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Supplementary Information

On the Electronic Structure Origin of Mechanochemically Induced Selectivity in Acid Catalyzed Chitin Hydrolysis

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Additional Details for the FMPES Implementation in G09

To implement FMPES formalism using Gaussian 09, we utilized the "External" keyword of Gaussian which is originally designed to interface Gaussian with other low-level calculator/s for ONIOM calculations. This allows us to call two Gaussian jobs simultaneously. In any geometry optimization job using external (Process A of main text), another daughter job/s of any calculator can be called. The daughter process performs a single point calculations for enenergy and forces at the structure given by the parent process. The daughter process also provides the calculated force plus external forces in a format specified by the parent process.

The total force in FMPES formalism as exactly written in the paper of Martinez and colleagues is

$$\mathbf{F}_{total} = \mathbf{F}_{abinitio} + \mathbf{F}_{ext} \quad (1)$$

In this case, we only need to call another process (Process B) to calculate the first term, $\mathbf{F}_{abinitio}$, of the previous equation.

The second term corresponds to the external applied force which is calculated as

$$\mathbf{F}_{ext} = \sum_i^N F_0 \mathbf{n}_i \quad (2)$$

where F_0 is a constant magnitude, N is the number of molecular attachment points and $\mathbf{n}_i$ is the unit vector from the attachment points (APs) to a constant pulling points (PPs) in Cartesian space. $\mathbf{n}_i$ can be easily calculated as

$$\mathbf{n}_i = \frac{\mathbf{r}_i^{fixed} - \mathbf{r}_i}{\|\mathbf{r}_i^{fixed} - \mathbf{r}_i\|} \quad (3)$$

In our implementation, this is calculated by a python code that is fed with geometry of the current optimization cycle, constant force and Cartersian coordinates of the constant pulling points. The pulling points in our implementation is chosen to have collinear points to the attachment points at described in Figure 2 of the main text.

The potential energy definition of FMPES is described as

$$V_{total} = V_{abinitio} + \sum_i^N F_0 (\|\mathbf{r}_i^{fixed} - \mathbf{r}_i\| - \|\mathbf{r}_i^{fixed} - \mathbf{r}_0\|) \quad (4)$$

As can be seen in the equation, the second term corresponds to the work done by the external force to the chemical system.

This is done in each cycle of geometry optimization because the geometry optimization algorithms decide the geometry for the next optimization cycle from the atomic forces from the previous cycle. Atomic forces are calculated as described above. Though this applied force is constant in magnitude, the normal vector is a function of the geometry given in that particular optimization cycle.

Note that without adding the force in each cycle, the geometry will then have the same as relaxed ($F=0$) system at convergence. This is similar to the restraining forces applied in molecular dynamics, that upon the release of the force, the geometry will go back to the original.

Our implementation of FMPES has been verified with simple molecular pulling (pushing) of a diatomic hydrogen leading longer(shorter) bond lengths. Units have been cross checked following the required inputs in G09 External.

Force vector diagram of a ball bombarding to a molecular plane

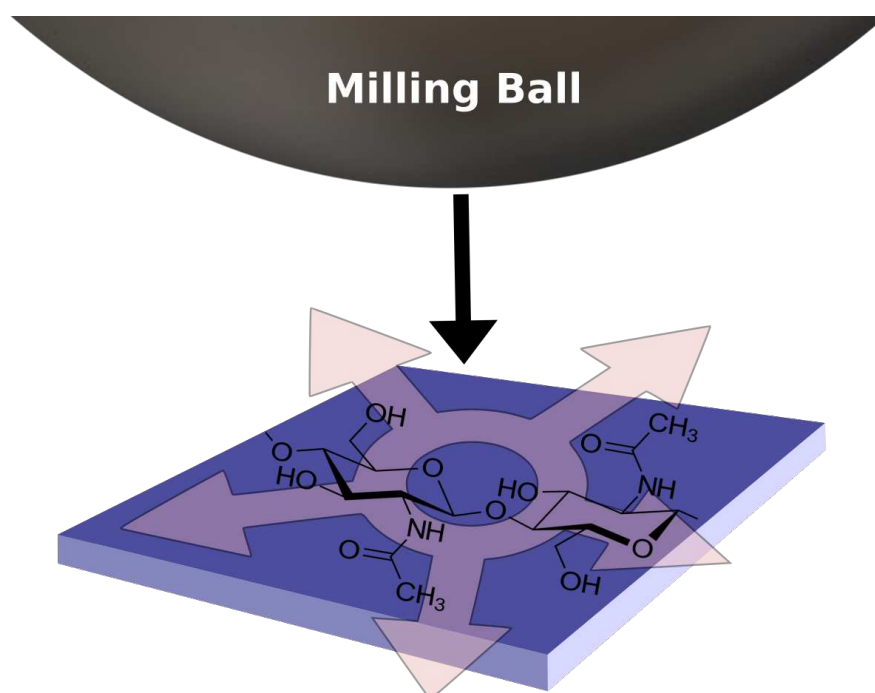


Fig. S1 Force Diagram in a Ball Bombarding to Plane

In ball milling, a ball pounds the sample inside an inert metallic cell. As the size of ball is much greater than any molecular size, the bombardment would introduce external forces both coplanar and noncoplanar to the molecular plane of chitin oligomer. The force diagram of the coplanar forces can be illustrated as above. As described in the main text, these forces can be added and hence a resultant linear vector can be expected.

