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Supporting Information
for
Azo-crosslinked double network hydrogels enabling highly efficient mechanoradical generation

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Experiments Methods

Materials: Azoalkane crosslinker, 2,2'-azobis-[2-methyl-N-(2-ethylpropenoate)]-propionamide] (AAC), was prepared by treatment of 2,2'-azobis[2-methyl-N-(2-hydroxyethyl) propionamide] (VA-086) and acryloyl chloride (Fig. S1). 2-acrylamido-2-methyl-1-propanesulfonic acid (AMPS) was provided by Toagosei. Acrylamide (AAm) was purchased from Junsei Chemical. *N,N'*-methylenebis (acrylamide) (MBA), *N,N',N''*-triacryloyl diethylenetriamine (TADETA), 2,2'-azobis(2,4-dimethyl) valeronitrile (ABVN), 2,2'-azobis[2-(2-imidazolin-2-yl)propane] dihydrochloride (VA-044), *N*-isopropyl acrylamide (NIPAm), ammonium iron(II) sulfate ((NH₄)₂Fe^{II}(SO₄)₂) hexahydrate, sulfuric acid (H₂SO₄), ammonium iron(III) sulfate (NH₄Fe^{III}(SO₄)₂) dodecahydrate, xylene orange (XO) were purchased from Wako Pure Chemical Industries. All reagents were used as received.

Procedure for the preparation of AAC

To a 100 mL three-necked round-bottomed flask equipped with a magnetic stirrer and rubber stopper and purged with Argon gas were added 2,2'-azobis[2-methyl-N-(2-hydroxyethyl) propionamide] (VA-086, 1 equiv.) and CH₂Cl₂ (5 mL/mmol VA-086). The resulting suspension was cooled in a liquid nitrogen/acetone bath, then added was triethylamine (16 equiv.). After that, a solution of acryloyl chloride (6 equiv.) in CH₂Cl₂ (1 mL/mmol) was added dropwise into the suspension. The reaction mixture was stirred for 5 hours, and it was allowed to warm slowly to room temperature, then poured onto saturated NaHCO₃ to quench the reaction and CH₂Cl₂ to extract the organic compound. The layers were separated, and the aqueous layer was extracted with CH₂Cl₂ twice. The combined organics was washed with saturated NaHCO₃ then dried over Na₂SO₄. After removal of solvent by evaporation, the crude product was then purified by silica gel chromatography eluted with Hexane: EtOAc = 1: 1 and EtOAc in turn to give product as white or light-yellow solid. ¹H NMR (DMSO 500 MHz) δ 7.68 (2H, s) 6.30 (2H, d) 6.13 (2H, q) 5.94 (2H, d) 4.15 (4H, t) 3.44 (4H, t) 1.26 (12H, s) ¹³C NMR (DMSO 500 MHz) δ 173.8, 165.8, 131.3, 127.7, 74.5, 62.9, 38.5, 22.7. FTMS-ESI (m/z): [M - H]⁻ calculated for C₁₈H₂₈N₄O₆, 396.20; found, 396.19.

Synthesis of DN gels with different crosslinkers

DN hydrogels with different crosslinkers were prepared by the conventional two-step procedure. To avoid the

decomposition of azo group during the polymerization process, low-temperature radical polymerization was adopted. After being bubbled with Argon gas for 15 minutes, the precursor *N,N*-dimethylformamide solution containing AMPS (1 mol/L, monomer), 2,2'-azobis(2,4-dimethyl) valeronitrile (1% mol/L, initiator, 10-hour half-life temperature: 45 °C) and different crosslinkers (MBA of 4-8 mol%, AAC of 4-12 mol% or MIX of 4-10 mol% in relative to monomer) was injected into the mold with two parallel glass plates and silicone spacers. Then the mold was kept at 44°C for 10 hours to form PAMPS single network (SN) hydrogel. The resulting PAMPS SN hydrogel was then immersed into aqueous solution containing AAM (2 mol/L, monomer), MBA (0.02% mol/L, crosslinker), 2,2'-azobis[2-(2-imidazolin-2-yl)propane] dihydrochloride (0.1% mol/L, initiator, 10-hour half-life temperature: 44 °C) for 1 day until equilibrium was reached. The equilibrated PAMPS SN hydrogel was sandwiched by two glass substrates and then kept at 44°C for 10 hours to form DN hydrogels. The as-prepared DN gel was then swelled in a large amount of water to remove the residual and to reach the equilibrium state.

Evaluation of mechanoradical concentration by Fenton color reaction

DN gels with different crosslinkers were cut into dumbbell-shaped strips (20 mm gauge length and 4 mm width). The cut gels were immersed in an aqueous solution of 500 μM $(\text{NH}_4)_2\text{Fe}^{\text{II}}(\text{SO}_4)_2$, 500 μM XO and 20 mM H_2SO_4 for 1 day. Then gels were stretched to the preset strain ($\epsilon_{\text{max}} = 4$) at a velocity of 100 mm/min and then immediately recovered to the initial position, during which the stress-strain curves were recorded. After 30 mins, when no further color change was observed, the gels were cut with scissors to obtain the gel in the necked region, which were used to test UV-Visible absorption spectroscopy (UV-1800, Shimadzu Co.). To quantify the Fe^{3+} concentration, a calibration experiment was done by immersing DN gels into an aqueous solution of 0-400 μM $\text{NH}_4\text{Fe}^{\text{III}}(\text{SO}_4)_2$ (as a Fe^{3+} source), 500 μM $(\text{NH}_4)_2\text{Fe}^{\text{II}}(\text{SO}_4)_2$, 500 μM XO and 20 mM H_2SO_4 to get the calibration curve of normalized absorbance at 580 nm as a function of Fe^{3+} . By comparing the normalized absorbance at 580 nm of DN gels after stretching with the calibration curve, we can evaluate the Fe^{3+} concentration, which is assumed to be equal to the mechanoradical concentration.

Repetitive loading-unloading test of DN gels fed with AMPS and TADETA. DN-10AAC, DN-7MBA gels were immersed in an aqueous solution of 0.6 M AMPS and 0.3 M TADETA for one day. Then the samples of ~1.5 mm-thick were cut into dumbbell-shaped strips (12 mm gauge length and 2 mm width). After that, dumbbell shaped DN gels in the solution were put into an argon glove box for 2 hours to remove oxygen. Then the gels were conducted cyclic tensile test with the preset strain of 4 at a velocity of 300 mm/min. After 3 minutes, the gels were conducted second cyclic tensile test at the same conditions.

Force-responsive functionalization of DN gels fed with NIPAm and MBA. DN-10AAC, DN-7MBA gels of ~1.5 mm-thick were cut into sheets with the size of 50 mm $\times$ 50 mm. Then the samples were immersed in an aqueous solution of 2.0 M NIPAm and 0.15 M MBA for one day. Next, the samples in the solution were placed in an argon glove box for 2 hours to remove oxygen. Then the gels were compressed by a polyacrylic resin stamp with the raised bear toe pattern. The height of the raised pattern was 2.0 mm. The compression strain was controlled at 0.8.

Mechanical measurement. The uniaxial tensile test and cyclic tensile test were performed at a velocity of 100 mm/min by using a universal testing machine (RTC-1150A, Orientec Co.). The Young's modulus was determined as the slope of stress-strain curves between the strain range of 0.03–0.1. The yield strain and yield stress were determined at the zero-slope point of the stress-strain curves or determined by the tangential lines method. The dissipated energy was calculated by the area between the loading curve and unloading curve up to $\epsilon_{\text{max}} = 4$. Each data point was the average of at least three measurements, and the error bars represented their standard deviations.

Computational Methods

All of the calculations were performed at the DFT level of theory with the B3LYP hybrid functional¹ as implemented in Gaussian 16.² To describe the dispersion properly, an explicit dispersion correction term called GD3,³ was also employed in the DFT calculations. The Def2-SV(P) basis set⁴ was used for all the atoms involved in this study during both the geometry optimization and the single-point calculation processes. To describe the open-shell singlet species involved in the homolysis process, the unrestricted DFT, as well as the procedure to test and optimize the wavefunction were used in this work.⁵ Also, to reduce the computational cost, the -CH₂SO₃Na group is simplified to -CH₃ group in the model molecule subjected to the computational study. To properly describe the solvation environment where the polymer stays, the implicit solvation model, IEFPCM,⁶ is applied to all the calculations involved in this study with water as the solvent ($\epsilon=78.3553$). All of the structures were fully optimized with the consideration and constraint of external tensile force. The external tensile force is properly simulated through our AFIR method.

The term of AFIR is the abbreviation for Artificial Force Induced Reaction⁷ and it has been extensively used for the exploration of organic and organocatalytic reactions.⁸ The original idea of AFIR is simple, as pulling two specific intramolecular (or intermolecular) fragments together by an artificial force can eventually lead to the reactions. The force is applied to the system by the following AFIR function $F(\mathbf{Q})$.

$$F^{AFIR}(\mathbf{Q}) = E(\mathbf{Q}) + \rho\alpha \frac{\sum_{i \in A} \sum_{j \in B} \omega_{ij} r_{ij}}{\sum_{i \in A} \sum_{j \in B} \omega_{ij}} \quad (1)$$

In Eq. (1), $E(\mathbf{Q})$ is the original Born-Oppenheimer potential energy surface of the given geometrical parameter $\mathbf{Q}$ and the second term applies the force to the system of interest. The parameter α controls the strength of the force added to the designated fragments inside the molecule of interest. Moreover, the force term is given as a weighted sum of the distances r_{ij} between atom i in the fragment A and atom j in the fragment B, and the formula of weight function ω_{ij} is shown in Eq. (2).

$$\omega_{ij} = \left[\frac{(R_i + R_j)}{r_{ij}} \right]^6 \quad (2)$$

In Eq. (2), the inverse distance $1/r_{ij}$ is scaled by $R_i + R_j$, the sum of covalent radii of atoms i and j , to treat all elements equivalently. Most importantly, the coefficient ρ shown in Eq. (1) can be set to either 1 or -1, of which the latter represents the repulsive interaction between two moieties of the system. To go a step further, if the repulsive force is added between the two terminal groups, it therefore turns to be a tensile force that stretches the polymer chain.

Determination of Rupture Forces

The minimization of the force modified potential energy surface (FMPES), which is constructed by the AFIR function, can be used to predict the site of bond cleavage when subjected to external force. It therefore allows us to screen the availability of the candidate molecules as a qualified cross-linker molecule. In fact, with the assistance of AFIR method, we are now able to locate the transition state of the homolysis process under the constraint of an external force. In this case, we have made our effort to locate the transition states associated with the homolytic cleavage of specific covalent bonds for both PAMPS-MBA and PAMPS-AAC networks under a variety of force levels. Once the TS structure on the FMPES is successfully optimized, we can realize the Gibbs energy barrier of C-C homolytical cleavage (i.e., the formation of mechanoradicals) under that certain level force. With the varying of force level, we can subsequently characterize how the Gibbs energy barrier changes accordingly.

For PAMPS-MBA network, two possible C-C cleavage patterns were considered and thus investigated. The cleavage of C₆-C₂₅ bond leaves an alpha-carbonyl radical and a CH₂ radical, while the cleavage of the linkage site

at C₂₈-C₁₁₉ generates an acyl radical and a secondary carbon radical (Fig. S3). For PAMPS-AAC network, the homolytic cleavage of the C=N=N bond forms a tertiary carbon radical and an N-radical, of which the latter immediately releases a dinitrogen molecule and turns into a tertiary carbon radical (Fig. S4).

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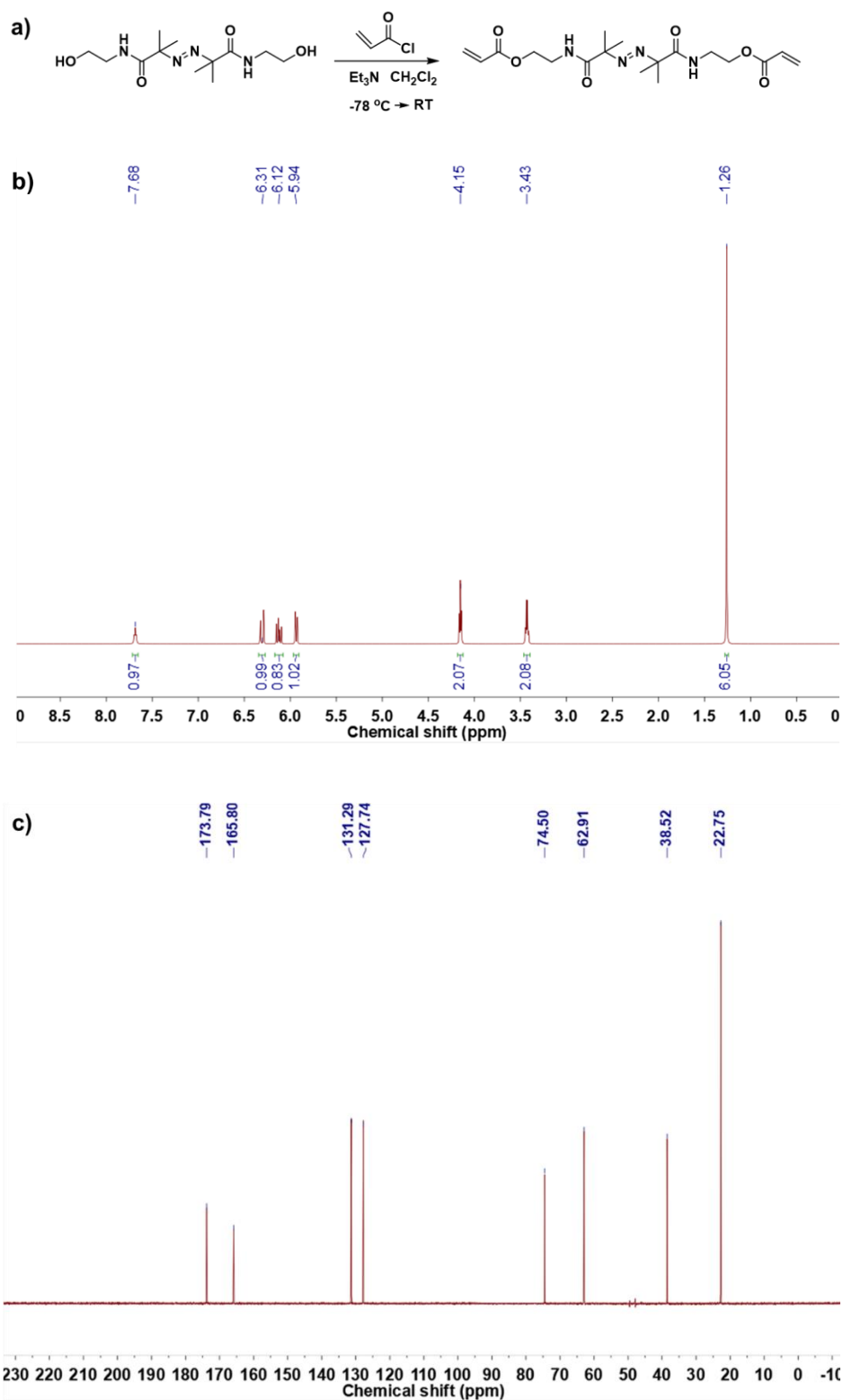


Figure S1. (a) Preparation of azoalkane crosslinker. (b) ^1H NMR and (c) CNMR (500 MHz, DMSO) spectrum of the azoalkane crosslinker

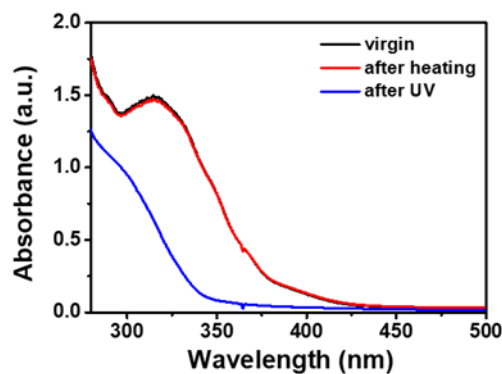


Figure S2. The UV-visible spectrum of azoalkane crosslinker (AAC) in DMF solution. Black: as-prepared AAC in DMF solution (0.01 g/ml). Red: after heating at 44°C for 10 hours. Blue: after UV irradiation for 2 hours. AAC had the absorbance peak at 320 nm due to the azoalkane group. After exposed to UV light for 2 hours, the absorbance peak at 320 nm disappeared. In contrast, after heating at 44 °C for 10 hours, the absorbance at 320 nm kept almost constant, indicating the thermal decomposition of the AAC during the polymerizations can be negligible.

