478864	0.37847641000319	3.01487208243476
H	-3.28518050133541	-0.66681307707657	1.75995331485203
H	-2.52962616787942	0.91900575911896	1.27675900101411
Cs	1.89262691837556	-2.27721288750004	1.13369162792433

### HF

H	0.000000	0.000000	0.032592
F	0.000000	0.000000	0.967408

### C2H4

C	-4.93157254171767	1.20388667810796	0.00000001322303
C	-3.59047745834284	1.20388667885153	0.00000001378480
H	-5.51142308638433	0.73415612586844	-0.81184557203880
H	-5.51142320851884	1.67361719561840	0.81184555828506
H	-3.01062691419078	0.73415612988081	-0.81184557543532
H	-3.01062679084554	1.67361719167286	0.81184556218122
18C6 (KOMs)			
O	-2.79368349498596	-0.41028917321035	-2.78837547231577
C	-4.11947559499481	-0.55774553061324	-2.31809561619178
C	-4.18888613966731	-1.73066043070494	-1.36174538583631
O	-3.41265836418309	-1.45561161404891	-0.20630462643131
O	-1.21927874660154	-1.98841305642615	1.53399050195626
C	-0.32815765126999	-1.75412690861991	2.61875818334026
C	1.06704767580955	-1.49465921585336	2.09148103954508
O	1.08726069611041	-0.23683439395722	1.42911788547777
C	2.37319027545701	0.08434137689714	0.89918939985127
C	2.28120409738488	1.36847496070719	0.10059103824521
O	1.43941648989563	1.15401037734826	-1.01792047634889
C	1.51256041896067	2.13794307109538	-2.03405035739158
C	0.86323510161217	1.59254353888322	-3.29016157006842
O	-0.52826611730720	1.38276516630796	-3.04984785704230
C	-1.18801471289386	0.75915988588625	-4.14341304671739
C	-2.65205936089002	0.57987121243508	-3.80075005786512
H	-5.25713342161997	-1.90810011828922	-1.08497690164445
H	-3.81398034711877	-2.65197749218873	-1.86995573798080
H	-0.67509538139117	-0.87783518245452	3.21896605196227
H	-0.30464440989579	-2.64449859966932	3.29388009863755
H	1.37519576783319	-2.30358133469893	1.38841092812488
H	1.77313803396176	-1.49247751748135	2.95828910716881
H	3.31022228680832	1.64363545936702	-0.23360922109089
H	1.89166314341991	2.20345597148888	0.73440987932613
H	1.34919887251503	0.62993414024196	-3.56991392946154
H	1.00533418083718	2.32756300541290	-4.12015439412237
H	-1.11862494163574	1.39707463726986	-5.05878260278132
H	-0.71603317187878	-0.22617590681341	-4.36761652948604
H	-3.20966643642840	0.27281195438993	-4.71887610498126
H	-3.07913704823875	1.55061586560516	-3.45081066239071
H	-4.82214230182205	-0.75347460890982	-3.16508231996426
H	-4.46288180611669	0.37493192888941	-1.80696552915227
H	1.01315494249538	3.08294803452779	-1.70631543119379
H	2.57724807487181	2.37580006507405	-2.26890605653278
H	3.10885096884283	0.22626044744509	1.72864335271655
H	2.72575154973062	-0.74012750141364	0.23802739404861
C	-2.56695345677999	-2.14896429715562	1.93126795196384
C	-3.40636275267724	-2.52409530961524	0.72780816434040
H	-2.95699246425563	-1.20832367864696	2.39130987370675
H	-2.66351763110331	-2.96129699597636	2.69378422361522
H	-4.44520004969893	-2.75217258404762	1.07048029292560
H	-2.99622586623770	-3.44954489817630	0.25614507859812
K	-0.56248182719466	-0.76904617600191	-0.99748139957009
O	0.80341910164625	-1.75429381798675	-3.24695451317251
H	1.31974280588380	-4.58082912620526	-3.04806228361830
C	2.24920611032378	-3.99261154355393	-3.15818638681710
H	2.51568389540877	-3.87021904583642	-4.22370131419452
S	1.97265329165581	-2.33781488145153	-2.46427302816188
O	1.57567681998053	-2.56340344944065	-1.01111737067291
H	3.08097346015402	-4.45874836136106	-2.59932097906813
O	3.26050543528803	-1.58994834846391	-2.63868328328379

TS-E2-anti (18C6-KF)

O	-2.61234034693518	-0.88339315037715	-2.38386586864322
C	-3.97753165794888	-1.12983167260317	-2.09646034256842
C	-4.09539807154152	-2.00936767862208	-0.86939307900927
O	-3.63820179719562	-1.28488651131647	0.26871733568831
O	-1.78899927124331	-1.15359784972361	2.44920919352753
C	-1.08300234203904	-0.51058907163023	3.49738971125301
C	0.40410406099345	-0.67695883519049	3.26097227438311
O	0.77785480454880	0.05408742529527	2.10177247198776
C	2.13617707804406	-0.15115731073921	1.72032286043041
C	2.47305537510006	0.77679217315506	0.57292205232838
O	1.73259329340264	0.41167446420506	-0.57970872920545
C	1.83682210885231	1.37131674477622	-1.63079764393369
C	1.13353979628915	0.88269308357970	-2.87499691851887
O	-0.26454373932461	0.72886440171004	-2.60817903933385
C	-0.95998603916921	0.22587367014270	-3.75283107918342
C	-2.42695164980177	0.07135430760988	-3.42719747492516
H	-5.16630611179184	-2.29913891555332	-0.74196014657741
H	-3.49553967115361	-2.94045204620620	-0.99565634338571
H	-1.35049676626844	0.57298191993575	3.54748236645415
H	-1.34374624935460	-0.96890627488608	4.48238598981292
H	0.64165700036339	-1.75790446085174	3.12799485998653
H	0.95815327476277	-0.30008105220363	4.15570617486307
H	3.57062844969585	0.72098915555705	0.36963441196919
H	2.23731757608352	1.82957835561901	0.86438648658955
H	1.55309331762056	-0.07636212720318	-3.26449159211682
H	1.28585287861711	1.65048984274249	-3.67321998731987
H	-0.87561086746353	0.95112472207262	-4.59922351669236
H	-0.48706657357424	-0.72565980143558	-4.09703330105463
H	-2.95787600015006	-0.25891474146945	-4.35234279506294
H	-2.86866239418329	1.04959164333258	-3.11445033478159
H	-4.47451224639023	-1.64048902432120	-2.95741303661630
H	-4.51700971919517	-0.16752877110818	-1.92018912643836
H	1.40554240978118	2.34267612232622	-1.28519093915297
H	2.90908197092341	1.54934005327976	-1.88434201428165
H	2.81884356132649	0.07941721756084	2.57371857097464
H	2.29218667320848	-1.21602204166166	1.42755755788395
C	-3.19561434695580	-1.19168530255801	2.61966909295249
C	-3.80650894895447	-1.99296123528864	1.48842850269178
H	-3.62065166358610	-0.15847485119693	2.63330099851028
H	-3.46012344361884	-1.67851111646098	3.59047390545633
H	-4.89201586491354	-2.15182293007235	1.70120938353102
H	-3.31102370846018	-2.98966613209829	1.42632829364599
K	-0.76411040320892	-0.88617225943766	-0.23142984593979
O	-1.28061140508121	-3.80843466682366	-0.02124056377172
H	-0.53159813867831	-6.53614113104547	0.61662403315369
H	-0.09292092477158	-3.30321985540308	-2.39291943592598
H	1.15636234132182	-4.72642118958804	-4.03308807465848
S	0.11908836791956	-4.26499926525261	0.28127574995338
C	0.03918598428971	-5.80335989673860	1.21430065080468
H	-0.47331955025664	-5.57622727379701	2.16701500565726
O	0.86402417912147	-4.73656221326406	-1.02391672531677
C	0.98510977102849	-3.50865817961675	-2.26330600869343
C	1.67282682013662	-3.94969074677992	-3.43982329252214
F	1.35202595667814	-1.66110281963861	-4.60548684768766
H	1.54977949786440	-2.82651131987858	-4.08799138288938
O	0.92610277301478	-3.26785115779806	1.05711697484774
H	1.07327360265297	-6.14868989793210	1.39073071183158



H	1.50773185864554	-2.72914555191092	-1.67866924985901
H	2.75388513092298	-4.14619497321728	-3.31999088510247
TS-E2-syn (18C6-KF)			
O	-2.59664755996869	-0.61096405639796	-2.77163035550431
C	-3.90968063161557	-0.91053235828877	-2.32983026356611
C	-3.86296480248899	-2.03594816264022	-1.31798549878078
O	-3.21246223947443	-1.58333925146184	-0.13974780997972
O	-1.02342482574875	-1.87644489390366	1.70062467833569
C	-0.18819428878970	-1.53338158318586	2.78738432408058
C	1.23053095770844	-1.35884828125782	2.28850949879295
O	1.27783406904774	-0.22871157983597	1.42897509836740
C	2.57908744545534	0.09744597508901	0.97938916706193
C	2.49872741337155	1.30702485510834	0.07101798642812
O	1.79025608751049	0.96338429812993	-1.10407696907064
C	1.65483847526691	2.04024694958474	-2.01992162979399
C	0.94856472246790	1.56448662262464	-3.27115518387903
O	-0.41422086875160	1.28200717993361	-2.97629858442585
C	-1.10285322319971	0.72385182574975	-4.09081526425860
C	-2.54192512310460	0.45052418117320	-3.71085032744707
H	-4.91131085681323	-2.35113664628565	-1.09114677674380
H	-3.32394098057491	-2.91626597646020	-1.74182898721100
H	-0.53742424170473	-0.58783247602174	3.27131163721649
H	-0.20070339917576	-2.33738369399216	3.56515851572666
H	1.55681997813683	-2.27806127530708	1.74492179753761
H	1.90726927868554	-1.21426988790254	3.16584428952513
H	3.53590740333180	1.64399233856170	-0.17592831264719
H	1.98986445557588	2.14548864351370	0.60602386235484
H	1.44726657181330	0.64729914723453	-3.66079814423505
H	1.01932718130325	2.36853807249276	-4.04564875855300
H	-1.09440820206073	1.43922696904099	-4.95004496519503
H	-0.60074938701369	-0.21903059460144	-4.41057031519518
H	-3.11268502537181	0.18395936634812	-4.63459475402555
H	-3.00685111169385	1.37121466062509	-3.28134471350952
H	-4.54979393142419	-1.22625495535796	-3.19035955465332
H	-4.38027575534764	-0.00647568991178	-1.87276099771838
H	1.08705462067227	2.87936222873361	-1.54893817292661
H	2.66115630238304	2.43226080629354	-2.30753571462705
H	3.25003353409555	0.33497274928347	1.84184617095415
H	3.03376446656224	-0.76121087696348	0.42763065192370
C	-2.38283338193964	-2.05336145945715	2.06140608233794
C	-3.15783668383341	-2.58180229331892	0.87405142463444
H	-2.82043244478517	-1.08804906949724	2.41624026262783
H	-2.47138617459470	-2.79226396480128	2.89528466080870
H	-4.18988354021711	-2.84747691994277	1.21112600039719
H	-2.66201672699317	-3.49827813472779	0.48176199510068
K	-0.31806354636674	-1.12123994869979	-1.10852730687615
H	3.80762401265269	-1.64334370030779	-2.62725183789631
F	0.99951079969997	-1.61965854882516	-3.46144664155326
H	3.51804549130049	-3.10449098062785	-3.73119155107523
C	3.26853106946039	-2.59426228351682	-2.78391624408256
H	2.04635344748082	-2.08644496761386	-3.11372193730049
C	3.11838317541793	-3.41935840270006	-1.64194111902754
H	0.30083617740800	-3.77223553911731	-3.62726562904126
H	1.43936607806498	-5.18283361263397	-3.41825110645453
C	0.44620981007970	-4.76793579306646	-3.16688106714102
H	3.43871245329092	-3.05299511453113	-0.65409471107142
H	3.16848044989597	-4.51834502985127	-1.72393665582281
O	1.31726455534979	-3.39333959417787	-1.01608798592474

H	-0.34745414624001	-5.48322824206195	-3.45071023829063
S	0.33233834437532	-4.57355157575938	-1.37316889306836
O	-1.05637047994490	-4.07465724346707	-1.09190617626679
O	0.75243475137233	-5.85912221104160	-0.75239694937215
TS-SN2 (18C6-KF)			
O	-1.70510878716433	-1.02661845062328	-2.98468627229190
C	-2.98046712894405	-1.58492499381570	-2.70625811537842
C	-2.84399808219038	-2.73325428344831	-1.73128282889974
O	-2.43764232427951	-2.23477955806202	-0.46393352721418
O	-0.61710499294841	-2.12832719505583	1.73170402000912
C	-0.15270814261414	-1.50967017508073	2.92390448182320
C	1.21548634063141	-0.90603023600546	2.69673425116515
O	1.09871803254025	0.22594224755547	1.84023449661623
C	2.36881227644790	0.79503060016260	1.53408447139774
C	2.18750418111468	1.94406969659298	0.56898151422098
O	1.81338751930321	1.44875841770984	-0.71023807113759
C	1.65586713617991	2.46286733959123	-1.67998054197832
C	1.32481055347737	1.83031312565443	-3.01508332990302
O	0.06176007858963	1.19486037127626	-2.92220396094922
C	-0.36842290503496	0.59174005529287	-4.12962527299644
C	-1.75772347482950	0.02518622609304	-3.92731932153778
H	-3.83599381418681	-3.24226398073886	-1.64962824581059
H	-2.09975375596306	-3.46948287933096	-2.11315219496880
H	-0.86973167310579	-0.71634408504798	3.24784998820850
H	-0.08420317456562	-2.26204790233970	3.74768086880943
H	1.90346455714917	-1.64992711483224	2.22923646896106
H	1.63551545729911	-0.60128970990051	3.68764626890298
H	3.15151299852827	2.50500252275548	0.49507716753624
H	1.41106048371728	2.65322030665810	0.94777783349745
H	2.11750601262405	1.09263841255447	-3.29105673705851
H	1.31066308881606	2.62549664233173	-3.80112517693517
H	-0.40217213099616	1.34140216045596	-4.95872448173353
H	0.33362014243554	-0.22157948831140	-4.43683010888661
H	-2.14540763360696	-0.34082500654920	-4.91081959174249
H	-2.44403360643167	0.83399565367061	-3.57604351400544
H	-3.44705318636499	-1.97026486882245	-3.64604508907977
H	-3.65930037860082	-0.80152657151362	-2.28875688664381
H	0.84118964089455	3.16972606040089	-1.38578489878765
H	2.59653143358269	3.05894684669586	-1.78896009228091
H	2.84892444702442	1.18853714909217	2.46422708625414
H	3.02547938644289	0.01108876069595	1.08474224044741
C	-1.94103526537209	-2.62756801783175	1.84276403898763
C	-2.36636188725860	-3.25127496247376	0.53211543216115
H	-2.64025635106551	-1.79956606089502	2.11657111165452
H	-2.00128883628446	-3.40401716694450	2.64449488717748
H	-3.37044976554862	-3.72150939248164	0.67628013614517
H	-1.65862632630550	-4.05648114518239	0.22578483868997
K	0.40940463064202	-1.17132033975981	-0.76586391541046
H	4.48286023921899	-4.88631869088283	-0.76964968410007
H	1.33615890176662	-5.99300725276734	-3.94606103886584
C	3.95438844827136	-4.34288657642725	0.03766096090791
C	0.58296913092561	-6.38035651294428	-3.23678875945258
H	2.57175326900453	-3.31720018933861	-1.40466224508623
O	2.01035207945433	-5.44862257889218	-1.24007792541807
H	4.56185276901115	-3.46657959556134	0.33558974270633
C	2.63549712764403	-3.83049187100249	-0.44398872320266
H	3.84086962463693	-5.01713342063765	0.90748257898978
S	0.55304138894680	-5.30441043086218	-1.78643814609061

H	-0.43032910079355	-6.36144400443426	-3.67842645230196
H	0.84217469790955	-7.39926219862923	-2.89718300602014
F	2.79155484172897	-1.88783142418947	0.18765795058162
H	1.78479507203467	-3.78281469340695	0.24076637326609
O	-0.47243012024631	-5.85165570590186	-0.84761772328976
O	0.28970685670781	-3.89925386431490	-2.26671332965907
[18C6 (KF) ]2			
O	-1.79098312787637	-1.30153252304493	-3.20953183976881
C	-3.09151694707178	-1.73765972988065	-2.83394422747987
C	-2.99887023249273	-2.78059407026418	-1.74310348007734
O	-2.66647704886815	-2.14885206857451	-0.51060635365773
O	-0.63352379766501	-1.96587712589127	1.55522369566975
C	-0.02147378282260	-1.33964439845320	2.66814477984530
C	1.41892729019617	-1.01944675987091	2.32847896275263
O	1.46263036021847	0.05817960284282	1.40038965605570
C	2.78271035492967	0.28711568416613	0.91559555124509
C	2.75156906070991	1.35909149979569	-0.15010084083782
O	2.20843403982185	0.83573564781349	-1.35625050607414
C	2.09648996467874	1.79889019758979	-2.38006969447725
C	1.55071671666744	1.14646949639987	-3.63344349567340
O	0.21766526072081	0.73324170797120	-3.40532491290073
C	-0.38506743900194	0.11388889771076	-4.52579486204338
C	-1.80650224072851	-0.27700742078071	-4.17836001988331
H	-3.99196100216919	-3.29066030380576	-1.65925250837812
H	-2.20854424500398	-3.53410101834824	-1.98758234404942
H	-0.57300316712598	-0.40863289270276	2.94925384346579
H	-0.03839007718684	-2.02232069460487	3.55418370137877
H	1.91380650831112	-1.91291017623958	1.87560693536728
H	1.95760565329771	-0.74233076177981	3.27002363782305
H	3.79332505484096	1.72361637512018	-0.32879811518796
H	2.14403900605257	2.23073423577262	0.19609031746232
H	2.19173968333262	0.27350247954467	-3.91340143882308
H	1.59875147637728	1.88266153689878	-4.47488446110375
H	-0.40432644488450	0.81028264318156	-5.40118124386115
H	0.19164628513429	-0.79468658321063	-4.83108453542832
H	-2.32205868138000	-0.61744344116407	-5.11221825901321
H	-2.35884878850979	0.61897186062974	-3.80138386778242
H	-3.61353046413513	-2.18006303794290	-3.71852409226640
H	-3.70104472167920	-0.86896336571106	-2.48360301976914
H	1.42287901898391	2.63465026423248	-2.06732085377295
H	3.09469190591909	2.24588517567039	-2.61879406622422
H	3.44466249232809	0.63611736343229	1.74810322806651
H	3.18395644687677	-0.66805453044397	0.49387701040068
C	-1.96893596911694	-2.38410962816563	1.77267110687320
C	-2.47564071622458	-3.09477401600686	0.53542817019800
H	-2.62003180621299	-1.50781524452889	2.01359813635371
H	-2.01781613538473	-3.09080512412624	2.63878095163834
H	-3.44435975955194	-3.59885027412552	0.78273443453260
H	-1.73609589473400	-3.86380071448531	0.20260957038877
F	2.65163895193454	-2.55946353138762	-0.16738028411761
K	0.41040199132960	-1.67021512263606	-1.04802346984693
H	5.38893974588986	-1.94803276484612	-2.90186750613206
H	3.71300024543707	-2.13018406904183	-4.59071739548499
C	4.54145962288053	-2.64136254146762	-2.66836464142391
H	3.81067718344873	-2.11369759625436	-2.00828402531432
H	6.37556093763489	-2.82124998868006	-0.73749868592151
C	3.87222194825080	-3.04532981078222	-3.96464161334091
C	5.48724168254474	-3.50069268260122	-0.68523421816682

H	4.53332900885257	-3.73606700600595	-4.54410407631099
H	4.66329383386939	-2.99875656352231	-0.11790860956092
O	5.02407946205314	-3.80151621414952	-2.00028182449043
H	1.70756265345336	-3.25184259164579	-5.51141192421278
O	2.63064941631674	-3.66960925398680	-3.68388891336917
C	1.93642002817381	-4.11631804690401	-4.83704422709359
H	6.50849054024941	-4.51444164913840	0.91414791299741
C	5.90716329524919	-4.77662640327454	0.00817570143877
H	2.56631188600979	-4.83520114198406	-5.41747648706420
H	6.55906982609834	-5.38638947677364	-0.66486983573834
C	0.63598591453891	-4.77146225854161	-4.42353024484884
K	2.15485858665552	-4.92087281493683	-1.09948023135039
H	0.10120829981684	-4.13058021247585	-3.68103292853003
O	4.76157803413324	-5.52825854808328	0.39006658574135
H	-0.00753118152510	-4.89572364665796	-5.33134035387156
F	-0.27377887668668	-4.11795513121566	-1.49217193704846
O	0.90300233834058	-6.03868427576018	-3.83418622085551
C	5.08489642887068	-6.75061755914645	1.01665760391045
H	5.73043609138918	-6.58066379982543	1.91545554405335
H	5.65139305863161	-7.41616820692017	0.31915896523704
C	-0.27265567914227	-6.60386256742996	-3.25815985415295
H	-0.70192504006831	-5.87506612426598	-2.52514543340690
C	3.81278039122767	-7.44242596161609	1.46130753076689
H	3.22529519372159	-6.75964514377899	2.12380206783137
H	-1.02617190237868	-6.81931872823134	-4.05715071380960
O	3.05736031040076	-7.80257081365446	0.32088539406885
O	0.76917279481105	-7.64857825996089	-1.35673774390165
C	0.07225171407518	-7.90404128428907	-2.56916207506584
H	4.08135818738974	-8.34668475536775	2.06322953692020
H	0.69470341010886	-8.54521448013396	-3.24067682855549
C	1.84013002694579	-8.45772431260891	0.62078027561635
C	1.14203642625066	-8.82428472748839	-0.67218860902689
H	1.17845796441336	-7.79884705186184	1.23562000598793
H	1.82262667665297	-9.45015570113568	-1.30114109923307
H	-0.87435947671017	-8.45991069361632	-2.35401885382841
H	2.02531555111835	-9.39133740663118	1.20908601509333
H	0.24437840777157	-9.44786784390360	-0.42936692557180
18C6 (KF)			
O	-2.64204159604815	-0.46177652440665	-2.63693798992662
C	-3.98262307619331	-0.59534440999546	-2.22499261056933
C	-4.08077508651659	-1.78001660377436	-1.28314845278294
O	-3.31343640837241	-1.52585617309598	-0.11391184720289
O	-1.13087602576801	-1.96144509783360	1.72545834284380
C	-0.40893697537256	-1.54099657299530	2.87302061309416
C	1.01027416327545	-1.17120438536985	2.49663471957009
O	1.00210434896065	-0.01497177800310	1.67923545609674
C	2.30326737704543	0.45414936933148	1.35252172159179
C	2.19922883064664	1.58597626047532	0.34798878584453
O	1.62947976002532	1.08048875937334	-0.83789206739919
C	1.74957889459230	1.92292854792935	-1.98169995926283
C	1.12074101763340	1.23409029647373	-3.17374081096775
O	-0.30179854661777	1.27617923992785	-3.04445993786876
C	-0.94734179538761	0.48102478923667	-4.04260486612366
C	-2.42831597637865	0.41479064611097	-3.74077879518307
H	-5.15194184386149	-1.95777282454681	-1.01748156363597
H	-3.69960587078416	-2.69218252784689	-1.80134180428978
H	-0.91063665975582	-0.66072412081649	3.34314833162267
H	-0.37585386289871	-2.35883245510415	3.63490910419714

H	1.50315316467751	-2.02403398074225	1.96800955989604
H	1.58457518330229	-0.98873877008426	3.43863161962723
H	3.22816252022060	1.98261312008993	0.16396479489560
H	1.58739841814582	2.42400472141389	0.76456412913491
H	1.44162527005482	0.15914054215491	-3.22237814865099
H	1.43936972690745	1.76890506738308	-4.10282460706211
H	-0.80909532584971	0.94506420699880	-5.05050710822173
H	-0.49224921479855	-0.54639897284600	-4.02539940995723
H	-2.97062350645663	0.03060117394796	-4.63848098011960
H	-2.82861079740370	1.43205448748088	-3.50712758133318
H	-4.65580148877446	-0.78735107972547	-3.09693493609027
H	-4.34621875049877	0.33480746542033	-1.72148539477614
H	1.25726436218775	2.90733502743013	-1.78890627434389
H	2.82848141503820	2.11455275372910	-2.19659275450900
H	2.83033526118643	0.81687903527642	2.26921072292533
H	2.91079370699695	-0.37214038939600	0.91202998383317
C	-2.48844828630448	-2.25794026616219	2.01495872180412
C	-3.22560050985460	-2.64395943289157	0.75024771495541
H	-2.98464462490711	-1.37242573582480	2.48024247623611
H	-2.55727057133583	-3.10536143017888	2.74126384103475
H	-4.24407176485077	-3.00447584369670	1.03742321024364
H	-2.70361386336688	-3.49284098822281	0.24418531610623
F	0.68974017329519	-1.73111235384435	-2.89743405925464
K	-0.42764116583549	-0.81796279278022	-0.95234720602186
18C6			
O	-2.57435959137768	-0.62366181360275	-2.85864898374966
C	-3.88390847802282	-0.85007642497456	-2.38277925353397
C	-3.88841953597656	-2.00300402530043	-1.39772895172812
O	-3.35845164721125	-1.58268502606353	-0.15824868481406
O	-1.16449347267059	-1.96605616648233	1.80926351604854
C	-0.47506945359252	-1.38582718168247	2.89695025859619
C	0.97501860018743	-1.14587828419863	2.52466122754118
O	1.07830502434612	-0.02002154694019	1.67918886200446
C	2.38780820369915	0.20662191068918	1.20331471888771
C	2.39197182403090	1.35900946088207	0.21764370871292
O	1.86216459306177	0.93786724452912	-1.02165440331422
C	1.73661111583796	1.98194960009601	-1.96394335014454
C	1.05435037330488	1.47114123845216	-3.21830696008062
O	-0.33101474662142	1.32163377377681	-2.98982534139561
C	-1.02106733805537	0.74159599764821	-4.07717449536300
C	-2.47107463698844	0.50209748366300	-3.70425069340574
H	-4.94045189680513	-2.36687855900080	-1.27453425950282
H	-3.29125710773473	-2.84831840455069	-1.81871157574246
H	-0.94318194958109	-0.41502683827310	3.19144172052058
H	-0.51101541787506	-2.05884358058919	3.79172827643685
H	1.38139733321782	-2.05793643107120	2.02243257001242
H	1.56824454637249	-0.99225641464092	3.46252107549331
H	3.44390705690000	1.72310108267931	0.09426106659814
H	1.79455117330830	2.20440598459115	0.63809199772681
H	1.51538186636262	0.49768160227447	-3.51506811780952
H	1.24094638747076	2.19708817438490	-4.05091944061542
H	-0.98530885254886	1.41454389625709	-4.97201327917878
H	-0.55343463649697	-0.22938402937312	-4.37184326124347
H	-3.06476947143461	0.34858569238580	-4.64182921535003
H	-2.87693881106721	1.41435465728366	-3.20195348456793
H	-4.57554213582471	-1.09564179996382	-3.22936397329581
H	-4.28701337744670	0.06312130930553	-1.88068494218275
H	1.14220200321645	2.82893309834091	-1.54203915563151

H	2.74349093587082	2.38649287824722	-2.24150032200807
H	3.07926868553193	0.45298176477348	2.04981414984330
H	2.79129478758691	-0.70671990873986	0.70180857633526
C	-2.54970194929056	-2.11714695671550	2.03775913584489
C	-3.23157197951486	-2.62752394317238	0.78300670256260
H	-3.01172262408361	-1.14443013778659	2.33540476696959
H	-2.73542884986884	-2.84402657804204	2.86975325514781
H	-4.23792277069023	-3.03355608750867	1.06032706028050
H	-2.63622777952648	-3.47338871158731	0.36014849909507
cryp (KOMs)			
C	28.22099909196255	-0.71336250920335	-0.68555717705074
C	28.15727603489711	0.46142207173625	0.29888471294676
O	27.01444713284574	-1.44606629892304	-0.84934568593122
N	27.32443164748590	1.59545441857494	-0.11720371539541
C	27.01666783959882	2.45848636628337	1.02664690417744
C	26.77031583234980	-2.46417296690279	0.11616454283568
C	25.91504558557535	3.48895177320836	0.80426651587739
O	24.72838885086385	2.83823140633887	0.38975667270372
C	23.56374657209417	3.64224294602933	0.41537909534216
C	25.59385706441169	-3.30209144288436	-0.35510601822604
C	22.33403128040842	2.76540552406065	0.28855049447243
O	22.30488104126628	2.14783997761859	-1.00412164185832
O	24.42864744531518	-2.49917608471643	-0.35060564386629
C	21.11711289733979	1.41901034217618	-1.27815089684926
C	23.23064754915577	-3.15060439955184	-0.71319043099150
C	21.07894960273504	-0.01923940128082	-0.75103502599916
N	22.06157644800500	-0.95450970740416	-1.32588168488355
C	22.05672040252196	-2.19086375434405	-0.53261311787475
H	29.03972954600625	-1.39575197558338	-0.35159164257767
H	28.49202853739417	-0.36244491449069	-1.70339648411260
H	25.74838284264027	4.01525948092833	1.77457543125561
H	26.21287137722789	4.26911588814568	0.05846504379929
H	20.23327353400991	1.95155460578698	-0.85251011327494
H	20.99104199107947	1.44612019816564	-2.38246495554121
H	23.04598142551938	-4.03056189137153	-0.04786269240623
H	23.29904395160301	-3.55455526436264	-1.75285388946393
H	20.02582374230174	-0.38820442050299	-0.90002341771416
H	21.25706589717770	0.00199221792746	0.34343212423835
H	22.05713574227735	-1.88434565309737	0.53354075853128
H	21.11778588270237	-2.78219384764354	-0.71585728310196
H	26.68870781969667	1.79842983456866	1.85609048169141
H	27.92628873999213	3.02000216181670	1.37663238393592
H	29.21829144036784	0.77604738033048	0.50421291196595
H	27.74769986343605	0.09777883810480	1.26290625295325
H	27.66344851586186	-3.12889343747017	0.21532004781716
H	26.53521086666787	-2.02554650212041	1.11432809183666
H	25.47312440080871	-4.17420876755314	0.33363775877500
H	25.79135427169440	-3.69875115326499	-1.38128782064189
H	23.49065376946520	4.18513434469087	1.38794630110354
H	23.59426952264836	4.40344073991710	-0.40510977068510
K	24.68932318902215	0.22582621119063	-0.46516737203343
C	27.82020596844868	2.29627253325366	-1.29916905635199
C	21.90195925226653	-1.15171277544939	-2.76612019087722
C	26.75767929080308	2.68336324877383	-2.33619263966899
H	28.54887429929210	1.64178424979326	-1.81950163123227
H	28.38864895779470	3.22438904038973	-1.02727028254658
H	21.41323622792649	-0.25087531163781	-3.18716397285933
H	21.20119479742993	-1.99911977863711	-2.99756659046522

C	23.19004438379418	-1.40175183007538	-3.57416984302001
O	24.23676577351712	-0.46652226210629	-3.39216001822941
H	22.89708135533877	-1.45218698523501	-4.65385288598910
H	23.63905794326198	-2.37956930044713	-3.31671837363726
O	25.99184413213005	1.54019478908552	-2.68263911915248
H	27.29072961423982	3.08823757752883	-3.23008595413339
H	26.08188750426974	3.48793592027335	-1.96275804228657
C	25.31484230494442	1.60572879186127	-3.92799063965218
C	23.99227024218728	0.85683778599742	-3.83994299135489
H	21.43019326044709	3.40907534123532	0.41604356768190
H	22.35175745687105	1.99658924229836	1.09464251083349
H	25.95741765901704	1.16848259045123	-4.72942065077435
H	25.08495218490820	2.65989641423717	-4.20996132466952
H	23.31750371854103	1.39855205344579	-3.13795589532850
H	23.51736408807617	0.85456994392681	-4.85269527834359
O	23.03685866723283	-0.00598447694624	1.92313409840897
S	24.17748635295900	0.15992793312840	2.91892854971646
C	23.87250726318165	-1.07505418482475	4.21411280591638
H	24.69141239768753	-1.00205276072255	4.95348678751993
H	23.85210612312142	-2.07681712797810	3.74706508568121
H	22.90100673655262	-0.84077958432485	4.68692745497648
O	24.19358596824983	1.49271786978064	3.60656115539742
O	25.50863688707621	-0.23051128200414	2.29329331866101
TS-E2-syn (crypKF)			
C	28.16091565807090	-0.35643318856628	-0.16500669964648
C	27.92137362779117	0.78142224557652	0.83123462933529
O	27.04686543988004	-1.21932842148386	-0.37286404202710
N	26.95357234276336	1.79657559605108	0.38443659887461
C	26.44001892436659	2.56546789354828	1.51970530987772
C	26.92388169410195	-2.30185117296127	0.54671306785916
C	25.24652754245826	3.46926457740771	1.22477029981969
O	24.18074300656916	2.70308710079089	0.69600206747812
C	22.95985396611482	3.39940298038549	0.54019626148449
C	25.85794945122089	-3.25162636095741	0.03130292917388
C	21.83776136122631	2.41068932730107	0.28689250175836
O	22.04421477505451	1.75546640903781	-0.96705149547273
O	24.59508887344459	-2.59885543808381	0.03052724638280
C	20.97580389793410	0.91132911030036	-1.37859282380607
C	23.52741032096963	-3.36905245048145	-0.48705681673403
C	21.02477297719056	-0.52332863072425	-0.84292324359088
N	22.17188554518463	-1.33989966880726	-1.27954848073178
C	22.23244855115538	-2.55949897351030	-0.46061611735267
H	29.04059591904667	-0.94631544386695	0.18681711621333
H	28.41787863532437	0.03868943178516	-1.17070329542438
H	24.93771541903282	3.94740038704480	2.18610653724260
H	25.51643590106785	4.30035682429188	0.52594810206719
H	19.99720549184261	1.35113049473172	-1.07118325312094
H	20.98792953036861	0.92752792612747	-2.49013613089599
H	23.36377965091297	-4.27935751849122	0.14147177051066
H	23.77603446185033	-3.73938417316711	-1.51104429918481
H	20.04683929815421	-1.00613710687191	-1.11812061027120
H	21.05964582182286	-0.48169965269425	0.26444224077611
H	22.06851863311253	-2.24538040042726	0.59053352579147
H	21.4034375554354	-3.26687332123667	-0.73416170895319
H	26.13151001790796	1.84217988532623	2.30208542845604
H	27.23599089054687	3.21994988812213	1.97120407362090
H	28.92117581352366	1.24082615818290	1.06293790036350
H	27.55172541794570	0.34507325118665	1.78524802546081

H	27.88631533415994	-2.86629149839757	0.61146404651292
H	26.68001828462454	-1.93645407361167	1.57227774331042
H	25.83049400371578	-4.15612343308218	0.68633065754822
H	26.11349105168161	-3.58610210002133	-1.00370183790780
H	22.71077987096436	3.96708950594543	1.46984285292326
H	23.03130405262714	4.13645843338451	-0.29920698699405
K	24.53557596446483	0.12526501469619	-0.18461828456568
C	27.43302723124529	2.60437790850145	-0.73502862429861
C	22.19512529940109	-1.57485287895866	-2.72324892194504
C	26.41093228612255	2.88761717899132	-1.84472823313092
H	28.28068066098955	2.07249123717920	-1.21174370925145
H	27.84884933079326	3.58815391519367	-0.39136979910038
H	21.62035336614179	-0.76651821994396	-3.21727770097067
H	21.65960336840275	-2.52324578447392	-2.99984677821519
C	23.58599044736320	-1.63459470191684	-3.38430397606759
O	24.45349605501995	-0.55011933376130	-3.10598258602106
H	23.42792037450229	-1.73535205122935	-4.48799937661580
H	24.14447214853744	-2.53096217031697	-3.05388571065232
O	25.79993528444357	1.67226599312395	-2.25002633222704
H	26.95860717662068	3.35919310299635	-2.69539812480874
H	25.62584519863402	3.60915281293829	-1.51936529646474
C	25.29246301941056	1.64265450752413	-3.57383023212243
C	24.08734862092039	0.71414218283553	-3.63619350736409
H	20.87199736836842	2.97096347426123	0.26651446485247
H	21.80809190907407	1.67025773854616	1.11812582938364
H	26.08853783810479	1.29924018645258	-4.27732745129272
H	24.95585850004503	2.65355144499616	-3.90397355813868
H	23.25442833395520	1.16770266604363	-3.05183890433944
H	23.76058187976114	0.62187583670802	-4.70144343374685
H	26.12311104919204	-0.30025901688557	6.20524807851651
H	26.89173647897913	1.24120320700854	5.53215885657711
C	26.04206037196877	0.53642954700216	5.48741731503835
F	26.73677480169155	-0.73031873851397	3.37367118310186
H	26.36726168406321	-0.11004861262868	4.34581331042074
C	24.75643087038195	1.13255171281336	5.37086327133538
H	23.88935536576098	0.70643780683944	5.90356277873861
H	24.67136265938522	2.22079273118505	5.22294193896251
O	24.03126557464875	0.88168973182455	3.65044149161072
H	23.95270482739999	-1.84000237309958	4.94834657336339
H	24.83981618267677	-1.77135516048300	3.36608378028808
C	23.84423107246592	-1.79688340720546	3.84922686214072
S	22.98401767579423	-0.26324366467447	3.43527393196894
O	21.80956022577982	-0.14479906483081	4.34585764000188
H	23.20767711067006	-2.62694689729940	3.49202586777473
O	22.68017337554563	-0.32134226052284	1.95961427653625
TS-E2-anti (crypKF)			
C	28.27297620655875	-0.15309114902885	-0.47143333533947
C	28.16927385478417	1.09522358416775	0.41241403865008
O	27.14769366755077	-1.02090497963949	-0.44422494124327
N	27.11416163335954	2.05429104120755	0.03332647856941
C	26.80086292207445	2.91869907707731	1.18181909294838
C	27.07087709791794	-1.90439388215840	0.67898788988202
C	25.51049533096753	3.73189421763453	1.12096459454203
O	24.38754656474847	2.87748535420550	0.96856605242486
C	23.15407136371597	3.55981191092401	0.79839618122196
C	25.97750439947873	-2.92642311049662	0.42698145043042
C	22.03177853705266	2.56533016172247	0.56564614208668
O	22.28728001312893	1.86068688085170	-0.64902308995092