Optimized Structures at the RDS of the Deacetylation

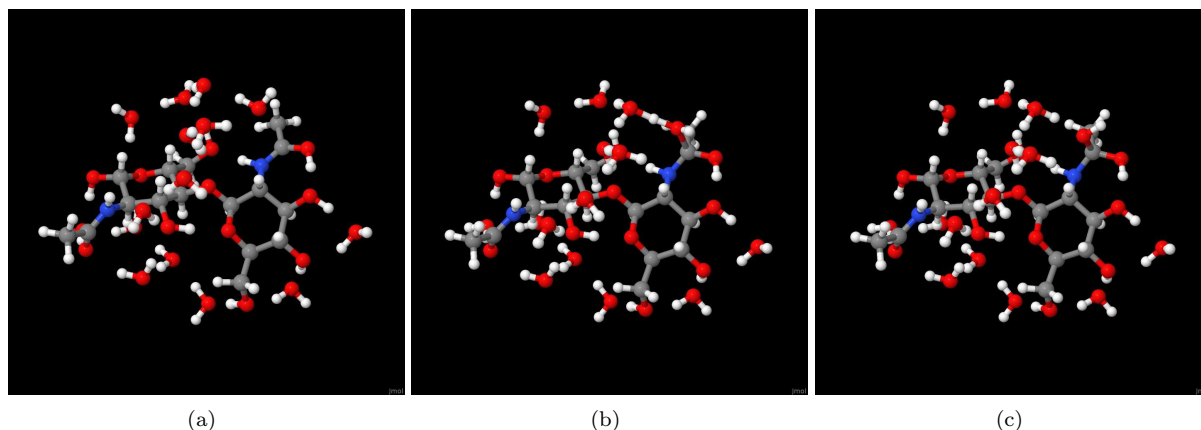


Fig. S2 Deacetylation RDS (Nucleophilic Attack of Water). Optimized structures of (a) A_Int1' (b) A_TS2 and (c) A_Int2. See Figure 1 for labels

This step starts with a protonated carboxyl oxygen (Fig. S2(a)) which has an increased reactivity towards the nucleophilic attack of water. In Fig. S2(c), it can be seen that the attacking water lost a proton and resulted to a protonated neighboring water molecule. This is captured in the imaginary frequency of the corresponding transition state, Fig. S2(b), which is characterized by $C_{GlcNAc}-O_{water}$ bond formation and $O_{water}-H_{water}$ bond breaking.

Optimized Structures at the RDS of the Depolymerization

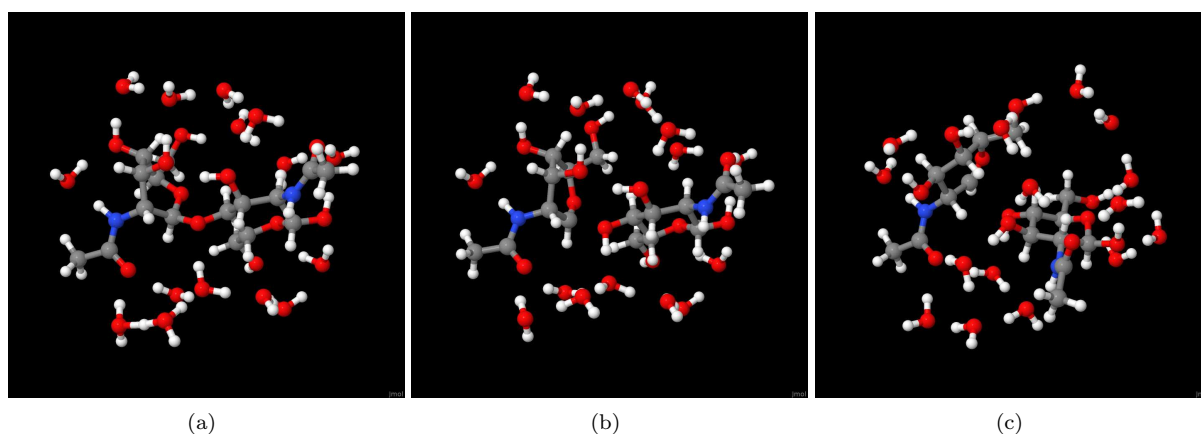


Fig. S3 Depolymerization RDS (Carbocation Formation). Optimized structures of (a) P_Int1 (b) P_TS2 and (c) P_Int2. See Figure 1 for labels

Depolymerization RDS is the formation of carbocation specie. In Fig. S3(a), the solvated proton is within the reaction center. The imaginary frequency of the transition state (Fig. S3(b)) shows protonation of the glycosidic oxygen and cleavage of the glycosidic bond. This occurs with a proton relay thru the nearest water molecule from the glycosidic oxygen.