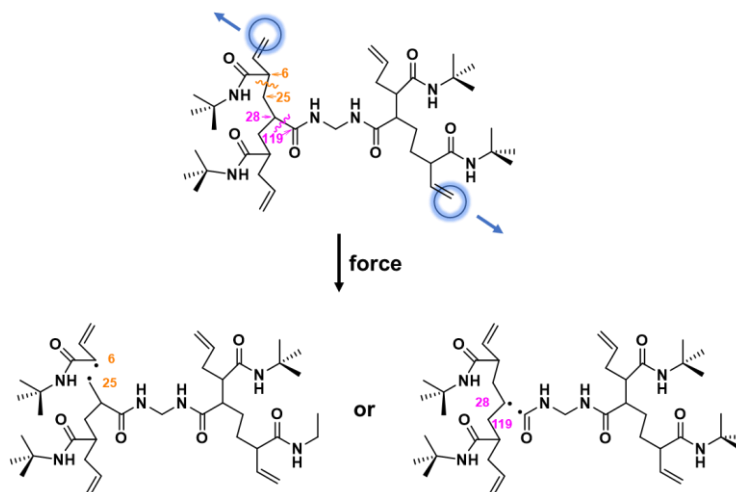


Figure S3. Mechanoradicals formed from the ruptured PAMPS-MBA network at C₆-C₂₅ site at C₂₈-C₁₁₉ site.

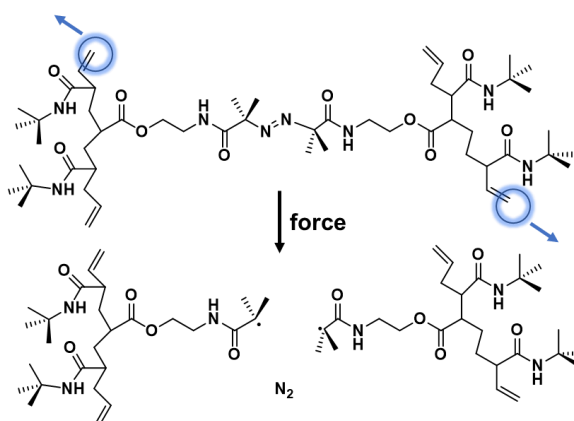


Figure S4. Mechanoradicals formed from the ruptured PAMPS-AAC network.

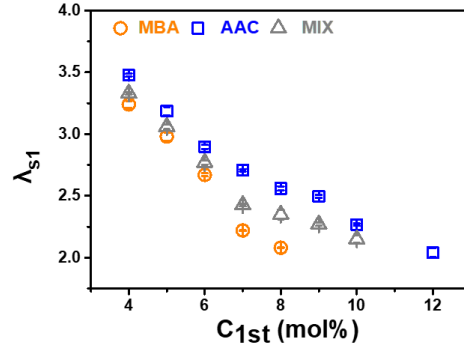


Figure S5. The length swelling ratio λ_{S1} of the three sets of PAMPS SN gels in the AAm monomer solution, which is determined by the thickness of the equilibrated PAMPS SN gels in AAm monomer solution divided by the thickness of the as-prepared PAMPS SN gels.

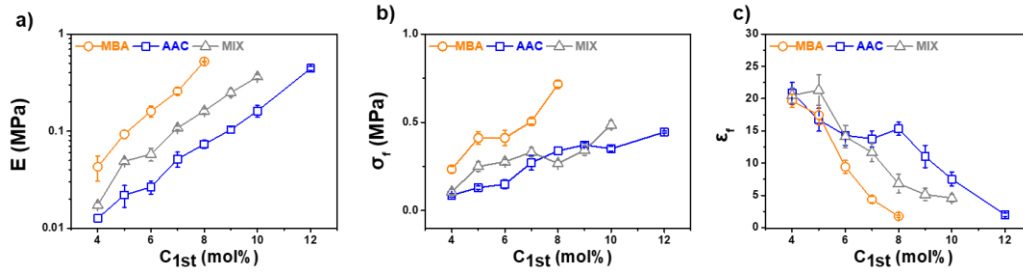


Figure S6. Young's modulus E (a), fracture stress σ_f (b), and fracture strain ϵ_f (c) of DN gels prepared with different in-feed concentration of crosslinkers C_{1st} .

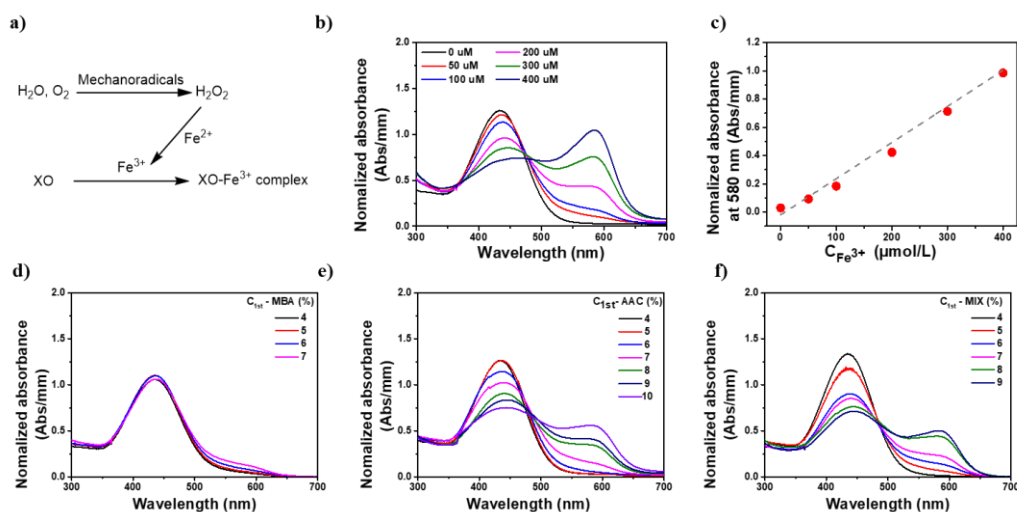


Figure S7. Quantification of mechanoradical concentration of DN gels with different crosslinkers. (a) Fenton color reaction induced by mechanoradicals that makes yellow XO form purple XO-Fe^{3+} complex. (b) The UV-Vis spectrum of DN gels fed with a specified concentration of $\text{NH}_4\text{Fe}^{\text{III}}(\text{SO}_4)_2$ (0-500 μM), 500 μM $(\text{NH}_4)_2\text{Fe}^{\text{II}}(\text{SO}_4)_2$, 500 μM XO and 20 mM H_2SO_4 . (c) Calibration curve of normalized absorbance at 580 nm as a function of Fe^{3+} concentration fed to DN gels. The calibration curve is independent of the species of DN gels. (d-g) UV-spectrum of DN-MBA (d), DN-AAC (e), DN-MIX (f) gels in the necked region after stretching to tensile strain at $\epsilon_{\text{max}} = 4$.

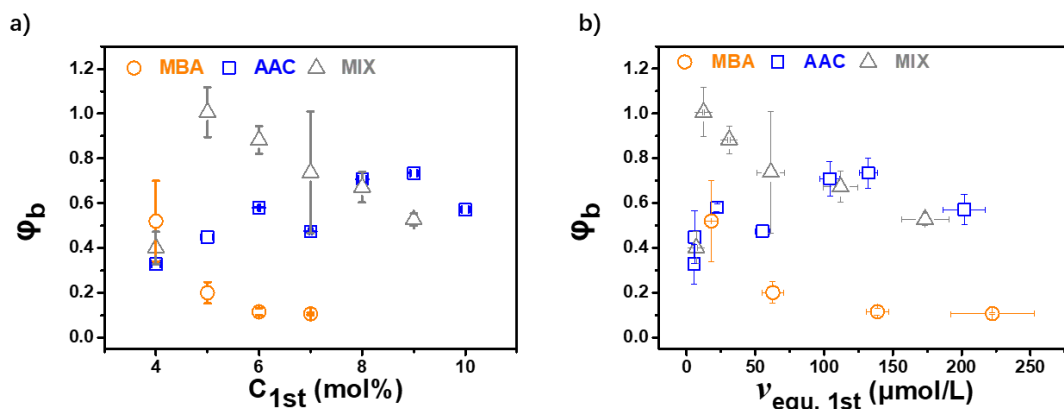


Figure S8. The ratio of broken strands to total strands of the PAMPS network ϕ_b , estimated from the relation of $\phi_b = C_{rad}/(2\nu_{equ,1st})$, as a function of C_{1st} (a) and $\nu_{equ,1st}$ (b). It should be mentioned that theoretically ϕ_b should be less than one and the absolute value of ϕ_b estimated from C_{rad} and $\nu_{equ,1st}$ should contain relatively large uncertainty due to experimental errors of related quantities. Except at the lowest C_{1st} (4 mol%), the ϕ_b values of DN-AAC and DN-MIX are much higher than those of DN-MBA, indicating the weak bond effect of the azoalkane group in AAC. ϕ_b of DN-AAC and DN-MIX gel show rising first and then falling with C_{1st} while ϕ_b of DN-MBA only decreases with C_{1st} . This different trend of ϕ_b is related to the $\nu_{equ,1st}$. At the extreme low C_{1st} , $\nu_{equ,1st}$ is too low to show DN effect, i.e. no extensive fracture of the first network. So ϕ_b will be relatively small. With the increase of C_{1st} and resultant increase of $\nu_{equ,1st}$, $\nu_{equ,1st}$ reaches a point to show DN effect, causing the increase of ϕ_b . With the further increase of C_{1st} , the strength of the first network is increased while the second network keeps constant, which will decrease the ϕ_b . The fact that DN-MBA only shows a decreasing trend should be attributed to the high $\nu_{equ,1st}$ at the C_{1st} of 4 mol% that already leads to the extensive fracture of the first network.

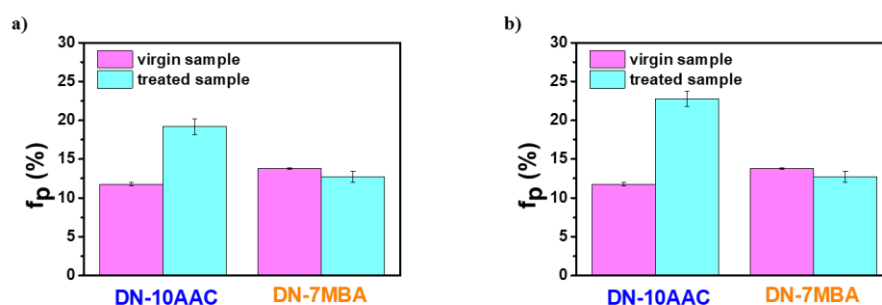


Figure S9. (a) Polymer weight fraction f_p of DN-10AAC and DN-7MBA gels before and after compression when fed with NIPAm and MBA. (b) f_p of DN-10AAC and DN-7MBA gels before and after stretching when fed with AMPS and TADETA. f_p was measured by the moisture meter (Moisture balance, MOC-120H). To test f_p of the gels after compression and after stretching, the gels in the compressed region and in the stretched region were cut and then immersed into a large amount of water for 2 days to remove unreacted monomers and crosslinkers.

Cartesian Coordinates of Optimized Structures under Tensile Force

R-PAMPS_MBA-1500pN (G = -2460.91676343 a.u.)

0 1

C	-7.180879699122	-1.978627223704	-0.484519708184
H	-7.984742043350	-2.070007485716	0.255028641916
H	-7.080696295126	-2.784753287645	-1.224101111308
C	-6.347919283628	-0.911927034412	-0.480673029730
H	-6.499484960917	-0.138948340432	0.285860591697
C	-5.216906516009	-0.666282348625	-1.484478086009
H	-4.840658499395	-1.662164198594	-1.772346776016
C	-5.652724818109	-0.067219547651	-2.842843614543
O	-4.905768958389	-0.180390820801	-3.812441755322
N	-6.826453095068	0.604525648941	-2.855265449228
H	-7.399876747557	0.521967522333	-2.021022188248
C	-7.483978600993	1.217759496537	-4.033198312676
C	-7.957686529379	0.104987971617	-4.985726196828
H	-8.464796517635	0.539051174040	-5.865876847543
H	-7.096022353116	-0.488647815122	-5.334489256160
H	-8.665952828881	-0.571046156224	-4.473525111657
C	-6.525735145854	2.182116357787	-4.753311462960
H	-7.060257503428	2.680465452771	-5.581888677741
H	-6.172396905710	2.951408734671	-4.048065091007
H	-5.658821585635	1.643343900225	-5.162159344033
C	-8.681796797119	2.011799800402	-3.487955195345
H	-9.235489710807	2.480168267390	-4.319466288956
H	-9.384073233807	1.354572157799	-2.941591911859
H	-8.333137411367	2.808478646344	-2.807087320208
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H	-3.724238510077	-0.160772599639	0.050432476005
H	-3.097353289085	-0.291038084200	-1.595261982685
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H	-4.031353207789	1.955420779093	-2.168430621009
C	-4.918087696346	2.349896373139	-0.229369284476
H	-5.911015839577	2.076247534129	-0.623019244880
H	-4.837916841341	1.935794400658	0.791310030065
C	-4.843230832503	3.882375487358	-0.129728211401
H	-3.865174040027	4.165310104569	0.297078530513
C	-5.019535952673	4.538606649889	-1.505496387575
O	-6.022643773421	4.315529026947	-2.182228640158
N	-4.021977889915	5.375090699616	-1.879917417299
H	-3.254273073341	5.480623805259	-1.227275182439
C	-3.963397924004	6.205874939772	-3.105407950010
C	-5.193857961744	7.127991246863	-3.177586412209
H	-5.126786877376	7.778440942080	-4.067435430673

H	-6.118816317804	6.534381939905	-3.239182159031
H	-5.248457429095	7.766747631586	-2.278412471140
C	-3.890071114698	5.299887168652	-4.347861406254
H	-2.988941791255	4.661030758545	-4.312740681607
H	-4.777547170047	4.651631455692	-4.409723776157
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C	-2.682591310680	7.049396921756	-2.998981278857
H	-2.573950798930	7.684958993509	-3.893754888676
H	-2.714591841263	7.708641671485	-2.112157289673
H	-1.787200534075	6.406066931529	-2.923157691481
C	-5.948883537366	4.422430835125	0.810659873519
H	-5.860390796314	3.890340349772	1.777054490017
H	-6.932168615500	4.166053523990	0.378908063659
C	-5.848887002319	5.905882022802	1.039898508416
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C	-6.753448345017	6.809298730458	0.644590110109
H	-7.668932098116	6.507738407355	0.117987708480
H	-6.613533211862	7.881444862120	0.828921950840
C	6.215630434790	11.206828085938	-2.592186981131
H	6.422047122338	12.231700262457	-2.262910519603
H	6.972147244688	10.702949157235	-3.206083785145
C	5.061367018495	10.595939613618	-2.244783774189
H	4.348465925435	11.164829812130	-1.629704199002
C	4.560799045677	9.176602333348	-2.616528678227
H	4.215564001998	9.214420519392	-3.665593947842
C	5.784593663431	8.243457655001	-2.656916501693
O	6.478868655874	8.207730363982	-3.674121794119
N	6.092215504757	7.586257643320	-1.511691202989
H	5.388751581763	7.526235422459	-0.776815152305
C	7.323993022272	6.790572409648	-1.292840786437
C	8.569189718368	7.654426543245	-1.567617680115
H	9.481786030090	7.085574129877	-1.315629334158
H	8.616838482206	7.953498585851	-2.625005193245
H	8.544827497251	8.567597552524	-0.946362940878
C	7.318669860315	5.546020284688	-2.200179054604
H	8.227847132865	4.941517502009	-2.031127207085
H	6.438274204132	4.915262008350	-1.985090200603
H	7.284789752815	5.847071888959	-3.259231871228
C	7.322247390553	6.367635097020	0.184488383519
H	8.211986594905	5.751869676118	0.400356465558
H	7.346194647356	7.253685332208	0.844617746128
H	6.419826433800	5.786089343534	0.430650183800
C	3.367883513822	8.707020922207	-1.728809594033
H	3.710248947002	8.689584213427	-0.684565983295