O	24.70603817359293	-2.28994303449653	0.38812071100105
C	21.20938829785558	1.07814964096902	-1.15115523963420
C	23.63599969540208	-3.15352994928234	0.03649117746097
C	21.13758037967475	-0.35135391838280	-0.60762481897892
N	22.28772018945071	-1.21169151734734	-0.94633704468623
C	22.32061475232260	-2.38145251998853	-0.05374462705760
H	29.19384164939951	-0.70844719976004	-0.16903874394808
H	28.40587309307923	0.12038761724187	-1.54068398850634
H	25.43323452171021	4.30666638058460	2.07645181650827
H	25.52372253150158	4.49296572689720	0.30185284542457
H	20.23520257701467	1.57652838412630	-0.93258538809570
H	21.32795583585765	1.08410585435694	-2.25729260187419
H	23.50178223920700	-3.94660188589762	0.81217785437480
H	23.88047446398100	-3.68692345234235	-0.91505848498778
H	20.17162467163129	-0.79456706227806	-0.97212644487502
H	21.04364173391614	-0.30135791268186	0.49701672696032
H	22.04747429568699	-2.04077692861144	0.96571243947529
H	21.53382238437372	-3.12988866443117	-0.33901236571593
H	26.73011083388290	2.24942557705768	2.06513470461936
H	27.62913787919286	3.65277842278458	1.37624562595599
H	29.18295351242211	1.58013364251123	0.42215183465710
H	27.95741156108711	0.77513579494666	1.45386029189353
H	28.03548431283888	-2.45530618038255	0.79790478904316
H	26.87062147158490	-1.33730481847943	1.61879359352272
H	26.00808095237297	-3.68894664099762	1.24345954098726
H	26.16335279170082	-3.45656702163320	-0.53955223372776
H	22.91032576317081	4.16736984430232	1.70409880205526
H	23.22546123027248	4.25867528634214	-0.07154161157948
K	24.70582212795530	0.38840053040093	-0.17592427656716
C	27.40873172942979	2.75540267395029	-1.21546039598477
C	22.33039212212474	-1.54159339336826	-2.37288940636143
C	26.19363992444438	3.14564017652771	-2.07559608232759
H	28.06044831520079	2.10248342622793	-1.83161490747554
H	28.00695569670659	3.69079141493066	-1.03724361842119
H	21.84160873287674	-0.71903832832800	-2.93264945842998
H	21.72238885824747	-2.45987763282559	-2.59912015822005
C	23.72482915763486	-1.75330255284056	-2.98410548673417
O	24.60583373803166	-0.64714705316752	-2.84471050094116
H	23.59703073279988	-2.01489338121021	-4.06197554150324
H	24.24235996411899	-2.60632936640772	-2.50653510735508
O	25.33944083154589	2.06223187399104	-2.41775728842237
H	26.56462401128815	3.65627641114123	-2.99664560153656
H	25.54838458261904	3.87263087680899	-1.54624254734487
C	25.65014183092497	1.35607821357582	-3.60578549229906
C	24.55465950239255	0.33583582499173	-3.86153434829788
H	21.07565173393569	3.13614192178535	0.48723435885656
H	21.91582741043701	1.86939422305609	1.42839710350744
H	26.63163958730461	0.82938256920835	-3.53019532831879
H	25.70210069683627	2.05599322862048	-4.47557849226136
H	23.56809179458274	0.85751368837851	-3.88378085711202
H	24.71980589422721	-0.12774372263416	-4.86487951023794
O	20.91031077039577	-1.97439223399198	2.97984364757738
H	23.51070806577346	-1.01370749393701	3.18124908112596
H	19.48455353785947	-1.53652152999517	5.45566495296519
H	24.94147150226911	-0.92338750478549	5.23841472500681
S	20.73752514442277	-0.63302295505108	3.62870362261292
C	19.30236469341287	-0.73051775004093	4.72226187186810
H	18.42752677078051	-0.96304634384569	4.08755345028318

C	23.59356568800600	-0.09157880564296	3.78070199226261
O	21.88912843428729	-0.30918628500612	4.62811618282763
C	24.65308373347618	-0.00176497597477	4.70307302661079
F	26.47120503627436	0.27799188639548	2.90182902723461
H	25.61972406074280	0.14909715074627	3.74454113738260
O	20.50202017542885	0.49902253827007	2.66500822347705
H	23.28928356804156	0.82692852255079	3.25234846180457
H	19.18069106315650	0.24642685221737	5.22330440722176
H	24.72441539448540	0.91750473368304	5.31039941903260
TS-SN2 (crypKF)			
C	28.22473954312287	-0.37997399844761	0.02971318329150
C	28.00858777045967	0.89804249687048	0.84980443961030
O	27.08523111374354	-1.21113736283768	-0.13981823989870
N	27.14671429945800	1.91979500563338	0.23348301058481
C	26.69586326722690	2.87890679545140	1.24610313683849
C	26.78671312764583	-2.07737240244553	0.95748531981044
C	25.52058618707362	3.77419807144426	0.86571930853693
O	24.35723083684740	2.99174213310679	0.65774108907997
C	23.20339379831039	3.73700899324362	0.31421725595149
C	25.71002512673221	-3.05657895507297	0.52693888230348
C	22.00625220428311	2.81436580665842	0.20790450466276
O	22.19053955089924	1.91966694598188	-0.89151369024542
O	24.48124790972263	-2.36708001700633	0.35828156538651
C	21.04560281766494	1.13813826158071	-1.22533424281697
C	23.40599515487706	-3.17016032846588	-0.08994889024160
C	21.01866539033529	-0.26386839075272	-0.61470336059570
N	22.12616433344960	-1.15536508352322	-1.00415898887596
C	22.12415074864930	-2.34361973104063	-0.13724074577018
H	29.04765143050108	-0.95628117914086	0.51873417981962
H	28.57028796474263	-0.14459210508368	-0.99932386851461
H	25.35489468517850	4.49152699300341	1.70726478184031
H	25.73603973618802	4.39526932184305	-0.03878583784470
H	20.11448690674775	1.66099031329964	-0.90735812025092
H	21.01452927370243	1.09281953981490	-2.33671712903878
H	23.22984980139730	-4.01609749442491	0.61923086781649
H	23.65509283716209	-3.63413483490227	-1.07613942676849
H	20.01940374584580	-0.70983945667480	-0.87763243910598
H	21.02318942713711	-0.16736051863083	0.48980703190332
H	21.89952153673205	-2.00927305495930	0.89690190019444
H	21.29651601834286	-3.04635561456019	-0.42632137954040
H	26.38102806980613	2.28028973187296	2.12803292611468
H	27.53206758119441	3.56074819865690	1.56309920001352
H	29.02691590502392	1.30967480615613	1.09211718299139
H	27.52779071762299	0.62333528727524	1.81111242741651
H	27.69755719485801	-2.65662677277635	1.24581258192779
H	26.42788814447875	-1.48631164692880	1.83482164301794
H	25.60688038926335	-3.84710280297830	1.31048920019769
H	26.00577699978510	-3.55883504116734	-0.42747212961311
H	22.98419086007722	4.50468963259542	1.09665207253750
H	23.36394323661494	4.27597317755195	-0.65302911065856
K	24.69139488294289	0.33379987939498	-0.09678188365766
C	27.71261774877088	2.50977536479381	-0.97588764552439
C	22.13439200920003	-1.46212197222640	-2.43540672110826
C	26.72103781828087	2.78902860930104	-2.11615457795402
H	28.47032978383492	1.80820088629304	-1.37880913341132
H	28.26629540898110	3.463044480695046	-0.76160768223327
H	21.60261062588328	-0.65091301403784	-2.97143610543004
H	21.54614844282165	-2.39288643913659	-2.66027721464949

C	23.51272251914519	-1.63667660746571	-3.09895441659605
O	24.42914480549580	-0.56829298966217	-2.93210308999787
H	23.33680556423386	-1.82773585050192	-4.18810211978273
H	24.03841045759317	-2.52140681578278	-2.69438583169599
O	25.88959989405638	1.65985704903014	-2.32116849297149
H	27.31734408873361	3.01473486937965	-3.03290231531275
H	26.09002514852855	3.68689812984268	-1.91323718944919
C	25.33847018831136	1.53545025650315	-3.62092776712693
C	24.09596732578696	0.65913838843769	-3.55753793794940
H	21.09977224657890	3.44308119521207	0.03710215009671
H	21.84693319058975	2.25696412954305	1.15944876680396
H	26.09637110031379	1.09703792566683	-4.31449482168511
H	25.03347821161111	2.52858023726042	-4.02999476734620
H	23.30382179760212	1.19762987712474	-2.98799812024387
H	23.72620075240855	0.49147337285949	-4.59935055565549
H	24.46791650031728	-0.77593350654508	5.56567626592823
O	21.03708249038205	-1.43754001331675	2.91962946194951
H	23.66358848022530	-0.72519064530980	3.19080689415170
O	22.11513734926864	0.15317467056528	4.57826829409725
C	24.59847706763305	0.18798333548119	5.03732947255456
C	23.84923036978063	0.20249833580395	3.74079490581645
S	20.92665807633136	-0.10744902347584	3.60348644784796
H	25.67211638709579	0.33488963011708	4.81433780088507
F	25.48236543489699	0.26559950268665	2.53527507504134
O	20.68487250799796	1.05533014068487	2.68327398939693
H	24.25313319198373	1.00326211460587	5.70229244925610
H	19.71450643449553	-1.02730172613981	5.45199869368290
H	23.62228589570633	1.15096556190505	3.24397742119701
C	19.53355544790023	-0.19254555865595	4.75129573999890
H	18.62713799297679	-0.37387246628953	4.14506049204168
H	19.46514671839908	0.77175363888271	5.28590397696754
[cryp (KF) ] <sup>2</sup>			
C	3.83582889929360	-0.89874541919479	-0.42615636223807
C	3.96159703619728	0.52591673891164	0.09565034172984
O	2.47168324572443	-1.28912209444464	-0.46682165681226
N	3.30093936518461	1.55055861748345	-0.71253163501112
C	3.09995952733032	2.76876589416208	0.07043889413654
C	2.25833958767253	-2.68378963013222	-0.52986734773143
C	2.11095427106968	3.76950133776316	-0.51149030278622
O	0.82893692747506	3.17896810079234	-0.62682868843805
C	-0.21357366865401	4.09979957856324	-0.88150892359706
C	0.92763837365595	-2.97741343399350	-1.19529601079276
C	-1.52924379100040	3.36091386800060	-0.99786654238090
O	-1.53258596074098	2.60405898124205	-2.20535577020164
O	-0.12819239770253	-2.32984094319976	-0.49279785648553
C	-2.76597307161224	1.95328691795112	-2.46801907255778
C	-1.43229937098400	-2.70558881498522	-0.91951795734622
C	-3.01526587087948	0.66392037062582	-1.68266818266633
N	-2.15056263302725	-0.48747167134761	-2.00593225181416
C	-2.38759338847426	-1.51716062432153	-0.98873491110507
H	4.41081371932457	-1.55679686237186	0.27012357942027
H	4.28558424993085	-1.02028233031449	-1.44252533573621
H	2.07076809567188	4.64691387799553	0.18117200824806
H	2.43882725139710	4.16940721131974	-1.50435529154421
H	-3.61660339412878	2.64327114749957	-2.24353577881436
H	-2.78503919946983	1.78524640105353	-3.56616836574784
H	-1.86515033236746	-3.43029616423176	-0.18666664069138
H	-1.38122542412050	-3.24398872320748	-1.88904943951185

H	-4.10042348315513	0.40043082566954	-1.83380104204540
H	-2.87922515000383	0.87188701666442	-0.59513253200262
H	-2.36526634120237	-0.99846904501503	-0.00500901459919
H	-3.42164489827722	-1.95352943729142	-1.09867073025818
H	2.71723478777654	2.44881953252477	1.06511880140493
H	4.06712192307134	3.32575880027640	0.22558436801247
H	5.05938913280084	0.73341317956317	0.23038386945927
H	3.48014152825983	0.56354406810284	1.09828013402025
H	3.04864274169909	-3.18759501161534	-1.13768720143690
H	2.29299958309849	-3.12800063993507	0.49713424629638
H	0.78296830541295	-4.08575299844131	-1.19617187662807
H	0.95322597369427	-2.61369640191548	-2.24753160590139
H	-0.29141492062172	4.83994741417668	-0.04442490032213
H	-0.01156100192763	4.67222549201292	-1.82107350583195
K	0.38046484500807	0.49576432210030	0.06896629583319
C	3.87139296597998	1.78019552859144	-2.03776734618230
C	-2.34041725936889	-0.92780835742191	-3.38460420272456
C	2.87150340316841	1.72351311134321	-3.19547252663653
H	4.66047110333143	1.02654278683370	-2.25136613072852
H	4.38726485569423	2.77252128866433	-2.07527618293310
H	-2.51570439590119	-0.02290561327092	-3.99895867268355
H	-3.27407335657074	-1.54829531970472	-3.49839321967156
C	-1.20585681871254	-1.71599532314473	-4.06907968031531
O	0.10644118925772	-1.21974469003967	-3.90885341331643
H	-1.47105844483291	-1.77130878086929	-5.15663911663869
H	-1.16122862652938	-2.76147949202591	-3.70720216114172
O	2.68479321640694	0.37344376590371	-3.60180510179691
H	3.27190259492857	2.31335237503087	-4.05973775303961
H	1.90627220411665	2.18704015484918	-2.88515636526780
C	1.85203626621435	0.21695257239407	-4.73610375730053
C	0.35894302633991	0.07131814234461	-4.44727417204788
H	-2.35467914942042	4.11619538120058	-1.02112641012036
H	-1.68681607935933	2.70195900772089	-0.10640953314327
H	2.19349450060045	-0.70374295824878	-5.25597889974026
H	1.99216231329188	1.07562862946193	-5.43860389797571
H	0.00112985332693	0.86977227113374	-3.75535788660410
H	-0.18580783298423	0.19231896489706	-5.41776157265207
F	-1.94278225125118	0.97907033277712	1.24667175859145
C	-4.21361075410421	0.14798844643800	4.27254867635235
C	-4.14449359466689	1.43621857809973	3.43862910794544
O	-3.04918178848219	-0.67458032476442	4.22673093219509
N	-3.34574053440930	2.51795713173377	4.03016495921815
C	-2.91128238584823	3.48601187929012	3.02067471119239
C	-2.90847685666720	-1.47072844537362	3.05580824943795
C	-1.77633964565257	4.41313282500820	3.45307218019458
O	-0.60301242389463	3.65404841471506	3.66791793597752
C	0.53977626405519	4.37044993207078	4.09651095400795
C	-1.76655013572458	-2.45118647065358	3.26963163843111
C	1.67661067062942	3.39030061868976	4.32831196274167
O	1.35338360318632	2.57390849637332	5.45469890892362
O	-0.55070329293506	-1.73390236198414	3.38117485861005
C	2.39812469357210	1.71724193364228	5.89765904779699
C	0.57088843691371	-2.48721130090035	3.79993553608981
C	2.63277302394855	0.44079333050961	5.08077082621897
N	1.55863919570300	-0.55420130242308	5.10984898909451
C	1.75375258656288	-1.55749409983162	4.06324979419108
H	-5.09665787240947	-0.44248955267446	3.92386392839602
H	-4.36114686906231	0.38212299996065	5.34588913730296

H	-1.61196107134463	5.16618012089786	2.64128105513625
H	-2.03468905569625	4.99472859860995	4.37420156072645
H	3.36510832609316	2.27828341776208	5.91721984286849
H	2.15224625975569	1.48042535681602	6.95441331565283
H	0.87359125789148	-3.21510310757661	3.00651324742695
H	0.30828717273994	-3.09585081615062	4.70221872471403
H	3.60968916637789	0.01134229820542	5.44386406206144
H	2.75803286291311	0.72158982813752	4.01026595093738
H	1.97025147195831	-0.99446322844580	3.12775786210999
H	2.63734670432710	-2.22063136244178	4.28220227755643
H	-2.56552130161620	2.90138719740652	2.13806121920804
H	-3.75790302936682	4.14598189203052	2.68184702376069
H	-5.20245704686369	1.76715288677009	3.24785927366587
H	-3.68812546319757	1.20059034611190	2.45154248557694
H	-3.84242423426395	-2.05692435180734	2.86600906639584
H	-2.69666293445490	-0.82725204144608	2.16589942381352
H	-1.72859887654216	-3.16523802725683	2.40875021604291
H	-1.94603287299550	-3.04727930805754	4.19893567300338
H	0.85536985763820	5.11001107689980	3.31855993765829
H	0.31464888835591	4.93676061541886	5.03462364783324
K	-0.62427416451369	0.97338450884659	3.67124220875715
C	-3.93121794467079	3.13692470013820	5.22252373941839
C	1.20304607184317	-1.07378372006911	6.42560973001813
C	-3.07960584256880	3.04151173600844	6.48975082242243
H	-4.91969514535320	2.67927632333630	5.44937514100851
H	-4.14219253462221	4.21671080774023	5.03324453972998
H	1.73976787388789	-0.49611281347563	7.20742133978451
H	1.53667484747102	-2.13486028302678	6.56397328096112
C	-0.30819460606336	-0.99063494626392	6.71572281929237
O	-0.81320070342005	0.31642795719898	6.51237123110126
H	-0.51231473307303	-1.35071158991093	7.75302683305260
H	-0.87609169494093	-1.64255192977794	6.02223791449790
O	-3.22640280566635	1.74045876291984	7.03866052476856
H	-3.41792245464676	3.80624266496699	7.23489385535085
H	-2.01759232483121	3.26219864243936	6.23624839531832
C	-2.32882641171834	1.39471077955312	8.07667968678317
C	-0.87951213761271	1.20083163304433	7.61345247781213
H	2.61015014595827	3.97205409948454	4.53011267371762
H	1.82660696468199	2.75454133061014	3.41873871072876
H	-2.71956722596389	0.44217662789145	8.49084705633596
H	-2.34603918532640	2.15571959303488	8.89953776019037
H	-0.42597766674176	2.16418527371387	7.29215722975849
H	-0.28068522246178	0.83652442296463	8.48241980711361
F	1.70449014780309	1.04605007190557	2.23862446015497
cryp (KF)			
C	3.35694644764549	-1.89537307534599	-0.00843195177309
C	3.71440715554504	-0.46259661678241	0.38532460216960
O	2.05459714457995	-1.96074426929443	-0.55730146503997
N	3.46435059865876	0.57425093036056	-0.62058103585808
C	3.76447196347107	1.90382410833759	-0.08532920225620
C	1.49710607612903	-3.26639058261730	-0.57414370430013
C	2.83415062042894	3.04795106036247	-0.49563335116679
O	1.50637483819876	2.73997700078157	-0.12976135532459
C	0.60817455296746	3.84731434910878	-0.19121811836288
C	0.21989906721758	-3.26928261428822	-1.39866373599886
C	-0.82591421501291	3.36258948179530	-0.23197988474270
O	-1.10260271579519	2.88023533847514	-1.55665317048342
O	-0.66081499992496	-2.29246829878057	-0.88996123746973

C	-2.47602683941811	2.60198197901002	-1.81006862333211
C	-2.01683549939799	-2.40539110662861	-1.31057437371274
C	-2.98930693562800	1.26527129200110	-1.27512858525262
N	-2.41137361155536	0.05570587841954	-1.89684018296245
C	-2.75430837042650	-1.09726368353312	-1.05159599630459
H	3.42782643136545	-2.51351985116744	0.91856294640616
H	4.09611274532197	-2.32593646679781	-0.73008477895212
H	3.19166596496218	3.96455285849282	0.03695397198817
H	2.88975004451977	3.27237965318214	-1.58719899294944
H	-3.11255897591317	3.40586901423206	-1.36716150437446
H	-2.59328770213976	2.68783526629740	-2.91395240811533
H	-2.52330223965895	-3.20812376938960	-0.72122783099510
H	-2.06364845711483	-2.71876968821773	-2.37840700853194
H	-4.11004012163695	1.27576654600236	-1.37164806851399
H	-2.71794599174914	1.19952581588388	-0.19071229663287
H	-2.52342949056535	-0.78397043433068	-0.00527712520518
H	-3.85370649768490	-1.32568930794925	-1.11780814206650
H	3.70719081184006	1.83885591303242	1.02038273304343
H	4.81676477113070	2.21389255592507	-0.32518955445498
H	4.78960187038528	-0.49164181602951	0.71512750862624
H	3.11898127477359	-0.19284206426693	1.28324913137715
H	2.21033577134305	-3.99920436660040	-1.02456065957944
H	1.28168247973282	-3.59647358447154	0.47083077864831
H	-0.22207241503904	-4.29452878829889	-1.33402719093357
H	0.45170450346005	-3.06482195177765	-2.47314839888066
H	0.75571457291333	4.49996327809328	0.70346628470229
H	0.82204043498337	4.45755259612153	-1.10181718820700
K	0.34366049144091	0.29835047454166	-0.73734935120898
C	4.04990016846953	0.28437807387812	-1.92260315304961
C	-2.74224723950175	-0.07311276351307	-3.31024365093351
C	3.44870888490796	1.03774806271066	-3.10939989671246
H	3.90180526605807	-0.79298097843011	-2.12914998639262
H	5.16032720019533	0.46955775243072	-1.93898109981922
H	-2.90299376734280	0.94732774784033	-3.71251683563892
H	-3.71935853017146	-0.60667363326009	-3.47511866046581
C	-1.69873543440401	-0.76500964595330	-4.21433039139241
O	-0.34773369507389	-0.38065913248000	-4.02658364777476
H	-2.00855857629985	-0.58494503649633	-5.27632042383579
H	-1.70041046601180	-1.86232894128737	-4.06677400977481
O	2.04842624898885	0.85015035541599	-3.14559901632127
H	3.92522702598701	0.63001188865650	-4.03463030681139
H	3.69791429247410	2.12737307041391	-3.08240337276286
C	1.46016738165125	1.14471073283818	-4.40127341652502
C	-0.04509007613634	0.97394723587752	-4.31807886787018
H	-1.49373444371239	4.23005743911964	-0.00925786597658
H	-1.00970142002907	2.54835179601448	0.52471268991707
H	1.88123178500963	0.46992254294259	-5.18679861206791
H	1.67707511807361	2.19834907237926	-4.70561103026247
H	-0.44817979429729	1.65906431817847	-3.53793037793727
H	-0.48019903444791	1.27385720931050	-5.30456576849650
F	-1.35759644874032	0.69640977952477	1.07080621788548
cryptand			
C	2.51244980095501	-1.61346109551770	2.06095010020656
C	3.26021635521908	-0.32213430223101	1.74407767057772
O	1.17825340263865	-1.33823361227785	2.45536840186307
N	2.95029698107037	0.27310506890478	0.45125316686303
C	3.03076713985661	1.72943316648502	0.42019807069922
C	0.38454643746000	-2.50149914300352	2.61180743440195

C	1.70314496244631	2.40997407391811	0.73877093838573
O	1.40901275719581	2.22444277491305	2.11763925036226
C	0.11121492798980	2.60848167461885	2.52530365484466
C	-0.25194809055494	-2.99611634658950	1.31761602885878
C	-1.04188954908746	1.74906698577549	2.00113088659999
O	-1.44545944823097	2.16524331875666	0.69500303682183
O	-1.37083150700012	-2.19442972300630	0.99728765151194
C	-2.82839702753181	2.04399267047776	0.42653576558336
C	-1.90018979109421	-2.47787873825348	-0.28882803207814
C	-3.40066879093340	0.62198399660342	0.34586475830262
N	-2.91446290535457	-0.22335014068612	-0.73643297023826
C	-3.15946283066997	-1.65023395475849	-0.51647127568095
H	3.04664771808669	-2.14328341962220	2.89060646050346
H	2.53200321658321	-2.30230286213240	1.18168478715593
H	1.76678309625509	3.50460374888450	0.50956627225000
H	0.90929228527294	1.96606353291460	0.09924976036872
H	-3.41931178447381	2.57927973279764	1.21369913194858
H	-2.99594374800075	2.59719236495311	-0.52096014405409
H	-2.15976049813388	-3.56605711249323	-0.36139706383134
H	-1.14884597290734	-2.24334479671258	-1.07962833381434
H	-4.52180729320976	0.74257996737881	0.31485578657065
H	-3.17502520438521	0.10188654273873	1.29887550910853
H	-3.83516188399352	-1.79538674279406	0.35678787840869
H	-3.70158968241072	-2.09311450230933	-1.38241939431355
H	3.82229465936642	2.12032454660208	1.10848482878045
H	3.32626795697891	2.06276363210004	-0.59467792984339
H	4.36143923794974	-0.53443208519262	1.84894751745737
H	2.99658653170295	0.40883712859896	2.53246262899749
H	0.98422385491866	-3.32982518184746	3.06292704009510
H	-0.42526360114996	-2.24711050519059	3.32718285428447
H	-0.56516615765003	-4.06514952364998	1.44308550756999
H	0.49837526560625	-2.97454679243457	0.48841508892275
H	0.12240309988884	2.52493094901760	3.63240285832439
H	-0.09017537608100	3.67853757929539	2.26408914172827
C	3.54572406921727	-0.43127129680416	-0.66951350979799
C	-3.25479069343596	0.24981144142901	-2.06605820146513
C	3.01486227744503	-0.03178589328858	-2.04485686476133
H	3.34778955992308	-1.51525945055107	-0.53125559104453
H	4.66958024350713	-0.32832341275400	-0.71443409392796
H	-3.01031715031712	1.33036576445784	-2.12527915029404
H	-4.36028256498815	0.18069041969644	-2.28640763800794
C	-2.54631504607689	-0.47546718327573	-3.22166330526530
O	-1.13983931937254	-0.58418172816904	-3.12986224662427
H	-2.84089390069621	0.05037652336465	-4.16669663987253
H	-2.91066431286070	-1.51906704672514	-3.31361754008279
O	1.60895740041467	-0.12289513335533	-2.08371434728537
H	3.49237948093590	-0.69345703223909	-2.81128670824494
H	3.33227883700909	1.01075931605010	-2.30385437164006
C	1.03699286806903	0.44488307193614	-3.24397223066928
C	-0.45369987728729	0.65334490514583	-3.05563767174018
H	-1.89816200487419	1.87436085163879	2.70863091928111
H	-0.74197631780576	0.67543837704341	2.00304279128325
H	1.22260296386593	-0.19474976580237	-4.14240637204450
H	1.49795570495738	1.44428182432778	-3.44724540137119
H	-0.62405735467934	1.14907927674446	-2.07145087045035
H	-0.81133340753830	1.34097329609846	-3.86431568047819
PEG			
H	6.73230724589164	-8.75036333836847	2.41812308891941

H	8.19748846705562	-9.46731817929294	0.07227447943595
O	7.37114143923469	-9.32235811154111	1.93146827364539
C	7.71079721188547	-8.69813311303644	0.71023925990706
H	9.59022586259129	-7.86794345713010	1.41433460261597
H	6.80515078100220	-8.34137846822265	0.16293772615312
C	8.67865836511093	-7.53266941748342	0.85992643460124
H	9.00725331033280	-7.19225388430623	-0.15481232884090
O	8.04070264887850	-6.47532473880875	1.55490191680044
H	4.03641043229195	-8.47659741994792	1.58549680026327
C	3.96271236306966	-8.08108396949725	2.62501206866664
H	9.79216762774517	-5.60611753654178	2.28958699130737
C	8.86537800985152	-5.34249560235882	1.71999912221434
H	3.03632916722996	-8.49799387394492	3.07803944849761
H	4.83034796226762	-6.12497329208251	2.22184509299454
C	3.87215864806134	-6.56016503791572	2.58567109275043
H	9.19061315879871	-4.94586249061615	0.72622432626661
H	7.74798817597766	-4.66593067129721	3.44615140093697
C	8.13330004350273	-4.25541031721588	2.48115845925986
H	3.69938956231352	-6.16463032455732	3.61421507659681
O	2.78309696610885	-6.22878843698412	1.73083559125543
O	7.07066648282495	-3.74681409227639	1.69941428294333
H	8.86964877117063	-3.44997590847532	2.72927353475253
H	2.02637117242409	-4.74909415702153	2.99653462445383
C	2.20923007318769	-4.94809291693020	1.91198579566165
H	6.20985249596559	-2.87609363239381	3.39600682742188
O	4.15932391481593	-3.56239125710879	2.11483151178791
C	6.36648326169722	-2.68189076208726	2.30764794397148
H	1.22462728619912	-4.98157868496220	1.40178152354322
C	3.00827645553325	-3.79070620631208	1.32617306659681
C	5.01200637056441	-2.53723907224628	1.64146379409976
H	6.93768496919759	-1.72397589523037	2.21576705728765
H	3.29356657729424	-4.02554136381517	0.27176629416122
H	5.14192663194980	-2.60674884424037	0.53462713824793
H	2.35280935457367	-2.88147850814022	1.30108160907100
H	4.58383188876697	-1.52881590229041	1.86975345003971
O	5.11553295654292	-8.44059911270842	3.39512644510541
H	5.01466388809008	-9.36407200261150	3.68514617660713
PEG (KF)			
H	6.68908848411109	-9.03323839457897	1.06849693345549
H	8.46588281348158	-9.22527768301371	2.17175763890740
O	7.40576506919691	-8.54333180807507	0.51458761553809
C	8.63012557646845	-8.76251989466051	1.17049859502023
H	10.41261109318625	-7.68957284608557	1.78939724955774
H	9.28758636949021	-9.46199456889399	0.59412852802846
C	9.41103493239889	-7.47134711801981	1.34409513777903
H	9.57841697585666	-6.98918041856354	0.35009062993732
H	3.09242045871057	-8.87283342488466	1.10585068739941
O	8.68617120791296	-6.57117846198538	2.18600586687978
H	1.90087263910180	-9.24264472639176	2.39048790276075
C	2.67892408074233	-8.50138224211854	2.07477603511842
H	10.26189968867205	-5.43066684119725	2.96415902761460
H	4.49232237889113	-8.92402079032373	2.73508261171487
C	9.33471511936201	-5.32796589869962	2.34702460477212
O	3.68984308403091	-8.35278927222320	3.03824708785798
H	1.58858498403545	-6.78599020587052	2.81252559591038
C	1.96437254722950	-7.18291135844473	1.83901363820875
H	9.64030867617885	-4.91690033365463	1.35406246368706
H	8.07102013566425	-4.73097781795475	4.01615138100741



C	8.40132391467164	-4.34340164710366	3.02181809260780
H	1.08640516679727	-7.33109095670705	1.16438545206900
O	2.86757559271670	-6.23410008881909	1.26336418088718
O	7.28161225899701	-4.11645677702231	2.17689119110524
H	8.95595449596914	-3.39108380639962	3.20132977280276
H	1.96628741213320	-4.62520286185248	2.22963494116109
C	2.33574964198160	-4.92749178076089	1.21957256494403
H	6.07920032447633	-3.10788628781893	3.56610361329324
O	4.46082698881486	-3.93447137882824	1.70751414387886
C	6.49454204001184	-2.99396516341878	2.53493778624687
H	1.46803469447667	-4.86597780991611	0.51610381938797
C	3.39729593771150	-3.94817227051803	0.76425293952805
C	5.36312869998760	-2.85545498478195	1.53902727209963
H	7.10985585058948	-2.06135777488730	2.51984973439540
H	3.77974290361343	-4.22439900766143	-0.24855896360313
H	5.78039227010251	-2.84396363801832	0.50306098657092
H	2.93227920117663	-2.93636815225247	0.68272851269052
H	4.84349982235064	-1.88032553615490	1.70581125947560
K	5.72384889547112	-6.68648808867646	1.89331138335415
F	5.71415757322896	-9.40103788276203	2.09294208594955
PEG (CsF)			
H	6.79543468567343	-9.22804778564166	1.18792919383149
H	8.42265794943711	-9.04573645009370	2.69509391893320
O	7.58268355115658	-8.68256837810314	0.80892957998922
C	8.70505783614117	-8.81950065593004	1.63656298445017
H	10.53146570327129	-7.73347553853709	2.11063230022423
H	9.37286249381816	-9.65830331057142	1.31019777469053
C	9.54942133694716	-7.55406256267292	1.60904140274206
H	9.74979310602992	-7.27528503785567	0.54722646081314
H	3.05707784456119	-8.69023959550393	0.59847348116981
O	8.86118524927414	-6.48084230593005	2.26045878161146
H	1.68056579547015	-9.36055970153542	1.52898063705529
C	2.50597842322372	-8.60401477032028	1.56657857935735
H	10.47919532281920	-5.17350910600300	2.49355496085495
H	4.20100643752144	-9.30446979998643	2.35928116552002
C	9.45391132141206	-5.21674445147838	2.04819904164312
O	3.35277025505351	-8.80896064421996	2.66717304732314
H	1.39689291154470	-7.09523582527612	2.64724118701939
C	1.84006216860476	-7.23745574370481	1.63213258906604
H	9.55826028515629	-5.01254775283246	0.95455175535848
H	8.44867899848124	-4.34778518261745	3.76644667581952
C	8.61597082277197	-4.12408274165982	2.68377945733098
H	1.01220798345744	-7.17613233134555	0.88308665625641
O	2.79454969102416	-6.20093964013503	1.37368691853660
O	7.37416630118856	-4.00027704695203	2.00247018393203
H	9.18532364067399	-3.16401399012196	2.62667920860482
H	2.02808840228856	-4.73677286105058	2.65187955121830
C	2.27683994857570	-4.90205561441059	1.57433964414948
H	6.32498610426579	-2.99004402094026	3.51005008217620
O	4.42979868067063	-3.84547201479820	1.92391025969257
C	6.59221742722891	-2.89661429472386	2.42823865256321
H	1.33233117575194	-4.75861667978069	0.99352470753198
C	3.26521827968587	-3.85190238320533	1.10521997092746
C	5.33154315384926	-2.80127669092977	1.59171071272392
H	7.16577718853905	-1.94435734871069	2.30916144439503
H	3.54479695676579	-4.04462391196555	0.04135319810839
H	5.60432107497450	-2.84759670764147	0.50953220598091
H	2.76087886372789	-2.85512788587685	1.14664960167683

H	4.85554537868191	-1.80616812783779	1.77514886828310
Cs	5.71603326400595	-6.77970349289829	2.45915577469025
F	5.56810398627491	-9.67028761620178	1.90226738374891
TS-SN2 (PEG-KF)			
H	6.49161122007550	-9.11826291817228	2.49250472306201
H	8.64463877169144	-8.90095766289782	2.75164903445420
O	6.84564994148072	-8.55289204040102	1.74037795203257
C	8.25599818558528	-8.64582381032423	1.73790421495749
H	9.99305100865328	-7.44809432685702	1.27939895146310
H	8.61486777438262	-9.44451575156351	1.04297984371009
C	8.88149409983585	-7.33375413671389	1.29672821639831
H	8.55204702204436	-7.07694765437923	0.25930113643912
H	3.68537779545799	-8.59779149862307	1.35328052809149
O	8.49371524009285	-6.30334824743878	2.19547490327227
H	2.38373320811178	-9.31872878801197	2.36080056339392
C	3.04497670631927	-8.42445136104567	2.25321166390481
H	10.22879213537265	-5.13723014813258	2.26720902675200
H	4.49554288151871	-8.91686888525913	3.55175687337884
C	9.15332271759229	-5.06674739497453	1.97395909299061
O	3.81680233399965	-8.18987297604611	3.41058478909547
H	1.57123421724255	-7.01086352272715	2.93915660028478
C	2.15356424349537	-7.22022693053707	2.01034997701279
H	9.11241221190575	-4.79596202072288	0.89030542226990
H	8.43715854473726	-4.28143826903351	3.86754891948721
C	8.48574103617753	-3.98291294894749	2.79417773859490
H	1.42928871820990	-7.43407190510237	1.18763628310607
O	2.95406388126028	-6.08482553425479	1.67958728289572
O	7.17783746075561	-3.76078845200941	2.26331207804478
H	9.09400281619526	-3.04896942721090	2.71951347955910
H	1.92700020544124	-4.73389874275515	2.88705317018485
C	2.27415407024741	-4.85213247907000	1.83225168517187
H	6.24130644215890	-3.04394651794162	3.99146578174127
O	4.31131444867899	-3.68341544298466	2.33153963443240
C	6.43964432120162	-2.75037008577150	2.93312414332973
H	1.37160511419448	-4.80685110830265	1.17444874107868
C	3.18872932564101	-3.69975171658989	1.46502134480357
C	5.13619989889371	-2.53431921678238	2.18949902646077
H	7.00650946571509	-1.78730910891184	2.94328649828056
H	3.52181818223579	-3.79133463651689	0.40229293370603
H	5.35300591818191	-2.34466529333153	1.11100648508099
H	2.60480951890225	-2.75112690583402	1.55449688025266
H	4.62006447555619	-1.63225327878947	2.59871804919372
K	5.65718774279247	-6.16369837558087	2.74414333037121
O	6.10496936907016	-5.58020961072407	5.32942514246480
H	5.72032604740470	-8.07128046105278	5.32883448068004
H	5.54318849806690	-5.65721799417245	8.14419955865520
S	7.16763632702752	-5.79184132128588	6.38334351083474
F	5.87085193022979	-9.69392112163641	3.85495091396838
H	5.88836317768979	-9.91661244690223	6.99127859891368
C	6.49687274116133	-5.14176584770514	7.93174333380739
H	6.34000393134312	-4.05583078640850	7.79732208279404
C	6.62672950888444	-8.68225909219006	5.37466628308230
O	7.36421586441827	-7.30001008309887	6.68408097460892
C	6.76249897324728	-9.82728350044583	6.32029912432902
H	6.86182746446598	-10.76152200545332	5.73434394922351
O	8.45422600530168	-5.07683617871675	6.12954726334450
H	7.45918133864776	-8.41828349627172	4.71497436004790
H	7.23870098987866	-5.33482309665632	8.72795884318915

H 7.67768453112783 -9.70437343673067 6.93141458131661

TS-E2-anti (PEG-KF)