A.Int1 Structure

C	-1.77735900	-0.04909800	0.71961900	C	3.90147200	2.44601900	-1.07011700
C	-3.22799900	-0.21609900	0.24526900	H	2.05083500	1.83330200	-1.42118000
C	-3.64522000	1.03520500	-0.56421800	O	5.04059200	2.35576100	-0.47435100
C	-1.37578400	1.39925600	-1.31943800	C	3.73172100	3.60979000	-1.98468300
C	-0.85773000	0.23157600	-0.46988500	H	3.57454000	4.48447300	-1.35007900
H	-3.29767000	-1.08304500	-0.41165300	H	4.64383000	3.74923100	-2.56448600
H	-1.71380600	0.80443400	1.40394500	H	2.87759900	3.48092300	-2.64567100
H	-1.34315100	2.31355800	-0.71553200	C	-5.78608500	-1.58513700	2.72556900
H	-0.76993000	-0.67555000	-1.07677100	H	-5.67767300	-2.60075800	3.11001500
H	-3.52670700	1.93897100	0.04406500	H	-5.48032200	-0.87135400	3.48952600
O	-4.93321600	1.02448400	-1.03039500	H	-6.84196000	-1.43051600	2.49217000
H	-5.15399100	0.16226600	-1.44821300	O	0.23163100	3.15655400	4.36242700
O	-2.73953100	1.14303100	-1.70165900	H	0.10159500	2.24353900	1.40612100
O	-1.37923800	-1.23651400	1.42964200	H	1.19493100	3.15291800	4.37656800
H	-0.41188600	-1.33596100	1.35939200	O	-5.53084400	-1.46741800	-2.03585800
O	0.44245700	0.60174400	0.04476300	H	-6.41734900	-1.59284900	-2.39303200
C	1.49086100	-0.25692700	-0.27627200	H	-5.49777900	-1.93030300	-1.17111800
C	2.80970100	0.46484000	0.03815700	O	-0.53433600	2.86295500	1.78762800
C	4.00559600	-0.51151800	0.01067400	H	-0.26748700	2.96022500	2.73507500
C	3.68901200	-1.86312800	0.68749700	H	-0.17206700	4.43898200	0.98937600
C	2.35234600	-2.41382500	0.16833900	O	0.22809600	5.21471200	0.54387900
H	1.45260700	-0.54182600	-1.33692900	H	-0.09865400	5.17205000	-0.37206400
H	4.29930900	-0.70525900	-1.02849300	H	5.14294600	1.50003500	0.08916300
H	3.58733900	-1.68976300	1.76273700	O	-0.67603800	4.82553700	-2.12393800
H	2.38179800	-2.50859400	-0.92458000	H	-1.62396900	4.59137900	-2.26162100
H	2.73342700	0.87666000	1.04896400	H	-0.46335700	5.49252300	-2.78664800