H	2.584700295300	9.485300446103	-1.780137970874
C	2.756854694233	7.326228244973	-2.098644248882
H	3.538241240050	6.555620979205	-2.017327145508
H	2.465329681302	7.344746568569	-3.164308599889
C	1.508009519570	6.828600239264	-1.297595307471
H	0.651811738380	7.494820966038	-1.511647211532
C	1.649898628667	6.794454927971	0.265018941094
H	0.756801130349	6.273680396443	0.646140651750
C	2.883130130815	5.964824734869	0.642224518569
O	4.019864988389	6.433852098952	0.562502659073
N	2.612997680966	4.688648458182	1.000258418569
H	1.634446978996	4.428986302389	1.055677162491
C	3.591933306181	3.595812406337	1.206171437123
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H	5.250471062714	3.119710556173	2.537642200029
H	5.092218069907	4.865481574788	2.161551135306
H	3.952855633918	4.090516595800	3.302466122781
C	4.379402803524	3.369018630415	-0.096928611266
H	3.688281373883	3.135644401463	-0.925203568322
H	4.944492377602	4.273158879120	-0.368936188867
H	5.089262962503	2.532264398219	0.025133687157
C	2.776628814221	2.338757713608	1.545785186939
H	3.453755432839	1.484726337997	1.714239773125
H	2.177723345700	2.488427578480	2.462454124887
H	2.093342278953	2.072436807545	0.718181444241
C	1.656032346505	8.162625847973	0.981461212521
H	0.874143438963	8.796293291498	0.523230678786
H	2.619726964809	8.668479238073	0.840636822620
C	1.386679153616	7.998663291584	2.454522227386
H	0.380068577366	7.645824190124	2.723404232898
C	2.285378348718	8.210208200062	3.423161530979
H	3.304224240754	8.548476516412	3.191204800816
H	2.039108669952	8.053473318217	4.480440626600
C	-2.433794715520	2.148978362000	-0.696361682588
O	-1.927584339197	1.744314849673	0.341571005976
N	-1.797020909810	3.068882216527	-1.512959418085
H	-2.235103186441	3.296184021665	-2.400728980584
C	-0.388940167180	3.425030390111	-1.355131617168
H	-0.059605244827	2.937006866365	-0.423751316004
H	0.206121064196	3.024398763184	-2.188883335508
N	-0.095993951988	4.870360290747	-1.310566369172
H	-0.635674894700	5.421731157809	-0.649718480684
C	1.110942530050	5.381906919114	-1.764486382812
O	1.862529386931	4.711884106031	-2.458395968534

R-PAMPS_MBA-2000pN (G = -2461.13547100 a.u.)

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H	-7.153885801049	-2.881567263014	-1.193789390283
C	-6.448859220561	-0.999487318047	-0.431517443931
H	-6.629003122303	-0.231309757054	0.334780318263
C	-5.291353285614	-0.722066859265	-1.408447703875
H	-4.890487521449	-1.710229841370	-1.687445284650
C	-5.714946316663	-0.137818232383	-2.776276759012
O	-4.976930769891	-0.290785813235	-3.747180648246
N	-6.866745433197	0.571574834412	-2.796528002717
H	-7.439991323707	0.523395383187	-1.959635183491
C	-7.510691522966	1.178372449458	-3.985588049999
C	-8.016932817923	0.059330267770	-4.913827516979
H	-8.515388068126	0.488717919625	-5.801186054281
H	-7.172623013472	-0.564093169643	-5.252843514872
H	-8.741165745470	-0.586882671718	-4.385704462498
C	-6.528177535195	2.100700762101	-4.728024190382
H	-7.050719808993	2.594826163044	-5.566736298298
H	-6.153412156331	2.875984104203	-4.040673963559
H	-5.677080612607	1.529477526612	-5.125916991205
C	-8.685488560575	2.015547339834	-3.454976656691
H	-9.227900989117	2.481191731292	-4.295448112040
H	-9.404179226264	1.388426058682	-2.894675236581
H	-8.314176673805	2.816356220183	-2.791371431111
C	-4.008143223687	0.083237372732	-0.912255118598
H	-3.832868801360	-0.152141973871	0.150812318378
H	-3.164089563240	-0.356639753331	-1.467595851687
C	-3.894405298688	1.639665305494	-1.089600363471
H	-4.078979119101	1.895810748454	-2.147041776053
C	-4.944774341837	2.356348410918	-0.210652561813
H	-5.942361516984	2.078645737813	-0.590699236951
H	-4.861261532618	1.963505775915	0.818310715328
C	-4.862568027808	3.889880966272	-0.138507579182
H	-3.882297588791	4.176193690996	0.280383209072
C	-5.041996148517	4.528332782412	-1.521802950423
O	-6.036876772209	4.281814823180	-2.202266922692
N	-4.057734611431	5.379956136359	-1.897999645234
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C	-4.009421372166	6.203243650128	-3.128978778688
C	-5.254615794707	7.104470600069	-3.211501790754
H	-5.195342276714	7.749937935508	-4.105541528164

H	-6.169296429632	6.494974762088	-3.272162330463
H	-5.323225691057	7.747929848236	-2.316674709442
C	-3.918095908031	5.289221439473	-4.364406686917
H	-3.007532675753	4.664298508942	-4.321755905099
H	-4.795598850697	4.627169813002	-4.424067839464
H	-3.871460797662	5.897256652702	-5.284980070889
C	-2.742612204000	7.067976557002	-3.024339349386
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H	-1.837357713532	6.440067106718	-2.935466467300
C	-5.963934475571	4.448180521270	0.797352995250
H	-5.873181114348	3.931310523886	1.771792867327
H	-6.949589008730	4.187159538898	0.373636985672
C	-5.860194347576	5.934743964647	1.003250829503
H	-4.945414364802	6.284143090624	1.504580447748
C	-6.766133242194	6.833436917097	0.600496336427
H	-7.685437385276	6.525518630838	0.084323011209
H	-6.623465413231	7.907999735827	0.767770625796
C	6.327286575096	11.237855609502	-2.566967226378
H	6.532562526667	12.256262702620	-2.217828184470
H	7.073110917865	10.752143599746	-3.207957497193
C	5.181162005183	10.609360778879	-2.205281351669
H	4.484539195759	11.164147884524	-1.559079677781
C	4.662300768307	9.188307164621	-2.587041090254
H	4.345730292177	9.229382067173	-3.644613408197
C	5.882999266161	8.250191485184	-2.595597487150
O	6.611086654729	8.223867261693	-3.589277791709
N	6.153199909608	7.581834368582	-1.447297673980
H	5.431773955986	7.523288907052	-0.729859174755
C	7.398096826003	6.820581976653	-1.182432254485
C	8.624500090073	7.730672092286	-1.384603710472
H	9.544823261765	7.186760387911	-1.107098109187
H	8.706082238224	8.055438979278	-2.432492956612
H	8.543335122307	8.627998106379	-0.745399130670
C	7.479528648751	5.591806665732	-2.107381589672
H	8.400326264299	5.016752864358	-1.902353800275
H	6.613125655289	4.927217860865	-1.944623119026
H	7.486133513277	5.908651064035	-3.162103079534
C	7.342213720888	6.372539736964	0.286183977638
H	8.245773575832	5.790597107854	0.535752885351
H	7.296221834609	7.246551041413	0.960925208005
H	6.455401682407	5.748938300075	0.479484633429
C	3.436196692698	8.722675911246	-1.727956330528
H	3.754804934263	8.699066853123	-0.676449901793

H	2.665729390671	9.512286402409	-1.794867999305
C	2.800116239736	7.343944595126	-2.106156271803
H	3.568734586549	6.560802550153	-2.015651530100
H	2.522330081026	7.367490672661	-3.175114900068
C	1.525476509185	6.858998148837	-1.318658940856
H	0.685789899034	7.544230490682	-1.537676338626
C	1.658826859277	6.820232673293	0.244921260747
H	0.764519576408	6.299787093033	0.623429927718
C	2.889456189249	5.984154397597	0.617315765216
O	4.024087538838	6.463750120593	0.590070550291
N	2.621093987096	4.688148007743	0.899447833479
H	1.643922631761	4.417276080398	0.905973204194
C	3.604773847498	3.589020757546	1.041042526767
C	4.530708597211	3.861445973581	2.238959605632
H	5.258052677568	3.038076041815	2.349911656557
H	5.080309362754	4.804458146810	2.099072417701
H	3.941823376584	3.935333948749	3.170531945125
C	4.404134588372	3.456858677091	-0.268050654479
H	3.720861292146	3.267293489418	-1.113781421040
H	4.955889764151	4.385294002078	-0.477960254488
H	5.126538468336	2.625138187819	-0.194997864239
C	2.795606790051	2.306521843416	1.286313323534
H	3.477832855741	1.448744376404	1.408999367936
H	2.181940485907	2.391558602620	2.201427788274
H	2.127409927571	2.088760378456	0.432799730919
C	1.666354501104	8.186903422987	0.962709711083
H	0.886881202447	8.822521853181	0.503074922921
H	2.631330541467	8.690911065256	0.824564674393
C	1.392084701771	8.023290366298	2.434898871550
H	0.383736527002	7.672730792009	2.700354054028
C	2.287558479166	8.233570164211	3.406748280738
H	3.307973091883	8.569327025394	3.178266812634
H	2.037007484538	8.077919698259	4.463197493265
C	-2.455908291033	2.123067629627	-0.697941843939
O	-1.912365880765	1.680017295183	0.304021108504
N	-1.850332018085	3.096477828838	-1.487001938824
H	-2.307837443620	3.344776792390	-2.359531670486
C	-0.433993783855	3.460653210199	-1.354692256785
H	-0.091200603210	2.973821194548	-0.427449075019
H	0.146864036726	3.055257796969	-2.196347891375
N	-0.120822754997	4.909464251630	-1.318013984560
H	-0.642000227896	5.465461652129	-0.646053278761
C	1.088346601953	5.415429526310	-1.792974396458
O	1.813871899667	4.744329839814	-2.511546391519

R-PAMPS_MBA-2500pN (G = -2461.35837935 a.u.)

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H	-7.197570342902	-3.007786174762	-1.265213033207
C	-6.509762577309	-1.138644526424	-0.440587250766
H	-6.706472832273	-0.402923125304	0.353726704286
C	-5.344010885274	-0.792586269421	-1.400712067756
H	-4.914105922253	-1.760833844372	-1.702472066009
C	-5.783126769190	-0.193561268652	-2.756306664736
O	-5.076912535587	-0.366742681886	-3.747135909183
N	-6.912157727463	0.552845338980	-2.745493753444
H	-7.464226433674	0.523362219390	-1.893806190314
C	-7.575223755184	1.169382518835	-3.919304030093
C	-8.148076049489	0.057535903153	-4.817155092236
H	-8.662904163889	0.493145583083	-5.692069574045
H	-7.335927503444	-0.595955421081	-5.177661954457
H	-8.873589697642	-0.559979494961	-4.257412558674
C	-6.589872475332	2.051097473205	-4.706227288822
H	-7.126585435197	2.554431465484	-5.530446819628
H	-6.164876242137	2.820447506364	-4.041881369506
H	-5.773723619485	1.447705819347	-5.128756848447
C	-8.704030067624	2.049640025472	-3.359248064348
H	-9.260055017578	2.522666368942	-4.186640951369
H	-9.422692771671	1.451785258094	-2.767680603503
H	-8.284535556903	2.845275153839	-2.718780224426
C	-4.064167068697	0.037980354287	-0.886647341280
H	-3.924521612611	-0.166076483998	0.188005487185
H	-3.207487848650	-0.430071763012	-1.396880101895
C	-3.910754273395	1.595696330168	-1.106622071470
H	-4.104413506850	1.832943032339	-2.167010256754
C	-4.940169859463	2.347038304512	-0.229051547117
H	-5.944750071090	2.076351528409	-0.595974255664
H	-4.853373681720	1.966720095129	0.804450555856
C	-4.841734061556	3.880404715571	-0.172085814942
H	-3.854762985874	4.161632316225	0.233482643665
C	-5.031769815929	4.511942649756	-1.556641610833
O	-6.024960483283	4.252563855915	-2.234317531059
N	-4.058341885740	5.374323635854	-1.938110955615
H	-3.308945895509	5.529267459636	-1.273680544236
C	-4.026101302712	6.196080666632	-3.170729892645
C	-5.281356489334	7.083677704973	-3.248985614069
H	-5.232701881195	7.729104504112	-4.143717264532

H	-6.189485604114	6.464055228013	-3.305647366571
H	-5.353765208517	7.726706590004	-2.354158116439
C	-3.931752944559	5.278971176524	-4.403682998691
H	-3.014590255772	4.663567387497	-4.363379031375
H	-4.802776412064	4.607571105951	-4.456241993052
H	-3.896440141821	5.884350931180	-5.326496619307
C	-2.767959056184	7.074358885272	-3.074546399555
H	-2.672720884134	7.697482995463	-3.979557673608
H	-2.821461893555	7.747744244497	-2.199444283526
H	-1.855723757754	6.456793259100	-2.983321567618
C	-5.928454050042	4.455532440867	0.771733310498
H	-5.830353690619	3.946273385684	1.749468744175
H	-6.921249895873	4.198702368771	0.362170501812
C	-5.810640596090	5.942843720181	0.964112151099
H	-4.887276582214	6.288910108708	1.451838774224
C	-6.714032755633	6.845487269823	0.564581268708
H	-7.641678587203	6.540916346176	0.061511150268
H	-6.560769338510	7.920176263068	0.721233740869
C	6.415720633939	11.306071205800	-2.523389276369
H	6.615489317325	12.317824238528	-2.152650853798
H	7.158627746756	10.839929532212	-3.182142842517
C	5.273879127220	10.659448304965	-2.161170188994
H	4.585575480595	11.200312606326	-1.494193250205
C	4.740096134770	9.237073706519	-2.558373680130
H	4.441110822692	9.289292550730	-3.620260959756
C	5.956556511381	8.293667161621	-2.556424657418
O	6.703122217487	8.276767941960	-3.536452919769
N	6.201597375411	7.608632348133	-1.412208114717
H	5.467507320088	7.546694269805	-0.708146947461
C	7.436973061427	6.836331461148	-1.134821005164
C	8.672475998785	7.740591429047	-1.305068822463
H	9.584471710350	7.186901835469	-1.019540841280
H	8.773183484610	8.078155069067	-2.347210815433
H	8.586741882351	8.630163725397	-0.655692176228
C	7.526249639909	5.618131955969	-2.072928752528
H	8.439762704649	5.034621773480	-1.859404187115
H	6.652958744043	4.957377939097	-1.932744233199
H	7.552747527699	5.947576612488	-3.123496717209
C	7.352830695192	6.371362815542	0.327101316236
H	8.248096124337	5.780410805049	0.585247289943
H	7.300825756511	7.237592352447	1.011370212980
H	6.458794346589	5.751553341440	0.497702009956
C	3.490714323899	8.760321666019	-1.721561922016
H	3.793415864880	8.727042633984	-0.665662729709