H	-4.64551	-5.86216	-0.32721
H	-5.64177	-3.65991	0.29600
H	-6.78940	-4.72560	-0.61256
C	-4.70237	-5.04624	-1.08378
C	-5.84768	-4.12868	-0.69529
O	-3.50600	-4.29143	-1.13477
H	-4.91890	-5.51861	-2.07221
H	-2.69329	-4.84507	-1.00579
H	-7.98968	-2.62081	-1.29466
H	-6.75088	-1.71150	-0.33684
O	-5.99322	-3.11151	-1.68391
C	-6.97673	-2.14891	-1.33827
F	-1.01955	-5.10862	-0.60832
K	-3.32687	-1.66031	-1.89316
C	-7.00040	-1.04894	-2.37991
H	-7.86910	-0.37939	-2.16966
H	-0.83775	-3.93077	-1.82228
H	-7.14074	-1.47885	-3.40159
O	-5.78669	-0.31480	-2.30822
O	-0.90616	-3.13734	-2.42057
H	0.58182	-2.11145	-1.35519
C	0.31222	-2.42292	-2.39363
C	-5.76643	0.88188	-3.06485
H	-6.66041	1.50907	-2.82626
H	-4.46428	1.79878	-1.60532
H	1.16322	-3.02922	-2.78818
C	-4.52061	1.67007	-2.71219
H	-5.78938	0.66350	-4.16091
O	-0.84552	-0.35471	-2.74015
O	-3.36803	0.98683	-3.18471
C	0.18693	-1.18342	-3.25848
H	-2.05773	1.70103	-1.72290
C	-2.15537	1.64353	-2.83311
H	-4.58837	2.68270	-3.17937
H	1.16219	-0.63777	-3.26317
H	-0.04768	-1.47200	-4.31228
C	-0.98221	0.88238	-3.41366
H	-1.13938	0.72118	-4.50836
H	-2.14728	2.68354	-3.24043
H	-0.05726	1.49930	-3.29330
H	-1.60924	-4.61917	2.27524
C	-1.03970	-3.87662	1.68936
H	-0.00257	-3.70965	2.02531
H	-0.97596	-4.52022	0.45867
C	-1.74012	-2.82598	1.09189
H	-2.76227	-3.02847	0.74041
O	-2.47092	-1.35947	2.34772
H	-4.28991	0.35168	3.69630
O	-4.84583	-1.38283	1.44313
H	-1.18432	-2.04715	0.54793
S	-3.58522	-0.58296	1.61107
C	-3.94812	0.78216	2.73806
H	-3.02501	1.37347	2.87489
H	-4.74611	1.38944	2.27220
O	-3.08599	0.02349	0.31834

TS-E2-anti (PEG-CsF)

H	6.79485575502199	-9.18279428996845	2.04109955486241
H	8.71084756773868	-8.26898834002997	3.26509699850401
O	7.24112788548620	-8.33948404638110	1.76047737095606
C	8.59745014174409	-8.33228750316493	2.15373986051443
H	10.39889963117295	-7.20672246329764	1.75631426139399
H	9.13289764433520	-9.25364548824917	1.82032823656217
C	9.30718707399758	-7.14794580213466	1.52226391998768
H	9.18737768381162	-7.19043694383661	0.41208305189937
H	3.39549022725687	-8.38562009659502	0.38336211811642
O	8.76179276597190	-5.92991895803779	2.01868703306815
H	2.18670118158292	-9.15646113089164	1.47151829376551
C	2.92561800350329	-8.32175588936566	1.39435834899250
H	10.41541329436298	-4.68439666322121	1.72438594281742
H	4.44457191668827	-9.19951005293697	2.35282338927078
C	9.33781561920839	-4.77656353588481	1.43838466875791
O	3.88900097410045	-8.37821112255347	2.42480985915267
H	1.77381513597506	-6.89408638536928	2.53634038674217
C	2.14984289547056	-7.02089138916245	1.49250115504556
H	9.28823181680761	-4.83165430542537	0.32310317762450
H	8.55625533106879	-3.52444136823905	3.02645910048079
C	8.60547417483636	-3.53479529194620	1.91003035142711
H	1.26453216880940	-7.06430029786793	0.81210905928783
O	2.98387782044781	-5.92054147469559	1.13320567945495
O	7.30055117757540	-3.50933417683255	1.34710993660501
H	9.18479932578182	-2.63476540861884	1.58815355040286
H	2.13273016722686	-4.44441935362830	2.34832503543535
C	2.34599152817245	-4.66432699120565	1.27294342203658
H	6.37316920273785	-2.26641368506954	2.75857332326112
O	4.38841784565175	-3.37763536135257	1.43920789966598
C	6.55614340042185	-2.34390860615183	1.65767607593144
H	1.36611429770730	-4.65795634674478	0.73542859501130
C	3.20536067163551	-3.56661716711670	0.67677415359366
C	5.23602908068396	-2.37006741011820	0.91152537805829
H	7.11540187012697	-1.42594027377755	1.34990480252120
H	3.46542621498951	-3.82852796547320	-0.37698442312530
H	5.43243162707503	-2.55534139051906	-0.17190718488343
H	2.60505670656803	-2.62352695584485	0.65256103636475
H	4.75210683457597	-1.36559076971233	1.00059764643588
Cs	5.68867074168613	-5.86639897812703	2.99417438330396
F	5.68869281706195	-10.35978941022255	2.61272752629610
H	6.67996615437322	-10.90385638359261	5.47480764327687
H	4.81396513086986	-10.91796227084293	5.48877016295351
C	5.74089701297240	-10.38486398138645	5.21894065624871
H	5.72066950611830	-10.37633550188236	3.82164461876054
C	5.72801585708388	-8.99276000384666	5.16713472667276
H	6.65831370543153	-8.46359895001557	4.91006314415711
H	4.78549274901455	-8.48350634449330	4.91511029143632
O	5.74390103439961	-7.98889682446179	6.98565490266669
S	5.85559472999086	-6.47328510560767	6.70925357671449
O	4.60284019549896	-5.89607912789199	6.10557827480091
H	5.14350286525541	-6.03502333941375	8.95154516481942
O	7.09866573037127	-6.13065271715184	5.92444455363353
C	6.04031622648147	-5.76873511140113	8.36292532309337
H	6.95412887003932	-6.19406796592650	8.81542963633452
H	6.12771001302196	-4.67287328231476	8.24569434883211

TS-SN2 (PEG-CsF)

H	6.68762295581351	-9.23958957720123	1.92501960196028
H	8.48335536842395	-8.43290567998613	3.26538467985572
O	7.20591651206864	-8.44706995402316	1.59360876305699
C	8.50601244026879	-8.44770795086853	2.14764033208057
H	10.33521199896169	-7.30442953863898	1.98826340609224
H	9.09296856725866	-9.34620556239514	1.83386653863790
C	9.26782149420943	-7.22613700056815	1.66621480394742
H	9.24409763561204	-7.18597994078714	0.54999728442518
H	3.62990011158594	-8.37882334151469	0.25086079230642
O	8.68157748176742	-6.04214974523338	2.20057214975441
H	2.26847243327278	-9.26572088982424	1.02201162745874
C	2.97922134997243	-8.41330876084047	1.15860553423075
H	10.35010136352731	-4.78870108178124	2.06464378835320
H	4.38317237660142	-9.30356610262370	2.29204425711054
C	9.28218980782387	-4.85257787209990	1.73657787450595
O	3.73137411569148	-8.53826708815671	2.34236329695398
H	1.58631024535913	-7.11810730166564	2.17875268322411
C	2.15212711400087	-7.14199952583334	1.21602329464039
H	9.27108824956718	-4.81357105033932	0.61916982889721
H	8.47086256067199	-3.72326156158869	3.40098875760466
C	8.53687567119250	-3.65205140137387	2.28744456633105
H	1.41006099763293	-7.13557599886050	0.37932991943784
O	3.00145899818406	-5.99966481498609	1.11741954767447
O	7.24113951461683	-3.59262516087032	1.70962037345362
H	9.11502592905880	-2.72686583272615	2.04296896403545
H	2.01658478410504	-4.64550382691707	2.37207823096320
C	2.32197740120846	-4.77334899087509	1.30397095279665
H	6.26673181744300	-2.46869760638659	3.18755153384334
O	4.32625453903704	-3.47411613303667	1.71305705479284
C	6.48428122207107	-2.45819652099790	2.09018943461122
H	1.38914872279881	-4.73981087089627	0.68958401371890
C	3.19565560638185	-3.61448844568890	0.86546473523137
C	5.19055371057035	-2.42768180178784	1.30070311462551
H	7.04812640240622	-1.51648642652727	1.87552264017734
H	3.52603813999478	-3.77988769462016	-0.18821247196080
H	5.42809017325501	-2.52720091476964	0.21423511780954
H	2.57910020178904	-2.68141838041784	0.88372881449368
H	4.69909560754273	-1.43384562788730	1.44911885213857
Cs	5.61318289783508	-6.17912750159277	3.11482316925919
O	4.98911343399260	-6.98813390847832	6.21401085824324
H	5.85433404661141	-7.85377935898729	8.83999753018580
H	4.84761610331212	-11.59687299944389	5.78652839508741
H	4.78769890701122	-9.45067720778281	4.44399658822238
C	6.70142744206981	-7.58267943702861	8.18428394516502
H	6.95313990836363	-6.51127396897994	8.28720541927421
C	5.55729352876322	-11.49843521056591	4.94284269045707
S	6.19351305718964	-7.85148541891595	6.47176356155996
C	5.68718991293765	-10.06778104742625	4.54237524422864
O	5.86257329191807	-9.36552987754390	6.45248383931081
F	5.61348988951709	-10.28449962706991	2.58384904877363
H	5.15382644168766	-12.06487156792449	4.08052316781717
H	7.58181442521402	-8.21854663961760	8.38650133242339
H	6.52947451106074	-11.93603932997116	5.23381960815264
H	6.66333770935879	-9.61244157881044	4.36009737439671
O	7.36394087141025	-7.52305934426554	5.58188353817229

TS-E2-syn (PEG-KF)

H	6.48483333738486	-9.38577300652228	1.60537840870788
---	------------------	-------------------	------------------

H	8.52278197437474	-9.12621297433150	2.43202070988442
O	6.98301442074828	-8.70203131448135	1.08148595059305
C	8.36078670018889	-8.87128094424404	1.35920608941031
H	10.21743808159233	-7.78399520248449	1.19737958000593
H	8.80687168343767	-9.69159460401233	0.74502018226502
C	9.12479747943603	-7.59649936454045	1.05331085116816
H	8.96996584043181	-7.29694532765981	-0.01300748228407
H	3.45997445516979	-8.69243173128561	0.96627248393466
O	8.67466191751211	-6.56623594702454	1.92055687105995
H	2.20442625639742	-9.28308088860391	2.10547183682356
C	2.94228744955411	-8.46309996680004	1.92932683468633
H	10.44648759647537	-5.48991214592128	2.19725567092026
H	4.46693524170842	-9.12396845497781	3.00737000195053
C	9.40081110657181	-5.35501300127853	1.82624538288643
O	3.85740631757273	-8.33464639392472	2.99832191064835
H	1.69876911366375	-6.91233467167332	2.76711256282705
C	2.16678956115789	-7.16827257500852	1.78576850601960
H	9.46022479809797	-5.01348592296135	0.76369997897528
H	8.54262963635827	-4.67284274957025	3.69938543306616
C	8.70615578677818	-4.29850638940965	2.66181050505343
H	1.34635191613087	-7.29394577058664	1.03799039044913
O	3.04656671320793	-6.12076649782182	1.38661344480062
O	7.46164878021072	-3.98508210687340	2.04689730347874
H	9.35438474898135	-3.39006142017363	2.71570254229642
H	2.12506354042384	-4.66561679928165	2.55680857900975
C	2.46897442391599	-4.83430140386308	1.50769623580412
H	6.45814319140790	-3.32695132225811	3.75989991833137
O	4.58519847113753	-3.83082193400266	2.01648103010151
C	6.71329734054264	-2.98715429908599	2.72887560690217
H	1.57779640287791	-4.73012312050243	0.84048976970145
C	3.47945394380790	-3.76906402365521	1.13228118051667
C	5.45333067129989	-2.70921587979571	1.93567625469326
H	7.30263704798201	-2.04092153436240	2.80842002402800
H	3.81678817100957	-3.90437419381576	0.07530730721678
H	5.72229474706439	-2.50080982745739	0.87234740958445
H	2.97250305607254	-2.77529833313153	1.19807105774587
H	4.95095936522083	-1.79962299424968	2.34541182947743
K	5.85468437593745	-6.42312107880824	2.38130169588354
F	5.63279497459163	-10.28284959798424	2.76281743872050
H	4.65139268291773	-8.15154306725789	6.93545970267594
O	7.20884994595463	-6.89734297571850	6.93985769257826
C	4.62633524193684	-7.22124237752873	6.33757220964935
O	6.60949845230850	-8.03488266282401	4.75347082504698
S	6.30653260715519	-6.88069981635275	5.75346193633123
H	4.30905855944020	-6.36740070843963	6.96456663789801
H	3.97717535642231	-7.34405396609457	5.44993369988961
H	7.01001564801746	-9.55677393439191	6.49968185217761
H	6.30703525481967	-10.47998942813963	3.75082878531035
C	7.47420596814239	-9.77761025506565	5.52756500280234
H	6.39049813073582	-11.60437635122057	5.23345665969673
C	7.09493947899693	-10.89149821532176	4.76862205448974
O	6.22530130243831	-5.58855003850442	4.97986621378093
H	8.43887439757255	-9.27656651243326	5.365111117417862
H	7.87295633670613	-11.34989397628136	4.13236426615021
TS-E2-syn (PEG-CsF)			
H	7.04691006989697	-9.47319570201633	1.31722516174276
H	8.68040425060238	-8.97464229041543	2.72007342740170
O	7.71907770374901	-8.91428325405940	0.85351468561324

C	8.90137494261205	-8.85059314446036	1.63453118306139
H	10.61840986644520	-7.57142847525481	1.91128892598775
H	9.61918170291589	-9.65607853785991	1.34244194245304
C	9.60662549873461	-7.51684457328497	1.44022542220877
H	9.74977947945941	-7.31809479380267	0.34947210776388
H	2.96040729603321	-8.67919290245525	0.65902774463526
O	8.84397183014507	-6.47909572597577	2.03713443343013
H	1.61377939629972	-9.29294405220385	1.67457317327100
C	2.42815338964727	-8.52800752757147	1.62891389003631
H	10.44118500701523	-5.21847674445926	2.50758821291998
H	4.02509291105634	-9.28375837022539	2.56366350948190
C	9.44860511921451	-5.19816579836457	1.99430425721240
O	3.30190348700339	-8.62867356360410	2.73448116894140
H	1.36712640954464	-6.94730642572396	2.63989394715115
C	1.76960011561768	-7.15942659694299	1.62029547900168
H	9.62289145080509	-4.88126466466782	0.93628252602785
H	8.30595389736175	-4.55815896397608	3.72121693886570
C	8.57005498431691	-4.18666350664371	2.70381112692299
H	0.90949886390896	-7.15882107998451	0.90637281254976
O	2.71391583387950	-6.15792634129996	1.25039588484136
O	7.38555183691085	-3.95308547933459	1.94217834398056
H	9.14611645875503	-3.23511300091554	2.81328404691549
H	1.97512098705128	-4.67346203446878	2.51682045784368
C	2.23282745643621	-4.84027017842075	1.44273265321357
H	6.24761380422002	-3.26330633322225	3.55737838632277
O	4.40039369862956	-3.86524873281492	1.85375409860479
C	6.54021944833760	-2.97003787300965	2.52127769664309
H	1.30330232809633	-4.66910706457405	0.84512508029101
C	3.26520791732295	-3.81824616186461	1.00606127429776
C	5.30191061165999	-2.78274047776017	1.66637755411998
H	7.07509241580626	-1.98987956723147	2.58399381402910
H	3.55970062718278	-3.99881252072691	-0.05730217574942
H	5.60163529579776	-2.70074841674008	0.59338404223231
H	2.78494734480627	-2.80950949028092	1.05137296929332
H	4.80690194220645	-1.82219206469275	1.95186729516993
Cs	5.77569158609535	-6.74085201910544	2.14966306309579
F	5.65753410004850	-9.95975281212343	2.33585817066471
H	5.75188983228270	-7.85181400525923	7.76805970525485
O	8.18512642641098	-7.22876707444382	6.37868549009052
C	5.67279952705411	-6.90765748807747	7.19775550681648
O	6.33448244252224	-8.16221671616143	4.92563701896712
S	6.83002966451075	-6.97719616904543	5.80568216195767
H	5.97018750535583	-6.05162207866155	7.83126619551045
H	4.65212869394609	-6.76904688450102	6.79800197668215
H	6.14602034010704	-10.00949321082075	6.32697587302010
H	6.10632619158849	-10.35222353499339	3.38934993904900
C	6.86960353363356	-10.09216990260799	5.50191460704902
H	5.80423102147905	-11.70845002990489	4.58708720675079
C	6.63796124491357	-10.99545679978080	4.45605268940465
O	6.63909765720383	-5.69298493467846	5.04420144290235
H	7.87277835771108	-9.69473137860595	5.71704766867093
H	7.52725619565270	-11.40145252991895	3.94203778538398
PEG (KOMs)			
H	7.51882053411127	-9.05903102356217	3.09825672242749
H	9.52955551337671	-8.09907187565416	3.36491296574743
O	7.85723111930103	-8.66422903692808	2.24007971650844
C	9.24446330091400	-8.44955192409851	2.34454411883329
H	10.78359993802458	-7.29886531915499	1.33925101312506

H	9.83028769399235	-9.38056271900144	2.14130566668752
C	9.67189745496103	-7.40727482011251	1.32899941733331
H	9.36788847367176	-7.72990329484130	0.30318954810934
H	3.10094168517036	-8.05624934731121	-0.15838319829156
O	9.05483920300653	-6.16272702941894	1.65251690560969
H	2.56700923219903	-9.39822217893438	0.90442327289772
C	3.17080722564583	-8.45999537998688	0.87519063813859
H	10.52662211281455	-4.99220053336672	0.73497150629906
H	4.58208471291027	-9.20638666205891	2.00550117222239
C	9.41505771461524	-5.09797969885642	0.79679998700701
O	4.53703232101583	-8.70687226409586	1.14080792185296
H	2.68201169674572	-7.82704543288398	2.89165238018556
C	2.54324140977130	-7.46814822890556	1.84542577164200
H	9.03882875918483	-5.27284705216168	-0.24135716407177
H	9.18233206819740	-3.68228592379602	2.40636749229443
C	8.84478430772366	-3.80895590076958	1.34979229615718
H	1.44567102198474	-7.38120031393032	1.64726574698915
O	3.16839675808199	-6.19530269543291	1.67775833048772
O	7.42538694072394	-3.83954006043206	1.28993158543560
H	9.24039699479952	-2.94612523221718	0.76038796369485
H	3.18657048310438	-5.55610694486333	3.66608854799326
C	2.79660923585759	-5.25031015097245	2.66518996211495
H	7.06187365977881	-2.75956746719270	3.03749101060801
O	4.75894345385223	-3.89697863228154	2.31798417482981
C	6.82856731166525	-2.73167110540317	1.94546646251552
H	1.68435071726812	-5.16984654243230	2.74227623618847
C	3.33633851989712	-3.89250414481961	2.26972283767799
C	5.33011743686790	-2.73979146764857	1.73480700778099
H	7.23226466791255	-1.77183536873928	1.53979082007372
H	2.99191156135678	-3.64790213833511	1.23664234465870
H	5.09599851253578	-2.70068361550897	0.64323552490356
H	2.93063268225456	-3.11334216623592	2.95955161890465
H	4.91142808516739	-1.81443838603824	2.20080951250342
K	6.10019868294746	-6.48327380300341	2.02019885772163
O	4.46020550660304	-9.74311911905407	3.66631868052646
O	6.78943605211414	-9.38909828326864	4.58217716405904
H	4.85958996354174	-10.43109762952375	6.42218504327076
S	5.33741547453195	-8.94755584243856	4.61404133187743
C	4.75574197160002	-9.34061276568898	6.27653997439215
H	3.69748596071343	-9.03099033173602	6.35118933081265
H	5.38345659600063	-8.78392065164390	6.99478521151343
O	5.17254527148561	-7.45153949525965	4.43541656775090
PEG (CsOMs)			
H	7.78963121719378	-9.33958907355074	2.76254903978551
H	9.39870404874569	-8.01424240982352	3.62476937400378
O	8.26276881919323	-8.80931611030228	2.05254938697939
C	9.49542814096777	-8.35775000232827	2.56746152348208
H	11.08179762321729	-6.99052218927785	2.01576324723550
H	10.26959851043732	-9.16546076449137	2.55431103393787
C	10.02573294838923	-7.21246875294400	1.72481031026955
H	10.02630093247812	-7.50976887548706	0.64723263857759
H	2.09832692687521	-8.17393737227585	0.33620961491662
O	9.21848919854978	-6.05008249593910	1.91145700158114
H	1.75879172582025	-9.25463952447641	1.72552067878821
C	2.42417438680752	-8.43336718269240	1.36766505208291
H	10.71326016158056	-4.75025110375400	1.24986794310418
H	3.99462465389626	-9.35424527183987	2.13449337790625
C	9.61935803669844	-4.94901671525560	1.12309442451997



O	3.77019057601236	-8.84643761375313	1.29930364232978
H	2.57245621543046	-7.43106780324449	3.29920399460390
C	2.18461747443004	-7.22748526933697	2.27182336756273
H	9.44720528973062	-5.14899247021812	0.03565437811848
H	8.98906919246159	-3.55947786433068	2.64942248503186
C	8.87487044582822	-3.69937593466494	1.54741923330053
H	1.08453968591578	-7.03886062824744	2.35027663165350
O	2.83253102018912	-6.07729733359187	1.72295597365219
O	7.49720246240250	-3.78092298197666	1.20351737169205
H	9.34337193659122	-2.81839747507313	1.04387330281670
H	2.97397176327929	-4.96909584914154	3.49470884454386
C	2.58720914807433	-4.88941785359407	2.44913826096959
H	6.82847315507240	-2.53567801772207	2.74102996984214
O	4.64902124145179	-3.75203821028811	1.91150472717617
C	6.77071109997465	-2.63909096313948	1.63035454519985
H	1.48828627492520	-4.69116281624723	2.51735735562600
C	3.23617209566820	-3.71247062130432	1.74881332425645
C	5.31921283489287	-2.72277666047492	1.20492648436696
H	7.20952887592094	-1.71293048622461	1.18370905477013
H	2.96700131003269	-3.73473194655076	0.66527339073856
H	5.24895668061818	-2.89053759818172	0.10202200353814
H	2.83054576683261	-2.76464508759155	2.17968127055456
H	4.84644808583990	-1.73264400052990	1.42016365417252
Cs	6.02621237290921	-6.70194660862118	1.68212110920769
O	4.42193504941377	-10.08601906983909	3.60699246260012
O	6.91508826653378	-9.98674480290241	4.04630497752048
H	5.31420702098614	-11.10637072892290	6.12746375654436
S	5.54190075546146	-9.45656302148660	4.41515384280135
C	5.26815350856640	-10.00217970010915	6.11580439177769
H	4.27191995934803	-9.64503146935845	6.43351663344689
H	6.06485772258310	-9.56677081861216	6.74547618298898
O	5.47801538177271	-7.94494045028199	4.41877872942522
PEGmet			
H	9.78600355168274	-8.81031697922058	3.64697341636147
H	5.33647246274495	-6.22644454224293	2.03745491346744
C	8.74564992375126	-8.81551802391479	3.26138247609787
H	8.21622572494617	-7.94494135255206	3.69504827895194
O	5.38828626625659	-7.16302286518227	2.32778457023876
H	8.24746248816867	-9.74128055057234	3.61119599532177
H	9.30341913104409	-7.44386650846034	0.10114921545663
H	4.95037160263189	-9.75900773428766	2.40964000481050
H	4.90535216856448	-8.62234567967598	0.12052685546240
H	10.47663514789697	-10.03765015100011	1.44217140784694
C	9.41303012643647	-7.48163217045936	1.21259900336690
C	8.71292972252470	-8.75673362991011	1.72489600500754
C	4.09888687203120	-9.12716462398402	2.73136607404749
C	9.42070572200294	-9.97194190454605	1.11283639885501
C	4.05385960082889	-8.00211344978037	0.46145011662203
C	4.13546262070271	-7.79450404944196	1.98208729193589
H	4.18049061098361	-8.96479607874123	3.82472183481775
H	8.89828833237105	-10.89760552376030	1.42386181547934
H	10.50737965303146	-7.52405731692447	1.44856811629557
H	4.09096717703453	-7.02894504589955	-0.06524775839924
H	9.17514634932294	-5.01940873128682	0.20824316668725
C	9.38242181471708	-5.12702679616698	1.30233609188622
O	8.83727936334622	-6.32828348800848	1.80263754573199
H	3.15755412145441	-9.67307297466621	2.51937522144485
O	7.37024673431156	-8.80027640431714	1.24722089388126

H	3.10884810650610	-8.51039617712381	0.17941939864273
H	9.39335412339519	-9.92120533352736	0.00544050937941
C	3.00507022473974	-6.87522036621815	2.47971574662009
H	10.49549630776128	-5.12184504801069	1.43015572590620
O	3.17448937197850	-5.61247913445755	1.85819048232354
H	6.83244403597895	-8.08643444386898	1.67632134904273
H	2.00542428984202	-7.31362603486372	2.24010726544092
H	3.27996542998029	-3.21409637499291	0.92074327801167
H	5.44684929616162	-2.36294947168772	0.75050000801626
O	7.48885116126696	-3.66691483204914	1.65433415637352
C	8.82437379051177	-3.92906982334591	2.04405002580987
H	3.08540102033055	-6.77113488003923	3.58756966558040
C	2.63801460373196	-4.49578070504094	2.53807244709464
C	3.34139613264504	-3.24964547481459	2.03604204736516
H	9.47244505438635	-3.04434616330984	1.81687386947335
C	5.51452187898817	-2.31149670967389	1.86488545902723
O	4.68861507733081	-3.29085858480208	2.46052811589382
H	1.53826953353628	-4.40002980844208	2.36017591608916
C	6.95211926789630	-2.52585688351409	2.29286991602472
H	8.88429968226347	-4.11230875478492	3.14522087425120
H	7.54377944474478	-1.61284073261017	2.02679835456081
H	2.81910229862469	-2.34235277538023	2.43153710315044
H	2.79978499049269	-4.59277249294380	3.63860726919668
H	5.19877875528622	-1.28312204104869	2.17465793591385
H	6.99385883283264	-2.63623037844736	3.40442412913604
PEGmet (KF)			
H	10.32783942415848	-7.83427308049175	4.26955242468343
H	5.19163539281970	-8.55582240453961	2.01300287737573
C	9.32256744938013	-7.98065128950015	3.82450698538371
H	8.72123302281857	-7.07051344920676	4.01473899673364
O	4.64852113049092	-8.33476891377429	1.17148773950571
H	8.82630305360954	-8.82370507843671	4.34307127601245
H	10.09417654819499	-7.32618552234390	0.48507537597207
H	2.99553403651264	-10.45128926788981	1.27785609330488
H	2.71193542256697	-8.69732492472118	-0.55108412722652
H	11.29026571705358	-9.45287563393349	2.47157768924784
C	10.09308586299593	-7.09691667024008	1.57728413819753
C	9.42229682621469	-8.26968334128934	2.31611085244749
C	2.82001067852492	-9.67725070487807	2.05093688938511
C	10.26064421711874	-9.53879478348126	2.06690379079459
C	2.50006576410542	-7.94501444733012	0.23420632351543
C	3.27056802993257	-8.30641943967851	1.51055316708882
H	3.40798411046852	-9.95370155730492	2.94947847320487
H	9.76717893004455	-10.40294054766385	2.55300716148427
H	11.15243156273527	-6.97013326590048	1.90876369135930
H	2.82138348847070	-6.95359181007681	-0.14032244891387
H	9.58387072041444	-4.95541785396617	-0.04253134296847
C	9.82164928387422	-4.79947492415213	1.03938083224634
O	9.37182377580303	-5.88840778601227	1.81575655708079
H	1.74293228880520	-9.68554489777875	2.31850039635928
O	8.14191780683718	-8.42471165691598	1.72252692273171
H	1.40611058717706	-7.91723030544303	0.41486328238705
H	10.31950387058586	-9.75346322560119	0.98106862464316
C	3.02677091620792	-7.25446627250977	2.61650287981461
H	10.93103099163048	-4.67829865159960	1.11861368564915
O	3.48832883216643	-5.97621207078441	2.17625933035969
H	7.40681186410791	-8.60217069029257	2.41821787305247
H	1.93866223210976	-7.19386973766923	2.86212860111106

H	3.25289787254573	-3.51123346409688	1.44382858046013
H	5.39098062695280	-2.58187646562563	0.61908280828550
O	7.77211063523465	-3.56218705681051	1.35631392518806
C	9.18247453434141	-3.52202403543604	1.54141008163669
H	3.57813186736525	-7.55624954967439	3.53852829255841
C	3.19840562911670	-4.92591208332869	3.07108093958096
C	3.68226959173651	-3.62382057619996	2.46795140386246
H	9.62001252341176	-2.65365235483380	0.99158830741678
C	5.63150887351080	-2.50800400624861	1.70780680709021
O	5.10443429133975	-3.62193997288710	2.40769183422431
H	2.09803610947157	-4.84426769136309	3.25392835696294
C	7.12854438009593	-2.42690942668758	1.91335997244979
H	9.41835312543404	-3.39283272861282	2.62479825767643
H	7.50167831688595	-1.49000356311196	1.43204875121867
H	3.32255381166553	-2.76711121868007	3.08784237252606
H	3.68620838771493	-5.09354256038366	4.06332002322639
H	5.18259260365925	-1.55676257252205	2.08479261581379
H	7.35278893883126	-2.35676060174421	3.00498469720902
K	6.42091166520956	-6.20802785781597	1.77412805162097
F	6.13266237754031	-8.44892800853083	3.19999890896912
PEGmet (CsF)			
H	10.07924031728337	-7.86046447944434	4.33078947667331
H	5.00811153454635	-8.72089611619910	1.64756691770084
C	9.17652151459688	-8.03933975411398	3.71173473383180
H	8.49480001749593	-7.17418980918755	3.82613204270280
O	4.27734142167547	-8.51116749050777	0.95007165012269
H	8.65253213839969	-8.93427223676462	4.10075211245735
H	10.44089783888949	-7.17391548438139	0.57644903735149
H	2.63812850900891	-10.52968581547341	1.57348652547608
H	1.99274540796000	-8.88776748932805	-0.26886991375622
H	11.45270545859627	-9.30825422135811	2.67886915910208
C	10.25920668721327	-7.00590750510109	1.66572649370938
C	9.55387712566136	-8.25297648007327	2.23578719878220
C	2.65262813933316	-9.70047428792571	2.30819275286088
C	10.51802945789490	-9.44813959410131	2.09746482488910
C	1.99132927790632	-8.07418956869156	0.48343132360050
C	3.01440449340028	-8.38895380647524	1.58313196108095
H	3.41674960954657	-9.93855240201377	3.07532353052951
H	10.01567313629959	-10.36512072775691	2.46274080438430
H	11.25055368568120	-6.85642377722878	2.15981933977124
H	2.25475992494515	-7.12695187097955	-0.02769749494934
H	9.94338793518930	-4.71944943440341	0.15574657906563
C	9.99931449912095	-4.67706310010288	1.27364388863875
O	9.45575047921056	-5.84240948925934	1.85287534946231
H	1.65849435714516	-9.65074671496716	2.79927389155330
O	8.40768405125973	-8.48256414451564	1.42946641503422
H	0.96725590887449	-7.97670988141071	0.89722125329277
H	10.78118157823498	-9.61175676114583	1.03306023828536
C	3.04232481106096	-7.26014123941536	2.64023174868277
H	11.07993741257687	-4.56339659359835	1.53964746365809
O	3.41313813693596	-6.01249193390821	2.04645153368427
H	7.57046340825251	-8.70688423655747	1.98685229373149
H	2.03342282874485	-7.16187403129943	3.11054552721721
H	3.32080571338429	-3.57614702891347	1.22525679980539
H	5.56121990621829	-2.52115266505648	0.50032786759293
O	7.91863527312346	-3.43633039097492	1.36447948573536
C	9.27483527701151	-3.45074643686741	1.79193027036430
H	3.77500853414719	-7.52439270044411	3.43885414463086

C	3.24573433814682	-4.91635412468542	2.92017571357105
C	3.73760862828940	-3.64362145085456	2.25956764463291
H	9.80648489724265	-2.53767481186313	1.42621487396032
C	5.71010587586982	-2.48236015560756	1.60828303001152
O	5.15991386574434	-3.62885179944369	2.23210126367306
H	2.16675810626228	-4.78478731803691	3.18395430796093
C	7.18437875886920	-2.37000988792904	1.94203808289865
H	9.31924336554026	-3.44594025288151	2.90772650682117
H	7.56123758984009	-1.38551751431373	1.56809136520302
H	3.35922542297544	-2.76374233577424	2.83492255625438
H	3.80200766213019	-5.07327997272743	3.87689599496552
H	5.20667461369233	-1.55512039574368	1.97615779124917
H	7.30604313268538	-2.37767596801535	3.05203918150867
Cs	6.38719120937677	-6.30087968416098	0.76388237186542
F	6.18690672650977	-8.68541462801708	2.56367208866827
TS-E2-anti (PEGmet-KF)			
H	10.91410898512902	-8.17967269804538	3.65477224138359
H	5.22296983632840	-8.72441203702892	2.92750844925263
C	9.80798580875478	-8.09798901569229	3.62285158296700
H	9.51063839014790	-7.17939929917741	4.16577012313607
O	4.79480882500113	-7.83848819245466	2.79870900893716
H	9.38521490070238	-8.97487790929505	4.15391005417070
H	9.45266049068055	-6.83306679483393	0.38273628415111
H	3.24188976255461	-10.07099439456545	2.73012403688422
H	4.05361399965216	-9.09539505939740	0.49842405825629
H	10.84592494166124	-9.39083098552996	1.35573636091180
C	9.79617187424218	-6.80689792965366	1.44518304362479
C	9.28691958495467	-8.05996536754404	2.17543594858641
C	2.72201215492525	-9.11317879459009	2.93782565788360
C	9.74023676006231	-9.30674591578743	1.39653231098464
C	3.53204171683238	-8.14733784138784	0.74071563153266
C	3.46993920847569	-7.95214675702189	2.26481434413623
H	2.68376416871742	-8.97351452516749	4.03730814974539
H	9.34692686560815	-10.21959153408764	1.88742587869310
H	10.91309779412140	-6.80815434625814	1.44474220457897
H	4.08453906030749	-7.31400834328835	0.26563077503930
H	9.75273880616657	-4.35667274595140	0.49192548081922
C	9.87430052871151	-4.43563357520815	1.60049969201600
O	9.30469744997355	-5.63743292650251	2.08447090191099
H	1.68474815623680	-9.20345233827047	2.55700491202679
O	7.86030278137833	-7.96107798915117	2.15871516454317
H	2.51695813609820	-8.18811250627377	0.29576749323851
H	9.34704269180952	-9.28158645649889	0.36106960594524
C	2.76883292310243	-6.63638025509737	2.63863802392211
H	10.96947344679270	-4.40137432358305	1.82318468572770
O	3.44160644336323	-5.52726771432694	2.05449862477676
H	7.46316193115382	-8.73752435047301	2.63998477880276
H	1.70665084646863	-6.66390652721108	2.29256394253027
H	3.55973041585520	-3.23726107661530	0.72384947334945
H	5.80407321089578	-1.92760618435150	0.69411536924972
O	7.86868073792674	-3.13534926666851	1.78336005594530
C	9.19851371614476	-3.25723662708779	2.27024104320299
H	2.77069305618604	-6.53441962286797	3.74975468091914
C	2.94549225387043	-4.28263821598638	2.53033816303481
C	3.66210347306917	-3.14548055194076	1.83262345061200
H	9.77958095110453	-2.32937746830692	2.04569232087940
C	5.75490793531432	-2.00104677024040	1.80788811514383
O	5.03102006156417	-3.15017228339073	2.20599258062377

H	1.85141707302686	-4.19063096953495	2.31747923431419
C	7.15190578256997	-2.06785475441047	2.38983969357508
H	9.19366689759777	-3.40348176092697	3.37667721889047
H	7.66870998550453	-1.09455249161759	2.20005397973784
H	3.18064431099316	-2.18586953926160	2.14146660585845
H	3.10057737995664	-4.20400376986039	3.63334451160996
H	5.25714879075888	-1.07472337065473	2.18684709776031
H	7.09100139510338	-2.22463039721948	3.49296791108337
K	6.40696744816269	-5.59517379719423	2.60985725360724
O	4.47134006325248	-4.70753943203324	5.73475596280105
H	5.59313705779486	-9.45474846589090	6.42996755679266
H	5.41614142302881	-3.78794699868866	8.31519519671608
H	5.40442467871514	-7.33870697066311	5.09890445713758
S	5.89240812604981	-4.80737303794808	6.20756934552814
C	6.48509739810746	-8.95499680914820	6.01544252228193
C	6.12742331422632	-3.56532721392339	7.49986224554342
C	6.36324096885667	-7.65008259120385	5.53704239194965
O	6.19838492877178	-6.13351454633758	6.94031398206546
F	6.47181847150735	-9.80001408479117	3.54806677890790
H	5.91635483511581	-2.57599902164018	7.05394614832063
H	6.49887188070820	-9.40850570912586	4.70886021489650
H	7.44906025417872	-9.27876694400955	6.44366780648768
H	7.17169260289988	-3.62814208171430	7.85575489458469
H	7.25920945839300	-7.13983261452634	5.15534280066021
O	6.91095039267401	-4.52196511086402	5.12422948481414
TS-SN2 (PEGmet-KF)			
H	10.94927881503728	-8.02975759564210	3.71430451472780
H	5.33745811498987	-8.78954643045597	2.69266078995121
C	9.84301614725536	-8.04262579726698	3.62543589180580
H	9.44327250840362	-7.12251356268132	4.09513573138056
O	4.90242569759627	-7.94570651716409	2.37693164955983
H	9.47038034388746	-8.92162321073727	4.18958521597758
H	9.59354538770627	-7.03386857250694	0.28862558830042
H	3.38497488660432	-10.20309573541778	2.57948378375792
H	3.69186401245098	-9.12384875761641	0.27168442469303
H	11.03202016190065	-9.48395005395975	1.53950694423488
C	9.91678731192798	-6.92943014226588	1.35264408220415
C	9.39543453634496	-8.13317855736293	2.15477761821388
C	2.92518665269599	-9.26179048366465	2.94233810446238
C	9.92433018129503	-9.42416546956550	1.50434246670755
C	3.21937365438098	-8.20013569563329	0.66050432664397
C	3.49292184377194	-8.06366352588640	2.16798010187142
H	3.13878776227362	-9.16992980797774	4.02728838777761
H	9.51700924455957	-10.30389444097398	2.04170745597593
H	11.03379750647770	-6.91671990783038	1.37479244684850
H	3.64930747514155	-7.33598408472061	0.11846998603809
H	9.68645200477784	-4.57402974287092	0.17098727943872
C	9.90053185162511	-4.55661842617907	1.26859903772603
O	9.40391816170114	-5.71995507243572	1.89710848733962
H	1.82725587040777	-9.34659196307096	2.81016648968814
O	7.97624172349930	-8.07011607200253	2.04902306444078
H	2.13202221994260	-8.24413520581524	0.44359895641253
H	9.59567364307132	-9.49162642288237	0.44793344442819
C	2.87172601943026	-6.77306520287228	2.73332414052366
H	11.01016615099935	-4.48016528070704	1.39262774122482
O	3.45203500447313	-5.63602680445004	2.09837137686369
H	7.53085776109394	-8.78979783013028	2.59374233456291
H	1.76570716668318	-6.77733039887730	2.56556170994090