O	5.06909600	0.15636800	0.70448200	O	-3.11192100	-1.33602600	-3.41472800
H	5.90215200	-0.39271800	0.71306600	H	-4.00506900	-1.54608800	-3.08386500
O	4.76090300	-2.77980200	0.52531800	H	-2.96566400	-0.43234500	-3.09808600
H	4.71420100	-3.21882100	-0.36039800	O	-3.22408300	3.91948900	-2.54202700
C	1.93564900	-3.78211000	0.73776900	H	-3.93222200	4.29682800	-2.00806500
H	0.86644300	-3.73894100	0.96464900	H	-3.30286900	2.95771500	-2.43132700
H	2.47538100	-3.99577100	1.66147900	O	-2.39209300	-0.48250200	3.95788800
O	2.20710100	-4.84783400	-0.16827400	H	-2.76893600	-1.20835300	4.46874300
H	1.49624600	-4.87805700	-0.85647300	H	-1.93554600	-0.90533700	3.20578400
O	1.35619800	-1.42754800	0.51101200	O	2.72594900	4.11892800	1.00941000
O	-0.59380500	0.86582400	5.57673400	H	1.88437700	4.57685600	0.79358900
H	0.13334800	0.24218100	5.67840100	H	3.25663400	4.78499400	1.45777300
H	-0.03987600	2.34111100	4.84615000	O	7.15244000	-1.48596200	0.84722600
O	-2.56182900	-3.60035300	0.29297900	H	7.53360100	-1.48491600	1.73293300
H	-2.15948400	-2.90630000	0.84287000	H	6.49414000	-2.20826100	0.84269700
H	-3.51016900	-3.39340700	0.30888800	O	4.38212800	-4.22089500	-1.70661300
H	-1.24004800	0.40455700	5.00049000	H	3.64209800	-4.65816700	-1.23142600
C	-0.56698000	1.62647200	-2.60910500	H	5.05441800	-4.89876400	-1.83767600
H	-0.24495500	0.67677200	-3.04001000	O	0.43788800	-4.95519300	-2.18876900
H	-1.21680000	2.11718900	-3.33934400	H	-0.14950000	-5.71735000	-2.14269200
O	0.59764500	2.41167900	-2.37976500	H	-0.16241100	-4.17519600	-2.25522500
H	0.29177700	3.33702800	-2.25531900	O	-1.24563800	-2.85977900	-2.02898100
N	-4.11037400	-0.45343100	1.37749700	H	-1.88222500	-2.40434800	-2.61880200
C	-4.99367100	-1.46900200	1.44920400	H	-1.77024200	-3.16252200	-1.25793000
H	-3.95375000	0.08845600	2.21856400				
O	-5.15629800	-2.28633800	0.52473100				
N	2.92076900	1.58302800	-0.92476000				