H	2.725726023352	9.554630982390	-1.793464409662
C	2.840290836954	7.379106953898	-2.112722345441
H	3.603859651368	6.590978912817	-2.020469445541
H	2.571347821346	7.411454575257	-3.183585149382
C	1.547478221688	6.887444777577	-1.337947116955
H	0.714245388402	7.578742319247	-1.561901132794
C	1.668654433882	6.843412294739	0.225765519417
H	0.770477860013	6.324576882480	0.597330282994
C	2.894546959282	6.002481079592	0.603486645354
O	4.030059536372	6.480425837097	0.591392956578
N	2.621330329059	4.704321109734	0.871338001355
H	1.643793723565	4.434729117621	0.863782185053
C	3.601840977663	3.602129669170	1.010924556015
C	4.518202422893	3.861795283481	2.218987685022
H	5.243821885129	3.036629587684	2.327786562651
H	5.069755446944	4.805590299000	2.093038931636
H	3.921702310249	3.927051014879	3.146349090419
C	4.411597628922	3.480545801109	-0.292862283609
H	3.734834741934	3.298280338697	-1.145464931496
H	4.965578754693	4.410345458898	-0.490707357367
H	5.132937482151	2.647770906434	-0.221303830378
C	2.788570032040	2.318820664531	1.237811074049
H	3.468363048655	1.458877947270	1.358845060804
H	2.167089790341	2.396815604895	2.148260263138
H	2.127516926986	2.109561553068	0.376660038276
C	1.675838237195	8.208368506383	0.946548516311
H	0.899234948077	8.846175615963	0.485063777284
H	2.642158103105	8.710925195781	0.812859496011
C	1.395387991557	8.042658752084	2.417322044550
H	0.385153426682	7.693986697652	2.678083615990
C	2.287389245003	8.249051226819	3.393189538247
H	3.309520416824	8.582724529927	3.169429069305
H	2.032187649400	8.092056052737	4.448331099084
C	-2.449270957630	2.072134437023	-0.745356888546
O	-1.866493479828	1.576176788485	0.207667894745
N	-1.872802482365	3.102967238505	-1.494030496619
H	-2.354856582790	3.388666473930	-2.341879907110
C	-0.448548823877	3.476142562686	-1.386381165761
H	-0.087644284342	2.979503184379	-0.471486193840
H	0.116401801469	3.078822508489	-2.242761942756
N	-0.122113139592	4.929991817201	-1.341588237964
H	-0.636480702474	5.483393010064	-0.662077162706
C	1.092146361377	5.439672370352	-1.818942787116
O	1.810034405740	4.771368354433	-2.546390064970

R-PAMPS_MBA-3000pN (G = -2461.58293063 a.u.)

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C	-7.387140078249	-2.367149198215	-0.549162550884
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H	-7.250390174640	-3.125146893030	-1.332424968533
C	-6.577217603457	-1.268156343996	-0.452933457245
H	-6.790565379648	-0.562811849295	0.364888671888
C	-5.401719372324	-0.855771641256	-1.392245784450
H	-4.942243764016	-1.802555871260	-1.715026014863
C	-5.853406606764	-0.241404204454	-2.735902867366
O	-5.173896521506	-0.425892353736	-3.743072979993
N	-6.964981073160	0.531006260943	-2.697869581230
H	-7.498291069020	0.510684953369	-1.834144945971
C	-7.649453981213	1.151455841526	-3.857623828569
C	-8.274280906327	0.043172558761	-4.724961683971
H	-8.807226213266	0.480647682741	-5.588026481004
H	-7.488286021068	-0.631607203741	-5.103966666857
H	-8.994583571736	-0.552812208547	-4.135909740215
C	-6.670751601108	2.002523127835	-4.685764145833
H	-7.224165467953	2.510420892558	-5.496059600126
H	-6.205576304320	2.768644285816	-4.044922979767
H	-5.884107808159	1.376149918730	-5.129992322477
C	-8.740986210878	2.062492691972	-3.273432423123
H	-9.312893848103	2.537142866276	-4.089004843025
H	-9.453236242730	1.487474489604	-2.652138916731
H	-8.284366337846	2.856589913404	-2.657133997765
C	-4.128668498242	0.002012657748	-0.851481130002
H	-4.038952508149	-0.165082897094	0.234801400040
H	-3.255910230050	-0.494688012212	-1.302888491755
C	-3.933419158255	1.559977860322	-1.116336089839
H	-4.133023170692	1.777076124289	-2.179975663168
C	-4.943502034954	2.347006317119	-0.245075754018
H	-5.954188306615	2.082463834159	-0.599806344163
H	-4.854865477315	1.981849343659	0.793744202611
C	-4.829768342455	3.880054289279	-0.206616271748
H	-3.837830633959	4.157223691965	0.188534488369
C	-5.025477973220	4.500522456799	-1.594709358383
O	-6.016262006981	4.229010780107	-2.270667511012
N	-4.058583015551	5.368122073600	-1.982961559007
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C	-4.035307443786	6.180636901214	-3.222004887816
C	-5.297235330358	7.058225373251	-3.305924721720
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H	-6.200795046967	6.431518991272	-3.357351740588
H	-5.373876636175	7.707282032360	-2.415816028996
C	-3.935901576453	5.252625794202	-4.446390292517
H	-3.013539674478	4.645333181025	-4.401485860750
H	-4.801607312011	4.573504995457	-4.490603306198
H	-3.907451603557	5.849367750357	-5.375037219780
C	-2.783609369239	7.068930548428	-3.135172075203
H	-2.692413047458	7.682509920507	-4.047101973191
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H	-1.866858609387	6.459312787126	-3.035968198473
C	-5.905382982492	4.473397519684	0.739591969015
H	-5.803437370885	3.973589279729	1.721791001769
H	-6.903460290291	4.219867718542	0.340818233219
C	-5.775071242252	5.961616353131	0.916053820564
H	-4.845996060468	6.305489550132	1.394394876309
C	-6.674201209685	6.867033882233	0.513244843956
H	-7.607339985624	6.564543090046	0.019154864443
H	-6.511773488399	7.942037908673	0.657974501092
C	6.498808177331	11.385376258963	-2.469639858686
H	6.691173703112	12.390900739024	-2.078816845233
H	7.241819154123	10.938154854352	-3.141316901475
C	5.359455236335	10.721463270864	-2.111121075714
H	4.676348977712	11.250047050076	-1.428798923293
C	4.811142779225	9.296546418836	-2.522622437145
H	4.523910417070	9.361312826913	-3.586777689371
C	6.024233757281	8.349236004345	-2.518140743148
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N	6.249923991524	7.645297642521	-1.381337365126
H	5.506287017878	7.577523556986	-0.688101034192
C	7.475743622226	6.859222655935	-1.100240071642
C	8.720704767955	7.755153028799	-1.243163084393
H	9.624519799888	7.189417446589	-0.955261688331
H	8.836249138297	8.106943154173	-2.279001811855
H	8.635110369714	8.635870074279	-0.581794080266
C	7.565500692492	5.653694857753	-2.054509163678
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H	6.685198569807	4.998454934157	-1.933272923224
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C	7.370270289421	6.374501530307	0.353816159668
H	8.256536666288	5.770878297442	0.613676192080
H	7.319069496014	7.231470391698	1.049723485799
H	6.468053027813	5.761678623655	0.505365852813
C	3.542826806460	8.804149639128	-1.703216801868
H	3.834508977774	8.759268459624	-0.644681292364

H	2.781342494640	9.601628429707	-1.774668973751
C	2.878558859803	7.419320637438	-2.108022442776
H	3.639177806706	6.627781086873	-2.019578645254
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C	1.571399775384	6.915097965525	-1.341899200990
H	0.742046833089	7.610900292326	-1.565451624890
C	1.686735099680	6.861159885379	0.221062070930
H	0.786196760429	6.342524550932	0.587386597500
C	2.909792717287	6.014883171565	0.596700837069
O	4.046043314725	6.491036110450	0.593485116386
N	2.633060523562	4.714737070695	0.851502743203
H	1.655111298564	4.446918333571	0.835442734960
C	3.610705029658	3.609087355309	0.983326466795
C	4.523518826545	3.854638640536	2.196992253965
H	5.247237340303	3.027034328028	2.299768357702
H	5.077252652555	4.798609139674	2.082528263577
H	3.924046070223	3.911566201630	3.122985038799
C	4.424683303431	3.498388088295	-0.318865212724
H	3.750295740815	3.326278968505	-1.175482588569
H	4.982058274585	4.428509986498	-0.505647381933
H	5.143456500263	2.662908417948	-0.253200700183
C	2.793807943666	2.325395356720	1.194736195760
H	3.471227085256	1.462724120492	1.309527402387
H	2.169416758238	2.395807484027	2.103807032492
H	2.135208280340	2.126201739267	0.329323207882
C	1.696333780090	8.222274359645	0.948793986502
H	0.920629748272	8.863579480060	0.490634456538
H	2.663443703900	8.723743853314	0.816905771019
C	1.416032315417	8.050079133115	2.418831256508
H	0.405071032724	7.702483305360	2.678223755429
C	2.308788319921	8.249574134565	3.395444009305
H	3.331651915219	8.581834614422	3.172982977661
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C	-2.449093744659	2.029189894411	-0.783179034856
O	-1.833776623989	1.487423040050	0.122230067151
N	-1.893522919193	3.106638894612	-1.494085254820
H	-2.396993829812	3.426034780836	-2.317595471611
C	-0.461298958437	3.488054188673	-1.408675974329
H	-0.083446991420	2.979703649937	-0.507379035041
H	0.087560045270	3.100697617775	-2.280026508049
N	-0.120010768979	4.947198341523	-1.352396201927
H	-0.630528854816	5.498149924323	-0.667812917697
C	1.099223006852	5.462047278613	-1.830988975208
O	1.811236924309	4.797424143269	-2.566205743584

R-PAMPS_MBA-3500pN (G = -2461.81099846 a.u.)

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C	-6.566414933543	-1.486223728343	-0.523132579472
H	-6.738572438590	-0.892389669889	0.388044201610
C	-5.438310536608	-0.913018732901	-1.459021494747
H	-4.941230248514	-1.792503741419	-1.894071390230
C	-5.985932752977	-0.209265084329	-2.721463131837
O	-5.375159130699	-0.313044915040	-3.782201271815
N	-7.106602016915	0.534148008901	-2.553025393219
H	-7.569377095308	0.439873192287	-1.653887588038
C	-7.935389781080	1.158279246813	-3.613418289622
C	-8.714857693421	0.050253614116	-4.346297879150
H	-9.362784054793	0.482494660592	-5.129767080416
H	-8.013971218076	-0.656024078294	-4.824167725903
H	-9.350961490589	-0.513161068736	-3.639805215761
C	-7.080642622112	1.963632549117	-4.607292741905
H	-7.751151100555	2.487810664901	-5.312102707891
H	-6.482109296636	2.716007562605	-4.069361026447
H	-6.407949242742	1.307267071546	-5.176126990216
C	-8.899633176716	2.114702978155	-2.892048469596
H	-9.584468091853	2.582326055176	-3.620135959551
H	-9.516636263669	1.577448940182	-2.147102467656
H	-8.330446119293	2.911049131351	-2.381448174209
C	-4.184365096357	-0.035431977913	-0.848722122749
H	-4.211755251842	-0.133887611135	0.249333237789
H	-3.281978578251	-0.576965623046	-1.169844841045
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H	-4.106257271248	1.701322608213	-2.248886664512
C	-4.906723570723	2.362852305085	-0.334393927079
H	-5.923740823961	2.098110897085	-0.668997127366
H	-4.815521058666	2.038703931558	0.717804359832
C	-4.776210823608	3.896099608897	-0.349584005656
H	-3.780969606574	4.177795169443	0.032276075318
C	-4.972960850304	4.473983062200	-1.754964374010
O	-5.968030725885	4.189665998900	-2.418160228832
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H	-3.269995195736	5.540198904459	-1.509686186845
C	-3.979198306374	6.082929247860	-3.448746439160
C	-5.229898278265	6.974243738651	-3.554952502948
H	-5.187296188505	7.576700005505	-4.479503692610

H	-6.142568001843	6.359007825590	-3.572586621290
H	-5.288246431059	7.659252447534	-2.690746731357
C	-3.904911994636	5.104150079845	-4.634865309775
H	-2.989244195120	4.488193650222	-4.573538374373
H	-4.779335047958	4.434244713588	-4.641616192955
H	-3.879935394619	5.662158248183	-5.587377643619
C	-2.715189788613	6.956952313556	-3.409864975487
H	-2.623919576354	7.530148522636	-4.347717923728
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H	-1.805078298971	6.341222613213	-3.290892749412
C	-5.843854229439	4.528327237626	0.581100013346
H	-5.739186418453	4.062923985285	1.579692703326
H	-6.845792074674	4.266938124410	0.197328465467
C	-5.703789665853	6.021041516510	0.703883379784
H	-4.774924136859	6.376068549377	1.174349034385
C	-6.594013029438	6.916919871319	0.261799786781
H	-7.526388951970	6.602374340698	-0.226145240875
H	-6.424676262920	7.995480372756	0.366663942258
C	6.566309990921	11.529926601885	-2.301666585611
H	6.742915368637	12.524960275184	-1.878108646806
H	7.314911264349	11.115310031714	-2.987932983787
C	5.432453242224	10.837077096740	-1.960009398651
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C	4.879491833541	9.410571529851	-2.405192718666
H	4.601182386118	9.501533424103	-3.469516029949
C	6.096042222901	8.468388995352	-2.414461994794
O	6.868401781156	8.495191478904	-3.373961733820
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C	7.530596980766	6.932626031857	-1.028128908110
C	8.779236206565	7.828837291816	-1.131336180076
H	9.678545076767	7.251665181697	-0.852122865611
H	8.905992092478	8.212242986997	-2.154533550788
H	8.689565036125	8.68852339558	-0.443757143835
C	7.625966421534	5.756541452950	-2.017939582729
H	8.528975292408	5.153723401228	-1.813583461463
H	6.743057135538	5.100197940913	-1.924174669455
H	7.676468335182	6.132466176445	-3.051961726676
C	7.409417808746	6.404052460606	0.409280434731
H	8.290092726350	5.787830598049	0.658424121893
H	7.356336674432	7.239530366588	1.130741689039
H	6.502469968477	5.792139177001	0.533655007488
C	3.596655187907	8.879819178404	-1.609303810346
H	3.878694477303	8.810368838812	-0.549520957463

H	2.831768979395	9.674785048220	-1.668235356245
C	2.929336001342	7.490913587072	-2.047498769216
H	3.693968844406	6.701628907624	-1.974912076614
H	2.666696702167	7.559230643707	-3.117990562760
C	1.612193076709	6.950483204169	-1.296838880281
H	0.780304289823	7.646422583955	-1.509057455417
C	1.723688582688	6.864014878849	0.263886935397
H	0.825186417271	6.333048325472	0.617720976444
C	2.951116008353	6.016766714532	0.623645923438
O	4.084344073684	6.499829868230	0.634030470957
N	2.681333160407	4.709497396732	0.848160661014
H	1.705103545524	4.436312664796	0.819777221801
C	3.664704267521	3.606134695540	0.954059748952
C	4.576064375228	3.827381239005	2.173430564017
H	5.303938537525	3.001215450520	2.256611396792
H	5.125086321924	4.776528565100	2.081643854032
H	3.976207935797	3.859207856222	3.100366645850
C	4.479620576594	3.530047895818	-0.350081871767
H	3.806171295867	3.375796849789	-1.210831388956
H	5.033617548359	4.466504071734	-0.514298764836
H	5.201632486606	2.696035428859	-0.304162558046
C	2.854259383393	2.313669716261	1.134938346452
H	3.535941220333	1.451741421784	1.228093219888
H	2.230436745635	2.358961367298	2.045995470629
H	2.195712405154	2.132489485759	0.265514387379
C	1.726030485232	8.210211174822	1.018644227951
H	0.946565588647	8.856204143023	0.573627126935
H	2.690361973048	8.719269788815	0.895780173070
C	1.447651592635	8.007697307122	2.485160249134
H	0.438725211553	7.649629953217	2.738197538264
C	2.339896874093	8.192626380496	3.465106451468
H	3.360881052980	8.534525727656	3.248720826432
H	2.086128806474	8.008877194122	4.516275749195
C	-2.410705348565	1.968337042044	-0.856195436832
O	-1.775820657007	1.378735198829	0.003446998153
N	-1.864723088014	3.089343491132	-1.519315492316
H	-2.379421856069	3.440939209661	-2.322904419315
C	-0.429020774513	3.489129016644	-1.432852968963
H	-0.041971392229	2.963166077718	-0.545916363661
H	0.117759064307	3.126055339180	-2.315838509716
N	-0.085031160530	4.956153786212	-1.345012098205
H	-0.601482203179	5.491550472066	-0.652065287222
C	1.135725832565	5.493789950151	-1.814818881791
O	1.850259569358	4.848931431505	-2.563687495140