H	3.51548345382784	-3.33972459183786	0.85261531414692
H	5.70842396669834	-2.19262864548773	0.54063860786564
O	7.88087718338025	-3.28404094743565	1.55037666265576
C	9.25936808219321	-3.33473073590047	1.89393867988114
H	3.06469330433511	-6.72382813207658	3.83032363325943
C	3.02235705919538	-4.41250270828709	2.67264261997883
C	3.68464936865536	-3.25574084589896	1.95374129637727
H	9.78334806870311	-2.42053932625870	1.52204120289318
C	5.76491042263480	-2.14923512913105	1.65626412629654
O	5.07851196277276	-3.24157954412773	2.23666561343967
H	1.91395673252443	-4.29696140008301	2.57017313916969
C	7.21289076369904	-2.15938741023860	2.10170842601898
H	9.38165193942318	-3.37353415516681	3.00328889574855
H	7.69739988537334	-1.21202196760244	1.75864412777512
H	3.21510076051536	-2.30250964678994	2.29917680390792
H	3.27519988114286	-4.38486990511848	3.75912310505232
H	5.30525743791036	-1.18186955939312	1.97818133510204
H	7.26417037087872	-2.18453317457387	3.21736928715853
K	6.47889008136587	-5.76215298563484	2.43789678125076
F	6.50033630360255	-9.63168198742375	3.53403462904963
H	5.22127037721923	-9.92464546716952	6.51394676135709
H	5.45345136765173	-8.17627878778664	4.75015585453992
H	6.62119989818175	-10.65302521899892	5.65060045626716
C	6.25742573241703	-9.74705486231970	6.17304087331224
O	4.49320084853715	-5.58176447330607	5.64524642158380
C	6.34226507965521	-8.59576828657607	5.22786089657500
O	6.17276004245687	-7.18909055508024	6.67264066903662
H	5.39190442748659	-5.06873391642571	8.35150091334462
H	6.90130147768476	-9.57120711722498	7.05561173887751
S	5.90357087793330	-5.76404032036215	6.12202007528762
H	7.31218945952160	-8.16104533769898	4.97167256674863
C	6.12237925732412	-4.73686595890277	7.59192280158390
H	5.93014360830110	-3.69106649730866	7.28967985811679
O	6.95204767988828	-5.34348750851819	5.12191056958096
H	7.15869301450310	-4.86295612223092	7.95333168303758
TS-E2-anti (PEGmet-Csf)			
H	11.19568550593403	-7.68869519536031	3.70119566656428
H	5.29873215949717	-8.57493323414683	2.84509868859015
C	10.08627069541104	-7.66729074804950	3.70971062242848
H	9.76502898957676	-6.69519827890901	4.13316687336061
O	4.87508489021225	-7.68072335867398	2.89504345531375
H	9.73331319191739	-8.47499148238697	4.38296009117435
H	9.51650118685691	-6.94199896514575	0.33743744773792
H	3.18732338791419	-9.78728446642975	3.05698917712696
H	3.83355141142162	-8.91749013786489	0.71351370320564
H	11.05268264454403	-9.29726892975248	1.65819971958661
C	9.96422346033234	-6.75253330196528	1.34212406283098
C	9.50158961993876	-7.86605734327291	2.29763884899449
C	2.73985390432966	-8.79459457947102	3.26877414975249
C	9.94796568640214	-9.21731641340226	1.71329004449831
C	3.39893884507538	-7.93216930134054	0.97826353077693
C	3.50018769767453	-7.70419270498466	2.49511363296475
H	2.79875631585365	-8.61555639779946	4.36167721499598
H	9.57618145695847	-10.04289756394735	2.35296378678861
H	11.07609679425895	-6.78943006502735	1.23738662513592
H	3.95503262299364	-7.14564514650809	0.43405786239601
H	9.57635382273808	-4.65070164362422	-0.11571017360710
C	9.92848289889695	-4.42595646706112	0.92057921863825

O	9.56421935913293	-5.46737521211974	1.80720717019845
H	1.67181497355560	-8.83615255166296	2.97396877836580
O	8.07842103537549	-7.78368717611490	2.33159176730556
H	2.34407378413408	-7.92091969074273	0.63574564156422
H	9.52957945636352	-9.36341883922253	0.69724142563577
C	2.93162565907814	-6.33416554615294	2.90452398135161
H	11.04109506605539	-4.31417655716423	0.87910174347679
O	3.56698590712269	-5.28480756406916	2.17684038026980
H	7.67082613828990	-8.61010087503584	2.71153231576103
H	1.83184611882867	-6.31608794035164	2.70481045231970
H	3.61989972286450	-3.23279434781307	0.59570478307856
H	5.71670209502911	-2.26897738475359	0.02172920166796
O	7.92695238416442	-3.10384314409442	1.14651856881910
C	9.33004331295842	-3.10529845831972	1.36858773278584
H	3.09650735444653	-6.19137242724356	3.99811315424737
C	3.12304258640663	-3.99441252062079	2.55723166496460
C	3.76037896934638	-2.94525703790921	1.66576051893282
H	9.81362905207111	-2.28321154738326	0.78667286120157
C	5.82725706832330	-1.92992879565356	1.08001054036464
O	5.14619615252681	-2.80901562844892	1.95677615828759
H	2.01314460124847	-3.91136727364028	2.44267020170410
C	7.30044933010410	-1.86516574954668	1.43890575356435
H	9.56138883273648	-2.92916609131730	2.44829817578222
H	7.77005114311925	-1.04024659312441	0.84906233310761
H	3.23792516151179	-1.97019503748105	1.82595789289567
H	3.36150599631284	-3.79237751030677	3.63054129213847
H	5.40245100301722	-0.89727053983801	1.14813034677886
H	7.41580403058034	-1.60728137995906	2.52068228990590
Cs	6.66342412782823	-5.22881547114036	3.27093294497989
O	4.53299257375295	-5.22826883997809	5.91339219899329
H	5.07995898818545	-9.87398968655025	5.88080097626120
H	4.21131480860120	-5.03562857518102	8.78983246854928
H	5.60101287914905	-7.56499073617129	5.11870183395441
S	5.62929699057405	-5.48462049994418	6.91611067180415
C	6.11400945556174	-9.48701513276555	5.89784841487063
C	5.18299798586292	-4.63624737998561	8.44782511860945
C	6.30192370026048	-8.10728230553140	5.76932691735139
O	5.69976295721646	-6.96806121632181	7.35248874293119
F	6.58620301561197	-9.76099326048338	3.35574218162120
H	5.11039124023497	-3.55741855478829	8.21696239504439
H	6.43729518973407	-9.64863894281650	4.56978100498630
H	6.82211474791488	-10.07311442275520	6.50742069308181
H	5.97744304016579	-4.83193955455401	9.19068089646861
H	7.31983739320289	-7.69494928658440	5.84973889596884
O	6.97073742270068	-4.95906698923457	6.47481226879359
TS-SN2 (PEGmet-CsF)			
H	10.82488901452048	-7.96393132154035	3.69130002054434
H	5.00861196522704	-8.56313323733868	3.22889737741885
C	9.71528309913756	-7.96171818031077	3.68818741132799
H	9.36520929630569	-7.06631274759790	4.23839475796308
O	4.40638942233888	-7.761947411111143	3.17263926917739
H	9.37728997122858	-8.85926593420190	4.24595176945624
H	9.25631591539777	-6.87560091147714	0.39626392709814
H	2.97135259829635	-9.99715538048909	2.67535892508871
H	4.55224938942030	-9.17128917254744	0.83494415169706
H	10.69900510329549	-9.39682184765421	1.50539456452075
C	9.67216282226520	-6.80314137780622	1.42994080723104
C	9.15885326376834	-7.99681286816591	2.25241084077116

C	2.41858005918243	-9.03895009485259	2.60189913428895
C	9.59510813731229	-9.29002751406112	1.53722611950046
C	4.00310241331629	-8.20885981374900	0.80757474327787
C	3.38795834205568	-7.91638517319581	2.18726215705004
H	1.97747431286695	-8.82429268313706	3.59616844566085
H	9.18296222434176	-10.16768793835131	2.07456823220315
H	10.78572056695595	-6.85775909532980	1.35734701467348
H	4.71658399967325	-7.41178411362854	0.52477191581262
H	9.54912719957420	-4.54951325840503	0.20668055479167
C	9.76594634461136	-4.44479026914779	1.29835629877084
O	9.28330135444830	-5.56438289081486	2.01235637423592
H	1.59706242076937	-9.17469431139507	1.86890820421610
O	7.73741645861259	-7.89156472541566	2.24660598996993
H	3.22135240448345	-8.27801122118850	0.02328047324895
H	9.20415933162556	-9.31359739939989	0.50046022778944
C	2.61415652142478	-6.58694234523255	2.18340861606135
H	10.87548555203709	-4.34818678829457	1.41231762084484
O	3.42845090158518	-5.51821404246228	1.70978092914503
H	7.30865252832131	-8.62907394897143	2.77459443320555
H	1.70683944347878	-6.67989103602470	1.53827119495427
H	3.80541848989512	-3.50636925315801	0.05981406320081
H	5.76038979113076	-2.22781573488715	0.04194298590461
O	7.74625253112955	-3.15551517375682	1.41551662005153
C	9.11252679575664	-3.17309068659740	1.80593031363218
H	2.27718419630848	-6.37773917094061	3.22639609412792
C	2.80915786752041	-4.25300269393601	1.82737780611810
C	3.62662336952126	-3.19236023320056	1.11637530286368
H	9.65087387510696	-2.29604468275670	1.37042946075402
C	5.66894764877916	-1.99910163220065	1.13093806659037
O	4.86628538693958	-2.97467430459701	1.77469276637540
H	1.79371016586331	-4.26391683459055	1.35926260324512
C	7.05640313968426	-1.96268626609498	1.74293627228625
H	9.21102853992863	-3.10982444630401	2.91799028814338
H	7.59439968799888	-1.07113910452362	1.33589355772604
H	3.02990398037528	-2.24699411089491	1.09155903491168
H	2.67023841967972	-3.97654387033896	2.90223045219392
H	5.20554598435894	-0.98505290030163	1.22518155861560
H	6.98578456981416	-1.82805481407883	2.85146462213507
Cs	6.31390199884853	-5.38980767776596	3.36673058911244
F	6.27087245011481	-9.49302795753670	3.72254282073112
H	5.55010482356583	-10.07770935290185	7.11844481969614
H	5.41843415285463	-8.27906691198776	5.34880202196125
H	5.98591999433769	-10.89819635331807	5.58096100515064
C	6.29605747444518	-10.11672975825414	6.30184624303311
O	5.48639835821514	-5.49223655398866	6.54064063281069
C	6.34732523284744	-8.81109020665222	5.58160015755202
O	6.48787094877086	-7.70781237081575	7.28948122718599
H	6.23617708057383	-5.76757638892209	9.32471708497128
H	7.27938215239484	-10.39278998794152	6.72478226648068
S	6.72185260709173	-6.19938457942320	7.02214478160071
H	7.29893850150101	-8.36643220511534	5.28063714693135
C	7.10543731394158	-5.56878480177770	8.67182715673800
H	7.28523055317662	-4.48300358310887	8.57062744268639
O	7.92544346768739	-5.96176598432349	6.14667094855605
H	8.00798607196365	-6.08896035970964	9.03930928393038
TS-E2-syn (PEGmet-KF)			
H	10.94959709840973	-8.05783984884482	3.40873617846021
H	5.31071963320160	-9.04946589559502	1.95954457658447



C	9.85006946442250	-8.14437859197047	3.28765418747019
H	9.36781596755490	-7.26675179512909	3.75928232344022
O	4.86454780181765	-8.44101153007287	1.31224320203185
H	9.51372790754729	-9.05492890317942	3.82320081133633
H	9.54469545955160	-7.04969872359366	-0.01768759754390
H	3.34273703880321	-10.63863078284430	0.96642278902685
H	3.17058823193430	-8.72048311395771	-0.69119526624340
H	11.24227695612353	-9.37144807619003	1.17352289611384
C	9.85597212009559	-6.95047895471040	1.05046422077900
C	9.45841759714558	-8.23210384258541	1.80307774598375
C	3.00483232783490	-9.95768590207175	1.77258833223003
C	10.13529943838133	-9.43661138878049	1.12576043809219
C	2.84542013356739	-8.04649058963266	0.12483862104440
C	3.44410829287159	-8.52006185855929	1.45552064077658
H	3.45042627732671	-10.31380420633408	2.72388114289726
H	9.82523614999839	-10.37274223559718	1.63177974168738
H	10.96585400005910	-6.82336412314630	1.07627062276853
H	3.19576855179171	-7.02244642368855	-0.10529090953932
H	9.19837379867258	-4.57779091340069	-0.03091362732465
C	9.53082201336873	-4.59133775797761	1.03644494820865
O	9.21989721351354	-5.82940494975886	1.64458969031900
H	1.90139796804231	-10.03674435362372	1.85526121974223
O	8.04194639272621	-8.31447193760723	1.65571761688329
H	1.73740679333724	-8.03848303017098	0.16446941887934
H	9.82529630618403	-9.50867293198153	0.06423369028983
C	2.99809201794966	-7.59150460709578	2.60901509412043
H	10.63515436010900	-4.41380797515097	1.04351132527621
O	3.41217765806687	-6.26528782331732	2.32256074316071
H	7.64271471405744	-8.99707037933984	2.25648217381092
H	1.88676233448919	-7.63080328131902	2.72848064306716
H	2.94808028531489	-3.77151063497932	1.70401289486144
H	5.04681014586671	-2.51069948502159	1.10080020117586
O	7.45392376633372	-3.51279363701845	1.62174838563606
C	8.86267031540351	-3.47068103770296	1.80677080463234
H	3.45462481590456	-7.94340045396125	3.56704015120058
C	2.97388858771223	-5.28770884644315	3.25000874299753
C	3.37542412731487	-3.92257462447438	2.72593164933169
H	9.26917476378477	-2.49385663323871	1.44539995746149
C	5.28635261174843	-2.61361756360954	2.18791663815896
O	4.78858575841037	-3.83918991565493	2.69274017613218
H	1.86254169174043	-5.31627851703774	3.36409104848114
C	6.78197862473225	-2.53998748685505	2.41369923768951
H	9.10907946511604	-3.56917420840800	2.89024190800834
H	7.13019905712263	-1.51358818012529	2.13941219853416
H	2.95135929767207	-3.13398926198144	3.39453284984166
H	3.42685200680253	-5.45689990823886	4.25685016534845
H	4.81570697329163	-1.75148024366564	2.72012732375544
H	7.00019695754349	-2.71428631690190	3.49282635111480
K	6.39546236576382	-6.20695862019563	2.31029855793562
O	6.54813639462394	-7.24126119169902	5.10785543812603
H	9.01532967230943	-6.47495682439254	6.39432422080487
H	4.74898808132657	-7.92171699515080	6.34737995776837
O	7.29967392529457	-4.90770901250277	4.72731807391600
H	4.38923138715294	-10.05263194473166	5.14031608803487
C	5.57727157781746	-8.63256764769644	6.20881158182150
F	6.36694671413918	-9.79541503296614	3.09557128645851
C	8.13854294875381	-6.09466102290923	6.94847645471203
S	6.78036714098950	-5.84661694935130	5.77664042469003

C	5.41885992719591	-9.81341557273657	5.46136943743192
H	5.96721769999568	-9.69785035520878	4.24316157573829
H	7.81577640480359	-6.81043264725858	7.72650088237077
H	8.35551099099306	-5.11085617055398	7.40299875384037
H	6.35799679375089	-8.57846446932188	6.98280689134934
H	6.01161993048209	-10.68591933306743	5.78801239165640
O	5.59573677383700	-5.40465252771196	6.56982966515382
TS-E2-syn (PEGmet-CsF)			
H	10.78357803376190	-8.07772001261628	3.70098530514757
H	4.84433137582355	-9.11271356072401	1.81351302771785
C	9.77454203595712	-8.31429880807023	3.30573464676262
H	9.04531466243381	-7.60518914387898	3.74200338992830
O	4.27468572887547	-8.63009455311997	1.16061452940300
H	9.50624671230015	-9.33302053739928	3.65256377881115
H	10.08763459256698	-6.86290387317326	0.14217007281034
H	2.61915398061780	-10.71230371960379	1.49618554337265
H	2.20967602257111	-9.07775806158868	-0.40955490883380
H	11.75833248867292	-9.17719856866959	1.53441819058944
C	10.18970564773312	-6.87250277785835	1.25488339544519
C	9.76043597416022	-8.26029705153283	1.77151709313076
C	2.47071622511604	-9.88650709592294	2.21965638069528
C	10.71615191398949	-9.31265422798813	1.17914961617037
C	2.09087167963520	-8.25553104323217	0.32319594199393
C	2.91053945120907	-8.55847102187005	1.58373165499287
H	3.06815366131462	-10.11605353224438	3.12667075226917
H	10.38151833148747	-10.32560390431816	1.47920136152574
H	11.26672052783984	-6.70164489724243	1.50040803734534
H	2.44911585390243	-7.31680668048793	-0.14114119970463
H	9.58577175787632	-4.42785443013762	0.30093651587047
C	9.73827679132640	-4.53957196676973	1.40355073033867
O	9.39333767047105	-5.84626432741515	1.82930107261131
H	1.40151399472372	-9.86610783925546	2.51167093191224
O	8.44138024376708	-8.47968624435440	1.25723841032175
H	1.01465044180449	-8.14134393706432	0.56262194466990
H	10.70709041073090	-9.26837004174704	0.07136829571297
C	2.72485567872148	-7.42746791685082	2.62511229207649
H	10.81910757466105	-4.33896710637023	1.61059748613351
O	3.11076151029890	-6.17639825404567	2.07363266921418
H	7.90873925390253	-9.06280310400977	1.85319661756504
H	1.65407125531524	-7.38960404741340	2.94292939144601
H	3.00593049255103	-3.73648706930177	1.17130225992065
H	5.28051449489890	-2.46449616230676	0.83038480285884
O	7.57593953239536	-3.46818693982635	1.68337204928070
C	8.92088288076046	-3.50139559902695	2.15012894072165
H	3.33149215159622	-7.65163734329120	3.53775889009587
C	2.76743381847094	-5.05797105636643	2.87711997861737
C	3.30710751461037	-3.78583539470835	2.24659602615772
H	9.40094715982580	-2.50274607209320	1.99642620310042
C	5.33915913436405	-2.55881691773388	1.94303077909401
O	4.71698888010051	-3.75385837461247	2.38256922076242
H	1.65631645966923	-4.97054341035550	2.96843843878162
C	6.78466610801494	-2.52734030695867	2.40413066129860
H	8.93957880006037	-3.72935689561522	3.24183426616214
H	7.18141370720634	-1.49406703358410	2.24050032262232
H	2.84827978095741	-2.91029376717189	2.76803248822263
H	3.18571276433452	-5.16101251620989	3.90744208466098
H	4.82381987826853	-1.67021182713659	2.38303246295029
H	6.82472936289664	-2.75268845959250	3.49476208611921

Cs	6.30726336271776	-6.37838253257183	1.99189336502071
O	6.81420624635324	-7.33081182160748	5.09395355786420
H	9.08068935616568	-6.08267013544770	6.35800211746432
H	5.29880917491452	-8.34481975669058	6.48383084946011
O	6.98602133678291	-4.86263154002997	4.83289479752103
H	4.83123987991584	-10.28301723368193	5.02314072425362
C	6.12465097363937	-8.95470724634897	6.08633378770561
F	6.34085135788367	-9.51445099476758	2.72706026808307
C	8.16107090470413	-5.94696111965019	6.95601859391414
S	6.74040373092732	-5.95404462286942	5.83130363760414
C	5.88982502305777	-10.01308707280476	5.18935424069864
H	6.17864629159897	-9.66113715950345	3.92471203362748
H	8.03865492525628	-6.76400214046847	7.69136733872017
H	8.16706624247282	-4.96881888505793	7.47162585624698
H	7.03775158802862	-8.95545243042514	6.70124890957206
H	6.57877515552301	-10.87426032906391	5.25225788490250
O	5.51448004550900	-5.84368754614386	6.67634710846812
PEGmet (KOMs)			
H	7.57706608992576	-8.93325888913460	3.25226419935481
C	9.81398459208587	-7.84528010491213	3.76994835982541
O	7.89394612648092	-8.49623136833714	2.40854631722050
C	9.31323191414285	-8.37005630651747	2.41274317335633
H	10.74028125028812	-7.25191837155631	1.18685201938304
C	9.96574341237331	-9.72389944349779	2.07868039668815
C	9.63483761983343	-7.37738030080312	1.28341878146989
H	9.24797420324513	-7.78898956075403	0.31978293293411
C	3.11978688728044	-7.82061138745999	-0.61446514236138
O	9.02560899013929	-6.12145557643011	1.56095239787615
C	2.35111053442867	-9.73746468953248	0.84640241227958
C	3.13961315432708	-8.41768497486338	0.79628257465675
H	10.41985831021836	-5.00664836738960	0.46952522687452
H	4.53912074298194	-9.12880818079040	1.99929687267521
C	9.31731743573724	-5.10570422180847	0.62507816853465
O	4.51524723574657	-8.64953662104435	1.12313839431040
H	2.65820559064153	-7.88009722525334	2.84270924837797
C	2.52975779352250	-7.44244273707507	1.82558458289137
H	8.86116581866707	-5.33062159338206	-0.37106649626151
H	9.21608669638556	-3.61819514142134	2.17823976118795
C	8.79151764297602	-3.78941681339711	1.16027672690913
H	1.43564962781497	-7.31013460902908	1.63707838564103
O	3.18303599209650	-6.17780368514329	1.74494740382218
O	7.37201471693141	-3.82072026072329	1.22125575213784
H	9.13465679346193	-2.95441547585981	0.50182104635746
H	3.31222874167066	-5.67658665563574	3.76721371605699
C	2.86231917428908	-5.30507686336973	2.81501320352086
H	7.14562215022056	-2.79096920699586	3.02088482340761
O	4.79196195945139	-3.91057870903610	2.43424666016377
C	6.83021239797464	-2.73131683293617	1.95108716806271
H	1.75630282780341	-5.23992643297116	2.95896999493972
C	3.36864984051456	-3.91759322762396	2.48032317113209
C	5.31970299644074	-2.73147078002074	1.85495144507077
H	7.20367871794626	-1.75980322265594	1.54440595697944
H	2.95691433382898	-3.60601186202584	1.49093040312868
H	5.00343356667730	-2.65127309992170	0.78669950129215
H	3.00527559064415	-3.19135691761729	3.24745633429221
H	4.94021380643953	-1.82412468270953	2.38542543527991
K	6.09118058774750	-6.46413248933372	2.01279764436420
O	4.43224635434033	-9.66064544461650	3.68286434440748

O	6.74124655535069	-9.38426357875373	4.68011976993512
H	4.71374224019180	-10.35385722389533	6.45303299415164
S	5.30603365774641	-8.89353867753909	4.65759050244104
C	4.65135717147602	-9.26109263955589	6.30066210357733
H	3.60176759239479	-8.91722373310163	6.33742206281765
H	5.27073940468616	-8.72302278822751	7.04018339599519
O	5.19617576159571	-7.39369761541081	4.46943495136236
H	2.81207926419714	-10.46634707634667	0.15126451150462
H	1.29189842555739	-9.59272645514885	0.55059738619899
H	2.37716220135297	-10.17322685752995	1.86570410735616
H	3.58445787464733	-8.52992648272882	-1.32705292915285
H	3.68703621821877	-6.87011668168857	-0.64154489245159
H	2.08261603553059	-7.61437814753595	-0.94540216667654
H	10.91777383275769	-7.73431448268878	3.77508098479951
H	9.52996404998722	-8.55094842313768	4.57573502991984
H	9.35917642417932	-6.86271280971301	4.00000234384935
H	9.58234691879319	-10.11054926435582	1.11355153003430
H	9.70771200247044	-10.46328897830961	2.86319005286884
H	11.07185215114476	-9.64963575074654	2.02349496322890
PEGmet (CsOMs)			
H	11.20797989313705	-6.22830448257810	4.56794655995413
H	4.28634790179098	-8.02429319899469	3.45432990095713
C	10.15029474728793	-6.53700749474130	4.44155542093608
H	9.51740276914377	-5.62999319119046	4.40985973997631
O	4.03086384214401	-7.81351338655043	2.50864572569532
H	9.85026439430231	-7.13115246081193	5.32655861532455
H	10.13223197950898	-7.17200800274146	1.00669385957037
H	1.89677080384824	-9.35108612900400	2.99288041786526
H	2.27956296711536	-8.47095693837772	0.64801765607479
H	11.92273240780556	-8.38852094180325	3.32771397108153
C	10.34967587965804	-6.55898612227652	1.91516405425350
C	9.96572265474411	-7.37252728551106	3.16330646995179
C	1.80571762790593	-8.31046711813942	3.36219296337023
C	10.84772243493262	-8.63539216965138	3.20577339319583
C	2.21224906855552	-7.43192409877752	1.02528273456137
C	2.66826594430323	-7.38257615402004	2.48817217678291
H	2.15274291290340	-8.29193415978149	4.41541876029326
H	10.54044243972039	-9.27001631508408	4.06087037334459
H	11.44595019725941	-6.34514728090801	1.93077081964882
H	2.85479988721256	-6.78673314239361	0.39525321615170
H	9.69640056167993	-4.93871078876691	-0.19033397874291
C	9.99317052539758	-4.49399484021550	0.79305497617718
O	9.62386584205975	-5.33478119052357	1.86574573127161
H	0.73515050949271	-8.02109566690404	3.33540592235036
O	8.59851506564353	-7.74491129033578	2.98749035827707
H	1.16443704778238	-7.08525021797484	0.92084391503457
H	10.71885993797529	-9.22917323504281	2.27857279298403
C	2.55675188234740	-5.94805557152701	3.05188612871304
H	11.10197506276812	-4.35064625461258	0.76693526679561
O	3.26219897563483	-5.02448715596373	2.22396384155646
H	8.19145999924567	-7.99908690214057	3.86722366092029
H	1.48107117326563	-5.64700626687474	3.10913785357182
H	3.39736586293871	-3.00794781792006	0.61651062794062
H	5.64587322896734	-2.42910722124166	-0.30807197761128
O	7.94983157349975	-3.19330413017868	0.75983894104181
C	9.35557195829161	-3.12962285201651	0.95988695293925
H	2.97390994499167	-5.93020785142083	4.08625681514095
C	3.13360306406265	-3.68344785656811	2.65032700182823

C	3.76731804291344	-2.74973371795602	1.63847426763437
H	9.81517437432251	-2.42629181936283	0.22230561691859
C	5.82758502795236	-2.02986089926840	0.71993714210103
O	5.18597782867594	-2.83765795134989	1.69091390492616
H	2.05435807506405	-3.40559153934735	2.74356756100911
C	7.31605851954832	-1.94477754178041	0.98971368762631
H	9.58313142761156	-2.74244889347859	1.98236395092400
H	7.74569620449390	-1.16134947450695	0.31775640349692
H	3.44392510719064	-1.70298682057717	1.86064596245861
H	3.60075729190723	-3.53279645224543	3.65465310812726
H	5.41785203644609	-0.99028911978004	0.74779471097084
H	7.48482052916938	-1.61257771585704	2.04241166613558
Cs	6.40316089449525	-5.83401972411725	2.04043213305397
O	4.78925723488306	-8.22223035656891	5.08940695379721
H	5.82452913441058	-8.44927097411298	7.74973805380050
S	6.02052909852544	-7.47881205568406	5.57508610773986
C	5.85944133752088	-7.41115744496414	7.37360056193507
O	7.31049853755060	-8.23698860331309	5.32041742137780
H	4.92419354184248	-6.87408717739676	7.61506216810575
H	6.73822389952314	-6.87601550469984	7.77681103809557
O	6.06739888662915	-6.05012903006851	5.08251592058728
PEGphen			
H	6.13449462876198	-8.60773276704031	1.54788145204173
O	6.66772025236388	-9.34551355948126	1.16739625023829
C	7.98057055728439	-9.37365937850045	1.71106729263584
H	9.79687605234037	-8.14675940275045	1.66626756345836
C	8.73216956057357	-8.07929219411876	1.33135574007987
H	8.74235045685677	-8.01494799355075	0.21729239173813
O	8.10761177667225	-6.93917046388222	1.89215558243599
C	3.09868568633280	-8.08184704631839	1.49581188074930
H	9.87630275898450	-5.84128392032361	1.86393006565854
H	4.48635444221192	-6.70004556663991	1.53005211292064
C	8.79974853605924	-5.74807280562253	1.57104085174900
O	4.43962293470936	-7.64712344040287	1.78522685009733
H	2.24890418650225	-6.91479709460651	3.10899079588319
C	2.14805995419900	-6.97328657545166	2.00025684552079
H	8.77519816392870	-5.55795436266919	0.46935688527430
H	8.07638765191359	-4.81490107841464	3.38323624765396
C	8.22050336170514	-4.55631809293969	2.30550275786102
H	1.08618322077447	-7.22499060203241	1.76765871999347
O	2.54452581683750	-5.75118008314646	1.40554528395937
C	7.00023932728934	-4.14359148898189	1.72152112754010
H	8.97109053628448	-3.72577372603719	2.25963265147477
H	2.07567422611480	-4.67857869011982	3.13291848524235
C	2.04058949570900	-4.57972482047649	2.02181673293075
H	6.37069087423775	-3.09498145955412	3.41788436864624
O	4.16890072532583	-3.53787168866412	2.19155759097029
C	6.48553969306865	-2.96729778455108	2.31354360027891
H	0.97847451169066	-4.39894520785718	1.72694394623717
C	2.89578636606878	-3.40325925540681	1.59626575868836
C	5.13759564494269	-2.62916354982748	1.71090428672416
H	7.18317442826023	-2.10694815630059	2.14720487489804
H	2.97899123153511	-3.38803965066539	0.48235327036993
H	5.20571670083865	-2.67542967162851	0.59619489993948
H	2.39863275149599	-2.45090485201754	1.91124862795489
H	4.87162526773099	-1.57800120721819	1.98962705860200
H	9.25599743633390	-8.69081627295006	6.25687431898447
C	8.64848454909604	-9.26094293092699	5.53683894409038

H	9.35238039242515	-8.10690447459184	3.84697324685251
C	8.70387590739284	-8.93354119572639	4.17043251605747
C	7.82404998124339	-10.30388789942394	5.98205969360113
C	7.93233870182602	-9.64072430778174	3.22813641849075
C	7.04901542753082	-11.01471111756112	5.04980582527370
C	7.10126440830012	-10.68400539859337	3.68883487899608
C	9.95142650941672	-11.00962934613246	1.52339135495260
H	6.48960892898031	-11.23691858361237	2.96032041225945
C	8.73792130362694	-10.51569912337266	1.00230029038073
C	10.67066148706389	-12.00440665393662	0.84363506321649
H	11.61507757561992	-12.37929703191116	1.26654630493389
C	8.25679815090284	-11.04312140203001	-0.21173139357797
C	10.18326252408811	-12.52666552980545	-0.36544072095536
C	8.97348269094038	-12.04397806923453	-0.88782756704364
H	10.74373671256027	-13.31178021951675	-0.89621205007778
H	8.58144473351460	-12.44855603148242	-1.83351486388659
H	10.33097605285922	-10.62541942533498	2.48270821605809
H	7.78516251983676	-10.56386958906431	7.05139878332680
H	6.40255525824609	-11.84126231379373	5.38514694031604
H	3.80244701556816	-10.90409266974896	5.21715373284314
C	3.20783124900062	-10.70329317935967	4.31279862822923
H	4.38103263471823	-8.95065956849689	3.77042822234931
C	3.53721664165227	-9.60326560022860	3.50507600063463
C	2.13309093420866	-11.53871977555517	3.97128461919376
C	2.80021107429908	-9.33133310560647	2.33616958541938
C	1.39255101755748	-11.27186856509015	2.80867126233974
C	1.72658166602543	-10.17917640512778	1.99423683453368
C	3.85828387585054	-9.28720565760815	-0.60077352064864
H	1.15364606631921	-9.99095950750779	1.07312395654575
C	2.95265287337515	-8.37933161955079	-0.00945655487596
C	3.75851804393955	-9.61641851886495	-1.95920747355924
H	4.47562283398238	-10.32727649404224	-2.39923255266301
C	1.94834012340918	-7.81220903796371	-0.81796919342065
C	2.74948913934824	-9.04958146155171	-2.75621623411516
C	1.84648620823604	-8.14518228913076	-2.18026670544076
H	2.66812908426487	-9.31349031385275	-3.82206425397087
H	1.05371673053762	-7.68814583948813	-2.79287730227825
H	4.65561531153388	-9.73492527920687	0.01109588015450
H	1.87656118202391	-12.40031460206905	4.60705486681281
H	0.55145948906193	-11.92489692169009	2.52809289907486
H	1.23598241032321	-7.08930808127505	-0.39559104331920
H	7.30914136335543	-10.66140095300284	-0.61448111653487
PEGphen (KF)			
H	6.74426319498441	-9.45444709672122	2.19722718228800
O	7.47537216198303	-9.33882242387071	1.46730310692520
C	8.79628284698633	-9.14551526006420	1.92789232290274
H	10.47314943396126	-7.88377089483365	1.22442482967847
C	9.38928253165098	-8.04497888441971	1.01639479933875
H	9.29346020233870	-8.41343224809123	-0.03048149291585
O	8.67495136444996	-6.81763542483462	1.17052198265593
C	2.45443951541181	-8.83702368852908	1.67410395661560
H	10.02515278082928	-5.77672812172331	-0.04649245067637
H	4.07025113252765	-9.52308454909949	2.70245890230201
C	8.92970645342884	-5.87459249659695	0.14758631013778
O	3.09722962903524	-9.77473773910041	2.48957161605091
H	1.51604325829285	-7.91151825036344	3.38342761188641
C	2.09590670370145	-7.57051563882246	2.49583003751758
H	8.44898738854781	-6.19146471009885	-0.81041991261284

H	8.89838088620036	-4.22338258403784	1.53940624520456
C	8.41508148377422	-4.51432433905023	0.57582262107974
H	1.44530783013297	-6.88397116790696	1.90512312179573
O	3.28306207074714	-6.90062270415995	2.91323977922128
O	7.00170410065514	-4.54353665755583	0.73206203090678
H	8.70380405272798	-3.75554687772723	-0.19198201774945
H	3.80219514670696	-5.68415818096974	4.48104420659211
C	3.07638917453848	-5.70006132156435	3.63835447436730
H	6.96120770659162	-3.11607529245727	2.25309973962042
O	4.67288167156406	-4.42734187643915	2.39475631688528
C	6.48564351674880	-3.33493576779040	1.26650510207041
H	2.05474719649540	-5.65967858543860	4.07824714883594
C	3.29959941817600	-4.47207140154184	2.76609610702191
C	4.98297436282114	-3.42995428096505	1.43719750863639
H	6.71111853279795	-2.47723647370495	0.58678922222314
H	2.65433538170446	-4.52266038368755	1.85642942291958
H	4.49520106967459	-3.66232436000745	0.45879782986818
H	3.02050179307873	-3.54673930125460	3.32843607179955
H	4.60866078474561	-2.43105012329390	1.76946656628089
K	5.89252255389827	-7.02429357932265	1.82583504805706
H	9.46843056961329	-13.46100692492556	0.10366271934752
H	8.08566369991645	-11.40581518581479	0.58503615540633
C	9.90185969052199	-12.62440584840182	0.67434060751855
C	9.12437337063648	-11.48424699264381	0.93697711014174
C	11.22415251040193	-12.70304754049381	1.13800671067679
H	11.83283350984142	-13.59730276267163	0.93188558417857
C	11.76387932960542	-11.63499772305387	1.87454334166595
C	10.98399239931801	-10.49982795685161	2.14325661373673
H	12.79640882254174	-11.69030106963397	2.25262215617064
H	11.40693146323865	-9.67939247286964	2.74499593038731
C	9.65678335410252	-10.41097748266958	1.67418078314102
F	5.52805268102914	-9.27605753282886	2.96787476438453
H	-1.59235810518571	-8.84856327067541	-0.82740412252302
H	0.60525471895568	-7.87324915960964	-0.20021000535412
C	-0.96187297719355	-9.36144382687248	-0.08413553952353
C	0.27598166258158	-8.80840286198814	0.27774523025431
C	-1.39024275112892	-10.56865184220366	0.49096494950708
H	-2.35938480148164	-11.00502515493103	0.20476255228583
C	-0.56899545620971	-11.21550713751472	1.42723832027491
C	0.66774983973171	-10.65997375800577	1.79273899390398
H	-0.89183485586128	-12.16640840847284	1.87854248964819
H	1.32479439681076	-11.15505526338270	2.52130044461633
C	1.10369264925860	-9.44837021724996	1.22300182559235
H	5.66553550982085	-9.97773685257513	-1.58118105610973
H	4.24107641030475	-10.43592873851272	0.42504186927295
C	4.98183740040875	-9.20001154709255	-1.20893212453082
C	4.18123882261098	-9.46565122598551	-0.08787691649530
C	4.92454118403840	-7.94722032771155	-1.84318758833486
H	5.55288912012757	-7.73926191018042	-2.72274768157070
C	4.05471438055278	-6.96416772721546	-1.34402440628435
C	3.25431365019325	-7.23333314699311	-0.21921235603958
H	3.99564535496448	-5.97904707775311	-1.83360537816546
H	2.58649159102593	-6.44224026016992	0.15469249250064
C	3.30641618344219	-8.48710688965882	0.42919127778622
H	7.77626603467625	-10.13756585935143	6.41086512624483
H	7.71750553793063	-10.57727400308518	3.96708858597786
C	8.26973500879300	-9.43526732499798	5.72185843162051
C	8.23644622735798	-9.68403638035852	4.34383690751968