A_TS2 Structure

C	-1.82545200	0.02604100	0.66913400	C	3.90562600	2.55564800	-0.79807500
C	-3.28934400	-0.04169300	0.21138300	H	2.15576300	1.80471400	-1.41938900
C	-3.66062000	1.29476100	-0.47080900	O	5.14962400	2.26708200	-0.36574400
C	-1.39012100	1.60148400	-1.27139100	C	3.93376700	3.49333600	-1.98659900
C	-0.90537800	0.35839200	-0.51021000	H	4.59064000	4.33106000	-1.76028900
H	-3.40860500	-0.84116600	-0.51959900	H	4.32369900	2.94999500	-2.84871800
H	-1.72346000	0.82371100	1.41472500	H	2.93929300	3.86788300	-2.22506700
H	-1.27534900	2.47141800	-0.61464000	C	-5.87560800	-1.51169400	2.60338500
H	-0.85069500	-0.51041000	-1.17447500	H	-5.81163700	-2.56147400	2.89471700
H	-3.48414200	2.13062500	0.21596900	H	-5.52800300	-0.88386200	3.42281500
O	-4.95909600	1.38809700	-0.89925500	H	-6.92531200	-1.28801900	2.39996900
H	-5.22635300	0.58240600	-1.39475500	O	0.64616900	2.32431700	4.67106100
O	-2.78032100	1.46239800	-1.61612100	H	0.29124400	1.81029800	1.62262200
O	-1.46701500	-1.22202500	1.28555100	H	1.56696100	2.05163200	4.74573200
H	-0.50486600	-1.35746700	1.18492800	O	-5.68091600	-0.97666600	-2.12308600
O	0.40931100	0.65635200	0.01609800	H	-6.57516800	-1.03200400	-2.47851400
C	1.43474100	-0.22375000	-0.33945700	H	-5.65818900	-1.52063100	-1.30654800
C	2.78232900	0.42491100	0.02114400	O	-0.03706500	2.58589100	2.10162100
C	3.91882300	-0.62854000	0.02855300	H	0.21559400	2.46899000	3.05489100
C	3.51114900	-1.98452500	0.63471100	H	0.64584600	3.81127400	1.36728700
C	2.17997800	-2.44475100	0.02693300	O	1.16676000	4.49869800	0.84290600
H	1.39658100	-0.44755200	-1.41444100	H	0.63926000	4.74576700	0.04740800
H	4.23834700	-0.79994400	-1.00748600	H	5.17796800	1.40218300	0.12821800
H	3.36495000	-1.85555900	1.71116600	O	-0.25456200	4.98594500	-1.43753800
H	2.25799800	-2.47945400	-1.06757000	H	-1.23567400	4.89317200	-1.48230700
H	2.69189700	0.81665600	1.04231200	H	-0.03038700	5.77823700	-1.93958400
O	4.98824900	-0.04552900	0.78099900	O	-3.26883100	-0.83939800	-3.50748300
H	5.78130300	-0.63647200	0.78499400	H	-4.16956000	-1.04002500	-3.19149900
O	4.54311900	-2.95355400	0.48341000	H	-3.08535800	0.02546600	-3.11069200
H	4.52016700	-3.34438600	-0.42395700	O	-2.92134900	4.46906100	-1.71200200
C	1.67566500	-3.82159300	0.49639100	H	-3.56121400	4.75240700	-1.04936600
H	0.60764300	-3.73549900	0.71706200	H	-3.16001200	3.55553600	-1.93080400
H	2.19203900	-4.12967100	1.40628000	O	-2.48490100	-0.79067800	3.88524300
O	1.89836100	-4.83900900	-0.47714600	H	-2.89444800	-1.58043300	4.25705200
H	1.23142800	-4.74599900	-1.20182400	H	-2.01644500	-1.09567900	3.08475100
O	1.21788600	-1.43081900	0.37947100	O	3.34958400	3.59254000	0.40201800
O	-0.81758500	0.32639500	5.77563000	H	2.24293700	4.02041200	0.57842700
H	-0.24701500	-0.40160800	6.04497500	H	3.83579100	3.41542000	1.21638200
H	0.12581900	1.60462500	5.10275400	O	7.00714500	-1.84590100	0.94228100
O	-2.76751000	-3.44378800	-0.01314300	H	7.31992900	-1.89059300	1.85305400
H	-2.33662100	-2.80851500	0.58415800	H	6.27811900	-2.49477600	0.88455200
H	-3.70740500	-3.20419300	0.02583100	O	4.20968900	-4.28321200	-1.83894200
H	-1.41864500	-0.06178600	5.10373800	H	3.41241100	-4.68833700	-1.43284200
C	-0.63940400	1.86543000	-2.58966500	H	4.84606500	-4.99849900	-1.94800800
H	-0.43452900	0.92660700	-3.10819000	O	0.26111400	-4.60971100	-2.60682000
H	-1.29703500	2.46063500	-3.23226800	H	-0.31287600	-5.37442900	-2.72364600
O	0.60319300	2.52330500	-2.39598700	H	-0.34691600	-3.83351300	-2.60690500
H	0.40255500	3.43804100	-2.11386300	O	-1.45500900	-2.55629300	-2.28488700
N	-4.16456600	-0.34221900	1.33367500	H	-2.07720600	-2.02735100	-2.82630500
C	-5.09215600	-1.32005200	1.33066000	H	-1.98392400	-2.90967000	-1.53898000
H	-3.97994600	0.12101600	2.21466700				
O	-5.30122100	-2.04626500	0.34176500				
N	3.01487600	1.49657700	-0.96147700				