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C	-8.176815196566	-2.394294750619	0.027845749657
H	-9.240976369790	-2.445554926053	0.282271215191
H	-7.558000251112	-3.276707545292	0.235863888708
C	-7.646545154989	-1.259757065866	-0.534954266215
H	-8.356908105809	-0.445057588352	-0.735538625150
C	-6.289398033665	-1.080215299424	-1.028557380636
H	-5.588401718625	-1.893094491203	-0.816579047455
C	-6.015405437498	-0.462625963812	-2.361754279359
O	-5.134669244018	-0.939545678311	-3.085546662201
N	-6.785092070433	0.600558710421	-2.730809495429
H	-7.459320574803	0.949650152922	-2.058987053648
C	-6.821962090419	1.218593384772	-4.076394150281
C	-7.244179390503	0.166705771337	-5.119425775465
H	-7.302509929240	0.625388242092	-6.122614955824
H	-6.516112587413	-0.659352252657	-5.150917610747
H	-8.236861842283	-0.248428320854	-4.867982372236
C	-5.447586345575	1.814282143223	-4.431821538871
H	-5.481953456153	2.275358947589	-5.435257480520
H	-5.180110462715	2.598099571724	-3.706165954273
H	-4.675077261011	1.030818583318	-4.423946653012
C	-7.867144731424	2.343388029065	-4.011748514590
H	-7.952097733100	2.832190920045	-4.997587703202
H	-8.863198156863	1.944108229702	-3.743784047798
H	-7.567708710352	3.108118453055	-3.274916232371
C	-4.325047364430	0.448887048126	-0.281667297041
H	-4.466071438511	0.251333939497	0.786365646522
H	-3.766233180604	-0.308137193298	-0.839907917571
C	-4.092813387029	1.893748000575	-0.686854508720
H	-4.152056985240	1.975275449058	-1.785714658850
C	-5.152546038887	2.826649946184	-0.049110552375
H	-6.127513184027	2.582615067274	-0.504195143841
H	-5.219971573186	2.584333020256	1.026358347049
C	-4.906638339584	4.340699690973	-0.174591387622
H	-3.941505541805	4.587774787668	0.299727687884
C	-4.901596500689	4.804240226417	-1.638177800680
O	-5.860126203091	4.565632882559	-2.371559152484
N	-3.808283924347	5.504252892490	-2.029262607716
H	-3.093178673685	5.663467399536	-1.327925830946
C	-3.616972492414	6.198292275630	-3.325695316885
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H	-4.564332747551	7.800032210575	-4.465259122359

H	-5.705981045361	6.805755629811	-3.503930986336
H	-4.663686919039	8.007767850394	-2.686566156152
C	-3.658989605943	5.183903446601	-4.482171362075
H	-2.900019862260	4.394150107348	-4.335145314560
H	-4.647951489479	4.707694385708	-4.547478391718
H	-3.445070266785	5.694170568604	-5.437844796924
C	-2.230894682465	6.860669564178	-3.269257115918
H	-2.047900853097	7.425534367869	-4.198714790986
H	-2.160052303123	7.566892595548	-2.421531561347
H	-1.430570547421	6.107902825023	-3.160389802002
C	-6.015278464701	5.129841168072	0.567973086463
H	-6.068291763635	4.744069018947	1.603891543523
H	-6.983511197404	4.915172361863	0.082799168597
C	-5.760088346651	6.612250432403	0.595642995950
H	-4.859008941378	6.930547769958	1.140506645126
C	-6.517567132671	7.536301714304	-0.006430153832
H	-7.416835800235	7.257706304096	-0.572115010771
H	-6.266953271900	8.603115888026	0.038745398251
C	5.966043110005	11.368956539619	-2.152160991715
H	6.267767563274	12.321599112142	-1.701819696296
H	6.596488036113	10.956730588319	-2.949470973268
C	4.850710328437	10.734570318320	-1.728313457273
H	4.266670478843	11.211355503175	-0.927174987892
C	4.232154779149	9.407064858287	-2.235695804951
H	3.715808216925	9.628513476511	-3.187319856435
C	5.385553587063	8.472974085740	-2.643327766519
O	5.886746229108	8.589369134947	-3.762844934891
N	5.858796444458	7.633200121284	-1.689997364140
H	5.295227725502	7.470896463949	-0.856544468951
C	7.061360094431	6.777871116083	-1.832189673249
C	8.283812127735	7.636364316879	-2.207248533062
H	9.191793853150	7.007613174866	-2.219941990320
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C	6.814072011258	5.694349214175	-2.898610288825
H	7.701620574167	5.044665543063	-3.002363316206
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H	6.600564854162	6.161781444165	-3.873073839461
C	7.307005642114	6.126895969362	-0.462090231688
H	8.180732777341	5.455258481932	-0.515874512457
H	7.508495502372	6.896227054927	0.305314198430
H	6.431373775423	5.544123604141	-0.135517141682
C	3.187219178650	8.813140715129	-1.242147499652
H	3.699330731048	8.622141237170	-0.288861454480

H	2.438126112032	9.598911621198	-1.034530734667
C	2.468437356770	7.516733515788	-1.711102352801
H	3.221351669031	6.733014264594	-1.884182737092
H	2.002303876345	7.706826998256	-2.694875275918
C	1.354973360218	6.914482529436	-0.791026885684
H	0.494080670989	7.607876216010	-0.762835010913
C	1.753426003706	6.653259650101	0.704903636843
H	0.920089110412	6.088937541294	1.153178563893
C	3.004379030631	5.766643292960	0.747585222632
O	4.127795011802	6.230527569700	0.544685469399
N	2.753299523308	4.455074705635	0.964305232996
H	1.786706406585	4.201095900625	1.135319794314
C	3.714547027789	3.333166847684	0.850997887360
C	4.852172564337	3.507139980146	1.872080420117
H	5.556609451557	2.659865490684	1.800302419251
H	5.401815281421	4.442423202429	1.687490853188
H	4.445496894537	3.537665666977	2.898571845866
C	4.258884784037	3.276848720851	-0.587705330273
H	3.429366827296	3.161560876560	-1.306573489762
H	4.795780689990	4.205273557343	-0.833404806174
H	4.953817721114	2.426552282677	-0.701987403936
C	2.927261319829	2.050576300122	1.159943820706
H	3.592994002150	1.174191527442	1.089313027745
H	2.504214966842	2.079405800297	2.180522548377
H	2.100603130184	1.907707370756	0.439716878532
C	1.921302131523	7.901611074617	1.598914865908
H	1.096181239842	8.602290453906	1.372914141469
H	2.864792446018	8.415207327814	1.374684126125
C	1.890947296116	7.524928566966	3.057306760436
H	0.931636716894	7.142330179656	3.435907400900
C	2.941543063607	7.587126481902	3.883775568601
H	3.918657237319	7.949734644101	3.537308222358
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C	-2.662034211329	2.354638735312	-0.229251726699
O	-2.233206445220	2.055160176350	0.875319810883
N	-1.953267927865	3.151144038527	-1.105954191019
H	-2.350493595010	3.327413782896	-2.023667835502
C	-0.560751940022	3.536359646248	-0.894545150478
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H	0.057289706296	3.171726431488	-1.727016462179
N	-0.279023771120	4.980662075952	-0.792571488045
H	-0.708401765153	5.467266714237	-0.010598486264
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O	1.449680901049	4.981369268025	-2.275338967035

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C	-7.537218026937	-1.364293713777	-0.541795885564
H	-8.222197981902	-0.503649312431	-0.536021075011
C	-6.206039052919	-1.133611712428	-1.133146538195
H	-5.502725565246	-1.967239286873	-1.042167869090
C	-6.081541051997	-0.489666956129	-2.480115884398
O	-5.265036132881	-0.930053779902	-3.295882073843
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C	-7.053772930450	1.235480748210	-4.059792005404
C	-7.533574619632	0.221511170468	-5.115183036268
H	-7.673663636393	0.722036520466	-6.089904820049
H	-6.795286792313	-0.587076234074	-5.235707633068
H	-8.497603406668	-0.224546021412	-4.810802486608
C	-5.719849651040	1.875096283037	-4.487116120196
H	-5.837307262525	2.382514224410	-5.461597750730
H	-5.412255300931	2.627284250581	-3.743773601191
H	-4.936156866514	1.107687306975	-4.575994554512
C	-8.110505862789	2.334685007364	-3.867045509009
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H	-7.771568666748	3.068547340095	-3.115994996997
C	-4.211754162901	0.336716535286	-0.544477802409
H	-4.191139516360	0.055551580430	0.513988254092
H	-3.711003627043	-0.357369212833	-1.226293918646
C	-4.024130564901	1.823084716106	-0.843476898212
H	-4.174914509161	2.000062958771	-1.922039456817
C	-5.055276036313	2.657457833079	-0.042821991498
H	-6.055494511731	2.393448474939	-0.426108834541
H	-5.011635442165	2.337340544857	1.013439259825
C	-4.898252743672	4.186021904520	-0.080566235187
H	-3.917616064645	4.457966043048	0.346481386456
C	-5.011058865766	4.731938752477	-1.509643666903
O	-5.975319965548	4.445111876545	-2.217664369632
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H	-3.285514273030	5.740908220331	-1.209157223927
C	-3.917643878903	6.318467850403	-3.163625552175
C	-5.133125212787	7.253332441910	-3.298215700425
H	-5.050494802617	7.851682567837	-4.222725275898

H	-6.066103985180	6.669584100791	-3.335119109589
H	-5.186920592586	7.941355233178	-2.436267929029
C	-3.844597661027	5.349921997470	-4.357576198829
H	-2.970987674218	4.679500073268	-4.263425207064
H	-4.754030204247	4.733229204484	-4.414288164645
H	-3.741273907575	5.917161780233	-5.299327150169
C	-2.623949237767	7.144412406823	-3.080922452871
H	-2.488727502357	7.728268949984	-4.006781399748
H	-2.659327967468	7.852285836139	-2.232372033645
H	-1.743025281872	6.490338453530	-2.950840493632
C	-5.998149742171	4.860974284674	0.778600768454
H	-5.958260165395	4.413316365012	1.789968648434
H	-6.983130735971	4.613677424663	0.345038625451
C	-5.831042236530	6.352568545786	0.880572496910
H	-4.914209535661	6.696635989674	1.381697771593
C	-6.684356936261	7.258712168294	0.389454622532
H	-7.603279935143	6.955222483085	-0.129995699299
H	-6.496510779400	8.335167609077	0.483634104169
C	6.296583331068	11.297627558460	-2.393295472922
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H	6.966163408515	10.856076687589	-3.141621131812
C	5.169761221881	10.664143910133	-1.983058482710
H	4.552021907856	11.173120494126	-1.228042470535
C	4.575758019911	9.295892668051	-2.439535937995
H	4.166276404521	9.440277536295	-3.455333203028
C	5.758194899861	8.332106086354	-2.645887784275
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N	6.113670626786	7.561947129998	-1.588196611989
H	5.460995323409	7.462053474652	-0.811998322310
C	7.331946369328	6.719044734744	-1.523483076182
C	8.583416103036	7.574445574168	-1.796925138087
H	9.492081074450	6.961229764890	-1.662149833799
H	8.572607911300	7.973832928010	-2.821728050299
H	8.627772741082	8.422949993543	-1.090888945503
C	7.232982504605	5.566431112063	-2.540325694789
H	8.133829283894	4.928887820858	-2.489378066615
H	6.351063663393	4.937441938120	-2.326903159587
H	7.139033371946	5.967600332460	-3.561876698173
C	7.409605390900	6.159213399051	-0.094642963565
H	8.293389299044	5.506332318427	0.005750919370
H	7.499060923160	6.978329465011	0.641845509211
H	6.508854932149	5.576795905873	0.154927933928
C	3.419332555962	8.779906760157	-1.514899446393
H	3.829910649604	8.660038405254	-0.502534286833

H	2.666453681192	9.585996595587	-1.444785630155
C	2.718028435011	7.449101667500	-1.946584916121
H	3.471269507876	6.647319812330	-1.986749109248
H	2.349435257627	7.566520845822	-2.981620188901
C	1.505011411520	6.923111681266	-1.091538348779
H	0.662460292716	7.632302722152	-1.187668024451
C	1.766544325024	6.763917045373	0.448690922669
H	0.891948021344	6.235327932445	0.860834916583
C	2.999731217087	5.875996091530	0.657824739134
O	4.141594925871	6.326419063267	0.550524783224
N	2.717246667034	4.574998096857	0.899584304195
H	1.736166291951	4.330782898837	0.975689253936
C	3.672909392961	3.442510304980	0.901756326058
C	4.712764438253	3.631829374577	2.019481448824
H	5.416659801516	2.781105390849	2.028604078462
H	5.281664724973	4.561595096707	1.868482249670
H	4.213929013169	3.683390907642	3.003636233477
C	4.345664743045	3.347273671102	-0.479548667725
H	3.582773947615	3.224045315110	-1.267397728458
H	4.912241548240	4.265258088910	-0.695957263064
H	5.038892553712	2.488532116344	-0.510693319388
C	2.846605940033	2.174420194857	1.165604408028
H	3.507259477835	1.291508091408	1.182952275078
H	2.326043234664	2.233527798652	2.138680639419
H	2.092998378094	2.018658601703	0.371627269899
C	1.870052703114	8.071687225972	1.262978713216
H	1.072781405112	8.756571771844	0.919291350897
H	2.833501716076	8.564892905177	1.082123903952
C	1.714035444546	7.800323773026	2.736652627405
H	0.720819845659	7.455159868535	3.059868123629
C	2.693940650792	7.910172140035	3.641315226693
H	3.701996249221	8.236761762765	3.352566362150
H	2.527700447330	7.677739432081	4.700288568703
C	-2.559857315096	2.288361943668	-0.459236440596
O	-2.032829852285	1.873641567775	0.561431641927
N	-1.937940951669	3.216465685827	-1.284185916933
H	-2.399150101571	3.463245926886	-2.155223485356
C	-0.518410820732	3.572417837769	-1.160417956903
H	-0.170865163353	3.071132949806	-0.242949892307
H	0.048093116703	3.173601401650	-2.014540815086
N	-0.189130621415	5.016952231695	-1.107439299740
H	-0.670786793906	5.562201537396	-0.397735126960
C	1.007014787908	5.519258011506	-1.619865535356
O	1.682880378887	4.866928691387	-2.401184865180

TS-C6C25-PAMPS_MBA-2500pN (G = -2461.31484859 a.u.)