C	8.92730940551043	-8.29850234258588	6.22163454842775
H	8.95559901280810	-8.10360090103712	7.30533152886950
C	9.54894961578730	-7.41537845375856	5.32753096889263
C	9.50923146704327	-7.66317538293731	3.94352473953476
H	10.06953907721760	-6.52121876671936	5.70568898145228
H	9.99499931409917	-6.95070915673645	3.26248432308421
C	8.85008663833221	-8.79888264477384	3.43029476317791
PEGphen (CsF)			
H	6.54219455679467	-9.75121644689932	1.31123425882367
O	7.25134534055119	-9.04226912876136	1.01194029124447
C	8.55104297552946	-9.16420711478436	1.54042264784382
H	10.39789440201505	-7.98733888760798	1.25580379619576
C	9.32097136807013	-7.95129747588806	0.96662696004594
H	9.26880056368088	-8.02342667797469	-0.14559277680671
O	8.73006097830400	-6.73547966439336	1.41732442904705
C	2.52886420332279	-8.50298990325769	1.85194764438062
H	10.46584480846615	-5.61440823267402	1.09576710954648
H	4.37615312875409	-9.47036746277822	1.99673687028800
C	9.35981957771753	-5.56943158277117	0.93275641115472
O	3.86551733955271	-8.60701433813946	2.28777798621022
H	2.14978485110425	-7.31766188559945	3.60241694596783
C	2.00623255553992	-7.20108098473507	2.50402111207368
H	9.19666306247522	-5.44883951424675	-0.16880377499346
H	8.95726278952385	-4.52310673129393	2.77528368976202
C	8.83757770638595	-4.35523686289335	1.67818740482200
H	0.91512213026299	-7.06451059095924	2.31419395043066
O	2.73546640211165	-6.07017183999001	2.03015451864561
O	7.46775497410042	-4.11565573287705	1.37141916093893
H	9.45549112788735	-3.46701725459268	1.39776622004724
H	2.86256039495601	-5.05367546100016	3.84942617457715
C	2.52685062656367	-4.90077950891063	2.79500350570012
H	7.02930662157377	-3.25870912103212	3.22493563247772
O	4.68141032983408	-3.93017153582066	2.30265269216270
C	6.91889876897230	-3.05169354230295	2.13324218982319
H	1.44127814743707	-4.63084427552986	2.82630946622172
C	3.27806062170646	-3.73405839731867	2.18164196053857
C	5.45191581199323	-2.84828214345332	1.80749295370381
H	7.46160897820668	-2.09837916882984	1.91546471941219
H	2.98985627032442	-3.62318932646226	1.10747228306649
H	5.31666872684321	-2.73527722412796	0.70324057637128
H	2.97266814495127	-2.79748371816728	2.70871371970056
H	5.12407395996910	-1.89009483739702	2.27989577413289
Cs	5.57539390386610	-6.64998626505009	0.77617272796867
F	5.33214157565902	-10.47639989947914	1.58549955716724
H	10.32806155677951	-8.08159103282292	5.82897002664616
C	9.54244792257175	-8.60087419191800	5.25732048911240
H	10.33447112682245	-7.94452475536227	3.35988160949144
C	9.54327825146345	-8.52902350038728	3.85375155294850
C	8.54546568229588	-9.32660812695542	5.92540456272081
C	8.55318344578383	-9.18049194098928	3.08828489408923
C	7.55107770612580	-9.97399745179921	5.17444659343291
C	7.55216440407669	-9.90391457096571	3.77273209757271
C	10.51358337224954	-10.85214371650314	1.51155865169950
H	6.75224709974843	-10.40655379598254	3.20464744466428
C	9.26820655089823	-10.43040812543491	1.00006591670279
C	11.16643561129512	-11.97443410206963	0.97948162458814
H	12.13615891719552	-12.28876360722421	1.39488235205009
C	8.68878540271725	-11.16587657887882	-0.05122505226621



C	10.57933740390584	-12.70185538755221	-0.06868106918293
C	9.33723318346892	-12.29448150285699	-0.57840037834470
H	11.08470042605533	-13.58942271933459	-0.47926710362177
H	8.86187482085475	-12.86265719461441	-1.39318916739101
H	10.97308751469147	-10.31031334723329	2.35285253439865
H	8.54266260822811	-9.38634382509801	7.02551622098073
H	6.75822583305508	-10.54429841938972	5.68384459480490
H	1.67528565153654	-11.97928936209311	4.93605559162018
C	1.29935759101469	-11.39950179963184	4.07871183288075
H	3.10176167224752	-10.18197312895291	3.92248401957421
C	2.10156663089810	-10.39309497672848	3.51827258937019
C	0.02845717292434	-11.67059435744304	3.54898172531301
C	1.64599766744250	-9.64512558205262	2.41571283277415
C	-0.43401639196362	-10.92954004109851	2.44985058276863
C	0.36942684105110	-9.92620432637281	1.88685029167607
C	3.22601367618053	-9.37100489154601	-0.44450990142544
H	0.00333190873738	-9.36841363635229	1.01099059492649
C	2.43540855589164	-8.46993924104027	0.30570981794186
C	3.16434888620279	-9.38177415378525	-1.84739190031443
H	3.78615163468468	-10.09712967374517	-2.40868467377917
C	1.58456063221850	-7.58803299944847	-0.39379675437510
C	2.31392161209371	-8.49734108163535	-2.53313319918603
C	1.52347885802395	-7.60014684930500	-1.79889048632321
H	2.26368625950874	-8.51113744485501	-3.63374790304266
H	0.85024210365912	-6.90151120867385	-2.32080087992884
H	3.91237866627598	-10.06131292468024	0.07787395027651
H	-0.59784927729835	-12.46376289388756	3.98612292213452
H	-1.42536690397811	-11.14005973750830	2.01980900556107
H	0.95760029027708	-6.87022597092153	0.15519756701914
H	7.71282969708159	-10.84683308687063	-0.44201480925136
TS-E2-anti (PEGphen-KF)			
H	6.41308441735777	-9.34590766200233	2.54186967701892
O	6.88628796293203	-8.60186810641708	2.08323433100164
C	8.29797797992879	-8.83560696270214	2.06518563130536
H	10.03961393960094	-7.57852861213476	1.71014740214150
C	8.93238190990171	-7.50316620529174	1.59898859289017
H	8.71268624770651	-7.37295725378710	0.51246646280747
O	8.42631654396770	-6.39259491028970	2.32367242958098
C	2.49575275904616	-8.27347598127544	1.92491739164168
H	10.18865148313195	-5.27842655136508	2.48894752635856
H	4.06295964425509	-9.00925351674933	2.96509910333991
C	9.15316205564423	-5.19628509094051	2.07820016611194
O	3.60641067663108	-8.13616940333019	2.80939973224734
H	1.48688348947591	-6.65840040894229	2.92629603714560
C	1.83992465245868	-6.87929503645153	1.89242648869425
H	9.23930725103218	-5.01488326421757	0.97881211002105
H	8.27018777084033	-4.25201199627586	3.81856726225710
C	8.45117614369121	-4.03093082216610	2.74062307395463
H	0.94180639551038	-6.89975178509552	1.23061799358376
O	2.75139942616936	-5.87355310662701	1.46782682538699
O	7.22331139220351	-3.78956968138195	2.05408619075314
H	9.11120835202906	-3.13166069627169	2.67301626597303
H	1.92776692300548	-4.36326629885721	2.64622039343151
C	2.20376228447538	-4.57088414314301	1.58446889309352
H	6.19853213981663	-2.89746347556322	3.63900904965308
O	4.35349734619541	-3.57707411609896	1.93369762861581
C	6.48554624248819	-2.69576147341740	2.58027488248225
H	1.27463490243297	-4.47520565656963	0.97060062723291

C	3.20453353725825	-3.53847982994554	1.10721583546003
C	5.24668989351986	-2.48961585358954	1.73474289777875
H	7.09737948257455	-1.76094167769276	2.54960218158897
H	3.48173688155152	-3.72689933318811	0.04112241563852
H	5.53132497632297	-2.41229447922510	0.65756984449638
H	2.71533584162663	-2.53461438853668	1.15466220822913
H	4.75708359322204	-1.52930906408615	2.02834663465706
K	5.54660156814259	-6.12898514195993	2.49983587767576
F	5.18406977004455	-10.15778272249057	3.49544492429690
H	10.06043797161303	-8.16487597544839	6.43352466791624
C	9.66673160524121	-8.88137365146704	5.69691569831305
H	9.40774005507046	-7.35167052825833	4.19193415966627
C	9.30462536621259	-8.42091515461726	4.41956563773611
C	9.50725134008889	-10.23408011318200	6.03441312263464
C	8.77260858917512	-9.30468139403414	3.45670441566123
C	8.97265916424320	-11.12341090112485	5.08715960568037
C	8.60808917150326	-10.66188300445335	3.81348832324450
C	10.00356579419766	-10.36193288207257	0.89879685804582
H	8.19240609721316	-11.36981051363991	3.08059356346410
C	8.68630627136486	-9.86195196755740	0.97782722046497
C	10.37400475435152	-11.24392233371576	-0.12787003653572
H	11.40467096474965	-11.62861034129148	-0.17133418177863
C	7.75048817864586	-10.26189944164815	0.00613721085136
C	9.43103633716583	-11.64486976207868	-1.08912573709795
C	8.11908100393305	-11.15224265102173	-1.01623077549905
H	9.71944778323732	-12.34283095696908	-1.89053806255619
H	7.36962530825746	-11.46064217035717	-1.76228100140634
H	10.74394615176318	-10.07232327132133	1.66100568998283
H	9.79251293375458	-10.59340577544797	7.03496721518317
H	8.83535772370809	-12.18628186164717	5.34006253592019
H	0.40692548959051	-10.56981994452678	5.50041921419182
C	0.39861089666751	-10.33780891182010	4.42392066770725
H	2.18446222081512	-9.09749088170634	4.53103352870570
C	1.39982939188918	-9.51465613804526	3.88318664800836
C	-0.60493381290047	-10.86607212541640	3.59774537773823
C	1.41969438482723	-9.22041704891133	2.50619039829536
C	-0.59910975737353	-10.56938300884472	2.22482992117435
C	0.40720776344092	-9.75528103113649	1.68292720971921
C	3.58938804528429	-10.05075001194209	0.48266862457979
H	0.41510242851721	-9.54411217953358	0.60213842518330
C	2.96317545113934	-8.78573682483947	0.54710788828181
C	4.02416293012478	-10.57817978074606	-0.74095173094146
H	4.50292412396096	-11.56915561155713	-0.76550208567675
C	2.78428279807873	-8.06706833850652	-0.65123047984963
C	3.84130639879449	-9.85131288939619	-1.93000459666746
C	3.22035116180358	-8.59524256755865	-1.87936168872812
H	4.17927237530095	-10.26512053331712	-2.89238136097303
H	3.07006690561263	-8.01597747105524	-2.80359669647273
H	3.73614339109306	-10.63679398539170	1.40354121256958
H	-1.38905205697410	-11.51275579539926	4.02165000611841
H	-1.37927088908053	-10.98324324541277	1.56719125499060
H	2.31109353093829	-7.07638578719372	-0.63455728349209
H	6.72393806596338	-9.87254691131404	0.06178916771751
H	4.62378564273017	-9.59154287668250	6.46445343712011
C	5.56413727772401	-9.34386119419189	5.94330425760138
H	5.36114383725949	-9.77423834353545	4.63640482638464
H	4.86864962842047	-4.17759032170103	7.60608997043188
H	6.45181470439618	-9.92713397168111	6.24083733511247

H	4.86926658463304	-7.45058532336506	5.17369505795855
C	5.74489900653917	-8.05694919184152	5.44810811264744
O	6.20148789240878	-6.58908507393227	6.88310170040863
C	5.95772005047752	-4.03521046298003	7.48703024917756
O	5.77930102521250	-4.96727550872905	4.99029317587991
S	6.56099936271242	-5.22540756254402	6.26491445679617
H	6.48803347711428	-4.22912598795913	8.43680730885949
H	6.19027264305588	-3.02119695860452	7.11164209227565
H	6.68877837382857	-7.82086176775165	4.93700820703819
O	8.03461081429211	-4.99602507149680	6.12245507169120
TS-SN2 (PEGphen-KF)			
H	6.47610210267467	-9.26638512168861	2.46169436322422
O	6.97121198048743	-8.70327032105264	1.78738134122599
C	8.36908835072802	-8.97282726622697	1.79533225235133
H	10.15451713177166	-7.79277094308259	1.34595688207479
C	9.04836347153437	-7.69745542819662	1.23577520986514
H	8.82405701858716	-7.63250559882250	0.14422678687146
O	8.57392795663631	-6.53075636148628	1.89155561114345
C	2.57867142584907	-8.25150656169385	1.82508138522165
H	10.36104504261140	-5.44529605487140	1.92236885205141
H	4.22933173906500	-8.94046153655187	2.83571749861015
C	9.30407964285470	-5.36074768229510	1.56766395706756
O	3.75244971712566	-8.08591196503508	2.60951003418090
H	1.64312942890570	-6.65397298810352	2.90857733710481
C	1.90301331050226	-6.86400730677163	1.84689071038949
H	9.33491615492411	-5.20626114276828	0.46087277303529
H	8.48374655557603	-4.38475391757943	3.31729022171857
C	8.65492521078445	-4.16647705891434	2.23721379830342
H	0.95318814855846	-6.88885406274985	1.26198831299705
O	2.76677474297124	-5.84507946244424	1.35331279988305
O	7.41672289121764	-3.88558180179688	1.59506018458250
H	9.34053021493435	-3.28741365390569	2.15468031572817
H	2.34118047159217	-4.46107662567200	2.85292242156312
C	2.33679694452528	-4.54766802967461	1.74033067585867
H	6.52223046385381	-2.97901306522951	3.24576956765601
O	4.55202572747218	-3.64075628235964	1.68915561438771
C	6.73040859334064	-2.78135187031564	2.16802924201008
H	1.29683556100035	-4.35186614557593	1.38024894235752
C	3.25092015741659	-3.49644439415179	1.14489717219957
C	5.42670358195676	-2.55713490434540	1.42919250221707
H	7.35090620154170	-1.85473157543580	2.08938749006644
H	3.27879423550857	-3.58279377864752	0.03126946251012
H	5.61570988773947	-2.45340278401321	0.33252395142266
H	2.83326770368676	-2.49094880007514	1.39697905224917
H	4.97588016056434	-1.59938400581908	1.78734401527340
H	10.26022820060647	-8.09070498572111	6.07978054395125
C	9.79656519322495	-8.82660665932145	5.40481192518414
H	9.59915591537941	-7.40121414735102	3.78642942981815
C	9.43305119640261	-8.43870298707744	4.10378552707544
C	9.56314822304481	-10.13780603511220	5.84579668072415
C	8.83318860581329	-9.35682546932936	3.21690679476887
C	8.95816379370732	-11.05947127526518	4.97514165144663
C	8.59883528266347	-10.67193643123213	3.67641884581451
C	10.04170563955337	-10.61607063531613	0.73695528862153
H	8.12909523388758	-11.40417260125048	3.00311870392124
C	8.73274449642799	-10.09199239251405	0.79183920620134
C	10.38351868804187	-11.59030045385392	-0.21334805740577
H	11.40788423178474	-11.99333535657878	-0.23849122657632

C	7.77519615201543	-10.56214609368344	-0.12497258682077
C	9.41913027495602	-12.06017626392586	-1.12054080998084
C	8.11509232787191	-11.54364661105389	-1.07086334673541
H	9.68416749403830	-12.83115215754876	-1.86090907165058
H	7.34992577633140	-11.90657249622246	-1.77532858545208
H	10.79862217427224	-10.273544461574310	1.46037807098209
H	9.84938575283603	-10.44059128534883	6.86449208421361
H	8.76508622450126	-12.09096255163972	5.30803107658757
H	0.71698268528399	-10.38531657713916	5.61275348707421
C	0.66511204580180	-10.23446266652272	4.52296630869957
H	2.38425427647354	-8.90174256511710	4.48417976923193
C	1.60603741657898	-9.40516244834422	3.89236814202201
C	-0.33522016613862	-10.86963941610415	3.77056125029009
C	1.57003333418585	-9.21021625986271	2.49742550056707
C	-0.38774656389623	-10.67039575837107	2.38159607501829
C	0.55912665959627	-9.84872885687649	1.75009969469594
C	3.59990949204792	-10.00837260964049	0.30890158869986
H	0.51968333088640	-9.70993466800209	0.65840678131826
C	2.94811010826300	-8.75928188051954	0.41686862669613
C	3.95996182333547	-10.52910658355388	-0.94125771549138
H	4.45813176617009	-11.50910076153572	-0.99980966534110
C	2.66732533670553	-8.04844559143661	-0.76619591203790
C	3.67686348140748	-9.80920340904181	-2.11502977934531
C	3.03034269820535	-8.56881134863316	-2.02164840929566
H	3.95781645473974	-10.21655772641339	-3.09827899138889
H	2.80179312745485	-7.99558645446278	-2.93346880712353
H	3.82319967065367	-10.58543512030256	1.21983500090515
H	-1.07213621881631	-11.52112160228161	4.26582262871942
H	-1.16771147224688	-11.16483064881080	1.78164896758377
H	2.17128303638671	-7.06967982025125	-0.71526649114950
H	6.75654828482857	-10.15076099866495	-0.08158346009430
K	5.67814598308321	-6.21632513051336	1.99615934893071
O	6.36212794282979	-5.29026150811508	4.51947883926709
S	5.44774221435542	-5.55202303640536	5.69558523942380
O	3.99613613121374	-5.34190611137658	5.39860571687623
O	5.74714023224732	-6.91896890555851	6.35765767342307
C	5.91744534949591	-4.38623061951149	6.99660543839621
H	5.28683507090040	-4.59166922178827	7.87993039047158
H	5.72870787874394	-3.36710841639809	6.61100137469224
H	6.98706158736175	-4.53394185217694	7.22969166599523
F	5.41172929329325	-9.77746045406080	3.55667465634053
H	4.67985401355242	-8.08893629407729	4.71797198318826
C	5.60366382708593	-8.54292440456175	5.08703426531654
H	4.61035262204859	-9.65011507790726	6.65954995591858
C	5.60444302832891	-9.54762735635843	6.18727344124065
H	6.34945667743818	-9.26640021316727	6.95573001742311
H	5.90848703415931	-10.52418173651709	5.76394942643982
H	6.55536770009587	-8.21749588717635	4.65314309431144
TS-E2-anti (PEGphen-CsF)			
H	6.65515167542456	-9.50986593972140	2.48080611960053
O	7.14264842936784	-8.86360838271058	1.90932712295179
C	8.56420974684322	-8.97234583045534	2.03681145457140
H	10.24096107465064	-7.61733762452032	1.70818324943023
C	9.13847351205829	-7.61819718402118	1.53580977579024
H	8.97399955419900	-7.56484949615530	0.43221618378858
O	8.53342998244654	-6.49718015357135	2.16366021231205
C	2.10681904155981	-8.24034165935402	2.02798791633724
H	10.21259354238161	-5.25547531830988	2.18153927057510

H	3.68994425032282	-9.04175905824723	3.03543995308080
C	9.15378164221414	-5.26241782798233	1.82533810230313
O	3.14609766553229	-8.20884918166703	3.00213551903919
H	1.18960725170702	-6.64622518069311	3.13898884628735
C	1.48640272601896	-6.82440809671417	2.07989377694259
H	9.17349714048468	-5.12847526210329	0.71520257586886
H	8.26246158773388	-4.31095131331393	3.55675205208200
C	8.42945633055185	-4.09761902082293	2.47544949226236
H	0.55796066890144	-6.79108883261416	1.46249040251383
O	2.40621744288066	-5.82883456499903	1.64682539421879
O	7.18909805715079	-3.84825857542744	1.80803070533083
H	9.08546124223282	-3.19608276532653	2.39582803100892
H	1.90243499968040	-4.35221093592992	3.03683991586745
C	1.98641750102234	-4.50426568852457	1.93354610184639
H	6.26373373848203	-2.95516986738437	3.45640038133459
O	4.20992383210058	-3.57379746564365	2.01415755294787
C	6.45983377488362	-2.76432909511954	2.37505954075471
H	0.97971003856145	-4.30613217917368	1.48968902529099
C	2.96004984826860	-3.49283776772024	1.35156183668976
C	5.14419259266876	-2.56869113061892	1.64087042698973
H	7.04979720340163	-1.81893688523547	2.28428778160791
H	3.08171463950633	-3.66714121983086	0.25388205888190
H	5.31979659261424	-2.58491260921484	0.53693208912752
H	2.51349817120124	-2.47516885912335	1.47953360660166
H	4.73986754843267	-1.55991623960628	1.90202457792646
Cs	5.45118899774920	-6.37150635043761	2.19652689922969
F	5.10675478016850	-10.02078391265596	3.41827392765860
H	9.88744741271589	-7.93871855363799	6.48452344035576
C	9.61382192231155	-8.72289735004340	5.76314114975533
H	9.37533176026770	-7.29481283126465	4.16098734253420
C	9.32924517173663	-8.35692519880414	4.43637453090248
C	9.52364112714249	-10.06490580087984	6.16257935134854
C	8.94609438967831	-9.32718997553137	3.48649948552170
C	9.13498482028705	-11.04005535426475	5.22876422786768
C	8.84806102548880	-10.67356367203133	3.90545532577056
C	10.47658876924437	-10.42250524509776	1.11337712053216
H	8.55410497536528	-11.44813490695240	3.18034058028878
C	9.12570709259465	-10.02067914473434	1.04835944097249
C	11.00003182456120	-11.32783588158554	0.17792464126687
H	12.05439220054526	-11.63700650134115	0.24824960450639
C	8.31271646207498	-10.54105785091038	0.02435669818791
C	10.17900994243435	-11.84889981867778	-0.83569824585325
C	8.83448895171488	-11.45367091050164	-0.90751401820396
H	10.58689477189136	-12.56562511148026	-1.56550460764548
H	8.18241121908207	-11.85981124900623	-1.69677745240180
H	11.12183407049326	-10.03798544229260	1.91887365415333
H	9.74847382976943	-10.35059595275022	7.20155911610478
H	9.05456930918542	-12.09601220980635	5.53052036206081
H	-0.20853384079777	-10.82231002728622	5.24378176013040
C	-0.15063356719373	-10.49866401870053	4.19302326016682
H	1.63002185484401	-9.28463004685039	4.51328707995301
C	0.88220355221901	-9.63749579146747	3.78809974664754
C	-1.10139264970138	-10.94936061321580	3.26457441861359
C	0.98430875845800	-9.22164802553077	2.44623648100707
C	-1.01146157960804	-10.53448084732898	1.92585538547036
C	0.02424821689138	-9.67898988805077	1.51992680382045
C	3.52338922822280	-9.72387772675025	0.51385248461909
H	0.09516547703867	-9.37508440594583	0.46431478100301

C	2.65270962733282	-8.61829441296170	0.63451342223937
C	4.01269420828472	-10.12127031345294	-0.73936976828293
H	4.68726669640280	-10.98931094185391	-0.80545254381749
C	2.28485814719914	-7.93003019680588	-0.54011837788743
C	3.64073644141447	-9.42581938512237	-1.90147343947666
C	2.77294609089961	-8.32923709265166	-1.79621685222195
H	4.02432847003777	-9.73889589537525	-2.88434357553202
H	2.47100962665582	-7.77387728935828	-2.69753145569065
H	3.83640452290199	-10.28812300081626	1.40685495950593
H	-1.90888520665092	-11.62754310864005	3.58175556620301
H	-1.74756075857113	-10.88759745898300	1.18710223476482
H	1.61303911418988	-7.06211332795622	-0.48199128221383
H	7.26133904477624	-10.22206543097462	-0.02788173858665
H	4.69281014846688	-9.55835262312039	6.47247112299814
C	5.59887907957137	-9.33220406461055	5.88499139332043
H	5.31135286980238	-9.70342481652600	4.57847152241294
H	5.33961531800217	-4.16641701151241	7.64378004439972
H	6.48251449102260	-9.95624732842965	6.10280881672838
H	4.93408769283220	-7.38194388219402	5.23511424260284
C	5.80166581071287	-8.03091315246041	5.42769835500614
O	6.44845363123613	-6.65696136243433	6.82755352519598
C	6.43065300408251	-4.10601358282148	7.48110186291612
O	6.07557640035152	-4.97452636456960	4.97451724874692
S	6.88780162015147	-5.31053532046055	6.20894092288173
H	6.98261828996563	-4.36069324700803	8.40360084206227
H	6.72545073145061	-3.10513537176546	7.11486518704154
H	6.70760686314981	-7.82978140069173	4.83926044854782
O	8.36772470196578	-5.19516078877186	6.00916148762766
TS-SN2 (PEGphen-CsF)			
H	6.92582743868750	-9.28626152001797	2.35634875869919
O	7.53094293966368	-8.97206748616895	1.62060765684634
C	8.91339496020541	-9.01797484305770	1.96452567004410
H	10.63379503023545	-7.68445908255234	1.72209457417228
C	9.55367371011751	-7.70318700655235	1.44036842247674
H	9.50294585082823	-7.72580951723017	0.32481717655167
O	8.89355900755490	-6.54489537615992	1.93056230116351
C	2.48251755118040	-8.28032791979615	1.50483613866071
H	10.57028441449609	-5.30111814538441	1.92005259681216
H	4.04734717164234	-8.85157716579804	2.71827272844355
C	9.52052693354287	-5.33350129652514	1.53665425060303
O	3.34646396177466	-8.14355490113007	2.62432372159881
H	1.36268054953607	-6.66431094316268	2.34905011995026
C	1.81679721904131	-6.88943115514878	1.35869742640026
H	9.57439039274198	-5.26217442224896	0.42183375584446
H	8.54404103576159	-4.30510852800840	3.17379189632883
C	8.77510893564729	-4.13514412462582	2.09652286851953
H	0.99292330549079	-6.93912150488667	0.60822594631416
O	2.75037978436709	-5.87351728251064	0.99993665548357
O	7.57170548168106	-3.90369772281105	1.36595698890956
H	9.44218670584678	-3.24122047078318	2.01612684431026
H	2.41089939690138	-4.53562643913074	2.56853860804849
C	2.38509304234177	-4.57518712576549	1.45359045080544
H	6.59802949509951	-2.96886269505373	2.95957735572784
O	4.61843038031492	-3.66325659413959	1.43939536426699
C	6.82464854062859	-2.80494485421443	1.87973670768018
H	1.35107425681586	-4.31998851252300	1.11634077577921
C	3.32207956137634	-3.52411091988353	0.88274014032366
C	5.52814476682654	-2.62701944142011	1.10952164685112

H	7.41878747648679	-1.86236770882976	1.78457715845575
H	3.35932525544498	-3.60409271328495	-0.23182454997562
H	5.73060480331959	-2.60981489102648	0.00988973137765
H	2.90111948310384	-2.51894812711703	1.13388232834599
H	5.09582199019035	-1.63379740758428	1.38661845655696
Cs	5.77636604776780	-6.44600871773972	1.74907909944646
H	9.10196185854043	-12.22965554492209	-1.50853655420579
H	7.93247661256691	-10.47602153175858	-0.12869301668240
C	9.62951483482869	-11.74327259681037	-0.67312271834851
C	8.97027515537052	-10.76545582443928	0.09053675769726
C	10.95386465326231	-12.10041271700597	-0.37657996388532
H	11.46973770940006	-12.86758170891967	-0.97462644233382
C	11.61588407200717	-11.47605329808456	0.69375677368056
C	10.95535572351800	-10.50339670277503	1.45987556001531
H	12.65177590758896	-11.75514243434394	0.94065734009838
H	11.47486449296520	-10.03729859539359	2.31193039439540
C	9.62510280533326	-10.13779940180366	1.16652940059761
F	5.53972393090869	-9.39758059352911	3.30655162002088
H	-1.22116323024360	-10.97975951695981	0.26351651883703
H	0.67592320767146	-9.44888081335723	-0.26000156809433
C	-0.57401937661205	-10.61531869601226	1.07624259957730
C	0.49042435903697	-9.74922458624969	0.78319114027227
C	-0.80632824789239	-11.02491763156802	2.39972214183086
H	-1.63747532619531	-11.70934958289247	2.63070581428921
C	0.03100766071328	-10.55904532875235	3.42482665928774
C	1.09209112776595	-9.68623486966066	3.13240793833239
H	-0.14077484938417	-10.87733653452132	4.46480985109645
H	1.75159425642852	-9.31422656773098	3.92990746106344
C	1.33546303458497	-9.27541470122046	1.80840537253393
H	5.33416979349210	-11.31588416694823	-0.69309231705666
H	4.10058261116025	-10.46877970479677	1.28264795506925
C	4.73170076109320	-10.39920613084897	-0.78482890315608
C	4.03250523841464	-9.91832291119493	0.33122775434127
C	4.65599483727393	-9.72152580959064	-2.01354576792771
H	5.20032639042078	-10.10006588520456	-2.89212667547764
C	3.87660638074925	-8.55944702061136	-2.11064365963642
C	3.18028992144978	-8.07475886574456	-0.98916329885981
H	3.80689710193839	-8.01958354287629	-3.06796842097561
H	2.58875483787275	-7.15413143679936	-1.08320526653361
C	3.24933427016219	-8.74505062678693	0.24971271958054
H	8.67129713481967	-11.81413425665430	5.73779397160754
H	8.48193660074131	-11.33424421902024	3.29996532062996
C	8.90432006755758	-10.80633168342828	5.36051718537431
C	8.79382120045397	-10.53563234196439	3.99015011589689
C	9.31531788879208	-9.79754724137726	6.24840711953002
H	9.40561035865850	-10.00851413616086	7.32517147409991
C	9.60811644844547	-8.51931827428934	5.75115987920737
C	9.49542924252873	-8.24789894942982	4.37624818337027
H	9.91928494391406	-7.71658272935121	6.43675089068529
H	9.70221383963851	-7.23432915755493	4.00920146926712
C	9.08962640369982	-9.25307851932954	3.47538499736081
O	4.18610667756952	-5.14718233910788	4.98826404765650
H	4.76159732773767	-7.73870309893582	4.49617013634943
S	5.55246526622121	-5.31999360055187	5.58031180898781
H	4.90022203749674	-4.42435415700266	7.70043281364372
C	5.61764696541132	-8.26694951518452	4.92672049144346
H	5.57092513235471	-3.15695146488718	6.57893902958934
C	5.69892178478725	-4.18031685989037	6.97693828030769

H	4.35072837960749	-9.48527838481473	6.18957114883424
O	5.73894195462129	-6.70070035954251	6.26145650877891
C	5.41870352077076	-9.32794695242346	5.95433118703136
O	6.67772400067929	-5.00188280833567	4.62504879106428
H	5.85621861534293	-10.27193335453337	5.57720706286427
H	6.63509437543357	-7.99727165453988	4.62500928507196
H	6.69860202152645	-4.30840608917730	7.43000321550659
H	5.96009841833744	-9.05440541012702	6.88050861457461
TS-E2-syn (PEGphen-KF)			
H	6.83972053689333	-9.55344224831062	2.58778928918971
O	7.25981739681419	-9.23051250653780	1.75088668819765
C	8.68229122111667	-9.18169813034837	1.80616586762474
H	10.18021327654814	-7.92104422141277	0.80938652793648
C	9.06980778060769	-8.02509481427225	0.85661087045229
H	8.71556054077132	-8.30507882318637	-0.16292443348718
O	8.46841967606649	-6.80682860640684	1.26603916563033
C	2.46228513638637	-9.06000902418738	1.57215177281019
H	9.76273261563326	-5.56229326847473	0.19508293721568
H	3.85041021153323	-9.68880742242581	2.86729999829849
C	8.67063534836983	-5.73839040385162	0.35500664798064
O	2.97821647453775	-9.99458291932727	2.50279755441606
H	1.18176939108752	-8.12066448793495	3.03622298499986
C	1.96915715470906	-7.79568658794239	2.31705736563394
H	8.22111359911776	-5.98086420880826	-0.63850832608124
H	8.41887997876142	-4.30184330422624	1.95268127851682
C	8.06086854839306	-4.46537869355864	0.90905323409731
H	1.49037984813010	-7.08977290605609	1.59889711373524
O	3.03842392792553	-7.17534639146011	3.01792316614314
O	6.64103549699727	-4.54611989727169	0.88846187847730
H	8.40755977317526	-3.60554870045651	0.28467932208700
H	3.39167035352763	-5.81884605056703	4.50865204627154
C	2.69308806261865	-5.94919060967387	3.65580290041569
H	6.40292181016116	-3.24750948068759	2.50169100017041
O	4.20127055484953	-4.63823431543049	2.37251551734197
C	6.02704108112108	-3.39650083250435	1.46366670402140
H	1.65577104144682	-5.98973303046188	4.06039238037959
C	2.83551730440383	-4.74745679520142	2.72881385881876
C	4.52211872987961	-3.57120683211039	1.49952229936653
H	6.26774680145269	-2.48760224012726	0.85959377195161
H	2.19747522413085	-4.86009009464394	1.81702360666428
H	4.11875141044874	-3.76636564721510	0.47454593222631
H	2.49098750988966	-3.82801797898283	3.26324219516823
H	4.07204877970686	-2.61601810346241	1.86302122180330
K	5.89377249509196	-6.90354741922797	2.50252041447106
H	8.40338923461056	-13.24833202872033	-0.60215635639278
H	7.40979816602170	-11.18337265665054	0.44440786514344
C	9.05205176825628	-12.53014262288609	-0.07622907791727
C	8.48959551614808	-11.38285662155160	0.50782169510838
C	10.43305444157971	-12.76474810180367	0.01043865377874
H	10.87284586880473	-13.66531601221603	-0.44532597526966
C	11.25027677098664	-11.84661295556303	0.69097639981584
C	10.68709708160307	-10.70620430722472	1.28299223362353
H	12.33395926170924	-12.02596034464566	0.77227840342177
H	11.33136874156261	-10.00456380947980	1.83688581599054
C	9.30088452133182	-10.46194648936158	1.19578580730050
F	5.39808431804606	-9.44428613503134	3.61191199641320
H	-1.04615110327203	-9.16861193532595	-1.61361324797559
H	1.02629306934335	-8.19276469624786	-0.64126446386828



C	-0.57803653582838	-9.64655156292519	-0.73947176969425
C	0.58579649643751	-9.09289142862669	-0.18468485778491
C	-1.13499202573535	-10.81315781973929	-0.19038011327623
H	-2.04537272447452	-11.25097821941242	-0.62713987229595
C	-0.51744895561818	-11.41872792515736	0.91486855939054
C	0.64413167589625	-10.86152099582642	1.47488830949935
H	-0.94120147793155	-12.33811266444947	1.34720275510042
H	1.13647289582331	-11.33075322571267	2.33708610945052
C	1.20754949173082	-9.69156230477983	0.93063406495822
H	5.66124344609839	-10.50784903640922	-1.55694143462163
H	4.02542657211355	-10.85326889668415	0.30640217004263
C	5.12380587365737	-9.64613974438505	-1.13239240214399
C	4.20647200573208	-9.84411512212628	-0.09223825947737
C	5.36361974390780	-8.35401259433502	-1.63058009747591
H	6.08691756069057	-8.19686251465447	-2.44568548891881
C	4.67146147409510	-7.26559628991914	-1.08048164840047
C	3.74132900483595	-7.46851713803002	-0.04440490322688
H	4.85404450109048	-6.24588536781155	-1.45308972084810
H	3.20991722942657	-6.59877239807658	0.36612290592898
C	3.49857674636443	-8.75896481149599	0.46784336932621
H	9.05942421683710	-10.75842801199190	6.21938509913887
H	8.30599447225226	-10.91628389030805	3.85489820323228
C	9.30725828990396	-9.94982400370439	5.51419106038066
C	8.87690737821446	-10.03351226491587	4.18354601631303
C	10.07059815690138	-8.84935708655194	5.94035697453915
H	10.42460272693496	-8.78878434336332	6.98094911658940
C	10.38475959954388	-7.83393041543924	5.02513926713095
C	9.93625787395650	-7.91090166767042	3.69490116736936
H	10.98832423224882	-6.96914691180749	5.34342151756816
H	10.17081077699428	-7.09157613588633	3.00200072567106
C	9.17956961007290	-9.01348819450954	3.25399335930366
H	3.68763864893932	-9.23543336874977	5.86787488748750
H	5.17720962290389	-9.22981334525053	4.80232606375613
C	4.77076205270445	-9.15924554652079	6.07141676346096
H	4.55931883807004	-7.09701982514293	6.78276642491916
C	5.22290870080041	-7.96603575766863	6.65447678320205
H	8.71774888952180	-5.81766625468247	6.40346376205836
O	6.30194568842140	-6.87773211996445	5.27746533717689
H	5.25536185047924	-10.08976256769905	6.41431778159124
H	7.45721895307819	-5.74841128789654	7.71938820741273
C	7.83365666295833	-5.28051346375115	6.79132158085891
S	6.53115575150195	-5.35813777702149	5.53792895090399
H	6.11448752241721	-7.97383420747702	7.29958746947622
O	7.09872504144920	-4.74474620750040	4.29022756519074
H	8.05769714219098	-4.21257394802476	6.96644711086867
O	5.31992955335481	-4.70749462248334	6.12671362675003
TS-E2-syn (PEGphen-CsF)			
H	6.95005986758219	-9.82268644183679	2.08127737876594
O	7.48515946398936	-9.18986744470044	1.53419074218860
C	8.89004423312483	-9.33209350712058	1.68895891183060
H	10.57679237016404	-8.35862211702953	0.66029381074619
C	9.46920041076458	-8.25335571814458	0.74502152771264
H	9.03621537579297	-8.43616778444529	-0.26589888864857
O	9.12433920517582	-6.95721282621900	1.21132153595072
C	2.63529011334198	-8.27911717476260	1.66622714436438
H	10.56201441586259	-5.94181244219406	0.08381471032599
H	4.36083342228331	-9.23762260280592	2.11363505742285
C	9.46658092735819	-5.92324297253173	0.30844321564015