A_Int2 Structure

C	-1.82311600	0.02629200	0.66950200	C	3.88786000	2.57398700	-0.80291600
C	-3.29723300	-0.04589200	0.24598900	H	2.15544800	1.79129100	-1.47691200
C	-3.68725700	1.28841100	-0.42960400	O	5.21062200	2.23779900	-0.56449300
C	-1.43664200	1.60003400	-1.28174400	C	3.85914300	3.55629800	-1.96704100
C	-0.92850000	0.35996300	-0.52950400	H	4.51888400	4.39474700	-1.74017100
H	-3.43051600	-0.84682300	-0.48091500	H	4.21515600	3.06001200	-2.87043000
H	-1.70910000	0.82731300	1.41031200	H	2.85287800	3.93546700	-2.14294200
H	-1.31472300	2.47178500	-0.62924900	C	-5.81663500	-1.52836900	2.70013900
H	-0.88360100	-0.50901300	-1.19411200	H	-5.70650100	-2.57046900	3.00577000
H	-3.49714200	2.12561500	0.25209100	H	-5.47443700	-0.87573700	3.50223600
O	-4.99543300	1.37818300	-0.82827000	H	-6.87818200	-1.34780600	2.51753200
H	-5.27087000	0.57220400	-1.31866800	O	0.88124300	2.28327400	4.48556500
O	-2.83347100	1.45563800	-1.59440300	H	0.35196000	1.82808700	1.49165100
O	-1.44848900	-1.21691200	1.28343300	H	1.77470800	1.92578400	4.53129200
H	-0.48903200	-1.35420400	1.15500200	O	-5.73485400	-0.98952200	-2.03778900
O	0.39548900	0.66363300	-0.02962700	H	-6.63540800	-1.04872300	-2.37625900
C	1.42062300	-0.22180000	-0.39183700	H	-5.69499500	-1.53118500	-1.22041700
C	2.77159700	0.42666600	-0.04968800	O	0.10509300	2.61076300	2.01428800
C	3.90691700	-0.62788500	0.00870500	H	0.40793200	2.46417700	2.96127800
C	3.48648400	-1.97403500	0.62576400	H	0.65682900	3.69649000	1.39357600
C	2.16575400	-2.43938300	0.00071100	O	1.15364900	4.48882000	0.84512800
H	1.36670700	-0.44922800	-1.46505200	H	0.61573000	4.74602600	0.04280700
H	4.24984200	-0.81737800	-1.01696600	H	5.24263700	1.43579600	0.00807200
H	3.32165500	-1.83258100	1.69794600	O	-0.25625700	4.99699200	-1.34563200
H	2.26021100	-2.47777100	-1.09246500	H	-1.23971100	4.90424200	-1.36346700
H	2.68238900	0.85598500	0.95608100	H	-0.04520400	5.80545400	-1.82792800
O	4.95877500	-0.03139300	0.77541900	O	-3.34871600	-0.84794600	-3.46626000
H	5.73598400	-0.63484300	0.82859500	H	-4.24279900	-1.05218000	-3.13419700
O	4.51722700	-2.95108900	0.50608600	H	-3.16061700	0.01626100	-3.06988900
H	4.51620900	-3.34378200	-0.40011900	O	-2.91862500	4.49750000	-1.57316000
C	1.65714000	-3.81570800	0.46672100	H	-3.56306200	4.77826600	-0.91396800
H	0.58869400	-3.72938500	0.68523400	H	-3.19343800	3.61020200	-1.84762700
H	2.17149600	-4.12643200	1.37674300	O	-2.40096000	-0.72062300	3.89393100
O	1.88067000	-4.83247700	-0.50787400	H	-2.79859100	-1.49535900	4.30800500
H	1.22015700	-4.73169100	-1.23712100	H	-1.94728000	-1.05716000	3.09752600
O	1.19778400	-1.42535000	0.33451500	O	3.39682900	3.26743500	0.42192600
O	-0.70715300	0.47992000	5.70849800	H	2.04479000	4.10026900	0.56537100
H	-0.18572800	-0.25108100	6.05774500	H	4.15833400	3.72760800	0.79881200
H	0.30974700	1.63210600	4.96408000	O	6.96257000	-1.87139200	1.09856600
O	-2.77172500	-3.44467200	0.01490200	H	7.18575700	-1.90194800	2.03582400
H	-2.33198700	-2.80621400	0.60228200	H	6.22147800	-2.50010900	0.98915500
H	-3.71159200	-3.20862400	0.07109900	O	4.22654100	-4.29465000	-1.82007000
H	-1.31485000	0.06660800	5.05771500	H	3.41590100	-4.68968700	-1.43061100
C	-0.71830800	1.87041800	-2.61643300	H	4.85892100	-5.01649900	-1.90664000
H	-0.52155300	0.93295000	-3.14055100	O	0.24756100	-4.58104900	-2.64182500
H	-1.39523400	2.46317400	-3.24154300	H	-0.31167000	-5.35431100	-2.77304000
O	0.52696700	2.52969800	-2.45227300	H	-0.37545200	-3.81709700	-2.62685800
H	0.33935600	3.43741400	-2.14843700	O	-1.50382500	-2.56261000	-2.28562800
N	-4.14468500	-0.34796800	1.38902200	H	-2.13806600	-2.03478300	-2.81385400
C	-5.06965500	-1.32820900	1.40695600	H	-2.01664300	-2.91720400	-1.52928600
H	-3.93250400	0.10690600	2.26854100				
O	-5.30273700	-2.05197800	0.42174000				
N	3.02917900	1.45488400	-1.07338500				