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C	-8.132771015320	-2.612317466295	-0.186913799999
H	-9.174761939710	-2.654609823908	0.148777828138
H	-7.584975614496	-3.559117077976	-0.280304417269
C	-7.550197272879	-1.402977479634	-0.480527595879
H	-8.207495095141	-0.526075529546	-0.380928090026
C	-6.208542258087	-1.141248684837	-1.081254524911
H	-5.507342285128	-1.978932195967	-1.011579186134
C	-6.134977359767	-0.528619878446	-2.449749221951
O	-5.338839349434	-0.975929530705	-3.280901739372
N	-6.978334084169	0.508475752763	-2.711611150340
H	-7.581493007904	0.826055725371	-1.961255259664
C	-7.155767545775	1.175007473580	-4.022011646115
C	-7.658921920629	0.154001735836	-5.059552112347
H	-7.820745568118	0.647507615134	-6.034500966775
H	-6.923083898933	-0.655266352192	-5.190721974672
H	-8.615714902770	-0.290226846585	-4.730659127072
C	-5.832257432591	1.812763154276	-4.484016308733
H	-5.974209543006	2.317427382963	-5.456698947207
H	-5.505483595609	2.566744425884	-3.750548782330
H	-5.051311339820	1.044896385526	-4.590891964404
C	-8.208028249130	2.275339878494	-3.811648025034
H	-8.395533289948	2.801709836422	-4.763322682658
H	-9.166977813932	1.846133923142	-3.466021769694
H	-7.851227984328	3.014779446619	-3.074320030099
C	-4.249672743054	0.316593044279	-0.548278469767
H	-4.196695523898	0.048598645762	0.512660715289
H	-3.742699605043	-0.378967353280	-1.224373936391
C	-4.036527418234	1.808074620197	-0.858343968596
H	-4.198061067154	1.983313470719	-1.935870001463
C	-5.052054695246	2.655323535278	-0.050348968836
H	-6.058066710810	2.384339156484	-0.413176109632
H	-4.991054738215	2.348199539124	1.009052393239
C	-4.904509373658	4.184336739416	-0.108543827340
H	-3.921469738982	4.468664276914	0.303813917716
C	-5.035788455809	4.709703957219	-1.543488801701
O	-5.996102502049	4.393573049622	-2.243860663467
N	-4.046360271824	5.543708895789	-1.947971295311
H	-3.339214984019	5.771825085257	-1.258011208848
C	-3.979752338176	6.292700945092	-3.225366683156
C	-5.215333254495	7.199279900843	-3.370373384327
H	-5.146195760518	7.788068157505	-4.302096403595

H	-6.135395224126	6.594932569148	-3.399488216372
H	-5.283677911852	7.896258816128	-2.516670293353
C	-3.889411219881	5.307007643258	-4.404109302949
H	-2.996464359031	4.662908415573	-4.307333914419
H	-4.781967406315	4.664462220936	-4.443352292191
H	-3.809850298372	5.861632869988	-5.355610750573
C	-2.703575838207	7.146987683527	-3.158673998368
H	-2.579399847821	7.714355453213	-4.096267847815
H	-2.755228985421	7.871525431556	-2.325137266194
H	-1.808631948984	6.514942951231	-3.014045491108
C	-6.001139955640	4.862289951200	0.752888155217
H	-5.947983725985	4.427993114962	1.769448903131
H	-6.988637836959	4.602244722906	0.332601626122
C	-5.844396339306	6.356330546327	0.833829895354
H	-4.926908134165	6.713968576882	1.324122548035
C	-6.707572587751	7.249378717068	0.335991270477
H	-7.627600191805	6.932096104771	-0.173158624598
H	-6.527035770784	8.328358755744	0.414091704656
C	6.424945173773	11.369589622050	-2.315370875128
H	6.695731283623	12.333777590531	-1.870375276362
H	7.084156500665	10.952443552240	-3.086647848379
C	5.301317653399	10.719688920009	-1.905352793625
H	4.700175960937	11.209020244199	-1.124073137212
C	4.681894816298	9.358740889213	-2.383723379587
H	4.284646495918	9.524684177677	-3.400769152031
C	5.855194420225	8.385187047186	-2.594745854471
O	6.495203905465	8.435517348142	-3.646275810710
N	6.187451368782	7.589545704824	-1.548311206644
H	5.524638546750	7.484138938029	-0.781597516358
C	7.394365309712	6.730315712112	-1.485082333037
C	8.659663284067	7.574783437387	-1.727123207890
H	9.558821958304	6.947146080893	-1.595008677888
H	8.665414130541	7.995190376268	-2.743526107085
H	8.707073262174	8.408004243683	-1.003290643246
C	7.293244009355	5.598523005280	-2.524851395058
H	8.184945324258	4.948163632705	-2.474927198595
H	6.400507560752	4.977411251477	-2.334284986307
H	7.217546863075	6.020080543329	-3.539710879392
C	7.447524783928	6.142528200481	-0.066440140259
H	8.321638950976	5.476465307816	0.032036835258
H	7.538300702170	6.946247458736	0.686660421274
H	6.536485934118	5.567217302716	0.161126421842
C	3.502719663304	8.831864331976	-1.477755291685
H	3.902499788853	8.691840089397	-0.463677726268

H	2.759069578583	9.645783127584	-1.401838565959
C	2.777661151789	7.506916523600	-1.928676969904
H	3.522108739456	6.697243562466	-1.977511679795
H	2.413424915944	7.643533827282	-2.962794951606
C	1.547186728842	6.973803766563	-1.083694461986
H	0.713620311530	7.693993896456	-1.174087869010
C	1.803309920788	6.794293190967	0.454612262663
H	0.924024905747	6.267671135307	0.859298042379
C	3.029452062047	5.894431953893	0.655243068407
O	4.174938229308	6.338028669213	0.559129916269
N	2.736492051036	4.591903349523	0.876152268006
H	1.753248133106	4.353299074829	0.942179297039
C	3.683925718217	3.452608225438	0.863226264804
C	4.722169306627	3.617243501052	1.986339772478
H	5.420823589336	2.762168237900	1.983322141596
H	5.297061793556	4.545821098594	1.851977756626
H	4.221144640477	3.655781542375	2.969980508716
C	4.359284858622	3.373451648388	-0.517920876261
H	3.597191049658	3.266979444279	-1.309013704241
H	4.932629044658	4.290649498750	-0.719585272425
H	5.046715109867	2.510542702870	-0.560494108778
C	2.848011751268	2.186583938919	1.105826194633
H	3.502531830692	1.298967069305	1.112584272620
H	2.324517977655	2.235181474454	2.077911022849
H	2.096133846640	2.047364708625	0.307177570465
C	1.915774092283	8.092254322055	1.283012163754
H	1.120390297376	8.784328945726	0.949360235077
H	2.880684342449	8.583139735322	1.103886171141
C	1.763163103396	7.806316210677	2.754252680357
H	0.769985352143	7.460226128716	3.076625960646
C	2.745450966031	7.905428281113	3.657558361553
H	3.753497349639	8.232637316737	3.369510915314
H	2.581281067747	7.663135175084	4.714648691693
C	-2.550285076799	2.266261851651	-0.497373177364
O	-1.984370425908	1.786040255433	0.471608444558
N	-1.957881761580	3.262668525271	-1.273714430584
H	-2.443777982484	3.554710621630	-2.117253140053
C	-0.529184639577	3.623226094872	-1.174318987190
H	-0.165788770342	3.110527972059	-0.269503518379
H	0.020236612310	3.230908671734	-2.042724885142
N	-0.182286660960	5.071280060976	-1.113520268281
H	-0.657215715898	5.614929719768	-0.397744170087
C	1.022474004804	5.572334192825	-1.624811115563
O	1.688813301107	4.921598653787	-2.414464783148

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C	-8.176915759385	-2.669565891283	-0.247837639056
H	-9.212749589288	-2.704269461477	0.107292368455
H	-7.663647418574	-3.622819000500	-0.429980346793
C	-7.562177653155	-1.455251403229	-0.455811428325
H	-8.193308123983	-0.573541491500	-0.266490606964
C	-6.216471409358	-1.160577600367	-1.076264138943
H	-5.516509221891	-2.001381879029	-1.036650696483
C	-6.201744523199	-0.565101626723	-2.457203771396
O	-5.439245755751	-1.017863324815	-3.315684630205
N	-7.056129102536	0.469052925628	-2.690498532154
H	-7.624642120447	0.792838245854	-1.915859487344
C	-7.270211026655	1.144213569887	-3.990866588887
C	-7.810109692121	0.131691773381	-5.018035561945
H	-7.999305629553	0.631471445607	-5.984834884704
H	-7.082398838435	-0.680125238701	-5.176172490597
H	-8.758439870102	-0.309992955088	-4.662329979629
C	-5.957829222595	1.777780990502	-4.489552253373
H	-6.127443029806	2.291102100255	-5.453257135224
H	-5.603097959260	2.523621767815	-3.760567239176
H	-5.185401701069	1.006184599200	-4.627525000807
C	-8.309277509819	2.249022366156	-3.742033317821
H	-8.525072520134	2.780194986111	-4.684989266609
H	-9.258549981394	1.823447233629	-3.366569556919
H	-7.924566983709	2.983775746813	-3.014013988932
C	-4.283189183693	0.276153089151	-0.592156610915
H	-4.189942804849	0.005109656660	0.465488651795
H	-3.777313797405	-0.411027651933	-1.278063509371
C	-4.048309407214	1.777665962293	-0.894021723756
H	-4.229165860194	1.966500573485	-1.966179296592
C	-5.040210298433	2.625770635916	-0.058186891871
H	-6.055204972494	2.354927582938	-0.395355718620
H	-4.952755418169	2.316349077396	0.998796889825
C	-4.899135394197	4.155465207653	-0.116447962125
H	-3.910301104721	4.443589861333	0.278400055568
C	-5.057394639484	4.679708677886	-1.548806036294
O	-6.019813668330	4.346692217435	-2.238102868998
N	-4.085943142739	5.529442514791	-1.965792470641
H	-3.382864649290	5.781490725492	-1.279646853987
C	-4.046847250113	6.275628411639	-3.246108296082
C	-5.301069377098	7.157684537727	-3.382655249128
H	-5.250241378529	7.746976033744	-4.315239777777

H	-6.209404620743	6.535615907327	-3.404579353195
H	-5.376677097952	7.853884210035	-2.528880945743
C	-3.948211215821	5.286423296027	-4.421324245740
H	-3.038791643796	4.664532116824	-4.332841812852
H	-4.825697459216	4.622463406281	-4.446021366819
H	-3.894255271983	5.837891319900	-5.376436991126
C	-2.787049221791	7.154978881136	-3.194587880889
H	-2.680400937954	7.717700131282	-4.137126549619
H	-2.847406166847	7.884698223983	-2.366170355826
H	-1.878374423123	6.542055608504	-3.051672278632
C	-5.984499411427	4.827251697124	0.764243207506
H	-5.914292072134	4.389730989824	1.778364891063
H	-6.977640503296	4.565344394609	0.358515552502
C	-5.831444837398	6.321546039241	0.847706733758
H	-4.910467157855	6.680787735535	1.330227916411
C	-6.701937158724	7.213157680452	0.360108090722
H	-7.625828727882	6.894273079632	-0.140973201900
H	-6.523864851763	8.292486356784	0.438946995919
C	6.558529268042	11.417301910443	-2.298698955667
H	6.819189235353	12.380253364275	-1.845239575696
H	7.226776515963	11.006832901256	-3.065822612251
C	5.429944153566	10.758738355027	-1.898753623178
H	4.825318759319	11.247597193339	-1.119568970709
C	4.798341838763	9.390741900154	-2.377322701705
H	4.424025007932	9.555223614599	-3.403015392464
C	5.969987930542	8.409929683156	-2.559755399479
O	6.637668405224	8.458174695009	-3.594015285378
N	6.269231214184	7.609441444631	-1.506951622222
H	5.587476474654	7.509261680132	-0.756439288926
C	7.468295090436	6.741763236497	-1.414409830262
C	8.745217522083	7.577435618491	-1.623675700031
H	9.636269862075	6.943326456731	-1.469313557371
H	8.779479347201	7.998298959233	-2.639321014395
H	8.780219067482	8.409858911745	-0.898202179498
C	7.385403306939	5.611845265631	-2.457803419101
H	8.271350393111	4.955603697560	-2.386690736408
H	6.484196110630	4.996379060640	-2.290130953805
H	7.337706440231	6.035109636982	-3.473669436380
C	7.481548669189	6.152115406711	0.004323774632
H	8.347521929659	5.478849821049	0.123639159665
H	7.560076527828	6.954230280773	0.760521735658
H	6.560514912154	5.584034256966	0.208439107168
C	3.587800451892	8.864604296604	-1.493800317581
H	3.965312633049	8.725863307970	-0.471090642965

H	2.848739030119	9.683991393762	-1.436362142233
C	2.849613221401	7.533204677574	-1.947821387754
H	3.589603114783	6.718571620497	-1.982395402508
H	2.500827874987	7.668338050047	-2.987283622007
C	1.593796274006	7.001684838649	-1.117482873773
H	0.767370766917	7.727762653658	-1.223463008225
C	1.828769510780	6.829345538469	0.424139507630
H	0.942773625534	6.308289774377	0.821532477468
C	3.049319268402	5.926024114906	0.643551259469
O	4.197327477606	6.366658137460	0.566572909715
N	2.749073487556	4.623675929245	0.856327974182
H	1.764072000054	4.387811729861	0.903930382571
C	3.692843289344	3.481299616318	0.850156003948
C	4.716139436461	3.636368770750	1.988211303816
H	5.412935439062	2.779775823685	1.989173295080
H	5.294762297981	4.564497248058	1.867702901260
H	4.201889486369	3.669666871231	2.965199599199
C	4.386352131223	3.407309066500	-0.522330454095
H	3.634183207127	3.307726469230	-1.323796247273
H	4.965463996419	4.323574191071	-0.711492045483
H	5.071355545345	2.542269588498	-0.560665715935
C	2.849745920204	2.216682565062	1.074454959527
H	3.501467732080	1.327057426312	1.086379087879
H	2.312294511825	2.262249024696	2.039025698142
H	2.109197861361	2.083554411703	0.264278064541
C	1.937110915159	8.132253701478	1.244946367742
H	1.146944105657	8.824246770430	0.898931995083
H	2.905111546224	8.618903747440	1.071117277289
C	1.769596915001	7.857320011533	2.716645964442
H	0.771949070538	7.517634470735	3.031991665134
C	2.743673800978	7.958594861323	3.628571743938
H	3.755825297421	8.279365192467	3.347814950373
H	2.568422801365	7.724382712846	4.685716623342
C	-2.537971284526	2.227129223572	-0.561188902507
O	-1.938903942231	1.691880303532	0.356706526789
N	-1.967138937469	3.277412163091	-1.293495316833
H	-2.473752947414	3.606941030787	-2.111113510831
C	-0.528761219798	3.640843321941	-1.216397088761
H	-0.151820150210	3.117358519401	-0.323566867040
H	0.004056409584	3.253822688788	-2.097547822813
N	-0.161948130577	5.092474655071	-1.148435740098
H	-0.637292437436	5.638603775289	-0.434626026883
C	1.052425839029	5.591801575152	-1.656528122137
O	1.716659765518	4.936815714643	-2.443336162350

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C	-8.233572998389	-2.708547844692	-0.287679061239
H	-9.264460626217	-2.733546512275	0.082330862720
H	-7.752023010170	-3.663339833057	-0.536256428260
C	-7.587997356541	-1.496687560765	-0.430945979853
H	-8.195923835456	-0.615703134199	-0.173329371543
C	-6.233586206556	-1.173842774449	-1.061769744860
H	-5.533713446472	-2.015320598039	-1.035998672131
C	-6.260504991943	-0.603889005878	-2.455907010996
O	-5.521880289922	-1.067833989953	-3.328445301000
N	-7.121734833654	0.426504427586	-2.677257693382
H	-7.664390161207	0.761314756796	-1.888680409125
C	-7.358056023082	1.100218535104	-3.974437955267
C	-7.919747508237	0.087509181879	-4.989492636182
H	-8.125140948313	0.586016996622	-5.953635718319
H	-7.197268242750	-0.726613147537	-5.159214573372
H	-8.862614752680	-0.350801602497	-4.615562333044
C	-6.052870585770	1.728852848723	-4.498166234771
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H	-5.285753970873	0.954456993778	-4.649875463088
C	-8.388630850079	2.208857263438	-3.708298618933
H	-8.621051481200	2.738355489027	-4.648231605986
H	-9.331656361602	1.787273865006	-3.313146476846
H	-7.987482328800	2.944346012955	-2.989809868056
C	-4.329662186798	0.249315727552	-0.610666688358
H	-4.208165082022	-0.018648109676	0.445178083731
H	-3.817383074947	-0.432267719731	-1.297895215322
C	-4.076465295861	1.760370474145	-0.911530981969
H	-4.264395585271	1.954512822212	-1.981390301332
C	-5.058557691890	2.608969686462	-0.065514819071
H	-6.076725943606	2.332766561227	-0.388736850600
H	-4.957241886783	2.303141317544	0.991355410862
C	-4.927795011662	4.139177388524	-0.130112295998
H	-3.938655348387	4.435437681817	0.257538378134
C	-5.096693962338	4.654338127218	-1.564268183927
O	-6.052880478415	4.301177729771	-2.252009582802
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H	-3.447397583957	5.793228048499	-1.296570995956
C	-4.110097854059	6.254878873224	-3.271339641574
C	-5.379211551105	7.113783931725	-3.417514289509
H	-5.335757068341	7.697884062075	-4.353721274259