O	4.02307249922329	-8.55598959071543	1.47152601043605
H	2.91645188968407	-7.34002209459768	3.63568581407854
C	2.49044970922065	-7.08210995320756	2.63995161971825
H	8.92444231318934	-6.04667397249654	-0.66063883656801
H	9.59052963010390	-4.49477137889545	1.92752381654718
C	9.13316023914584	-4.57162648404320	0.91038457953826
H	1.41164549746856	-6.83909154814469	2.79229550873756
O	3.17484115681161	-5.96581365199599	2.08819217951582
O	7.72752166412011	-4.38895498877940	0.97636478382504
H	9.59651025499869	-3.77724264479917	0.27452143421536
H	3.44706514081280	-4.90527935732353	3.87407667989422
C	3.03127408509647	-4.77639736088723	2.84589825286816
H	7.64939186568040	-3.03306185882774	2.56922903339509
O	5.14735133832571	-3.80866148166256	2.19136709954177
C	7.35076196231506	-3.12351151947552	1.49529201842011
H	1.95264702364168	-4.50433811270958	2.95584443836051
C	3.73302992769071	-3.64418843177941	2.12272709093125
C	5.85529216500180	-2.91471529454506	1.35451161861318
H	7.86816164125966	-2.30523671604041	0.93721587113356
H	3.40297751257790	-3.62877286697762	1.05707924284769
H	5.55651754826225	-3.05982618215033	0.28773000476548
H	3.43876740571303	-2.67221130086283	2.58860355654044
H	5.62758749119415	-1.85377566995608	1.62688655860748
Cs	6.24829748716086	-6.71383807533996	2.84569995012191
F	5.48913617237549	-10.18782382166293	2.97497577574218
H	12.01189699727260	-7.99690855338781	5.01589407997652
C	11.00888984666147	-8.39562560084954	4.79793098798542
H	11.32228187518817	-8.33373035225831	2.66207831486919
C	10.61491299818765	-8.59071847325071	3.46469722192654
C	10.12680409062130	-8.69666242594275	5.84775530951353
C	9.33584883388906	-9.09885469714474	3.14869143050326
C	8.85040161456238	-9.19624288156322	5.54834685850350
C	8.46137847863248	-9.39880585110481	4.21364259901747
C	10.54179987573283	-11.33461340521076	1.60108844359769
H	7.44862934405841	-9.78077890199067	4.01405880928055
C	9.36346922791338	-10.70587522351336	1.15152846895891
C	10.96115663989970	-12.55416170211177	1.04592284790435
H	11.88170320398397	-13.03124203022161	1.41565907537896
C	8.61286374409357	-11.33080713405858	0.13340910310340
C	10.20875563592084	-13.16673141170326	0.03224485698306
C	9.03158100514175	-12.55022468563811	-0.42029001138118
H	10.53480128823735	-14.12563361157301	-0.39821011205008
H	8.42895334391544	-13.02420827661306	-1.21045724532827
H	11.13363882361457	-10.87498384385725	2.40579681323930
H	10.43296340247598	-8.53554744089174	6.89305377380151
H	8.13264526908430	-9.42470840430805	6.35077140002851
H	0.47099246563690	-10.89511985714233	5.00916882283161
C	0.84670693040271	-10.83564333584959	3.97615771528018
H	1.54134863632075	-8.81040234151426	4.24216566468357
C	1.44252021839239	-9.64186304167094	3.52885438695831
C	0.73482847593003	-11.94012823744383	3.11912514456343
C	1.92665618164862	-9.53516361820005	2.20880429481261
C	1.22359625652528	-11.84581544230760	1.80431073285829
C	1.80881023490419	-10.65477538296004	1.35543890504796
C	2.85205804651932	-7.71782221434173	-0.82994042307026
H	2.18417526918171	-10.58211023821039	0.32368644080450
C	2.03680477519609	-7.87229220528860	0.30550466693506
C	2.29654255668075	-7.31918909437696	-2.05789665490953

H	2.94825506676367	-7.20435192436181	-2.93861882603526
C	0.65374489292067	-7.62568033150356	0.18624829395288
C	0.92049066380112	-7.06757625647302	-2.16699256647092
C	0.09883137461274	-7.22467887274683	-1.03782747566255
H	0.48659320775527	-6.75418645439602	-3.12926261089970
H	-0.98405738148413	-7.03783715360969	-1.11194797959066
H	3.92743016027164	-7.92165512616173	-0.73368489134635
H	0.26754684201645	-12.87271143241414	3.47163939886582
H	1.14116176470486	-12.70587226889922	1.12154268747550
H	-0.00256506898139	-7.76492384718657	1.06025519530749
H	7.68269886059768	-10.85472258214544	-0.21004883656212
H	3.65477892101449	-11.75457795305102	4.45583600053915
H	3.42720356931690	-10.25604952325952	6.38144466442073
H	5.86394732235546	-7.03300034502460	8.08399584706321
O	5.20487824225645	-8.82905294029403	5.92764386470912
C	4.58210266476420	-11.47766847178520	4.99051770719015
H	5.06789349700021	-10.74227827718514	4.02545506835120
C	4.40496265221739	-10.70837585186675	6.15442240713275
C	4.78010070090923	-7.24317923489186	8.04252368285644
H	4.52152792735838	-8.12204022633779	8.66188704320456
O	4.75238869690365	-6.40571301383233	5.52035378094240
S	4.33543517902886	-7.60637991955309	6.32549225530332
H	5.35728971680486	-12.26376973023726	5.03111959158187
H	5.08937753423531	-10.81709175767600	7.00920764779554
H	4.19467615774846	-6.36071548209176	8.35912409835822
O	2.87260782216769	-7.92360571684941	6.31553198078274
PEGphen (KOMs)			
H	6.99439180075369	-9.03608740084250	2.59985655503911
O	7.25020284622356	-8.87689576483989	1.64072454272681
C	8.66903384799903	-8.89627939391393	1.51197723312671
H	10.27803889209632	-7.39680785772991	1.45332073581004
C	9.16587303109778	-7.43202916628772	1.38464972122178
H	8.88676679656175	-7.05350991763982	0.37223264578752
O	8.56220180774105	-6.62564647643361	2.38276398701314
C	2.26131166781743	-8.08027256289836	2.10799253032260
H	10.06136693041422	-5.44352073159995	3.24118916574068
H	3.38629297479596	-8.05263172816660	3.82747307860563
C	9.17776818332607	-5.36411858850443	2.56113371821937
O	3.14438069084323	-7.47519556451105	3.04130939657531
H	1.15126060523768	-6.24759778928508	2.01335830658539
C	1.70838568744043	-6.88983901639167	1.29527258053112
H	9.53728363902465	-4.95573964780699	1.58680689092917
H	7.70589417977150	-4.82503289953276	4.06820581641942
C	8.17233281774974	-4.39469478315733	3.15078122742591
H	0.98389065819233	-7.23443413369701	0.52062883264606
O	2.76832621771234	-6.14270675683925	0.70760562501972
O	7.18159321741816	-4.13552574210947	2.15831386164765
H	8.69727283043365	-3.44970952863695	3.42941435468360
H	1.86556617751048	-4.35442580278738	1.26449975076340
C	2.40284744626236	-4.81247441739263	0.39979105134701
H	5.75284828793078	-3.19596913294346	3.37024653154668
O	4.47767070615388	-3.94994984518408	1.23738324573286
C	6.33416361080375	-3.03383706136443	2.43068232703081
H	1.71624644827772	-4.77177782037432	-0.48284445524951
C	3.63503876704829	-3.98574324117894	0.09342887007409
C	5.38763390963008	-2.86204257736494	1.25987669003024
H	6.93137754213031	-2.09759635405351	2.55639673089417
H	4.18810553083188	-4.40480099809321	-0.78219508392784

H	5.97901497278915	-2.81742200522010	0.31382692538394
H	3.29947345561801	-2.95800003528949	-0.18248084989911
H	4.83742109152561	-1.89566074127693	1.36607108639655
K	5.54214444013950	-6.56908645302588	2.04283456075397
H	11.31874750519211	-9.31779556805979	5.45265139966783
C	10.65844502124963	-9.80620552232993	4.71854394018600
H	10.39401342151884	-7.99330294373144	3.56898236235600
C	10.13947070712512	-9.05940772928313	3.64669362572002
C	10.33480890841699	-11.163422269948862	4.85727866869894
C	9.29442211802592	-9.65864042011719	2.69447309075847
C	9.48875074934556	-11.77128203660530	3.91401134422457
C	8.97843390995049	-11.02605543096400	2.84406028740226
C	10.40071138264234	-9.81915270916798	-0.13449629550891
H	8.31736109564413	-11.50621405192535	2.10608803458911
C	9.04749899766822	-9.58340281197045	0.18566421952772
C	10.75464927372903	-10.39383539938974	-1.36447394381532
H	11.81528217795860	-10.57843452274565	-1.59669630293830
C	8.05490881535585	-9.94106678660803	-0.74580243467125
C	9.75922780990179	-10.74699245024328	-2.29077008800364
C	8.41046686707455	-10.52256394086706	-1.97461581266607
H	10.03659396188280	-11.20282118141139	-3.25372940286806
H	7.62236761677451	-10.80523333434332	-2.69014571570810
H	11.18604162468278	-9.56860998593663	0.59640279029331
H	10.74048277822531	-11.74740336287835	5.69792795820063
H	9.22446898500418	-12.83538688795329	4.01351485519318
H	-0.73398875812249	-8.54780974267966	5.73690084208058
C	-0.46952530799312	-8.86318836973976	4.71614661633835
H	1.29406415841513	-7.59251373353877	4.63395399562786
C	0.67107705951064	-8.32487035952360	4.09940957571916
C	-1.26568323434608	-9.79996359521319	4.03905255946906
C	1.03879087519422	-8.72483681322928	2.79877516893365
C	-0.90929038265990	-10.20033740060878	2.74140667520413
C	0.23560012772961	-9.66948086402539	2.12750570083255
C	3.79733667166801	-10.09374097412896	1.88273822809715
H	0.51756439019544	-10.00551593435003	1.11850328348018
C	3.00202821496645	-9.11995656483718	1.24061276788686
C	4.46482710468857	-11.07891721981406	1.14172029985333
H	5.08674173366987	-11.81859131417926	1.66845848605828
C	2.90080081591609	-9.16039033892563	-0.16547351550295
C	4.34815863255233	-11.11698935141553	-0.25781315411330
C	3.56556647462275	-10.15154840411483	-0.90882435061402
H	4.87124914656158	-11.89298733121910	-0.83790869620378
H	3.46918038968572	-10.16442780910662	-2.00636363633109
H	3.91097875451733	-10.07914192555946	2.97795430791306
H	-2.15964607300700	-10.22196547961973	4.52312160693227
H	-1.52248664771154	-10.94003398952143	2.20323426506645
H	2.29905347325301	-8.41083240302665	-0.69939221426576
H	7.00022025259885	-9.77244082254781	-0.48419098827484
O	5.96664135460337	-6.88320170667384	4.77053231584448
H	7.45477617509305	-8.47398057091547	6.67172573964196
S	5.68086371801164	-8.33458529999169	5.08292061246638
C	6.36796260952350	-8.67049353141634	6.71732950668029
O	6.38870134605015	-9.28530921003260	4.13426270776248
O	4.19653926853469	-8.64292493749114	5.19500720953924
H	6.16836068874185	-9.73067062608779	6.95635005135903
H	5.86815153086527	-8.00153166407291	7.44033326492664
PEGphen (CsOMs)			
H	7.26732223290694	-9.66219188947730	2.40115483908190

O	7.60438583659791	-8.95801095463481	1.76721507398079
C	9.01952776013944	-8.94742799811092	1.65900649809295
H	10.45911960167677	-7.60109563920626	0.71736218086630
C	9.35278616329285	-7.68780510357680	0.83222256604020
H	8.92077470282545	-7.82544493048068	-0.18684673868267
O	8.82482069194476	-6.50533531906490	1.42516358884050
C	1.95042298630908	-8.03224170907459	2.32600653580691
H	10.36295137668434	-5.26241854597789	0.74932731637070
H	3.26544614134837	-8.90422975709048	3.61856057980938
C	9.24549467641647	-5.33239832740795	0.75765383013498
O	2.97273916931312	-7.99426613732585	3.30795342785263
H	1.11076255790363	-6.30203563188060	3.27056114781729
C	1.44524315237661	-6.57716350360651	2.24489369892581
H	8.90754287497053	-5.33548482968234	-0.30790036016188
H	8.92366575219010	-4.16476879162219	2.55140686580088
C	8.70049302834607	-4.10439549989177	1.45800018318310
H	0.56059612943502	-6.50291434770627	1.56904647909439
O	2.47601367696964	-5.69665386687556	1.80816046879519
O	7.30359331039940	-3.98639414891467	1.23377315130841
H	9.22817193046667	-3.20455083324032	1.05635103892983
H	2.18721919630135	-4.11408221679961	3.14125850152750
C	2.16926325628519	-4.33790414896458	2.04596379640621
H	6.75681519008393	-2.80888411028325	2.87969934086429
O	4.45113478731082	-3.54077133970536	1.84004752076397
C	6.74938268512825	-2.79305612536165	1.76176709580624
H	1.14266133128146	-4.09317546268317	1.67634044288382
C	3.13593934446200	-3.43233042166931	1.31213541784374
C	5.33637622600689	-2.60282086712764	1.25186876412576
H	7.35376783416983	-1.91006043460247	1.43843212512527
H	3.13745501670371	-3.68450747079075	0.22384453545662
H	5.33281175656285	-2.70493091090017	0.13905414822742
H	2.76819113575022	-2.38089646227808	1.41302716201945
H	5.01012562089645	-1.56006337410452	1.49346937316719
Cs	5.63813863896078	-6.67481800850523	2.43223046215101
H	11.63297458708097	-7.15032158587699	5.22540814242094
C	11.04052029445384	-7.99661037136339	4.84354183415181
H	10.59289825265533	-6.99510415505512	2.97942899537312
C	10.45516393966528	-7.91256222045213	3.56802400047586
C	10.86939175796714	-9.14694657378150	5.62666327895310
C	9.69081241434633	-8.97627622279386	3.04937373465465
C	10.11552899980700	-10.21805706397587	5.11776509904898
C	9.53929613290866	-10.13533076252207	3.84291709239207
C	10.90285087207742	-10.45688132736267	0.75750974137794
H	8.95610171278079	-10.98513640992418	3.45807438147258
C	9.52979967662939	-10.13823675051404	0.80937951856489
C	11.36381833451874	-11.50684772243877	-0.05085464112915
H	12.43847201574574	-11.74720216733295	-0.07440261206266
C	8.62813990556935	-10.89331622448545	0.03664227268807
C	10.45658522773467	-12.25928763957012	-0.81459666781057
C	9.08843062534531	-11.95021225834586	-0.76593198192948
H	10.81646440514359	-13.09150972962008	-1.43956822538340
H	8.36894431832709	-12.54035843892816	-1.35486758516678
H	11.61739515021307	-9.88916152309931	1.37449755014133
H	11.32413384561823	-9.21099464073835	6.62683104506773
H	9.98039046085715	-11.13246904309575	5.71672015238610
H	-0.66187949155091	-10.11796484166848	5.67198778803292
C	-0.54994522039570	-9.89201534567459	4.60004686807215
H	1.32296135902106	-8.81933988520970	4.87914660498439

C	0.56654797932636	-9.16313616340136	4.15905111552845
C	-1.51327338292068	-10.33844176157724	3.68258025921829
C	0.74075710050387	-8.87822812002704	2.79031609901550
C	-1.35017911545101	-10.05519487179005	2.31686635872444
C	-0.23081698506770	-9.33310743922253	1.87462485887442
C	3.29757738616722	-9.72516520385954	0.98770350146100
H	-0.10332105036947	-9.13360708474699	0.79938135452266
C	2.49610990874689	-8.56176723856681	0.98120122752713
C	3.81103267113585	-10.25079281340552	-0.20711776155277
H	4.43333344797090	-11.15813007289073	-0.17140380256837
C	2.22036863063727	-7.94727914719621	-0.25760071268970
C	3.53092424957850	-9.62927179987742	-1.43549960761455
C	2.73180368645407	-8.47651488740002	-1.45547159650143
H	3.93273759295488	-10.04245040321860	-2.37329883496083
H	2.50384847771876	-7.97845929382002	-2.41076015186914
H	3.52955527859213	-10.22862893620580	1.93956781400066
H	-2.38652517222382	-10.91234309231597	4.02990099236535
H	-2.09478532758537	-10.40814780531134	1.58653617433271
H	1.60815281262916	-7.03500493794203	-0.29971234371842
H	7.55691625022048	-10.64683558398468	0.08336728480770
O	5.90846237175439	-8.63257835159323	4.80699373810479
H	6.98930593108262	-10.91194781312837	6.20238461112114
S	5.53337580742309	-10.06196805471116	4.51357547999525
C	5.90844965880036	-11.02121384483141	5.99758301444242
O	6.37196709665303	-10.68101896329273	3.40649281331163
O	4.04267038941171	-10.25148274000657	4.27839214156559
H	5.64404725071384	-12.07606683258432	5.80071188139375
H	5.30570170620616	-10.61102472063847	6.82773664612965

TCE (KOMs)

O	-1.69417620336885	-0.27455596810387	-2.35366554801989
C	-2.89305569951538	-0.93516006963537	-2.31984823155948
C	-3.08861897695325	-1.80682217091697	-1.20601692671353
O	-2.05144351264557	-1.86727967928762	-0.31277418002851
C	0.90353175882895	-0.19626799013336	3.32142559947325
O	0.96115095257027	0.77280373818136	2.27054670098111
C	1.26755943297181	2.07685674950612	2.55830338845276
C	1.50919238594081	2.91338800035740	1.42793305008266
O	1.39660415026497	2.30112129897601	0.20659998011121
C	1.81117121590154	2.98638770278423	-0.97722631078887
C	1.77260572955026	2.00213903675427	-2.13839099969444
O	0.39374082509080	1.66855433669453	-2.38278851205226
C	0.20630062080432	0.70529961048911	-3.44722165521676
C	-1.28331043407642	0.40645020932466	-3.54490829218622
H	-1.45878966512642	-0.24327010176562	-4.42985238991342
H	-1.86335186430990	1.34896447253665	-3.66948231552670
H	1.13554887306324	3.84697663265138	-1.18410442305806
H	2.84932040540112	3.36499683706958	-0.85184909199857
C	-2.02855889349142	-2.88459102434883	0.69023239786722
C	-3.90285642205270	-0.80841438239234	-3.28413246982840
C	-4.28741745813308	-2.52441099599649	-1.09020904280023
C	-5.29279491749149	-2.39010847587503	-2.06742206907181
C	-5.10132728139156	-1.53681323493560	-3.15793005295299
H	-4.44726253164592	-3.19180557968600	-0.23180290524841
H	-3.75932745982725	-0.13623856967670	-4.14126270810502
H	-6.22830939476309	-2.95906822067676	-1.96251831930592
H	-5.88398260495288	-1.42560969955285	-3.92337403705648
C	1.35573704263896	2.61464882253259	3.84966761607491
C	1.83841391709238	4.26197893039610	1.62061602905043

C	1.68652313506904	3.97142316235914	4.03045155164180
C	1.92755888880653	4.78975070156234	2.92320620604235
H	2.02927836399402	4.91010303353588	0.75481378606745
H	2.19091508037352	5.84872281911359	3.06025861963838
H	1.16759360563519	1.97757187267099	4.72460199895045
H	1.75506508060502	4.37935916827487	5.04963853107554
C	2.43647986417147	2.56246606305630	-3.40247275014253
H	2.31533467895006	1.08045040774879	-1.81360254605454
C	0.79061264915525	1.22797000170405	-4.75972904530318
H	0.72350037883350	-0.24152324551025	-3.15944428835583
C	2.28509770872789	1.58568409462881	-4.58113508086887
H	3.51057021383126	2.76121964486919	-3.21228841795716
H	1.95200446959844	3.52608054086842	-3.66792940389628
H	0.23112297530133	2.13188530326394	-5.08484074636236
H	0.70143186282742	0.46779723600301	-5.56267915146265
N	3.12020312560985	0.41178130513272	-4.38452921489667
H	2.64124371831807	2.05713508885564	-5.52103851760926
C	3.70580453166120	-0.29162114959878	-5.40839270585202
N	4.41833773991067	-1.37741236221303	-4.99633180755085
S	3.55729039129806	0.14264467743622	-7.04161253863742
C	5.18931899975112	-2.21776290599810	-5.88583412555570
H	4.56438254009727	-2.58815642523067	-6.72433245042939
H	5.57540122712205	-3.08014939748287	-5.30882673715500
H	6.04816363441071	-1.67437438313115	-6.33660405709936
H	3.23025242445239	0.01013878343612	-3.44025270835022
H	4.48550290471758	-1.53282583942669	-3.97889011319906
C	0.82936001959496	-1.57943529376273	2.69178182431740
H	0.01389675007941	-0.01603786987369	3.96646368098362
H	1.82111488561714	-0.13090878641291	3.94673874919150
C	-0.63898419598770	-2.92753319120586	1.31542145370918
H	-2.24974990881354	-3.87385640914445	0.23185119875582
H	-2.79165088074852	-2.67463516932424	1.47367690200845
O	-0.44766583618291	-1.68639862936998	2.02670239834761
C	1.00871955820930	-2.70943399239365	3.70669478937922
H	1.64329433438568	-1.64268146578541	1.92708927880700
C	-0.46488003279062	-4.13270197221930	2.24745012197618
H	0.10232094118674	-2.97896107643560	0.47971421188773
C	0.87594860578811	-4.07945937976426	3.00347695798515
H	-0.52418811684999	-5.07434306622329	1.66420864172330
H	-1.29215281112035	-4.13687121292920	2.98974255618384
H	0.23791068325040	-2.61574974342801	4.50242738261913
H	2.00506060671518	-2.64604424407905	4.18996331845889
N	4.15662358911409	-5.00155314635234	1.66671790707407
H	4.08015308236687	-4.32637886548381	0.89095599333826
H	5.87958375625616	-5.42505124437154	2.83445913978817
C	3.10164638835289	-5.09006286696123	2.51824120506481
C	5.41004947915060	-5.69516806384085	1.86391590742776
H	5.27034343517677	-6.79719085457860	1.86766833062727
S	3.13826455550774	-6.04501989333855	3.92049419709659
H	6.09600388728997	-5.41796501269146	1.03991715197063
N	2.00415131251213	-4.34970262612342	2.12685792080801
H	0.90752951218075	-4.88243925764634	3.77014303815436
H	2.17409432349303	-3.71939880763305	1.32714801243214
H	2.39805678057164	-3.43873262183788	-3.48093265384408
H	1.99515487027988	-4.46902456199750	-2.03631002353226
O	1.44340245507895	-1.73533298109475	-1.35361704926072
C	2.72889365782654	-3.77130631286178	-2.47981662005117
S	2.84170027514372	-2.31410468929754	-1.41245620337697

H	3.73002839139460	-4.23721785113886	-2.53057840265287
O	3.82742857095822	-1.38094382167678	-2.08368296062773
O	3.30610123160158	-2.81333067589523	-0.06076822111302
K	-0.10586834019254	0.04226724597408	-0.16136870330249
TS-E2syn (TCE-KF)			
O	-1.90143560644402	-0.80227035332909	-2.39408838150730
C	-3.21213694174028	-1.10055101690404	-2.09847694378340
C	-3.44254839333355	-1.77771201854549	-0.86480058805066
O	-2.33213821652082	-2.05174708523990	-0.11013875298265
C	1.34314853919278	-0.80563111354225	3.02599675194851
O	1.54041552339618	0.01112360378275	1.86388206955475
C	1.99272009409785	1.29486477171583	2.05100417955553
C	2.13166971150955	2.09308793626975	0.87774991019008
O	1.81061020094453	1.48764684108904	-0.31477111899066
C	1.92414012466998	2.27235842067372	-1.50767901037703
C	1.64694860581956	1.41680184987336	-2.73106749774937
O	0.26937067667216	0.99111120894658	-2.66574292672103
C	-0.15126108876828	0.16766666400709	-3.76922508440690
C	-1.64241344768815	-0.08475394743350	-3.60304404659268
H	-2.00390042675635	-0.66923850237734	-4.47862972552411
H	-2.17660181944022	0.89139254639200	-3.58115583915015
H	1.20739398898089	3.12338529027162	-1.46791808583789
H	2.95453808021143	2.68144587228282	-1.59481390907826
C	-2.48652951556736	-2.84580119197197	1.07257077199135
C	-4.30169914170339	-0.78472360451649	-2.92463764811848
C	-4.75398694453607	-2.11540957434897	-0.49684543824154
C	-5.83688828207834	-1.79500816042122	-1.33629892609795
C	-5.61181904425888	-1.13220399018191	-2.54502876939134
H	-4.94181069272197	-2.62840655476217	0.45507473671496
H	-4.14013729490186	-0.26636075032490	-3.87809905776675
H	-6.85671668917632	-2.07073392206058	-1.03087348291615
H	-6.45089504621192	-0.87685308642383	-3.20836804644107
C	2.31683912923873	1.84464959999831	3.30127787198198
C	2.58172254308055	3.41758766478571	0.99565617027091
C	2.77249261956400	3.17197610501168	3.40381930440175
C	2.90291178133322	3.95609277142806	2.25548694452309
H	2.69012420749465	4.04509027529957	0.10231211371532
H	3.25753131635237	4.99453772588805	2.32362818855806
H	2.22032798372931	1.23961225819872	4.21217873107266
H	3.02415388390347	3.58138555674950	4.39289016474232
C	1.92838170662682	2.18850598460262	-4.02193258319140
H	2.30216503697005	0.51347911196371	-2.69111059887004
C	0.11852581232340	0.84238067249760	-5.12342519000960
H	0.39465779383134	-0.80741662020104	-3.72112175383386
C	1.56778987715691	1.33604010600337	-5.25858694348708
H	2.99851757228431	2.47186628510071	-4.08620017095329
H	1.33136479115187	3.12554238758695	-4.02480617566323
H	-0.56199651519723	1.71470075073325	-5.22254261252314
H	-0.11351658438157	0.13522861916120	-5.94558120952377
N	2.48839934179571	0.23437228874773	-5.4556522236531
H	1.66648642566703	1.97540281412004	-6.16104247088573
C	3.64663118424052	0.34403228956461	-6.19102662839546
N	4.46442219804266	-0.73530211620865	-6.07963726308598
S	4.02548987949042	1.68853768622667	-7.15792405868163
C	5.72499553154549	-0.87076168114028	-6.77250227692215
H	5.59008334484984	-0.83166290983668	-7.87415723956168
H	6.17260677268448	-1.84547147842581	-6.49752307406907
H	6.43281510820551	-0.05617629037095	-6.50481812627935



H	2.46864552585249	-0.57357009185327	-4.80416547801672
H	4.17694748010425	-1.45589656293022	-5.39920494621709
C	0.82474728464350	-2.17020212709647	2.61187552565640
H	0.61162130063697	-0.31772489336011	3.70830000541818
H	2.30658552914077	-0.93183448588502	3.56693165654032
C	-1.11196161488483	-3.20225281363436	1.60811584933305
H	-3.03073313107694	-3.78376278550399	0.82583441831210
H	-3.06710489644226	-2.28126956607119	1.83694738882268
O	-0.49858169088179	-1.98146907967333	2.07074243188928
C	0.81004908510865	-3.15220801646519	3.78273202577314
H	1.48477825491424	-2.57718062456653	1.80607412005622
C	-1.17982856624442	-4.25653954820689	2.72136620151283
H	-0.51402447600937	-3.61153986402725	0.76044309940419
C	0.20138241177534	-4.50471429149677	3.34921448341791
H	-1.58666004166163	-5.20470152627301	2.31286715507954
H	-1.87230356861316	-3.90937296133325	3.51719682310804
H	0.21331521424792	-2.72661077397282	4.61805822023141
H	1.83608814355505	-3.33756872352166	4.16144600602016
N	2.92405373937544	-6.46238977645697	1.83430379452105
H	2.78645755626150	-6.10963663408085	0.87661128865021
H	4.87327913483654	-6.72973228082729	2.64815927889130
C	2.15424374220250	-5.96410802089463	2.83850354061328
C	4.10182228160146	-7.27334881983022	2.06002303204856
H	3.85270714806997	-8.19489777989088	2.62494818024031
S	2.50668694687770	-6.24162049801159	4.47769712250698
H	4.52226191239564	-7.55254576932347	1.07552826367438
N	1.07275022247039	-5.22121248280418	2.42772429380207
H	0.10300004354397	-5.13956215211707	4.25485487087453
H	0.87600622875988	-5.16708653625085	1.41606668319014
K	0.13809028958824	-0.79480288783096	-0.45612603475242
F	3.10396936807939	-1.95802704873216	-3.86318292224169
H	5.34824355609995	-2.09441307484526	-2.05546651608471
H	4.55892540825423	-0.45083671751646	-1.71310308759602
C	4.45017565796689	-1.55165079950364	-1.71032452006655
H	3.72227828286677	-1.73144116297041	-2.75941335527601
C	3.82723175713474	-2.09483421967730	-0.56167228517490
H	4.12844193866451	-3.08268238399814	-0.18135110712208
H	3.35487461470380	-1.43097756265557	0.18034748640075
O	1.98713277993660	-2.79467751821878	-0.92772305943124
H	2.33446552658075	-3.83012510320079	-3.50878377633875
H	0.55780663769894	-4.07057715886389	-3.20681928644454
C	1.57311727095621	-4.45604538157854	-2.99988773689449
S	1.84580855467112	-4.32967336785260	-1.22954145654773
O	3.10707423149450	-5.06213661624787	-0.88559950791138
O	0.61085166150661	-4.85673676427852	-0.54831596978652
H	1.64489156760600	-5.52841273607533	-3.25755623128025
TS-E2anti (TCE-KF)			
O	-1.48654451009023	-0.79447814134396	-2.33963984647496
C	-2.75133433104479	-1.29918992365700	-2.16960358833241
C	-2.98585386466993	-2.02728287608928	-0.96636828604758
O	-1.91303610622660	-2.14963300146465	-0.11868330366587
C	0.93627161835631	-0.07563711327696	3.36948817771026
O	1.09068978084661	0.72089258077898	2.19212500215061
C	1.35538557810011	2.05957555376085	2.32688966766688
C	1.65831738888867	2.75744832427710	1.12137858557101
O	1.64957008922778	2.01009205509792	-0.03084784237139
C	1.91567013398954	2.68761572557047	-1.26360435709811
C	1.83899465280640	1.72175330096605	-2.43402120733077

O	0.49189780119327	1.21113374902789	-2.48519994254944
C	0.24105312474297	0.33803574526222	-3.60202650584306
C	-1.21620931597622	-0.08474317340286	-3.55629640270586
H	-1.40428553049809	-0.74898012709518	-4.42619410882894
H	-1.87028393748175	0.81416092785867	-3.61505586610303
H	1.16882392833445	3.49954519387444	-1.41184725805066
H	2.93256799883891	3.13687447056602	-1.23865132466308
C	-2.06791101209960	-2.92891382092246	1.07138833080930
C	-3.80022252903844	-1.14135047790097	-3.08912958672657
C	-4.25633764852431	-2.56685378354533	-0.71642370627488
C	-5.29881441255398	-2.39828341172666	-1.64681522018234
C	-5.07005414616058	-1.68891391947122	-2.82828033851649
H	-4.44449666223438	-3.12309668819862	0.21117093715593
H	-3.63351715935554	-0.59169189992108	-4.02386779601644
H	-6.28801452699516	-2.82945781797880	-1.43507919640349
H	-5.87659672123266	-1.55278700377902	-3.56400295174689
C	1.34358165708748	2.75118105784219	3.54677634369765
C	1.94525909775116	4.13036485576857	1.17716960289782
C	1.63175548479846	4.12820776083015	3.58755510527623
C	1.93295555058616	4.81341467231743	2.40786856441253
H	2.18854071597401	4.68135650518054	0.26000025716204
H	2.16606886297767	5.88793599295187	2.42969721149022
H	1.10375009123920	2.22154189465149	4.47828800452972
H	1.61784630377587	4.65541394494195	4.55283097382905
C	2.23229643051004	2.43633929488222	-3.72530700495314
H	2.54221376396723	0.86802883328920	-2.26556095200297
C	0.56302051089066	1.02272705024192	-4.93915056899121
H	0.87137802980272	-0.57659641765353	-3.49913113743181
C	2.00273388774117	1.56309444521441	-4.97500909917017
H	3.29983963945402	2.73478346107364	-3.69961886949545
H	1.62312315605856	3.35951635500388	-3.83148071755277
H	-0.13613047804611	1.87307668560611	-5.07997374442391
H	0.39307624993864	0.30428788502503	-5.76765515752938
N	2.93029749281215	0.43755956479725	-5.07412985966211
H	2.13399401681662	2.22139000222824	-5.86430520972468
C	4.25041226769934	0.56260500271424	-5.45965914213476
N	4.82518682102547	-0.61473471072170	-5.82481551961231
S	5.09866729445745	2.03231980193426	-5.47878783326281
C	6.19172797640359	-0.73271065384188	-6.28183784563339
H	6.36952081401487	-0.15717227192209	-7.21623925736644
H	6.40692855167092	-1.80218069567268	-6.46947168130342
H	6.90212055693995	-0.34526149173806	-5.52262384303554
H	2.50673548204228	-0.45351641318133	-5.38767623862110
H	4.19608911547045	-1.42519859228899	-5.93489257212467
C	0.82449602098848	-1.52638260683481	2.93561019590696
H	0.02372063202907	0.22970812575646	3.92960554809550
H	1.82317198356807	0.04876968284651	4.03006080453654
C	-0.72372317919227	-2.99505505506699	1.77068509144928
H	-2.39754932989269	-3.95898003446619	0.81124645942902
H	-2.82860430704384	-2.46588048445225	1.73961413271045
O	-0.43994522810575	-1.66594608915142	2.26055716058362
C	0.95868549276169	-2.52515844895250	4.08854720902210
H	1.64579490073711	-1.71279463114085	2.20330483991018
C	-0.66026307723376	-4.02770744241842	2.89474468866331
H	0.04206660822681	-3.26245203637480	1.00501006820607
C	0.72405694599232	-3.95845758079934	3.58017215796563
H	-0.81341234846769	-5.05171785174939	2.49533532655302
H	-1.45722179573020	-3.82950794660903	3.64277873976219

H	0.20876274260999	-2.29301136877081	4.87406166139839
H	1.96789486561476	-2.44397115528542	4.54208589625909
N	3.11847979210681	-5.82565496412034	1.50961667717221
H	3.46346888129469	-4.98333839264868	1.04166517079456
H	4.59806639447032	-7.30623591040418	1.93568921910064
C	2.22273274820239	-5.65432388329128	2.52699547491223
C	3.78642087518161	-7.07512164517770	1.21093716498954
H	3.05892449207764	-7.90887041475135	1.25319028879498
S	1.69776762765409	-6.93319367919107	3.50416349319548
H	4.21824226747244	-7.01382236319343	0.19343906299594
N	1.79653211951677	-4.35719806023061	2.67719061182004
H	0.74602196260591	-4.68129134378705	4.42116445364166
H	2.02700765857941	-3.70851488051837	1.90769766583109
K	0.39915355892575	-0.52275002752912	-0.23424433605897
F	2.15684866111431	-2.65841106573279	0.22504183492047
H	2.39082330294599	-3.29252881004874	-0.74021740666604
H	2.05241043784366	-5.05472800643650	-1.49504990889784
C	2.64726619634540	-4.17743288774071	-1.80177461124571
H	3.74201712766093	-4.31927432035028	-1.78213801515310
C	2.11282621406468	-3.30379102347117	-2.74589084247766
H	1.02229718202222	-3.16699497032012	-2.81652053972422
H	2.72558615549986	-2.45777794311310	-3.09597997534657
O	2.10358480197640	-4.11971248894634	-4.63982570024598
S	1.44815162298313	-3.21107682111862	-5.69943623139505
O	0.16935278421621	-2.58995177357399	-5.21806349986840
O	2.42793117195536	-2.19981943514677	-6.26143259739872
C	1.05469846099787	-4.34128621114051	-7.04915822937615
H	0.33940641555737	-5.09116919322256	-6.66646196845190
H	1.99347267476299	-4.81818969181013	-7.38284193110803
H	0.60629846010097	-3.74087313625609	-7.86163717960075
TS-SN2 (TCE-KF)			
O	-1.77718041425976	-0.46161015416402	-2.30967662033360
C	-3.06177410412405	-0.89852852019821	-2.10941535750720
C	-3.26966497830975	-1.71084215556126	-0.95627508033681
O	-2.15981116313607	-1.94683551175874	-0.18976317421103
C	0.93598187010775	-0.27402289293428	3.26802263849304
O	1.06265832203764	0.60214754485904	2.14259329859876
C	1.39206285846565	1.91486876469120	2.34631372676287
C	1.68148217083279	2.66873601433051	1.17112278360027
O	1.59575893413890	1.98451184281550	-0.01592415443405
C	1.90245987201588	2.67989538022816	-1.22721798007636
C	1.74900117578155	1.72878721621345	-2.40267829511383
O	0.35601948210122	1.36897546865269	-2.47533052290826
C	0.01861830365571	0.50127685218682	-3.57105395306267
C	-1.47901510415151	0.25308615904816	-3.51136018169749
H	-1.77765979824575	-0.35112467755489	-4.39602955130673
H	-2.02450040342499	1.22352423374689	-3.52632223569858
H	1.21237422788640	3.54344758099763	-1.35675897560135
H	2.94827236766624	3.05698624393094	-1.19736811274688
C	-2.24379975431875	-2.86752364781785	0.90066873382740
C	-4.14501736577446	-0.60466623956697	-2.95036957680036
C	-4.55149075669086	-2.20713377365553	-0.67922135553157
C	-5.63045123261897	-1.90460560360940	-1.53165900280882
C	-5.42822583766291	-1.10659037934771	-2.66065380020284
H	-4.71880455922734	-2.83340614484383	0.20729985499151
H	-3.99536969884687	0.01655999666615	-3.84309415115062
H	-6.62924798921302	-2.30266172895367	-1.30089997941578
H	-6.26554628151087	-0.86623972008736	-3.33214523746077