P_Int1 Structure

C	1.50765300	0.08644800	-1.10012800	C	-4.49318700	1.94114300	-0.40985800
C	3.00671000	-0.15616500	-0.83433600	H	-4.94853700	-0.02251200	-0.32005100
C	3.56052400	0.91877900	0.12397100	O	-3.62869700	2.82839800	-0.59118700
C	1.42917600	1.37353300	1.08337100	C	-5.94385000	2.29185200	-0.19933700
C	0.70506300	0.35702400	0.18598000	H	-6.56537600	1.41360100	-0.03253700
H	3.11859600	-1.13253100	-0.36279900	H	-6.02175200	2.96515000	0.65702000
H	1.41194700	0.97522100	-1.73934400	H	-6.30432600	2.83298800	-1.07751500
H	1.51372000	2.32787000	0.55725600	C	5.26583400	-1.01284200	-3.79978500
H	0.56156500	-0.57950200	0.72300200	H	5.01372800	-0.08318400	-4.30899100
H	3.46362000	1.91590400	-0.31682500	H	6.34611700	-1.06369200	-3.65102500
O	4.88856600	0.76172100	0.47790200	H	4.97882500	-1.85826100	-4.42874700
H	5.09245100	-0.17622200	0.69535300	O	-1.65043000	4.98279200	-2.75779200
O	2.75531800	0.87262000	1.31889500	H	-2.62761000	5.14918600	-2.29393200
O	0.99599400	-1.04388200	-1.78961100	H	-1.22281400	5.82445700	-2.96842200
H	0.01717000	-1.05812000	-1.74015200	O	5.35633500	-1.91431300	0.87944200
O	-0.56384300	0.85188800	-0.27595800	H	6.23291500	-2.19596700	1.16440700
C	-1.78566000	0.51134500	0.39887900	H	5.24839200	-2.18938000	-0.05745800
C	-2.82519800	0.15472300	-0.70457800	O	-3.83007900	5.19526800	-1.67934300
C	-2.87924800	-1.36505700	-0.93956500	H	-3.90189100	4.32640400	-1.19156100
C	-3.02887800	-2.17736400	0.38474400	H	-3.88403500	5.89642700	-1.01848000
C	-2.71848500	-1.32142800	1.61058400	O	-1.81965700	3.97967100	1.38816700
H	-2.11262700	1.39572100	0.95280400	H	-1.17077500	4.05183800	0.67042900
H	-3.75206200	-1.58935800	-1.56303800	H	-2.59434300	3.63629200	0.92003100
H	-2.28666000	-2.97551800	0.36170900	O	2.95024400	4.68592400	1.58406900
H	-3.55056700	-0.64156200	1.83076100	H	3.72768700	4.15533800	1.85723800
H	-2.48453200	0.63847700	-1.62118800	H	2.24052800	4.26420100	2.09653400
O	-1.68644100	-1.71406300	-1.63996900	O	3.03363200	-1.83402500	2.39834000
H	-1.63708700	-2.69378200	-1.71018500	H	3.87827900	-2.04365500	1.95755500
O	-4.32081900	-2.76427300	0.53734600	H	2.89168200	-0.89171800	2.21419300
H	-4.24663100	-3.70563100	0.24877300	O	4.62560300	2.73664200	2.65395700
C	-2.45340700	-2.14368000	2.87271300	H	3.77206600	2.35933700	2.91855500
H	-3.42306400	-2.46153800	3.26143900	H	4.94351300	2.10455500	1.98860300
H	-1.99119800	-1.48280400	3.61640600	O	2.31438900	4.08065300	-0.95797300
O	-1.69936400	-3.32271100	2.66823100	H	2.59953100	4.39545700	-0.06155800
H	-0.76186800	-3.12073000	2.49287700	H	2.77042600	4.62441400	-1.60890200
O	-1.54311900	-0.54341200	1.29721400	O	-6.38919300	-1.15896600	-0.17124200
O	-0.29862900	3.70350300	-1.07588800	H	-5.78179500	-1.87631200	0.11087800
H	-0.43854800	2.74084000	-1.03476900	H	-6.70497300	-1.42309200	-1.04255300
H	-1.05054400	4.44427700	-2.09659100	O	-1.49534800	-4.46960400	-1.65115700
O	2.27075400	-3.54493600	-2.01321900	H	-1.35478400	-4.86968200	-2.51716900
H	1.81100800	-2.68477400	-1.97525600	H	-0.67492200	-4.67611900	-1.10945500
H	3.20340900	-3.32280500	-1.86834400	O	-3.76873200	-5.26516300	-0.29996300
H	0.68509700	3.87238100	-1.08238600	H	-2.96449500	-5.08693300	-0.83485700
C	0.77978900	1.63669300	2.42705000	H	-3.45671000	-5.78772300	0.44754100
H	-0.23304600	2.01474000	2.26717300	O	0.99782700	-3.56373700	2.16164500
H	0.73986200	0.72196400	3.02621000	H	1.19278100	-4.21116600	2.84924400
O	1.57528200	2.63541200	3.08944700	H	1.73839300	-2.90857600	2.20650700
H	1.18015600	2.81804600	3.94939300	O	0.70853100	-4.93070500	-0.27760900
N	3.74998900	-0.18500900	-2.08748000	H	0.77978700	-4.45934600	0.57642800
C	4.59074000	-1.16779100	-2.46139100	H	1.38358800	-4.50963600	-0.85503100
H	3.63572100	0.59914100	-2.71480900				
O	4.79792500	-2.17699600	-1.76216500				
N	-4.16982500	0.64396900	-0.38922100				