H	-6.276398659588	6.475727932554	-3.438160924540
H	-5.469687255606	7.814107488128	-2.568545177204
C	-3.990968595211	5.257850992529	-4.438014980129
H	-3.068256958594	4.656671151594	-4.344268538760
H	-4.854193712546	4.575004416415	-4.456417358960
H	-3.949187398523	5.801897763459	-5.397964084726
C	-2.866033978760	7.156577536052	-3.223617586261
H	-2.765128292104	7.711492965959	-4.171409140062
H	-2.942873167032	7.893556660369	-2.403052323492
H	-1.947157417386	6.561329935111	-3.070693492208
C	-6.013320743719	4.807099780365	0.753413374402
H	-5.936431169212	4.372497989721	1.768306598950
H	-7.006776150669	4.538542736695	0.352683614736
C	-5.868462500736	6.302456421098	0.832577787110
H	-4.948461673559	6.668184980995	1.312121342860
C	-6.745050740260	7.187876153944	0.344601134729
H	-7.668333774655	6.862490452140	-0.153426773823
H	-6.572826946553	8.268389936630	0.420120809212
C	6.688266842832	11.478468847236	-2.261056626749
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C	4.904501802180	9.440145093335	-2.352376045051
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C	6.069807241463	8.451404334744	-2.529007110381
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N	6.346240274865	7.636521705873	-1.480898199317
H	5.653735477309	7.536620765527	-0.740444942115
C	7.533213003573	6.753071074793	-1.382317380222
C	8.823116310884	7.574030962466	-1.568827286568
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H	8.874759108758	8.003893734795	-2.579920400951
H	8.860283301537	8.399065919633	-0.835076545858
C	7.447822001086	5.633966951481	-2.437073545803
H	8.324334049094	4.965614753819	-2.362129885690
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H	8.376624597769	5.463358865843	0.153563073290
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C	3.671198881250	8.906719373811	-1.483202543972
H	4.037218259339	8.759819984204	-0.457533346104

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H	2.569532686879	7.715470562118	-2.984379790442
C	1.639842097126	7.035354022403	-1.120746668493
H	0.819679091931	7.767830493977	-1.229089643502
C	1.868425059164	6.858324593791	0.420176302560
H	0.978722652212	6.341103510128	0.814587442080
C	3.084204517047	5.948527744454	0.640487909547
O	4.234380502514	6.384320520368	0.569686386300
N	2.776943451381	4.646589617823	0.846123824569
H	1.790574122461	4.415292634309	0.887346669892
C	3.714840887772	3.499494085474	0.836027637032
C	4.736110203185	3.643014590908	1.977398683683
H	5.428778113158	2.783075477286	1.975091753098
H	5.319482304828	4.569025046520	1.863758828356
H	4.219624565977	3.673088707867	2.953314525047
C	4.411265306418	3.429059432825	-0.535250346078
H	3.660275836921	3.338403177175	-1.338909009161
H	4.996597178463	4.342738396827	-0.718085514804
H	5.090998751355	2.560016236593	-0.576895095589
C	2.864654662013	2.238072640429	1.051538786646
H	3.511656378816	1.344969658919	1.060405736821
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C	1.982426020968	8.159842444641	1.242161134766
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H	2.951766276699	8.643180987494	1.066695449696
C	1.816162777730	7.884907383892	2.713944456237
H	0.818028984855	7.547683589543	3.030397297692
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H	3.804091244603	8.301951326371	3.343042889611
H	2.616745637906	7.749787843517	4.682134474790
C	-2.547274646546	2.212927244841	-0.591688368255
O	-1.931411605382	1.645395417229	0.293889434909
N	-1.985419805295	3.299516374924	-1.290979307839
H	-2.501500683163	3.649817196172	-2.094347411855
C	-0.537488777711	3.667650063111	-1.224608942179
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H	-0.014752179150	3.282015973268	-2.112343964338
N	-0.147230302497	5.122834247242	-1.152433206091
H	-0.616552027241	5.671793575180	-0.436637632956
C	1.075559872213	5.619552306958	-1.662004688948
O	1.732594627410	4.962489769586	-2.451772216214

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C	-7.142508442687	-0.976750318193	-0.177669064868
H	-7.527909048228	-0.022445859877	0.212292380835
C	-5.775658972814	-0.926574354632	-0.862282457799
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C	-5.840372791629	-0.695038909556	-2.386836199757
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C	-5.683672039332	1.339223581826	-4.705739139474
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C	-8.103632791661	1.703476316360	-4.141584461739
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C	-4.679051132205	0.087241934780	-0.281854003048
H	-4.720402011391	0.023053295966	0.820734872399
H	-3.707364864528	-0.334869069068	-0.594516506456
C	-4.721766678037	1.532076152366	-0.726265629578
H	-4.555398541000	1.713339393139	-1.792249368845
C	-5.656775952501	2.477842141971	-0.032533590729
H	-6.671845716848	2.333997161453	-0.465526218877
H	-5.738210830230	2.206438305178	1.035328366577
C	-5.332245700374	3.976998188209	-0.122108681047
H	-4.354275266303	4.143116969726	0.363092812654
C	-5.255075231577	4.442372154772	-1.580844064601
O	-5.958993374364	3.946762331518	-2.452678282633
N	-4.345713442333	5.440107916488	-1.817621941259
H	-4.048260645801	5.949097751024	-0.987972286307
C	-4.212616129595	6.199783769786	-3.089812897354
C	-5.541440246124	6.893485336013	-3.440162913370
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H	-6.337114147936	6.147751138540	-3.594760531224
H	-5.849239504901	7.569797855041	-2.623295808148
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H	-2.825806091232	4.748653221917	-3.965918667173
H	-4.540902321539	4.470410058630	-4.389568125559
H	-3.633619279216	5.815045407993	-5.151300232493
C	-3.118020841548	7.251716888966	-2.848365559209
H	-2.950028497968	7.838799253165	-3.766732421315
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H	-2.160554011641	6.779174368650	-2.563313865246
C	-6.407869846922	4.819247691549	0.620394182103
H	-6.566928917385	4.350873752860	1.610254968457
H	-7.362395298857	4.746616931448	0.068453761354
C	-6.020611333346	6.259669336942	0.815520487772
H	-5.144033556544	6.432409364705	1.457646134292
C	-6.638783017666	7.309802767781	0.262333173178
H	-7.510171576386	7.179501873120	-0.393139081949
H	-6.296716286876	8.336508382128	0.439696298608
C	6.696133964657	11.453682883516	-2.243011567462
H	7.034115176957	12.396562800855	-1.797777682584
H	7.299723849902	11.020680659776	-3.050183528199
C	5.572064436871	10.849272239978	-1.799198766241
H	5.017551761009	11.336399568095	-0.983555978276
C	4.919510464110	9.534384863650	-2.297741062601
H	4.518407360250	9.724172560945	-3.309323484525
C	6.044048249322	8.507993908067	-2.534058717110
O	6.672856621095	8.539890424817	-3.592767328153
N	6.341412003551	7.674118985033	-1.506504417189
H	5.677697343251	7.589621404076	-0.738602340785
C	7.448205685192	6.686827942574	-1.505048007005
C	8.789540222534	7.390929408118	-1.780459267897
H	9.617011364650	6.664218235820	-1.696139782080
H	8.803453400601	7.832767123553	-2.787537930610
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C	7.178815758854	5.597338403247	-2.560091057911
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H	7.111454314295	6.045827693928	-3.564096314298
C	7.484397104883	6.061779932018	-0.101653303883
H	8.280953017007	5.299940566072	-0.050615309021
H	7.693332165735	6.831693655772	0.663397223095
H	6.520804014384	5.588180456067	0.146162540863
C	3.746471285739	9.058484558298	-1.387961939815
H	4.147580837923	8.898611876127	-0.376586919757

H	3.028921673647	9.894445219258	-1.298781277689
C	3.004503104946	7.780552504006	-1.869234128181
H	3.719887009818	6.946340117976	-1.921182926624
H	2.664259984321	7.945462115733	-2.907370108492
C	1.757953956884	7.291738876937	-1.061393658420
H	0.958187087925	8.051107228849	-1.138896889782
C	1.964707775619	7.035098170448	0.470943492450
H	1.023125278107	6.596438219044	0.838097472341
C	3.083140626711	6.003271836113	0.659047028229
O	4.268590425836	6.324964505916	0.561607262236
N	2.649384607766	4.740431149632	0.876728652708
H	1.644123154998	4.609830174918	0.910367751466
C	3.462030621139	3.501890918652	0.876134105841
C	4.530325543251	3.568019454138	1.981255976103
H	5.108214648953	2.627319943193	2.002373984214
H	5.222381825722	4.405524977982	1.805795944728
H	4.054577579037	3.708080926307	2.968186590921
C	4.108577094050	3.318008676703	-0.508793437497
H	3.332916524988	3.294526954968	-1.293584797033
H	4.792726660434	4.152998928660	-0.728290441616
H	4.681968725806	2.374969329984	-0.542059522144
C	2.490120997348	2.345674928029	1.162156272899
H	3.034815444673	1.386683990939	1.160059491828
H	2.012513329830	2.467812494759	2.151204015093
H	1.692752262774	2.285145263848	0.398049128116
C	2.208262851840	8.279174284936	1.352648160329
H	1.539602058338	9.089307404562	1.007609425262
H	3.242849470035	8.628807078664	1.240878151861
C	1.939856277080	7.971040302409	2.802655447685
H	0.892121114351	7.762241297304	3.064794426992
C	2.878458990117	7.896399742037	3.753576859694
H	3.936414167006	8.084317861923	3.526018862551
H	2.627284888634	7.645118807443	4.791293831790
C	-2.121827486084	2.599074056383	-0.635597786936
O	-1.364007090922	1.745642975372	-0.255865556875
N	-1.806705065878	3.796404945968	-1.202269807254
H	-2.592633576111	4.351031823798	-1.550615696941
C	-0.465722637766	4.142402846175	-1.688379595316
H	0.221326746469	3.346592822433	-1.359129958509
H	-0.455582735135	4.154531310724	-2.791490168137
N	0.017677700243	5.456144456468	-1.218694786972
H	-0.526878334993	5.944546831040	-0.514308930580
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O	1.843281174185	5.345294593814	-2.537763604062

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H	-7.760994543596	-3.145753253827	-0.508548626392
C	-7.324810428257	-1.069321136316	-0.164538628742
H	-7.723761503704	-0.144708546873	0.280074637320
C	-5.958354801167	-0.945886178704	-0.861583996186
H	-5.474877394657	-1.932430679308	-0.795660407691
C	-6.066835220269	-0.698940785688	-2.381048649243
O	-5.299199165472	-1.264645577621	-3.155972846901
N	-6.991672840418	0.214286421872	-2.761811091680
H	-7.598398093111	0.588170157785	-2.039739174486
C	-7.245990886099	0.689377949386	-4.142302117564
C	-7.761688731318	-0.478652023537	-5.001892714025
H	-7.976744939353	-0.133014431574	-6.028760110780
H	-7.007706690940	-1.280906835011	-5.049668516230
H	-8.690808535159	-0.894305224860	-4.572019393710
C	-5.961652584692	1.288052907467	-4.746312982575
H	-6.166315535261	1.655709974296	-5.767868884949
H	-5.616298475919	2.136103295462	-4.131854501094
H	-5.166646731170	0.528664314182	-4.796790306088
C	-8.316267984955	1.786386522056	-4.030437381018
H	-8.559703161352	2.178172999603	-5.032837669193
H	-9.247720545777	1.389787236685	-3.585014457994
H	-7.944334755975	2.621287123441	-3.411072674186
C	-4.859105417579	0.086820860578	-0.278646529454
H	-4.941474020092	0.065438039620	0.823009548145
H	-3.886193271373	-0.369987095786	-0.534270338710
C	-4.825398750596	1.525260991970	-0.771088977383
H	-4.676162467971	1.656180676702	-1.847040276276
C	-5.741997778611	2.517428658841	-0.113913403390
H	-6.754187137250	2.381870936609	-0.555575355302
H	-5.842469276302	2.276106606879	0.959471814688
C	-5.384973604423	4.006954418277	-0.231706184273
H	-4.421966485334	4.167035485946	0.284133307351
C	-5.246911466045	4.436323318416	-1.696184396002
O	-5.939084537430	3.942347892778	-2.578894837361
N	-4.302429273343	5.400702762523	-1.925508682266
H	-4.011054260767	5.918746485557	-1.099577674827
C	-4.090679021441	6.111614931958	-3.214189555168
C	-5.380726068704	6.830774641575	-3.647949083385
H	-5.208700732298	7.388457485282	-4.585457803240

H	-6.191016610581	6.103280977602	-3.813025488128
H	-5.703437350553	7.544120801524	-2.869174163660
C	-3.637596569429	5.105362893397	-4.286462520453
H	-2.711690862542	4.590199823624	-3.973675866272
H	-4.414312296312	4.346486326352	-4.466407672868
H	-3.432715566133	5.635104892136	-5.233031949900
C	-2.975491432087	7.138133007562	-2.958440841607
H	-2.748201156232	7.687707359969	-3.887275970467
H	-3.283456822234	7.875531228873	-2.194213163317
H	-2.047934310482	6.646542140489	-2.612762208985
C	-6.469703675442	4.887035253554	0.451491066222
H	-6.674368971433	4.445734576521	1.445429630865
H	-7.404518099640	4.819635138313	-0.133852073211
C	-6.060415885239	6.323964573361	0.626277708903
H	-5.208703864367	6.496088191667	1.301202599385
C	-6.630457278696	7.370999746816	0.018264302012
H	-7.475441934989	7.240866903384	-0.670993786380
H	-6.273771264284	8.394873212657	0.182822348601
C	6.624401351492	11.516817209066	-2.157212633987
H	6.935724594090	12.461008628081	-1.695888873901
H	7.248481990335	11.104662840498	-2.959656031326
C	5.500666271112	10.886407541195	-1.734045919247
H	4.930754993063	11.362656749292	-0.922209588504
C	4.854277384979	9.560883238725	-2.242273286043
H	4.433421813893	9.763908058352	-3.243169403253
C	6.000227576467	8.568743410545	-2.513464187054
O	6.613066835322	8.636363598642	-3.580059675561
N	6.340364164340	7.733203456341	-1.501148927638
H	5.692245427135	7.615388152034	-0.723864591631
C	7.516390031055	6.830033816033	-1.503782433367
C	8.803379023257	7.637023489446	-1.757563842386
H	9.682779493282	6.973656548626	-1.677010377064
H	8.792061087293	8.093616613430	-2.758178933918
H	8.903772374888	8.441312074972	-1.006898639517
C	7.341583674101	5.737947699816	-2.575774172197
H	8.208045506481	5.052515991741	-2.572929576809
H	6.430748100906	5.145812389063	-2.377853000248
H	7.253547059096	6.194548436399	-3.574379488712
C	7.589999794959	6.192274118413	-0.107714731671
H	8.440757216313	5.491371017284	-0.059072812762
H	7.734407027497	6.965890657976	0.668243577347
H	6.664045043150	5.644625267006	0.128567476250
C	3.697673400447	9.037899294614	-1.321802903188
H	4.121094965336	8.858210910654	-0.323385077403