C	1.46063866963348	2.53422864779871	3.60247830398728
C	2.03398381127667	4.02129813845166	1.28872196428220
C	1.81448206673798	3.89278045550068	3.70659018423163
C	2.10037784190965	4.63192447409415	2.55574799753198
H	2.26617050214001	4.61059912649081	0.39246508551838
H	2.38325114846681	5.69202695943506	2.62914531167020
H	1.23519574994852	1.96052603192321	4.51149105575433
H	1.86492920130853	4.36374706212791	4.69935531510185
C	2.24920425264356	2.34855672219221	-3.70486416804229
H	2.34979208577573	0.80681893540784	-2.19780141579390
C	0.45849496516117	1.08671952020528	-4.91879601542060
H	0.52555559854877	-0.48478305338571	-3.43463893612850
C	1.95850098587725	1.42643570010408	-4.90799414439115
H	3.34137626226733	2.53323014060968	-3.65619066054155
H	1.74751020357028	3.32560786743650	-3.87405916813707
H	-0.11433639481874	2.01588170614697	-5.12099008240173
H	0.22849887151069	0.36142622946272	-5.72577998189381
N	2.73046113666537	0.18685930588477	-4.85229474904088
H	2.23426678652346	1.98087882294428	-5.83336713783970
C	4.06964852664498	0.10962358232693	-5.16170488111502
N	4.57512287259175	-1.15571801551223	-5.13401184485066
S	5.02204780960307	1.45983329077057	-5.54498600656399
C	5.95025837271066	-1.47246944409996	-5.45594478222697
H	6.20762189055744	-1.16205837793833	-6.49037335194416
H	6.08664241086249	-2.56741707445101	-5.36001050078438
H	6.66251906283139	-0.95483876525172	-4.77841146322420
H	2.18575270326131	-0.68526792790062	-4.97966423134471
H	3.96734218927057	-1.91914178555585	-4.79447166227568
C	0.76450430402288	-1.68452029746119	2.73459660928502
H	0.05931617122661	0.01693894032893	3.88939733599335
H	1.85528005025582	-0.22203653347826	3.89274107353722
C	-0.85329096216610	-3.00836228969812	1.49486928801387
H	-2.59716111979755	-3.85699996317236	0.53434185776280
H	-2.95298296721683	-2.49291760848954	1.67287197741540
O	-0.53816645120986	-1.74515710160561	2.11514998166235
C	0.92100010217376	-2.77821170506464	3.78915044892459
H	1.54210854263126	-1.83906876587964	1.94764534819243
C	-0.72102910944196	-4.16621459819372	2.48761315433383
H	-0.14072664899474	-3.17971230704094	0.65139154850856
C	0.67892248906981	-4.15559158163063	3.12897817342214
H	-0.88719229525175	-5.13060832300122	1.96491229338134
H	-1.48827864779980	-4.06829624925197	3.28472494353450
H	0.19416080231406	-2.62121091446973	4.61502953153979
H	1.94177585192021	-2.75820991564000	4.22311847313943
N	3.74794680012887	-5.17164161136965	1.40193511809720
H	3.50977817931519	-4.64036637980694	0.56067407065894
H	5.60316191374173	-5.62367740886716	2.31733868047789
C	2.83696673236703	-5.17138849736388	2.41663247178189
C	4.99814484397543	-5.89848482903088	1.42785503850770
H	4.83798718603514	-6.99757387276619	1.46925355503430
S	3.10906373820569	-5.99898624552146	3.87132033264197
H	5.56758293951630	-5.65113425128480	0.51005785586862
N	1.70131359554811	-4.45595952446354	2.13701513497195
H	0.76335149923913	-4.94932391186208	3.89991664683352
H	1.72157158348496	-3.88744117606332	1.26764164864815
F	1.91962502005213	-2.67300809551984	-0.17409805429292
H	1.07509522318435	-4.70884239759612	-6.77758282856886
H	2.34439537614541	-5.50892831249648	-5.74677791960050

O	0.46729612199813	-4.22493531245636	-3.97068167444581
C	1.97757094563469	-4.55196289531729	-6.15833817552578
S	1.48199889123314	-3.49917910378567	-4.78088450216210
H	2.76303613759075	-4.03188343620699	-6.73609327802882
O	1.05134960244415	-2.17967707884548	-5.36563829983731
H	1.82936029432421	-3.80338387911203	-2.02565027400491
O	2.83071670787822	-3.30485748074728	-3.98795915246494
C	2.58648666706154	-3.01477476391058	-2.04438494931683
H	4.28873614042520	-4.32801974631130	-1.78984230351901
C	4.02342123222692	-3.25662345940836	-1.71009563326675
H	4.68695311750422	-2.67772577966494	-2.38022869526407
H	4.21000581723149	-2.90158920597276	-0.67759072922236
H	2.25550361698382	-1.99201009280964	-2.24473861572686
K	0.24193023813435	-0.49649246122212	-0.30556127890597

[TCE (KF) ]2

O	-1.49850572692350	-1.73016082413128	-1.71451108796822
C	-2.61606312157315	-2.17569628378785	-1.05901024912894
C	-2.45059319181934	-2.45735139025713	0.33025336382909
O	-1.19085435071015	-2.25616439399268	0.83066935295670
C	2.53524652287274	0.55241167374447	2.47665659439563
O	2.10662976119237	1.06012178244814	1.20686770117572
C	2.24792504783747	2.38954862237019	0.91645269319333
C	2.02120375341201	2.75046569741046	-0.44534128740417
O	1.71220317040607	1.71574954729666	-1.29270733683984
C	1.59787359873971	1.97354113681276	-2.69703746842167
C	1.43137029778416	0.64679732082884	-3.42054368562207
O	0.15125622670586	0.10631774666611	-3.04127132197224
C	-0.13427414894695	-1.18624759591057	-3.60223531407471
C	-1.52968028219919	-1.58029802990054	-3.13800494984224
H	-1.81672999821627	-2.54164714155228	-3.62107168559079
H	-2.25772771868982	-0.78843367807666	-3.42459735471451
H	0.72200826151248	2.63058719050129	-2.89784160773342
H	2.51841690371795	2.47600036422352	-3.06725278436511
C	-0.85403358957706	-2.74005343740435	2.13834261746572
C	-3.86878806706170	-2.37047303653958	-1.65830713497251
C	-3.54250180609968	-2.91580312647866	1.08047000982516
C	-4.79618401999185	-3.10293079874396	0.46741857306264
C	-4.95718314746538	-2.83306044015636	-0.89441364929034
H	-3.41982313560960	-3.13100511606555	2.15063437576609
H	-4.00258950241606	-2.16650339584810	-2.72917310977252
H	-5.64338051994010	-3.46460555875218	1.06833408612970
H	-5.93187616522190	-2.98496318734185	-1.38110351692021
C	2.59413659212290	3.37812451184710	1.84819155757017
C	2.13221055158826	4.09394288252086	-0.83130512687379
C	2.70705473167579	4.72309722321219	1.44709563296545
C	2.47460670275044	5.07865509028475	0.11530024653806
H	1.95499961179279	4.38462521942924	-1.87544734984364
H	2.56209653496632	6.12706680007154	-0.20541783505303
H	2.77892974722551	3.10230206822114	2.89510262002707
H	2.98007810358811	5.48750799151923	2.18924198398288
C	1.54885301413136	0.76497431278548	-4.93547345907199
H	2.23879312973384	-0.04424033984413	-3.06692231271937
C	-0.00332224034954	-1.19710163227636	-5.13154694915369
H	0.58632755228415	-1.93169104213830	-3.17892119244029
C	1.34778081167320	-0.62188572048319	-5.58973444505338
H	2.54604608054505	1.15006446212243	-5.23123712800306
H	0.78115064910979	1.46846226313863	-5.32214567988953
H	-0.80996067088560	-0.57251532325296	-5.56877415682675

H	-0.14666144788070	-2.23302648730068	-5.50514025355170
N	2.43302437218254	-1.53950512196266	-5.24880710456396
H	1.35035265968883	-0.48398854844964	-6.69231776227844
C	3.71280375704575	-1.44518155081954	-5.74404600527889
N	4.59493206327137	-2.35732437161362	-5.26223573376210
S	4.15776008080301	-0.26230315360127	-6.88398195650497
C	6.00010695163627	-2.32837108849751	-5.60947647831801
H	6.15942759424234	-2.42948320903675	-6.70404876905948
H	6.50356509083516	-3.16557682291021	-5.09256703337911
H	6.47384419922192	-1.36974450097821	-5.30705694328240
H	2.20701107395016	-2.35618226732847	-4.67362608923429
H	4.28764252585357	-3.11344985546040	-4.60530848033819
C	2.40014370982118	-0.96001162749746	2.39821518760282
H	1.90205436299050	0.96108393878077	3.29586947411547
H	3.59601382778619	0.83361137292031	2.65800416674645
C	0.65684407807914	-2.64254456821377	2.27002166482512
H	-1.16712179323561	-3.80238301854730	2.23978166066543
H	-1.36163921718671	-2.13393726356678	2.92161317179423
O	0.98717900003810	-1.24406808208139	2.38356886501077
C	3.13278090385799	-1.75005272544547	3.48855904324647
H	2.83546595179843	-1.25338443884130	1.41443246766592
C	1.28488180896359	-3.44877318959671	3.40413956470614
H	1.08208928315719	-3.03345905800855	1.31532692067721
C	2.82314860984586	-3.25387123988738	3.34062577890818
H	1.05482418889181	-4.52861848094955	3.29311646299176
H	0.89674121741332	-3.11193223245352	4.38900046409139
H	2.80598440433150	-1.41154593743531	4.49422014411823
H	4.22481426568786	-1.57436840611713	3.40215726056775
N	3.40158638640272	-5.21468143900618	0.32345740882746
H	3.14390798284092	-4.35403115946230	-0.20933421570470
H	3.77816982849403	-7.28205797531585	0.14876727187781
C	3.37327039098274	-5.05317585627331	1.68942300542066
C	3.15618723516995	-6.49261278593706	-0.31412311882233
H	2.09705234439494	-6.82035439716441	-0.20588740263100
S	3.38894450658045	-6.34772166808795	2.78302705413035
H	3.39705544046495	-6.41039035650426	-1.39116555209546
N	3.35630708926349	-3.73360843630619	2.06611927946959
H	3.30178905618141	-3.83636239932796	4.15333837537792
H	3.22741379189444	-3.10248355966399	1.24681377043643
F	2.80659029779107	-2.58233356923532	-0.39317420398978
K	0.83277720415080	-0.82386542141834	-0.48459783233442
O	5.83393722299882	-8.17933356787683	-1.96694469797674
C	5.44822393824947	-9.49315865430689	-2.03935077039768
C	4.65928629612691	-9.84468771195768	-3.17565189049454
O	4.39784487362177	-8.82579545683111	-4.05283193378168
C	5.43930729262650	-5.59231127841809	-7.65871521758616
O	6.50518510025893	-5.58121846722871	-6.70074544267279
C	7.77465744363966	-5.23672961548092	-7.07502852222539
C	8.68788319282722	-4.99702239391363	-6.00436884387450
O	8.16896898147479	-5.12726087337731	-4.73925242207761
C	8.93476541589021	-4.68632462416229	-3.61083105092501
C	8.03268841792508	-4.68439661654439	-2.38512985848379
O	7.68547883699398	-6.05596897273154	-2.10443097871092
C	6.79222378259822	-6.22134971929252	-0.99087197885727
C	6.56421840393413	-7.71812595488873	-0.82602860369586
H	5.98452987698725	-7.90466606420798	0.10464803746270
H	7.54380186673956	-8.24208514872788	-0.75799921587145
H	9.80288269639920	-5.36328111330709	-3.44667499505175

H	9.30831760351789	-3.65419174718265	-3.78706529099084
C	3.36339375881939	-8.96097000529761	-5.03766529510298
C	5.76406164050024	-10.47372741016586	-1.08817077495939
C	4.20899585136254	-11.16310306551408	-3.32833860392473
C	4.53273337368451	-12.13861461043538	-2.36583170595702
C	5.30678432820591	-11.79541719645934	-1.25315758039266
H	3.60632040141343	-11.43762871996462	-4.20521107150126
H	6.36231327966284	-10.21229762064260	-0.20516049287332
H	4.17176398368235	-13.16906456902922	-2.49760496573377
H	5.56165820087342	-12.55161180376414	-0.49618845660982
C	8.20990834203978	-5.10159451180523	-8.40057448248975
C	10.01279221598045	-4.64064566927210	-6.29100131221720
C	9.54204315705291	-4.73884864040215	-8.67516590130251
C	10.43878047119008	-4.51248265022159	-7.62699509589689
H	10.72170141238648	-4.45530836096192	-5.47271792479197
H	11.47964227211411	-4.22594083459808	-7.83681638932607
H	7.50814488966114	-5.27615782936353	-9.22761462076034
H	9.86871455550162	-4.63189532453447	-9.72000501964109
C	8.66989178592517	-4.01743155516325	-1.17157217159054
H	7.09813928496748	-4.12281804006161	-2.63849880284520
C	7.33338127194040	-5.56059826861861	0.28606535679950
H	5.80794710475455	-5.75648208793172	-1.24695362048353
C	7.71322605208944	-4.08965104181269	0.04221619783894
H	8.89474471304150	-2.95088680389220	-1.37501725273042
H	9.62359060471209	-4.52688364823547	-0.91557449047333
H	8.24312864856090	-6.10307591763871	0.61749249924542
H	6.57988796032392	-5.64660814800088	1.09740040410184
N	6.50973179221511	-3.28616820737140	-0.16462335018838
H	8.25243564934959	-3.68239817013921	0.92586154132081
C	6.48571795173066	-1.90874394225361	-0.14451279554997
N	5.27552102685276	-1.34102408725013	-0.37464246875082
S	7.88454640821354	-0.98440472600760	0.14611018982050
C	5.09665937770758	0.09304768882769	-0.45318157796221
H	5.36012841270811	0.60055059111807	0.50070225994049
H	4.03637178580422	0.29982992842497	-0.69202125049532
H	5.74365712253754	0.54112691153481	-1.23660997416565
H	5.60817363132664	-3.77598466458004	-0.17676529539902
H	4.41221116437706	-1.92344030827149	-0.49192441008127
C	4.16159472482264	-5.81716504751948	-6.86379655519615
H	5.59006414196085	-6.40480913010465	-8.40450797410693
H	5.39297115201816	-4.61311828048221	-8.18519934819233
C	3.08512909538120	-7.56069044793483	-5.56169986301467
H	2.44544162167841	-9.37368290365345	-4.56513729949627
H	3.68837658887041	-9.63846042003089	-5.85814341007205
O	4.19855424265199	-7.18148876103973	-6.39554691592321
C	2.85043844084696	-5.50035879348819	-7.59127901720285
H	4.23288230290999	-5.13118574654996	-5.98603982101567
C	1.75938344372194	-7.35406467797705	-6.28921100997774
H	3.06982093088115	-6.90169332105775	-4.65918740957892
C	1.65787748611566	-5.85494520750821	-6.67791535026212
H	0.90621051036532	-7.61191552331225	-5.62849034124348
H	1.70193615695697	-7.99227900835724	-7.19575998046273
H	2.77739807607633	-6.08630254432241	-8.53034508073148
H	2.82554986018372	-4.42234769201596	-7.85230865738250
N	1.17037445656448	-4.56309368650453	-3.31023910545607
H	2.21330613234749	-4.53805638072731	-3.22343853203240
H	-0.64135779320077	-4.27280006322791	-2.27137103590240
C	0.71005744114172	-4.97165719439281	-4.53274002875355

C	0.38809083329635	-4.63322005655860	-2.09321285102909
H	0.30423188065526	-5.67678991493302	-1.71383842213639
S	-0.91505804066977	-5.34367315720469	-4.85326095748001
H	0.87724973706527	-4.00856596932833	-1.32137146489826
N	1.70051685788921	-5.00725423080873	-5.48630792547937
H	0.69478778156606	-5.67369405627076	-7.19638860241059
H	2.64264005964356	-4.86513174813801	-5.06004611605845
K	5.79507191814392	-6.42673199579328	-4.14304551285495
F	3.89856380266240	-4.63797419648462	-3.83847478777464
TCE (KF)			
O	-2.28887457694121	-0.11111456579284	-2.09413101905931
C	-3.49486781995725	-0.74135324858646	-1.93157271750949
C	-3.66681368974851	-1.42969708150950	-0.69363821653893
O	-2.60535338641007	-1.37276065026042	0.17059470802107
C	1.12941029933751	0.17497917831072	3.07052578642564
O	0.86802075572091	1.20247234596966	2.10505276946621
C	1.39246550486596	2.45919206807748	2.25590959985441
C	1.46037805048495	3.24298583719594	1.06569651701199
O	0.98635517438022	2.64205654555789	-0.07034482096508
C	1.46750787182027	3.03683342186055	-1.36595840479543
C	1.37657403530211	1.81594842456817	-2.27029761757803
O	-0.02335989307312	1.56763617728063	-2.54100905422863
C	-0.27680067668246	0.34938650143697	-3.27385862561141
C	-1.78803258694264	0.19966719324827	-3.40154033303870
H	-2.02057129650803	-0.63147883365464	-4.10245479912388
H	-2.24687007261126	1.13872633465057	-3.78316279028793
H	0.85902832251428	3.87805376214944	-1.76409146682592
H	2.52851444806368	3.35642959861686	-1.29249299487592
C	-2.40733461055179	-2.39910548055207	1.15786468660808
C	-4.52848897919220	-0.74538849364554	-2.87834054114957
C	-4.86964521313781	-2.10159920647266	-0.43472957777458
C	-5.89923984113525	-2.10287070666101	-1.39462716148552
C	-5.72938906781222	-1.42897728412018	-2.60924210482746
H	-5.00599208376227	-2.62464871824258	0.52215691658170
H	-4.39948563897839	-0.21213309455702	-3.83057737878188
H	-6.83798952916220	-2.63438038676506	-1.18046073204164
H	-6.53341622000359	-1.42635952379851	-3.36044144924412
C	1.85391555744088	2.99312393268849	3.46715253179198
C	1.98835271647244	4.54049413286433	1.11964803122774
C	2.38704443162198	4.29562572950902	3.50731304219271
C	2.45456546143308	5.06475649349078	2.34023398939098
H	2.03501758001373	5.14850976082840	0.20513147709691
H	2.86859513907202	6.08292729764482	2.36838828158849
H	1.80068750253048	2.39227633964725	4.38646215257792
H	2.74895867092371	4.70193393728310	4.46299732791505
C	2.17671194348967	1.88533701893981	-3.56678637634368
H	1.78508922266808	0.96092706486365	-1.67853042778239
C	0.49687903369479	0.32274959951788	-4.59533926835662
H	0.06673221190941	-0.51992347560492	-2.65676838856770
C	1.99646577017396	0.53920874053138	-4.31724384425573
H	3.25660891950411	2.03096157027923	-3.35585473208447
H	1.83023270196290	2.73018483122908	-4.19991021314364
H	0.12832333645475	1.12536250446088	-5.26842899571795
H	0.34219677906127	-0.65214148595413	-5.10222038515265
N	2.51779788868007	-0.57659086409302	-3.54042057882827
H	2.57250784056477	0.57274901577141	-5.26407238007293
C	3.86090629500528	-0.85561555373920	-3.41585730831526
N	4.13453043669309	-1.65019758566248	-2.34365300360793



S	5.04132345230606	-0.29092894907746	-4.49230291232632
C	5.45010166138146	-2.14985757326662	-2.01454861707369
H	5.94671318355428	-2.55279852281812	-2.91997138661838
H	5.34376529659347	-2.95841984586037	-1.26483502637360
H	6.11568000994787	-1.35671530206022	-1.60509455906688
H	1.95425458923139	-0.92940706402729	-2.74143651664935
H	3.36705387289715	-1.76032295411504	-1.65827280043853
C	0.89438895519990	-1.15827937786053	2.37136131114718
H	0.45894699946495	0.28442879928784	3.95136729960536
H	2.18689587154329	0.23530451179670	3.40726424550371
C	-0.91160482848669	-2.48014304015224	1.42924115639350
H	-2.75558463377794	-3.37600706457288	0.75990389281774
H	-2.97353269241796	-2.15929912632811	2.08520210636415
O	-0.52784660419420	-1.28946584509018	2.15838471075037
C	1.46987560996653	-2.38539910997090	3.08271811180239
H	1.39893038714227	-1.07388319868616	1.37745226763954
C	-0.43256402791363	-3.73675037765922	2.14908988760116
H	-0.41347082675900	-2.46584945232374	0.42919605017201
C	1.10978392381550	-3.65395252710222	2.28516959435202
H	-0.68944811624672	-4.64561567808591	1.56674211290518
H	-0.90637233675910	-3.82156544203724	3.14988055202969
H	1.05211484596362	-2.46492650505138	4.10781005761790
H	2.57171722510894	-2.28793885890242	3.16375477495568
N	2.16783389640560	-4.40221912125564	-1.11959438222641
H	1.97402451780666	-3.41966707127546	-1.38095764334913
H	3.21176943554970	-6.09170155463036	-1.82321814626643
C	1.92961290670278	-4.72337721990292	0.18250590691129
C	2.44169473986915	-5.36883888051063	-2.15905587504463
H	1.54065476038414	-5.95939536043459	-2.43975014046072
S	1.87345208650921	-6.31493746079102	0.76191687712997
H	2.81236520055020	-4.83057249335942	-3.05279990997090
N	1.75623018650997	-3.61445600222094	0.98055633376860
H	1.47886662760136	-4.56323620818713	2.80182842457629
H	1.71855796225493	-2.72702706923421	0.44106866976751
K	-0.43584066449113	0.28652055617951	-0.12093638194011
F	1.51208780753591	-1.53378872921388	-1.00507015578433
TCE			
O	-2.05159255732882	-0.34292110355136	-2.33818753055852
C	-3.34464832640633	-0.61241125847864	-2.00010930346417
C	-3.52672743470452	-1.41722958914012	-0.83323125548461
O	-2.38435451240343	-1.81836755776223	-0.20720307124895
C	1.05099647773044	-0.30189552360440	3.14487470024968
O	1.27001686479426	0.55525069153179	2.03683548955747
C	1.53325433566258	1.87080324191758	2.27683984007519
C	1.71159090182546	2.69039793153247	1.11964747057766
O	1.59367746900799	2.05560369095576	-0.08112903959274
C	1.72026149041670	2.82530951518714	-1.26543873377714
C	1.46185707946797	1.93285749902812	-2.46925019269646
O	0.05696698452018	1.67145016091021	-2.52779702222138
C	-0.30770224977942	0.75787751152132	-3.55418756812257
C	-1.80488169748547	0.50326050208753	-3.44830322777599
H	-2.16813349927270	0.02507369155169	-4.38841883714790
H	-2.32710158896256	1.48039113523992	-3.32894114853557
H	0.98810950716654	3.66566060212353	-1.27150637931469
H	2.74596809485038	3.25538634149489	-1.34099305665403
C	-2.49529498251275	-2.59263494328867	0.97522768572629
C	-4.46995159003846	-0.16913991735943	-2.71300146226345
C	-4.82769768381214	-1.74330171347849	-0.41820961869508

C	-5.94730815609058	-1.28704756606253	-1.14138650256951
C	-5.76942929981957	-0.50477229588106	-2.28444001552470
H	-4.97985530151389	-2.35564663870267	0.48061823831703
H	-4.34071932424166	0.44253319488127	-3.61577260543748
H	-6.95768363107197	-1.55315426427272	-0.79762050775970
H	-6.63698502522200	-0.14528611073863	-2.85687945484071
C	1.64567728058350	2.44767711059463	3.55209304993830
C	1.99936491060999	4.05525715770131	1.28052723405745
C	1.93069697931189	3.81961948096208	3.69726818795223
C	2.10775386763864	4.61976617567710	2.56668646538333
H	2.14630985674139	4.69178051958803	0.39834422383444
H	2.33720764736889	5.69076487055311	2.66997445149897
H	1.51436063547331	1.82844372879940	4.44974803972543
H	2.01525879701396	4.25067412873505	4.70599526282095
C	1.94603086877561	2.56680654058002	-3.77793523029948
H	2.00312948072679	0.96868043840424	-2.29482974787183
C	0.08729412009804	1.30693213242038	-4.93587603725166
H	0.20320603845286	-0.22421291249479	-3.36832864205175
C	1.57639467188389	1.68911986893307	-4.99314968019159
H	3.04390870893113	2.72295537615829	-3.76911151557497
H	1.47067803809857	3.56419485488402	-3.89638554964842
H	-0.51682924726287	2.21723984896089	-5.13519329779615
H	-0.14599573477604	0.57026256128186	-5.73239399585069
N	2.40366999736018	0.48742938722864	-5.08292064168101
H	1.79300559641383	2.26190504712879	-5.91805218933690
C	3.63001540952036	0.43769098891095	-5.69640836961115
N	4.26205669352777	-0.77208002035595	-5.61016204445423
S	4.31752332676514	1.75547528899373	-6.50137129890570
C	5.52864771202394	-1.06572378731296	-6.25001304707264
H	5.44704567527929	-1.08847629224816	-7.35914495392006
H	5.88433510524049	-2.05037039653905	-5.89063194220236
H	6.27606964118657	-0.29000207631066	-5.99125248074950
H	2.12950888616160	-0.30617837385873	-4.49894714661141
H	3.72520483908858	-1.56753374736270	-5.25836579825831
C	0.68086838613809	-1.68577781079423	2.63615707609951
H	0.22241860386617	0.08063049660889	3.78447103465441
H	1.97207958066652	-0.37211795550578	3.76964201534257
C	-1.10090728122969	-2.832115111053591	1.53706881706845
H	-2.98227856818651	-3.57175609923764	0.75397010506411
H	-3.10522760233393	-2.06212958715208	1.74190041125348
O	-0.65859829639694	-1.62191128387534	2.13825284791383
C	0.80040192575256	-2.75866434432369	3.72371326984726
H	1.37077577784670	-1.93023721444703	1.78898944418406
C	-1.07166751012583	-3.98583611177673	2.55259388467284
H	-0.43761576495483	-3.07013313233449	0.66360399218569
C	0.31212487874118	-4.13027991463493	3.20992539878141
H	-1.36347742729879	-4.94199220143576	2.06973267274598
H	-1.81634460008155	-3.77127608459652	3.34711801295054
H	0.18345388111517	-2.45915773336125	4.59833636382619
H	1.84664692514060	-2.86183922943582	4.07698706979374
N	3.11586049985937	-5.92872467339571	1.61216906039048
H	2.74958302898129	-5.81922784907890	0.66411142837876
H	4.94067602564613	-6.39746930652390	2.55297926239312
C	2.33295221102882	-5.50281882634921	2.64997214313830
C	4.26286034674987	-6.79957312266643	1.77404555581288
H	3.97401775189126	-7.82688299702043	2.08825994846288
S	2.67712411201293	-5.89493322361481	4.25718993020838
H	4.80410036593420	-6.85339342432196	0.80966982142652

N	1.25458787331213	-4.74091205748848	2.27432138477766
H	0.25957091465577	-4.82869432482203	4.06951941191420
H	1.22112181425579	-4.40990200553469	1.30697944002351
TCEbut			
O	-2.08368536541057	-0.33477839267315	-2.32413942045618
C	-3.37588198016383	-0.61092613607766	-1.98828102726397
C	-3.55604664949553	-1.40687254538575	-0.81502912015270
O	-2.41272110648670	-1.79451324992287	-0.18223989804833
C	1.01501923147543	-0.24458798091070	3.16312803918388
O	1.22541770162405	0.61251464172780	2.05334969345085
C	1.47449127284161	1.93130052189067	2.29064499123508
C	1.64167712238174	2.75052418729101	1.13153395401876
O	1.53012157072289	2.11146040812608	-0.06743770582010
C	1.64684691340786	2.87916567689242	-1.25417787573892
C	1.40519481630895	1.97784562251583	-2.45485473607560
O	0.00395579556607	1.69803547232851	-2.51828377746257
C	-0.34394297768114	0.77285025289702	-3.54019977081212
C	-1.83899390780960	0.50333114817936	-3.44091393436848
H	-2.19233007019041	0.01296254717288	-4.37857945116252
H	-2.37159613964152	1.47623186669734	-3.33364185963874
H	0.90174949041364	3.70812521600472	-1.26443848883882
H	2.66588983476614	3.32498924258556	-1.32919368741217
C	-2.52120344709120	-2.56153071420808	1.00516350392202
C	-4.50199401812556	-0.18199952426519	-2.70862621833255
C	-4.85587666970373	-1.73841504361706	-0.40092141572243
C	-5.97641345449705	-1.29647544477218	-1.13165335898586
C	-5.80041996505987	-0.52311969329153	-2.28105858780910
H	-5.00646615413315	-2.34349373214136	0.50307262043003
H	-4.37437067358526	0.42281706602829	-3.61622818473677
H	-6.98600086009780	-1.56666998828913	-0.78870298632473
H	-6.66870918165070	-0.17479608014555	-2.85932768881312
C	1.58309913448425	2.51179964858404	3.56455425367476
C	1.91362600667827	4.11899549924510	1.28895371590388
C	1.85270412815776	3.88726040416899	3.70637443538404
C	2.01801959643333	4.68723084955231	2.57385922613884
H	2.05106623709228	4.75553884484215	0.40519802528130
H	2.23511762456982	5.76109805892932	2.67467940526281
H	1.46105980875729	1.89292645877391	4.46378423241408
H	1.93456605540511	4.32126267618042	4.71408782357889
C	1.88674346794607	2.61080026775802	-3.76470253456619
H	1.95803157264406	1.02168363289400	-2.27266638033304
C	0.05257861393057	1.31648706257162	-4.92374089703941
H	0.17671370612913	-0.20198694958954	-3.34397537265805
C	1.53665615453244	1.71913361915193	-4.97583112051063
H	2.98215576766008	2.78278122709531	-3.75214406520041
H	1.39736030029147	3.60033526924448	-3.89222343522598
H	-0.56224201759148	2.21739276463420	-5.13310901466189
H	-0.16639278245285	0.57102894604747	-5.71619639702008
N	2.38079287934668	0.52859253711974	-5.05061892476648
H	1.75064123341880	2.28853481915186	-5.90335243718647
C	3.61899323545846	0.48413066859110	-5.64990141435295
N	4.22891691703584	-0.73509538780461	-5.54596172443877
S	4.26953289655196	1.83625784232246	-6.43628253772164
C	5.55018074263054	-1.19591971204904	-6.04820605991025
C	5.59958489428775	-1.14021937169166	-7.58721470349193
C	5.67268043577399	-2.65840837374872	-5.58125247429187
C	6.68887344222831	-0.36713097445438	-5.42486752561675
H	2.10827032344356	-0.26346634248226	-4.46363367051236

H	3.65553223947254	-1.48489046375573	-5.15113048247893
C	0.65270810400944	-1.63185636222799	2.65808523094101
H	0.18568401154963	0.13350007450091	3.80442105410334
H	1.93800481632578	-0.30748425532200	3.78590822476508
C	-1.12562934422517	-2.79199110413808	1.56799433988433
H	-3.00459769964512	-3.54386946685726	0.79032615523690
H	-3.13338618753538	-2.02859586596318	1.76843516368488
O	-0.68810027231514	-1.57678693947419	2.16219148498184
C	0.78050573507892	-2.69992989879718	3.74916208500994
H	1.34271258714980	-1.87516201812258	1.81078073560599
C	-1.09005157256467	-3.93997456638517	2.58989835729083
H	-0.46234317084320	-3.03176638010996	0.69497373223763
C	0.29657264075535	-4.07599992613865	3.24358108539255
H	-1.38073553875749	-4.89968112414849	2.11337746242411
H	-1.83263469808372	-3.72297373579634	3.38576078846254
H	0.16488678135480	-2.40019107859440	4.62476065634213
H	1.82817102612005	-2.79791451265232	4.09937997200845
N	3.04795320461867	-5.89887075363335	1.59804803442364
H	2.62331667805389	-5.74351231596090	0.68009690445989
C	5.44257892587058	-6.00318602175258	2.26807599352114
C	2.32416093006834	-5.44754732057398	2.66713321420634
C	4.28413682902669	-6.72237142930718	1.55149015013937
C	4.03750392293147	-8.11901708287161	2.15597144317319
S	2.67713311034519	-5.77139701393424	4.29190792103791
C	4.62196356364077	-6.86258199914900	0.05518853260145
N	1.23567964655180	-4.68691869854228	2.30505974827635
H	0.25008956521582	-4.76974957600435	4.10726074818171
H	1.17799929422300	-4.37407909773655	1.33276297909446
H	6.57455516238380	-1.52191114851675	-7.95226773557734
H	5.47063707309697	-0.09927241833386	-7.93964100319901
H	4.79573849594643	-1.76330830801949	-8.02904313061638
H	7.66786824977471	-0.76431788001553	-5.76044130976731
H	6.65083164400879	-0.41987263558147	-4.31751580985453
H	6.61297331964004	0.69372050190610	-5.72992193725965
H	6.63590789154954	-3.08427835148064	-5.92133599851068
H	4.86101512643256	-3.28697425866033	-6.00572273964890
H	5.63899470292151	-2.73277448828375	-4.47373248966648
H	5.63400580151048	-5.01328535083501	1.80667817560097
H	6.36752027094403	-6.60911924677063	2.18930062002030
H	5.20609238617746	-5.85273188155870	3.33824169735984
H	3.80617113048474	-7.37566757235409	-0.49714555780415
H	5.54090859795112	-7.46702501727281	-0.06918019256742
H	4.80013772020591	-5.87143403336452	-0.41142631830583
H	3.21584480831687	-8.63751810317643	1.62104231177041
H	3.76242125723911	-8.03510767326407	3.22473701378267
H	4.95414972949506	-8.73643253064487	2.06826865283713
TCEbut (KF)			
O	-2.21874039231105	-0.30022523963697	-2.09027913514966
C	-3.43385132857489	-0.90432804792893	-1.90632257315301
C	-3.64287698908223	-1.48418582497458	-0.61956338641557
O	-2.61109627200917	-1.35079852717080	0.27396745820158
C	1.30977123858141	0.15928068699027	2.96432597914851
O	1.01320651284517	1.18157861860422	2.00336565476339
C	1.52019254334927	2.44632659977290	2.13954063010787
C	1.48901292431587	3.25061592074194	0.96167353241292
O	0.94191789307115	2.66572741818646	-0.15108274679646
C	1.39494772312224	3.03425902306130	-1.46648757991913
C	1.35947851299429	1.78202572396840	-2.33084600991341

O	-0.02597641734211	1.45557006264981	-2.59229830908053
C	-0.21308942370446	0.19132493745205	-3.26705179715403
C	-1.71424572825222	-0.03235188182646	-3.40481962051595
H	-1.90053317425508	-0.90670109577949	-4.06624860754717
H	-2.20874272965673	0.86496081718488	-3.83938389722744
H	0.74348190601892	3.83161756173534	-1.88566285885857
H	2.43945362061682	3.40645753198478	-1.41338462173260
C	-2.38399769569543	-2.35413447423821	1.28158775940412
C	-4.44320172148121	-0.98423250921286	-2.87642304467505
C	-4.85473820321662	-2.13012926569643	-0.33821064793489
C	-5.85837464431039	-2.21123556163361	-1.32150728224210
C	-5.65347789645624	-1.64046618068832	-2.58280243232969
H	-5.01739135146033	-2.56878272820050	0.65638035268239
H	-4.28812750892693	-0.53397510779663	-3.86659189398920
H	-6.80435704231151	-2.72172646353440	-1.08906089927963
H	-6.43719876194120	-1.69935601741497	-3.35283292299699
C	2.05489476780725	2.97123786014562	3.32486275503465
C	1.99391480570203	4.55781735971604	1.00143906716390
C	2.56398566238351	4.28351151461493	3.34991166152841
C	2.53560317467404	5.07256423924504	2.19440442620824
H	1.96027127375032	5.17987367540854	0.09563330772702
H	2.93054034343993	6.09855580150032	2.21145387309828
H	2.07925333737439	2.35553430033942	4.23542215785706
H	2.98449822124423	4.68148638441957	4.28500932407306
C	2.15115607958793	1.84841468536726	-3.63191418469500
H	1.81070913382453	0.96725610306032	-1.71385202975203
C	0.57231690537540	0.13832733917448	-4.58209906170433
H	0.16498393415235	-0.62817931896542	-2.60376903129685
C	2.05526822567515	0.46202941296252	-4.32190417665761
H	3.22083309898658	2.06894472915569	-3.43524664362261
H	1.74972066865719	2.64189897773917	-4.29796317688931
H	0.16013573271363	0.87828344613686	-5.30028024413668
H	0.47684531701954	-0.87007780817319	-5.03599080508865
N	2.65165263058641	-0.58187191658588	-3.49568980440292
H	2.62292345678681	0.49315586445647	-5.27387405678262
C	4.01232161812186	-0.69514886079593	-3.28713598426093
N	4.30074756539993	-1.39583244704996	-2.15319337965701
S	5.13573682406436	-0.01534995296992	-4.36620936894275
C	5.60924315403192	-1.84965710112390	-1.62270532545162
C	6.31204573209827	-2.77518291663461	-2.63441999226037
C	5.28809862985356	-2.63957019069481	-0.34114281344820
C	6.50353761531611	-0.64339627800622	-1.27064892873919
H	2.08224559933662	-0.96463997438914	-2.71475379027742
H	3.47597547289523	-1.60669748417729	-1.56350897033144
C	1.00814609181861	-1.17528484647161	2.29357194653350
H	0.69314099341875	0.29181418495383	3.88074158326328
H	2.38600438471405	0.20141921647051	3.23917531701221
C	-0.87901944095980	-2.46947720221704	1.48063404193719
H	-2.77794005034896	-3.33219900459230	0.93405879818463
H	-2.89394801118733	-2.06823916067316	2.22769831246200
O	-0.42702175071510	-1.27557294093060	2.16257008234988
C	1.59794575610487	-2.40659190439734	2.98702513919468
H	1.45946220552290	-1.11322221703194	1.27225284470854
C	-0.39489612115705	-3.72142592202292	2.20442250486512
H	-0.43337688056320	-2.49204250754728	0.45596982052942
C	1.15456739475562	-3.68136317613424	2.24410670234928
H	-0.71135398794085	-4.63729176913899	1.66383178339817
H	-0.81081874708024	-3.76691732537581	3.23321500150983