H	2.971810579033	9.862330618931	-1.199520262906
C	2.948945321595	7.752105356884	-1.805897221161
H	3.675719547915	6.930754809000	-1.898643977974
H	2.569844257122	7.932691529078	-2.827873421475
C	1.731173099653	7.220302327073	-0.961337966079
H	0.913876779610	7.963246525888	-1.003557631814
C	2.004481336107	6.961240956985	0.561462696494
H	1.108772584858	6.455715911278	0.956733473076
C	3.194127412682	6.003670590371	0.701693121142
O	4.354274672496	6.402948516443	0.587808223223
N	2.851530180452	4.709222366068	0.895163897480
H	1.860341772400	4.509613066521	0.974159564722
C	3.750746924837	3.532818912980	0.844333093103
C	4.819719278064	3.636635582320	1.945914011151
H	5.477341992846	2.750027011103	1.918340884878
H	5.434577707229	4.538823338575	1.808370186395
H	4.342569114354	3.687105845095	2.940796829459
C	4.393700782900	3.446822567938	-0.551761152423
H	3.611840014108	3.394093003618	-1.329017362125
H	5.010022678427	4.337414354843	-0.747971434083
H	5.034763795307	2.550848746053	-0.624674030581
C	2.868618456947	2.298857544232	1.089276914027
H	3.485308121792	1.384839404987	1.067574454840
H	2.371428954358	2.355012173734	2.074617375460
H	2.091301116918	2.201369038645	0.308676550076
C	2.189604932773	8.212734812246	1.446829551341
H	1.430931395368	8.961417150806	1.152518078394
H	3.178980392654	8.657965962142	1.281593655260
C	2.033214519887	7.867662313812	2.904963230525
H	1.024818779792	7.563744319011	3.222494141114
C	3.027739031953	7.867716358852	3.800293907199
H	4.050239684565	8.150512177523	3.516129489358
H	2.859594952195	7.585312005590	4.846760034290
C	-2.296661383227	2.483554653711	-0.607822557359
O	-1.604014221186	1.599090706423	-0.176262251318
N	-1.863874548742	3.690665258460	-1.091826234910
H	-2.570362688018	4.278230126871	-1.539719996968
C	-0.443315330490	3.978073452612	-1.386900891742
H	0.145675199790	3.241267174434	-0.814781444826
H	-0.229435771732	3.822530851613	-2.456206430215
N	-0.011222345711	5.356829962607	-1.065492739365
H	-0.486733595038	5.825753685191	-0.299647585532
C	1.175488404756	5.872843843303	-1.570702434285
O	1.801277813590	5.262009020050	-2.426531239780

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C	-8.134342522431	-2.309528986374	-0.127361401233
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H	-7.810621613243	-3.236342239189	-0.620291555506
C	-7.370692051716	-1.180621256013	-0.141692605822
H	-7.770848885804	-0.297332907958	0.379095027230
C	-6.012327470685	-0.975528554638	-0.858844640670
H	-5.495388731379	-1.946146971140	-0.831777083121
C	-6.165318438156	-0.699492693821	-2.368934755706
O	-5.427046402626	-1.255417028139	-3.178532890486
N	-7.097879988753	0.224215375809	-2.703894720305
H	-7.693113941185	0.571470399249	-1.959200448159
C	-7.419297278534	0.695879328445	-4.071641838598
C	-8.000930116124	-0.469303936254	-4.892583887518
H	-8.267022202110	-0.128052307686	-5.908929706631
H	-7.263067752172	-1.283936422945	-4.975964819195
H	-8.911140099679	-0.867238155843	-4.408782640531
C	-6.161904149475	1.269055250417	-4.751799515209
H	-6.422704594248	1.643679183756	-5.757943591285
H	-5.761974447801	2.107929860815	-4.158493476563
H	-5.387715997546	0.493796678050	-4.852835207378
C	-8.462804534315	1.812208344046	-3.908561562200
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C	-4.909552535374	0.076185923707	-0.269587923944
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H	-3.938415112213	-0.406461807555	-0.479504042936
C	-4.814667338408	1.512939650566	-0.791952672632
H	-4.685949956525	1.610770590883	-1.874489045915
C	-5.724105491627	2.528778064634	-0.155487050928
H	-6.735673903716	2.385986348167	-0.594751632226
H	-5.825563922559	2.308837137452	0.922344418834
C	-5.366840707007	4.015200768708	-0.298006064173
H	-4.405474810190	4.184548933948	0.217518417655
C	-5.228669500274	4.424514456471	-1.767774155409
O	-5.929709956375	3.927272403429	-2.641890538644
N	-4.276000112927	5.375836557045	-2.011531846093
H	-3.968206629815	5.895246586222	-1.192738654200
C	-4.054425051089	6.065878041228	-3.309186535549
C	-5.335841464776	6.793234305802	-3.754686751926
H	-5.156347240237	7.336380197758	-4.699317998794

H	-6.153764300242	6.072355953624	-3.911124075573
H	-5.651949120850	7.520322370338	-2.985984169373
C	-3.611423971429	5.039553610918	-4.366490415696
H	-2.689111168390	4.522450536548	-4.046623692227
H	-4.394881101211	4.284402101648	-4.533245043560
H	-3.404150943893	5.552771029262	-5.321662578101
C	-2.927791988211	7.082762700570	-3.065423008747
H	-2.688774934253	7.613449612036	-4.002281605379
H	-3.230652003300	7.836914457771	-2.315610410835
H	-2.008867820645	6.585083762435	-2.705456337901
C	-6.453172766526	4.904879766152	0.370271843722
H	-6.656564898189	4.481022562483	1.372052223775
H	-7.388049402070	4.825367379622	-0.213394917764
C	-6.046472934082	6.345467740270	0.518881941606
H	-5.194255130173	6.531410460325	1.189517286923
C	-6.619709962884	7.380270510707	-0.106729727171
H	-7.465322155859	7.236072638202	-0.792420323358
H	-6.265024437220	8.407683108638	0.039043865276
C	6.663998880531	11.571047054902	-2.091768796885
H	6.963899615436	12.509862673447	-1.612491766308
H	7.292443871475	11.179603371524	-2.901166676737
C	5.542895896129	10.920059093672	-1.676551710561
H	4.974249455023	11.382068587038	-0.855354161781
C	4.887737715816	9.590850514512	-2.195260685423
H	4.472709978965	9.803988618584	-3.196237351486
C	6.038706815986	8.606016892526	-2.469323115620
O	6.661373136684	8.690734278136	-3.529026377955
N	6.374261473780	7.759509861203	-1.464640805012
H	5.722981287904	7.631627746860	-0.691523190498
C	7.569461313424	6.881735066392	-1.458438974563
C	8.842676587865	7.720848719558	-1.676392193899
H	9.735143301383	7.075856823785	-1.590687955983
H	8.838965206644	8.192907428050	-2.669926006639
H	8.912068470789	8.515104981589	-0.911697192321
C	7.440241506361	5.802075490235	-2.549270810076
H	8.322735444298	5.137466613977	-2.539962510668
H	6.540587216698	5.185368494590	-2.377593866655
H	7.359912401852	6.271845444671	-3.542310650446
C	7.632367305346	6.225639152924	-0.070531321792
H	8.499573412440	5.545717487465	-0.015280282466
H	7.741720276512	6.990818916565	0.719337886848
H	6.717137077945	5.650645000589	0.140258518082
C	3.718243829839	9.049277038058	-1.285406524330
H	4.137161875999	8.858710980150	-0.287307505924

H	2.993260680224	9.873575722508	-1.158176258848
C	2.956427215425	7.759923884646	-1.776343056537
H	3.682622187985	6.938817081884	-1.879008886083
H	2.572096759959	7.949371489611	-2.794636264439
C	1.733692037182	7.213967557392	-0.927938722313
H	0.916677896264	7.957435276361	-0.962815863361
C	2.019686995202	6.951999781724	0.592307290482
H	1.136996803845	6.427040204278	0.991577373038
C	3.227813596482	6.015445071536	0.718262982293
O	4.380760437461	6.438580607019	0.618805456481
N	2.909904456980	4.709784729131	0.878375795591
H	1.922739806447	4.488202899182	0.949990650368
C	3.832914799588	3.554129980428	0.787163436060
C	4.899101180973	3.641819030136	1.892723670988
H	5.580018523152	2.774771217567	1.830523115241
H	5.489465425641	4.564876752363	1.792031895192
H	4.420862490465	3.639789640276	2.888379558393
C	4.475566484846	3.531267536375	-0.611662038698
H	3.693412762735	3.480861979851	-1.388724624855
H	5.064418991585	4.445417558154	-0.780287150980
H	5.142446892241	2.657341139919	-0.714371267781
C	2.977575372257	2.293661734601	0.986731388016
H	3.614880860654	1.394911676037	0.937895085386
H	2.474492452974	2.305326175332	1.970619537810
H	2.207596359015	2.205646807726	0.198021530190
C	2.184943361068	8.204097555393	1.480127865793
H	1.399086574062	8.930724292585	1.201895269345
H	3.157135132608	8.679961425709	1.299650419150
C	2.062753644522	7.850427508392	2.939386831695
H	1.070868381433	7.508806399427	3.270383387403
C	3.068692474485	7.887376897648	3.821043085642
H	4.075842487545	8.208517857395	3.523242556491
H	2.925575766235	7.598218129228	4.869386752989
C	-2.356865806597	2.434799803643	-0.588590060963
O	-1.673976727059	1.570018927786	-0.103923388319
N	-1.894882229617	3.646237532009	-1.059361199665
H	-2.567611448685	4.220192689147	-1.570988845871
C	-0.449290109461	3.937349228433	-1.263728432376
H	0.091041148690	3.243073354709	-0.598316692629
H	-0.153089852234	3.713846631604	-2.300340286891
N	-0.027055225542	5.339613846053	-1.008535442671
H	-0.479920651882	5.818162673235	-0.234623445961
C	1.160672071372	5.858524721742	-1.532496363157
O	1.776694047299	5.250332689544	-2.395120815342

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C	-8.158878235027	-2.401390360718	-0.149607785475
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H	-7.839674712814	-3.311060967407	-0.676169417180
C	-7.396565738973	-1.265218957460	-0.133655644806
H	-7.801680000611	-0.404814875599	0.420845479125
C	-6.039072573426	-1.004341103919	-0.857563369628
H	-5.500960218416	-1.963162269438	-0.855507285358
C	-6.222379515777	-0.709988774197	-2.360175652059
O	-5.514326196768	-1.269177323432	-3.194095029690
N	-7.151492584933	0.228679819502	-2.663048198987
H	-7.727465842516	0.570833936729	-1.900801865433
C	-7.517201786296	0.697695835124	-4.020643050626
C	-8.148405648740	-0.463446481646	-4.810303094715
H	-8.446928912049	-0.125524311343	-5.818729960962
H	-7.427164018272	-1.290506119282	-4.914795427586
H	-9.046015167492	-0.843100604727	-4.289620252238
C	-6.278095807142	1.245555058572	-4.753358118410
H	-6.573854928269	1.623498405320	-5.748572978073
H	-5.837774127220	2.077386813182	-4.179161932497
H	-5.523761906878	0.455523032903	-4.884796314760
C	-8.535709771601	1.831872291014	-3.825912152438
H	-8.862362852587	2.216675470992	-4.807144935425
H	-9.432830353716	1.474357602107	-3.286531927860
H	-8.078755232976	2.662474484124	-3.259993294790
C	-4.925523170671	0.061515236682	-0.263756084512
H	-5.063836464022	0.092769548587	0.831360056421
H	-3.960343039836	-0.443972219368	-0.443347841499
C	-4.781341270380	1.500365924853	-0.802980776001
H	-4.669903514946	1.577327521650	-1.889452578531
C	-5.697243097489	2.522803988592	-0.181210965188
H	-6.706360171543	2.360147155312	-0.618251022272
H	-5.796747035367	2.316437706845	0.899448355770
C	-5.357814258127	4.011029303748	-0.339367715329
H	-4.401978188682	4.198276102160	0.180096448307
C	-5.217786769982	4.409183482418	-1.811560621610
O	-5.914695551651	3.902072739325	-2.683371856669
N	-4.268539491040	5.361840486195	-2.059857998662
H	-3.960243210015	5.885963418096	-1.244458511511
C	-4.036604761900	6.036605643856	-3.363224252136
C	-5.316208875621	6.753175068637	-3.830743363868
H	-5.128955352639	7.285847935697	-4.779825857426

H	-6.129471636201	6.027007146212	-3.987015455511
H	-5.643320292330	7.487947677658	-3.074019743075
C	-3.578897862435	4.998542753210	-4.402718434347
H	-2.656059611868	4.491723721083	-4.068146292845
H	-4.356669414494	4.236439751079	-4.565021210466
H	-3.367195562209	5.499489258441	-5.363429505740
C	-2.916245228005	7.060602156664	-3.120229726872
H	-2.666667105454	7.578199956685	-4.061645152810
H	-3.231181598157	7.824644723514	-2.385575598122
H	-2.000819716847	6.570919206434	-2.740702673863
C	-6.458892397602	4.893283787150	0.314584358834
H	-6.659419957569	4.479455002236	1.321118915020
H	-7.390575156909	4.792914858622	-0.270940073894
C	-6.073144009522	6.341365248910	0.445281371084
H	-5.226563844362	6.548659487749	1.116799555008
C	-6.658273067640	7.359130493152	-0.197005794168
H	-7.498786510818	7.193467084041	-0.884138132260
H	-6.318770125654	8.393400978396	-0.064118169713
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H	8.954615185962	8.518196692536	-0.870609658653
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H	3.702032564710	3.512605257719	-1.412054561469
H	5.076704481811	4.468872495124	-0.798459469439
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C	2.210739910658	8.211114585513	1.502287700104
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H	-7.623632559149	-1.321741100468	-4.814931800264
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C	-4.764457391396	1.497491844264	-0.797550874438
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C	-5.696091398027	2.529767628400	-0.211597914508
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H	-5.806122555158	2.348408614760	0.872539563966
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O	-5.899880991183	3.859327002597	-2.746179657732
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H	-7.422406154502	4.759633162718	-0.375256385212
C	-6.144907265040	6.357035129093	0.303351547259
H	-5.309089336087	6.604395607094	0.974733914380
C	-6.745775271355	7.340589779270	-0.376545231099
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C	5.689637640418	11.041615765762	-1.542253649472
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C	6.140719090826	8.729535027170	-2.387608171843
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C	7.688908658282	6.237626200179	-0.073885996235
H	8.546654448887	5.544422035960	-0.040255321776
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H	0.956357977105	8.013585142503	-0.856655564656
C	2.077718288241	6.965625439410	0.656916120353
H	1.202975592075	6.430796597867	1.061172202390
C	3.289489011200	6.028031700084	0.737563463348
O	4.440283895089	6.456573604448	0.638400429569
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H	1.989370472393	4.491729199179	0.929126689609
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H	5.661456248989	2.747878486717	1.686089020983
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H	4.518257430415	3.566320264413	2.797019561941
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H	3.722073997545	3.576463549191	-1.470654712606
H	5.100126513623	4.522251495189	-0.848501654342
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C	3.045005642511	2.298687017715	0.866116730039
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H	2.260742854056	2.244130257185	0.088592980691
C	2.260303961826	8.198599389248	1.567382569188
H	1.465214870557	8.927691880817	1.324241825595
H	3.225956603023	8.681793785388	1.372331960078
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H	-3.755336320880	10.351524249733	-2.936527661368
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C	-0.452298113071	7.585059077199	0.545589365439
H	-0.151084435202	8.365966365672	1.256654155653
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H	-16.611117638848	8.856985780504	-14.748537244340
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C	-14.839374775992	7.699183735384	-14.867552630356
H	-14.434695098445	8.139347425057	-13.944819856574
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