H	1.24882584978875	-2.45822052552365	4.03950705192616
H	2.70507986848426	-2.33533983796605	2.99167917541257
N	1.84380976332134	-4.50074658833241	-1.22638978532226
H	1.76220512712652	-3.48719811215109	-1.42514840289310
C	3.27579780559318	-6.21570617581924	-2.32009914954883
C	1.73709236790534	-4.81626206599214	0.09625611873117
C	1.98301486877730	-5.38256502730942	-2.40979891124050
C	0.75363344499389	-6.30238727071022	-2.55830004224774
S	1.64640598698543	-6.38127905202964	0.75375820395100
C	2.06069384485000	-4.43960647450412	-3.62438073986534
N	1.71489188718439	-3.69116786300608	0.89775213222572
H	1.52794494343766	-4.58838263048083	2.76115428676107
H	1.68973430845482	-2.80148063398218	0.35855947963240
K	-0.42509928831983	0.27469689989453	-0.13229375751873
F	1.53354218440433	-1.55817801567708	-1.01333249069722
H	0.85086674571761	-6.91750413981182	-3.47587405610624
H	-0.17499816255041	-5.70075730304075	-2.64116075511046
H	0.66035593004737	-6.97313285017142	-1.68241823130918
H	3.37682381162676	-6.86029548413848	-3.21718748312132
H	3.26254383951112	-6.86018354817590	-1.41958880148615
H	4.16474445819669	-5.55388405335993	-2.26826135122300
H	2.18751287208314	-5.02907816621084	-4.55344680285756
H	2.91440598281347	-3.73512240564588	-3.54424513293065
H	1.13010753384324	-3.84252938277585	-3.72609218064493
H	4.62624645122929	-3.50478958984266	-0.54884664479924
H	4.78421747018115	-1.99526842709435	0.40916137292301
H	6.22272216686793	-3.02217223621643	0.11237640046873
H	6.71461291084068	-0.04174857815404	-2.17526184173220
H	7.46336750802424	-0.99414331459352	-0.84088106616560
H	6.00346925995387	0.00490886305638	-0.52183118521933
H	6.51633218613497	-2.23801132783695	-3.58047581113196
H	5.67927272773487	-3.65744365652449	-2.86020016967046
H	7.27306693358792	-3.13618987123969	-2.21672921159038
[TCEbut (KF) ]2			
O	-0.80849064039257	-2.91300135917179	-1.71302294639576
C	-1.87527765813541	-3.61916308824372	-1.21590478662315
C	-1.72237866024845	-4.13737762155180	0.10306319703476
O	-0.53662390803823	-3.85064730318002	0.72492860368873
C	1.57315892193213	-0.11669403046250	3.18527554024054
O	1.54209430006072	0.30425814543703	1.81627546787668
C	1.47950339103491	1.64636086804281	1.54871018624604
C	1.61498502613788	2.02072415502700	0.17975432287133
O	1.77735682926763	0.99483769853242	-0.71972226053017
C	1.79164349612195	1.34262783637641	-2.10641214383068
C	1.81926599054489	0.09716793574120	-2.97721521997851
O	0.64644179278276	-0.66823530338974	-2.64848523303619
C	0.41779546351796	-1.81774995814849	-3.47146325703632
C	-0.92159910741026	-2.39031649597468	-3.03984055460998
H	-1.22021906157986	-3.19553136765341	-3.74084169902029
H	-1.69206800046227	-1.58682700200826	-3.06750826696618
H	0.87838977776341	1.93075456350802	-2.34877590641372
H	2.68614925310395	1.96187851614188	-2.34054032560711
C	-0.35249480405520	-4.29126125879034	2.07325135345776
C	-3.07066932905633	-3.85276707533073	-1.91373449774349
C	-2.76021803006643	-4.88926861232372	0.67547387280035
C	-3.95043336242263	-5.12303239939937	-0.03860842717566
C	-4.10594455620528	-4.60466102799807	-1.32616124010918
H	-2.65023887153697	-5.29825401451387	1.68802920933029

H	-3.20862877922017	-3.44878948414600	-2.92503051790831
H	-4.75419126621720	-5.71225665128151	0.42700760845159
H	-5.03386346885982	-4.77744170265349	-1.89087769926694
C	1.29470395087985	2.63949445140540	2.52293553856878
C	1.57995474300574	3.38096492699511	-0.16654837973252
C	1.25471201081388	3.99874837050491	2.16036883546529
C	1.40092957812963	4.36748395945968	0.82091690989795
H	1.69972412168482	3.68764249787428	-1.21354597273840
H	1.37630929855605	5.42683210410720	0.52585580121748
H	1.16969767180099	2.35794650381679	3.57654161978405
H	1.10689440029923	4.76184882708503	2.93860267968460
C	1.84765820557557	0.49445287802218	-4.44978441738834
H	2.72872388924011	-0.51204696542767	-2.74246534410634
C	0.42731094066160	-1.48770297432623	-4.97270177590295
H	1.21366029845111	-2.57815393171537	-3.26532184038323
C	1.68287241507749	-0.71252631873154	-5.39677362693676
H	2.79725434014726	1.00877389065244	-4.70205650042145
H	1.01868885633493	1.20566834408390	-4.65289699443422
H	-0.45999180184342	-0.86382117894622	-5.20992794802364
H	0.33515544298080	-2.42447805504405	-5.56066611659551
N	2.85287031425104	-1.58747018776400	-5.40478363232943
H	1.53995628650559	-0.30429018079576	-6.42270742532194
C	4.04826592710300	-1.23700891744304	-6.00874860008096
N	4.95991335344188	-2.24436754532129	-6.01303660244799
S	4.28279555665785	0.31389852884506	-6.67388910324946
C	6.37912655318612	-2.21149807202867	-6.44457025570376
C	6.47343881084665	-2.08632788265117	-7.97958429668862
C	6.97477502397451	-3.55206824245968	-5.98445468819568
C	7.16211210803713	-1.07897340918676	-5.75420291009481
H	2.70658768096998	-2.60651224895813	-5.31130210263546
H	4.55820563040162	-3.18910723993328	-5.84245683574453
C	1.91725730901847	-1.59193233664420	3.22162547900839
H	0.58698053773245	0.06913545321669	3.66789978559927
H	2.35502355086455	0.45120724758702	3.73568201363039
C	0.96174236196280	-3.73621931143014	2.58662226694775
H	-0.33058997572308	-5.40384516801847	2.11060530448374
H	-1.18838822236209	-3.92644239032593	2.71090924531636
O	0.78709248711804	-2.30741412582858	2.68068826881192
C	2.27290358125204	-2.10978201134716	4.61417071542347
H	2.79266057533302	-1.75407079848822	2.54826730344378
C	1.37362035853751	-4.34966237537797	3.92859377091803
H	1.76117749015951	-3.94751334006057	1.83502353536559
C	2.58756766929762	-3.61892258914304	4.52590065103351
H	1.60836490386441	-5.42556586176518	3.79299502924405
H	0.52979679190189	-4.27432626138276	4.64902667755971
H	1.42490164189552	-1.93932225525172	5.31248201435752
H	3.15852306950420	-1.57791144824087	5.01882296131865
N	6.08538016381189	-3.97164456145177	3.48860503262348
H	5.85293519191265	-3.65835768056052	2.54009486959575
C	7.98529250351375	-2.82620289904229	4.62732493619786
C	5.03366502211285	-4.00215828673548	4.36352449452681
C	7.54729847618007	-4.02876139837513	3.76639797749085
C	7.92773663895164	-5.36115784827077	4.44014732127310
S	5.18752279884264	-4.21013906885475	6.04590655453242
C	8.24068256757287	-3.95003744698755	2.39511384070080
N	3.80468781852438	-3.86083910389834	3.75970324117576
H	2.79920505600644	-4.00697023124992	5.54373557644200
H	3.77465057737561	-3.65507464737750	2.73791327695172

F	3.53138898032117	-3.13456269644435	0.93909945786882
K	1.37450848629617	-1.82251066506817	-0.07177326644275
O	3.24928985734193	-8.42614169464443	-3.37099328417759
C	2.68698603687706	-9.64690205167051	-3.65831506346818
C	2.61432790852138	-10.00113244649847	-5.03835998082562
O	3.10464614181772	-9.08012615832445	-5.92170226555966
C	6.37491490381361	-6.39625075702189	-8.54327185526625
O	6.85857341460279	-6.64009154851529	-7.22181355288466
C	8.17877962191593	-6.92615248569406	-7.01517705662160
C	8.56147670542819	-7.10784272160985	-5.65323188826056
O	7.56918910731206	-6.93446537659099	-4.72183675979187
C	7.93264796510964	-6.92820551342157	-3.33754646966845
C	6.77610178020899	-6.39818806001023	-2.50964215853149
O	5.67292388743022	-7.31836033580695	-2.63643531450295
C	4.49575554889838	-6.94880027460659	-1.91041950336341
C	3.54677042735549	-8.13789113902960	-2.00537655440805
H	2.61158012180607	-7.91635063243981	-1.44201029636314
H	4.04095470949496	-9.01897767280775	-1.53976880446027
H	8.20650317651710	-7.95669993676088	-3.01105571474008
H	8.80148855524475	-6.25381191924599	-3.17912211575924
C	2.79987040933034	-9.20818014654522	-7.32136326193374
C	2.18749980891468	-10.53659375845925	-2.69411720777828
C	2.06102324289166	-11.23653447326849	-5.40788374801385
C	1.57077861261698	-12.12146736015826	-4.42989617216953
C	1.63081430931083	-11.77121097746052	-3.07852325988053
H	2.02078476048471	-11.52165029458788	-6.46836755274294
H	2.21795502984264	-10.26843129074869	-1.62992983230950
H	1.14396590198401	-13.08632994073938	-4.73988383331266
H	1.24510332029924	-12.45328689747550	-2.30692676444079
C	9.13937800789664	-7.04332974826143	-8.02961258792868
C	9.89062007727062	-7.44011769700226	-5.35237273597609
C	10.47180698046524	-7.36827225277034	-7.71216106949227
C	10.84324691502734	-7.57218665284892	-6.38061512038367
H	10.19556046042180	-7.60331952289256	-4.31010260600498
H	11.87981702249061	-7.83534029689715	-6.12387563993039
H	8.85195873212932	-6.87908850287643	-9.07681671527031
H	11.21334650218924	-7.46040504259589	-8.51934600576583
C	7.16094040400167	-6.22213243391229	-1.04418254533233
H	6.48720112766132	-5.39769877651336	-2.91198068996726
C	4.78200314813089	-6.62187397820847	-0.43486592208065
H	4.03227406379234	-6.05065403930173	-2.39284244780806
C	5.97582845599900	-5.66140901261493	-0.24814245727550
H	8.03114598072576	-5.54579104572254	-0.96253014305668
H	7.42714006475606	-7.21072112591262	-0.61196441011789
H	5.01765313378486	-7.56250412001746	0.10738275534200
H	3.86878761492697	-6.19690455453021	0.03304286402372
N	5.54590325233631	-4.29623155136738	-0.59586020647294
H	6.25088759433279	-5.68762603126864	0.83326732207594
C	6.33758026267503	-3.16456641859237	-0.77327708571514
N	5.77436750144730	-2.05661963532590	-0.21461331617952
S	7.80101847506188	-3.14513292668585	-1.64914114112988
C	6.16824812328238	-0.62834769370859	-0.31408569562924
C	7.54545932253719	-0.38647541603316	0.33781037260954
C	5.10154954755878	0.15175986052767	0.47691978524450
C	6.16859582858875	-0.15128580942947	-1.77886862662062
H	4.66679039501836	-4.05300654176430	-0.08530166414537
H	4.88898767315843	-2.25165090720849	0.30620782099847
C	4.86063211740425	-6.32426972536889	-8.43222702620135



H	6.65918786642203	-7.22904717576866	-9.22444872512025
H	6.78990056643921	-5.44086034641281	-8.93742596960161
C	3.04051946669407	-7.84397808637935	-7.93882836202034
H	1.73196114898010	-9.48635197723908	-7.44894611785069
H	3.44085952881575	-9.98808455593653	-7.78783052467751
O	4.45998454372944	-7.64367064812390	-8.02142193565273
C	4.14527852378005	-5.84385163745824	-9.70472741678678
H	4.61451335020892	-5.60244968213434	-7.61512781741920
C	2.38201653673048	-7.56172212344612	-9.28283522035245
H	2.61517539865959	-7.11997815898472	-7.20609625860662
C	2.62248172063513	-6.06029213639592	-9.60032860343706
H	1.29144719584740	-7.75201469932242	-9.23878114181724
H	2.81830545724432	-8.20018896034596	-10.07954499967741
H	4.51578457223157	-6.40562977265795	-10.58717956672292
H	4.37636312152160	-4.77030424398310	-9.86690058405221
N	0.68530566724357	-5.30608622830670	-6.71240331378008
H	1.59527303250741	-5.09151870428265	-6.23932276439825
C	-1.66344049318691	-4.80572121503749	-6.03929525562718
C	0.77631487419804	-5.40517525576192	-8.07202518031740
C	-0.43469826894787	-5.71234917033252	-5.82828427366918
C	-0.82632784488196	-7.18731210368038	-6.06491083931901
S	-0.49684999774881	-5.76859620224399	-9.13432028308630
C	0.10892999906378	-5.59019115619652	-4.39128668827730
N	2.06586617583773	-5.20033001865575	-8.54237168986875
H	2.13483663447891	-5.80602749824743	-10.56390307749130
H	2.72183807728123	-4.93304277828681	-7.78502710701687
K	4.75561259217323	-6.82644612761833	-5.24459460123597
F	3.31463240934076	-4.66571673039574	-5.92238286955045
H	8.00987224619089	-4.83831204382672	1.77306248963644
H	9.33865051501872	-3.911111096003631	2.52906092039512
H	7.94147200066237	-3.04508356976087	1.82667038516153
H	7.75333139574082	-1.87165492791873	4.11067095498941
H	9.07894274240361	-2.86349460021727	4.80630588988285
H	7.46436219686878	-2.83764051553152	5.60330768647119
H	7.60551574259127	-6.21768471661174	3.81339636312622
H	7.45016307135476	-5.45423243424755	5.43273846283896
H	9.02821835786771	-5.41514113900863	4.56363968460592
H	8.22932815760452	-1.14461110850090	-6.04793533628199
H	7.10042793150679	-1.18357220627718	-4.65254571949675
H	6.77357500853405	-0.08495945446063	-6.04251827330857
H	6.42103841141007	-4.40804824896831	-6.41388746519628
H	6.95894021170096	-3.63602619507657	-4.87760898025500
H	8.02799429708038	-3.64135520188812	-6.31581540452889
H	5.94269843545504	-2.92580648616278	-8.47494018514731
H	7.53362937680046	-2.10245071731266	-8.30505895686192
H	6.01210208359011	-1.13778269849905	-8.31705695995045
H	4.09556686908490	0.05455646797405	0.02124905425405
H	5.35462797141764	1.22963646072648	0.49343984506847
H	5.04402025920429	-0.20139810538602	1.52740295278682
H	8.32637464500971	-0.98734636871438	-0.16547750575051
H	7.52186309622494	-0.65763579910432	1.41323326224187
H	7.81583336190198	0.68619977694769	0.26203028314004
H	5.18006329423395	-0.32239904024215	-2.25323462742420
H	6.93244515471269	-0.69388127958064	-2.36715249708802
H	6.38947723676490	0.93420614615674	-1.82673493287258
H	-1.39590556819296	-3.73712583785678	-5.91854813015881
H	-2.46095646351454	-5.06070760289706	-5.31161490366229
H	-2.05610268889894	-4.93581006804366	-7.06626437623942

H	0.49930547640953	-4.57532599216460	-4.18028719127421
H	0.94122694187811	-6.30605192482992	-4.22697349882747
H	-0.68833535874689	-5.81555167006264	-3.65550764843168
H	-1.16963010904604	-7.33922181353591	-7.10610850717750
H	-1.64454918457347	-7.47431023516941	-5.37375670566687
H	0.03806822069653	-7.85482282091678	-5.86982276274692
TS-SN2 (TCEbutKF)			
O	-1.65249545751129	-0.60890236487198	-2.29309402662005
C	-2.95250854466161	-1.01193180762478	-2.12956000976962
C	-3.23108128674092	-1.76750048625594	-0.95289528244282
O	-2.16240557505772	-2.00066861168058	-0.12843778159479
C	0.86599712590738	-0.31889342579644	3.39032989755632
O	1.06720069275271	0.51781044199927	2.24580866479993
C	1.39664351631602	1.83360271224661	2.43295416703277
C	1.72027234254792	2.56645777533314	1.25360869284162
O	1.66585619531683	1.86679574018542	0.07265804872334
C	1.96908713338139	2.57113422722560	-1.13494084388887
C	1.85022159082231	1.63744995112455	-2.32776251330586
O	0.47489287073237	1.21741136439844	-2.40665265120131
C	0.18206711220589	0.35797586252783	-3.52162774592724
C	-1.31114353521919	0.07537816596964	-3.50070291053790
H	-1.56214357840139	-0.56059628771715	-4.37720023731469
H	-1.87330041169571	1.03450428499412	-3.56322216904358
H	1.26288395983495	3.42196934242942	-1.26263069617245
H	3.00629518925534	2.97016329981074	-1.09400638491099
C	-2.32702695375491	-2.86584388517482	0.99790222374405
C	-3.99359398151311	-0.73304211136379	-3.02818606190056
C	-4.53630221210770	-2.21844998386087	-0.70868044183079
C	-5.57124665279671	-1.92989360798651	-1.61836319440102
C	-5.30029717696067	-1.19023918731089	-2.77234544605625
H	-4.75709054438528	-2.79723149366549	0.19794890966935
H	-3.79337062378589	-0.15743658759368	-3.94086504529211
H	-6.58901201530239	-2.29197404578789	-1.41225633937457
H	-6.10170315518433	-0.96014661068297	-3.48982898216163
C	1.43350988385367	2.47423083861585	3.68012604887932
C	2.07246702862875	3.92065787224723	1.36042820129940
C	1.78819755140042	3.83314449169644	3.77260188735223
C	2.10684934614405	4.55234739396728	2.61806667210716
H	2.32991636322549	4.49654946703378	0.46260679102057
H	2.39028964430219	5.61295949191484	2.68079950743914
H	1.18210286909442	1.91753632242691	4.59267022048847
H	1.81268043809298	4.31967052209632	4.75884198245969
C	2.30813895685891	2.33038305588451	-3.60784911854516
H	2.49374323444061	0.73821781469800	-2.15699828542581
C	0.60176661098857	0.99002887722210	-4.85776502275821
H	0.71124364045551	-0.61575785818112	-3.39226740097171
C	2.06932558348629	1.45184129963299	-4.85395129293463
H	3.38747106740207	2.57825680298355	-3.56011818153027
H	1.74771645099310	3.28170533903953	-3.73399374162661
H	-0.03760190321821	1.87710294051172	-5.05048521720848
H	0.42237526414781	0.26614496062993	-5.68012418757978
N	2.95436653370506	0.29023532996983	-4.90625381569575
H	2.26737036116065	2.08601296729880	-5.74723322675517
C	4.27953866442574	0.35242907720084	-5.29995013622505
N	4.82191145936571	-0.87645714265323	-5.52294916294384
S	5.09113734141516	1.83753354217666	-5.46621728161060
C	6.20300741011345	-1.25770431634182	-5.90518465302705
C	6.56202170198097	-0.70212001005669	-7.29851302487332

C	6.20234772710734	-2.79702311774565	-5.95192501992735
C	7.21626232775319	-0.78064680596615	-4.84641230815166
H	2.50505196019584	-0.62443647598770	-5.07942023058830
H	4.15088580735910	-1.65930772272856	-5.48626389267281
C	0.66399983575141	-1.73743330470293	2.89259712339178
H	-0.02372674505125	0.02116613321687	3.96652093370170
H	1.76110112770897	-0.27959478101032	4.05039753926906
C	-0.96461295963618	-3.04083529930972	1.64329322176514
H	-2.71331429512125	-3.85456018176404	0.66394313521976
H	-3.04463886854974	-2.42471537866586	1.72608680794118
O	-0.61767508037362	-1.76982098639380	2.22909903026365
C	0.75096424407185	-2.80631744665545	3.97998845178618
H	1.46286245526879	-1.941481444482676	2.13981400541657
C	-0.90058404483380	-4.17209096002856	2.67220687446203
H	-0.23777103743181	-3.26472801794470	0.82536963659050
C	0.48337468468021	-4.19216702230154	3.34601093550324
H	-1.09080012835136	-5.14461045479337	2.17285409770860
H	-1.68157763065040	-4.02406905993409	3.44766470687114
H	0.00619060864775	-2.60448516844568	4.77977886266321
H	1.75893782548176	-2.80896852051567	4.44386577589108
N	3.59032092647503	-5.15203380169275	1.67948283202084
H	3.33424345927308	-4.52394291675933	0.90822776224415
C	5.88850920950230	-5.27738240013889	2.62592452318414
C	2.67381407304456	-5.20306132133673	2.69115031690768
C	4.91497780346682	-5.80567794775197	1.55364903867221
C	4.77610308059037	-7.33770981864460	1.63928679764655
S	2.88943998400310	-5.99137553257617	4.18136641049183
C	5.43557578836075	-5.42057338360530	0.15642996137214
N	1.51191075377663	-4.53830353952780	2.37628857902096
H	0.52728466513943	-4.97055399995479	4.13546063984010
H	1.52767633893703	-4.01303868940871	1.48056705951022
F	1.83721055989808	-2.92721997168383	0.02163720037475
H	0.58996989308843	-4.46631493031944	-6.69964389792692
H	0.61435114163002	-5.62513934161123	-5.29222332141761
O	0.30793331819508	-2.96389486546795	-4.20470192057553
C	1.19019068860123	-4.87880406870720	-5.86826146654508
S	1.58604372137205	-3.50990599136603	-4.76509968350704
H	2.13895964827967	-5.30597897923899	-6.23890784874354
O	2.37028211878088	-2.51203520393937	-5.58590120159920
H	2.46157132435908	-4.43545636721151	-1.48668005542370
O	2.46858859602210	-4.17584261916641	-3.67631429684088
C	2.33963912342258	-3.40804226200950	-1.84474186773166
H	4.39510133393282	-3.04116067541201	-2.36828886717778
C	3.52535952805445	-2.49987735568303	-1.94957157878379
H	3.32764938138562	-1.61937816023304	-2.59112631452625
H	3.79501769459587	-2.14741778802798	-0.93465602207346
H	1.31992956904643	-3.08800675916473	-2.07970492453396
K	0.31454017896712	-0.63988755690241	-0.21924874301052
H	6.01064981725721	-4.17873523113532	2.53375509570125
H	6.88384851754643	-5.75063514062612	2.50652699938479
H	5.50377030925026	-5.50537172941114	3.63859000742738
H	4.76140359331719	-5.79435098297416	-0.64263956809763
H	6.43615394899034	-5.86296567891746	-0.01258366176746
H	5.53154237690208	-4.31906912055824	0.05165392677976
H	4.10708308311786	-7.71399624880081	0.83888801203032
H	4.35336793053396	-7.63462334599911	2.61800777864232
H	5.76864776565013	-7.81721109995311	1.52146447046658
H	8.23548650417115	-1.12200911981599	-5.11882723740030

H	6.96616923328248	-1.19996936637893	-3.85036506995736
H	7.21794725754076	0.32381631305846	-4.77284819996079
H	5.48195799488897	-3.17657531663526	-6.70563458618302
H	5.93118808750149	-3.22888234987146	-4.96642507271974
H	7.20891018611519	-3.16954271420299	-6.22401973218158
H	5.84356284060466	-1.06804466618871	-8.05991109306647
H	7.57825273725194	-1.03569754318070	-7.59111430717247
H	6.53644457339290	0.40486385475106	-7.29348596185399
TS-E2anti (TCEbutKF)			
O	-1.50954549904853	-0.74106902265644	-2.35522663614677
C	-2.77277753522795	-1.25504325921235	-2.20085227051460
C	-3.01615382446106	-1.99166887398061	-1.00465901173589
O	-1.95244494184479	-2.11388299079624	-0.14508853027519
C	0.91263016053122	-0.10075151971547	3.36880686779791
O	1.08497931790643	0.70431881650891	2.20037403120371
C	1.35102576839038	2.04081186086083	2.35337065388889
C	1.64962977719021	2.75574227448960	1.15706213344130
O	1.63383265638260	2.02526613203503	-0.00571361259488
C	1.89975354499127	2.72060507206853	-1.22827949667769
C	1.81958151149681	1.77357658514678	-2.41345115330640
O	0.47188362459069	1.26532728385491	-2.46938325026351
C	0.21843791226217	0.41234983379004	-3.60069048109970
C	-1.23846160331500	-0.01186135586712	-3.56111477201321
H	-1.42354305711919	-0.66334030256462	-4.44094794543952
H	-1.89335396732961	0.88722380051004	-3.60552704545460
H	1.15427893009636	3.53608620035371	-1.36363692356637
H	2.91740133017571	3.16775896280845	-1.19782067339945
C	-2.12017271501139	-2.90097293422008	1.03778191387764
C	-3.81279314939896	-1.09843657227459	-3.13077497120929
C	-4.28650967865878	-2.53946096254629	-0.77167616788460
C	-5.31968942445766	-2.37235453474018	-1.71252624620257
C	-5.08192241931922	-1.65535132405381	-2.88753198480708
H	-4.48229490762729	-3.10090705416102	0.15116253567178
H	-3.63913744526223	-0.54319101399944	-4.06083432082647
H	-6.30861276003590	-2.81036712239471	-1.51385615449572
H	-5.88072898158319	-1.52027199062920	-3.63186053674179
C	1.34525193576075	2.71504743153455	3.58309327660893
C	1.93852184086989	4.12736056250520	1.23112636619557
C	1.63511779180931	4.09103673611455	3.64229305593062
C	1.93216767224201	4.79280184925749	2.47143595276517
H	2.17787353757392	4.69125620811562	0.32085545888014
H	2.16638273554730	5.86669961266112	2.50770515706237
H	1.10980927995700	2.17278873277078	4.50837054578742
H	1.62592770804110	4.60432733398818	4.61510636001119
C	2.21077947763335	2.50996506496342	-3.69289415537373
H	2.52221862768564	0.91626075267344	-2.26095772675392
C	0.53869014639340	1.11858357402765	-4.92748926226436
H	0.84970919221848	-0.50320093687488	-3.51240262840343
C	1.97830867466119	1.66043901558287	-4.95846334329602
H	3.27848542383339	2.80707279871735	-3.66470271263018
H	1.60198167413536	3.43530224476976	-3.78049097434417
H	-0.16103630277580	1.97086282942247	-5.05251232599474
H	0.36679357087641	0.41322836763463	-5.76665989829828
N	2.90659020917023	0.53790232543467	-5.08568608577727
H	2.10742868990202	2.33589896085128	-5.83483125922681
C	4.21995325800306	0.66332901042639	-5.50172789512055
N	4.76115188178550	-0.52390709323813	-5.89254940732078
S	5.02404700122720	2.16264602392916	-5.50706721364025

C	6.13459591790638	-0.84360369137277	-6.34998896273976
C	6.46597992526154	-0.10067790557370	-7.66015870298325
C	6.13592484916833	-2.36174540465559	-6.61055055195210
C	7.16572986626757	-0.51466887178602	-5.25320585494489
H	2.47140812776040	-0.35488412870441	-5.37965745722170
H	4.08718548345033	-1.30159453672531	-5.96984977233670
C	0.77821630822727	-1.54743235442446	2.92939129274807
H	0.00267440372057	0.21517122359997	3.92732502674176
H	1.79788943116595	0.00406358301551	4.03514681949132
C	-0.78261219068066	-2.98748704678068	1.74701110715922
H	-2.45688121414825	-3.92618285277510	0.76754843679669
H	-2.88225421300416	-2.43713724345582	1.70409308445781
O	-0.48074142851286	-1.66304828775702	2.23935013562203
C	0.87329972695711	-2.54276576286797	4.08890862244127
H	1.60397671696889	-1.75756842460078	2.20833622210557
C	-0.75132187852590	-4.01983652832729	2.87357790068128
H	-0.01373144553223	-3.26774456492410	0.98945620495328
C	0.61971228889012	-3.97452990557443	3.58459399662301
H	-0.91891636876971	-5.04058639398174	2.47210962314899
H	-1.55628016493572	-3.80525394899836	3.60843283762862
H	0.11450253705070	-2.28952861055306	4.85963908732791
H	1.87550847952157	-2.47970569460378	4.56031876385299
N	3.18264237386524	-5.86480278537812	1.75483336912187
H	3.43365882194310	-5.02430558554947	1.22560524989352
C	4.88639837742449	-7.46104112279299	2.62657957187225
C	2.22042610759551	-5.68892605190915	2.70736168390761
C	4.00500333670265	-7.05857171212416	1.42761239461414
C	3.11099827868845	-8.23079787729903	0.98100030911579
S	1.69056009225440	-6.88012022118001	3.79458669514465
C	4.90480042811383	-6.62757605670124	0.25465829349439
N	1.70231460757141	-4.41197748557505	2.71433329773455
H	0.61041718421889	-4.69126445974383	4.43149942478958
H	1.93741134891563	-3.80680217533857	1.91206893231918
K	0.37444284147287	-0.50808819477462	-0.23888555631927
F	2.04728452184800	-2.72608892679681	0.19166137488189
H	2.26421411524501	-3.31306277654096	-0.80590870333562
H	1.93070141203021	-5.03891572419819	-1.63029333924928
C	2.50178800006339	-4.13867207757666	-1.91565376302847
H	3.59872122899848	-4.26065710636001	-1.92398359992641
C	1.93186610386098	-3.24850687262235	-2.82318484591832
H	0.83787438498388	-3.12896839137911	-2.86910053714370
H	2.52273740182594	-2.38094601068480	-3.15785594868611
O	1.91122452906837	-4.01766351648235	-4.73163283469117
S	1.28045595390713	-3.07686995987178	-5.77902635327008
O	-0.01972469917714	-2.48630315664786	-5.31939775084515
O	2.26899209526248	-2.03937111714850	-6.27306687438960
C	0.94451636061552	-4.16535751771874	-7.17816841966686
H	0.22752682704172	-4.93589709726292	-6.84285945678902
H	1.89947141119607	-4.61925180660724	-7.49764632634737
H	0.51299844077816	-3.54322012352372	-7.98343931597458
H	4.30289154434211	-6.32866098483671	-0.62830179787724
H	5.55607906491337	-7.46869846891063	-0.05074648334970
H	5.56180494164522	-5.77893582825466	0.54005266266869
H	2.48804987812556	-7.9393376855372	0.11090896106068
H	2.44163909593343	-8.54383188278961	1.80410819939617
H	3.74114478766698	-9.09305741483318	0.68398127140734
H	5.53112594095329	-8.32018465008172	2.35154112958682
H	4.25904620883239	-7.74936613176319	3.49147568256673

H	5.54031199116493	-6.61880416465062	2.93090626629014
H	5.74364406382889	-0.37640312041846	-8.45522341347959
H	7.48361669516265	-0.37578697349278	-8.00462505521378
H	6.42262618700178	0.99503194837262	-7.50724249070880
H	5.38723143275528	-2.63491059065234	-7.38277185046438
H	5.90554143417260	-2.93101383699979	-5.68643285869071
H	7.13227953613629	-2.68303243355155	-6.97118507585113
H	8.18106100348621	-0.80597574972059	-5.59074374886685
H	6.93598754510927	-1.07378709159064	-4.32341629867806
H	7.16405495338385	0.56790092746053	-5.02335716672890
TCEbut (KOMs)			
O	-1.94335106402936	-0.15052336244327	-2.22054094260432
C	-3.14020417312266	-0.81454792563688	-2.16045267713825
C	-3.32887584553992	-1.64235677765407	-1.01214048688963
O	-2.28995535287824	-1.66215509170016	-0.12015135360215
C	0.72949401846354	0.14199189803778	3.41686612212109
O	0.68972087408373	1.11667246892953	2.37222544033644
C	1.03735017874916	2.41655670500627	2.63006918735520
C	1.24418419476203	3.23351228097223	1.47883855390776
O	1.06979912204153	2.60609555843990	0.27337428405489
C	1.48960986324179	3.24585360689830	-0.93401931264851
C	1.46685763143227	2.22095833546403	-2.06027349507003
O	0.09346559516931	1.85641879292657	-2.29859040634200
C	-0.06791194109839	0.85819738252394	-3.33296135966678
C	-1.54871942557916	0.51533990490434	-3.42482182277428
H	-1.70658258016381	-0.15668511942572	-4.29653536425968
H	-2.15315783921122	1.43938716869536	-3.57099483395842
H	0.81389893781893	4.09730622997917	-1.17593288228124
H	2.52613846765553	3.63122443336608	-0.81696192108411
C	-2.25869994688887	-2.63581648144733	0.92808031501022
C	-4.15239425837053	-0.72964059394947	-3.12656425092684
C	-4.52453603793958	-2.35945767917026	-0.86485516930713
C	-5.53246646457690	-2.26786955927380	-1.84422572508314
C	-5.34735431246141	-1.45768441147494	-2.96832115750144
H	-4.67893888146170	-2.99260447309962	0.01998409338692
H	-4.01368574235632	-0.09139371861590	-4.01000773241980
H	-6.46526651862110	-2.83619951944826	-1.71473233489583
H	-6.13243180620981	-1.38062763007405	-3.73552151758010
C	1.19436619266150	2.96695299286151	3.90939354848301
C	1.60458991764720	4.57845023711184	1.63922056438726
C	1.55856211749356	4.31922103790596	4.05761959729583
C	1.76269005148468	5.11969312435811	2.92971514623332
H	1.76654725891888	5.21225966584715	0.75698914895129
H	2.05072915799067	6.17519294780761	3.04096239176643
H	1.03330360232008	2.34311586500958	4.79945476620243
H	1.68225511630445	4.73819544757865	5.06703879628365
C	2.12346118764206	2.75721225790691	-3.33894734387440
H	2.01972723071402	1.31786326689714	-1.70408650780069
C	0.50120482815125	1.35839436088412	-4.66105843641357
H	0.47708582880504	-0.06365713634646	-3.01591570152831
C	1.98677942910334	1.75775641760101	-4.50009484250135
H	3.19491852563017	2.97414552240730	-3.15393848248147
H	1.62755431119895	3.70901254270511	-3.62578322082865
H	-0.08238030534902	2.23930626854160	-5.00646630894114
H	0.42783440845448	0.57599469123623	-5.44406874501008
N	2.85594622637743	0.60899053959632	-4.30273554606237
H	2.32007217335556	2.22609844599433	-5.45013054231466
C	3.48050685405220	-0.06869896421884	-5.32620691360100

N	4.22300237248670	-1.12602888119343	-4.88906826986121
S	3.29586912204192	0.40931705191612	-6.94883064622904
C	5.11790959561291	-2.03441325327780	-5.64658298675262
C	4.32854934522371	-2.84357054372730	-6.69433536916588
C	5.70967647027317	-2.99961218464229	-4.60291166868097
C	6.26243182242758	-1.24418781652223	-6.31179896196786
H	2.98378908205720	0.22120606564268	-3.35411041335112
H	4.22652143771259	-1.25925597092022	-3.86553291996945
C	0.64932657442476	-1.24202778269277	2.78602997307209
H	-0.11758555546740	0.29390126318932	4.12405583894754
H	1.68598907966011	0.23001937555756	3.977644448567220
C	-0.86236960975331	-2.65264629114880	1.53626904798592
H	-2.48408625063082	-3.64404398834124	0.51627335437307
H	-3.01522322234345	-2.39068999494852	1.70752662527124
O	-0.66245834804765	-1.38742916864263	2.20852025219957
C	0.93274724997893	-2.35948951565280	3.79719123897185
H	1.40883951564427	-1.27726279979463	1.96622880294124
C	-0.65528516317485	-3.82000131401497	2.50209787154514
H	-0.12724882785038	-2.72529813719094	0.69797698949492
C	0.74330232174249	-3.74632564552349	3.15821890196379
H	-0.74641234817432	-4.79084680357409	1.97358308226297
H	-1.43470563827938	-3.78939240741640	3.29420132814402
H	0.23228879505943	-2.25789783016720	4.65323995852045
H	1.96624804816901	-2.26423664382010	4.18816725767874
N	3.38931216841318	-5.29033524455851	1.13741312618154
H	3.59086440994230	-4.37472201733687	0.70725107985393
C	5.10336725040546	-6.93021098792269	1.89943422721647
C	2.38201177617242	-5.28238579628561	2.05531007691862
C	4.28055455627282	-6.39566509514294	0.71044051086969
C	3.47449621937231	-7.52808101746446	0.04455162413548
S	1.82694780865551	-6.63261621177516	2.92995149612632
C	5.23805087333720	-5.77548773553296	-0.32457922356490
N	1.81792088801690	-4.03596658051906	2.22277285884488
H	0.80047603287401	-4.53906854373401	3.93380379063341
H	2.18103968770267	-3.28503434347928	1.61396021629363
H	5.00337641813027	-3.55901832130283	-7.20767598934688
H	3.87865918329935	-2.17088100716947	-7.44906811691660
H	3.51467364054058	-3.42007996605212	-6.20907718885486
H	6.94498958003295	-1.93806061205942	-6.84380063854578
H	6.85044119779258	-0.69427472023502	-5.54860588221476
H	5.86124060739733	-0.51346933454070	-7.04068712021749
H	6.41977459229031	-3.69552668816164	-5.09080543552253
H	4.91617702432134	-3.60961418274221	-4.12355379055560
H	6.25669167222090	-2.45417618862633	-3.80601440661095
H	5.70412570742802	-6.11551863590439	2.35239974642293
H	5.79662999575988	-7.72535819759822	1.55675664317697
H	4.43756357977499	-7.35031911867176	2.67745713992117
H	4.68636219339162	-5.39599291954416	-1.20954745220069
H	5.95841696065640	-6.53768444832763	-0.67922172268566
H	5.81307336879541	-4.93249519599061	0.11044253509827
H	2.89686815081249	-7.13870578544694	-0.81875484075478
H	2.76506035598308	-7.98031953233961	0.76383226535209
H	4.16090197174243	-8.31642891155161	-0.32492257800382
H	1.61282459952170	-4.07222467690078	-1.65715536914722
H	1.83908952154256	-3.04917465294451	-3.14457707081012
C	2.30048688176765	-3.40097717234686	-2.20368512496632
H	3.26140593300035	-3.90866981837463	-2.40678335670179
O	1.28074825936456	-1.30541132990428	-0.94091578717431

S	2.63066021927804	-1.95523466912245	-1.16370395920540
O	3.23442917810212	-2.48337812070166	0.11898246013339
O	3.57022519982264	-1.07329526688732	-1.95743178625414
K	-0.46517433859298	0.35881430968996	0.00661865162489