P_TS2 Structure

C	1.55027800	-0.38114500	1.01513300	C	-4.83880400	-1.84046300	0.43966600
C	3.03949000	-0.06999200	0.78022300	H	-5.05629700	0.05634500	-0.28394700
C	3.63050500	-1.05642100	-0.24861500	O	-4.07336000	-2.70773400	0.89029400
C	1.52566000	-1.49603300	-1.26431600	C	-6.30746200	-2.10103400	0.22708600
C	0.77448500	-0.55745600	-0.30630500	H	-6.78459700	-1.32539000	-0.36929400
H	3.11402100	0.93874900	0.37477700	H	-6.42571200	-3.07175700	-0.25591700
H	1.47488100	-1.33111100	1.56248900	H	-6.79419300	-2.15351700	1.20475000
H	1.60441000	-2.48832700	-0.81057600	C	5.22413600	0.64701600	3.83693700
H	0.64663700	0.41702300	-0.77481300	H	5.02944100	-0.34043800	4.25415200
H	3.57853100	-2.08285600	0.13209200	H	6.30052300	0.79195100	3.73047700
O	4.95290300	-0.81621500	-0.58345300	H	4.85416600	1.40825000	4.52763200
H	5.08765800	0.13633100	-0.78401800	O	-1.47279900	-3.86877400	3.25125900
O	2.83729000	-0.95838700	-1.43811700	H	-2.35404900	-4.28043100	3.08709700
O	0.99468900	0.66468000	1.79629100	H	-0.99223300	-4.49471800	3.80359000
H	0.02357600	0.68456700	1.68736900	O	5.26594600	1.92687700	-0.78133000
O	-0.53695100	-1.03558100	0.05681200	H	6.09938500	2.30460700	-1.08428300
C	-2.17823500	-0.68843300	-0.80113300	H	5.21086800	2.07068900	0.19059900
C	-3.00198900	-0.22559300	0.38997700	O	-3.92818400	-4.85218200	2.59646900
C	-2.84790500	1.27306500	0.67188300	H	-4.17201900	-4.14372800	1.96832300
C	-2.86208300	2.16622300	-0.59601100	H	-3.84552700	-5.64587200	2.05643900
C	-2.20996300	1.55381500	-1.84095100	O	-2.33734500	-3.97118700	-1.06055400
H	-2.26652000	-1.73522400	-1.08395400	H	-1.57723000	-3.97501600	-0.45142000
H	-3.69533200	1.58190500	1.29208600	H	-3.07615000	-3.76842800	-0.46805700
H	-2.27980600	3.05579900	-0.35656000	O	2.98259700	-4.76457400	-1.84516700
H	-2.90270000	1.66374900	-2.67382900	H	3.77204400	-4.22413900	-2.05498800
H	-2.66735600	-0.78289300	1.26271300	H	2.30204500	-4.33393400	-2.38754100
O	-1.62584100	1.45124000	1.37840400	O	2.75037300	2.51236700	-1.71017800
H	-1.58991900	2.39722800	1.65502200	H	3.69413600	2.44647900	-1.45642500
O	-4.17927500	2.60259800	-0.92481100	H	2.62012700	1.82976600	-2.37735500
H	-4.29652200	3.46058900	-0.45153300	O	4.72774000	-2.78604800	-2.77474200
C	-0.88284100	2.21188100	-2.20820100	H	3.89000300	-2.38367100	-3.05184100
H	-0.43446200	1.66604300	-3.04725200	H	5.05176700	-2.16328400	-2.10364100
H	-0.20022900	2.16389400	-1.35289700	O	2.20939700	-4.25077600	0.70309900
O	-1.16769800	3.55370200	-2.54658600	H	2.52323900	-4.54248400	-0.18803900
H	-0.37237400	4.07645800	-2.32029300	H	2.59970700	-4.85200200	1.34594200
O	-1.96494700	0.08876200	-1.81382900	O	-6.41798300	1.04745700	-1.11217500
O	-0.35748500	-3.43839000	0.87687300	H	-5.71666800	1.72122000	-1.20821600
H	-0.48498300	-2.00723300	0.40602400	H	-6.99286400	1.39459600	-0.42039900
H	-0.74129600	-3.61294100	1.78029400	O	-1.71232900	4.13550900	1.90995100
O	2.17912100	3.19807800	2.26760500	H	-1.74715400	4.36731900	2.84542500
H	1.75227900	2.33284700	2.12734900	H	-0.85593700	4.52621500	1.55641800
H	3.11479400	3.03771800	2.07249400	O	-3.99419800	4.90660000	0.48390500
H	0.55314400	-3.82369400	0.85291200	H	-3.20909700	4.73554600	1.04612900
C	0.91258200	-1.65057000	-2.64227200	H	-3.73281100	5.63329400	-0.09290100
H	-0.12742600	-1.97408400	-2.55337300	O	1.18023500	4.69322700	-1.69215900
H	0.94888200	-0.69751500	-3.17910700	H	1.56296800	5.43454400	-2.17424000
O	1.68622600	-2.64224500	-3.33333900	H	1.83509800	3.95524200	-1.74241200
H	1.33756800	-2.73713600	-4.22689800	O	0.59349500	5.03807900	1.03171900
N	3.76984600	-0.10751000	2.04050800	H	0.76052600	4.97883900	0.07120500
C	4.57413700	0.87100700	2.49582500	H	1.24723400	4.43205100	1.44644500
H	3.66929900	-0.93420200	2.61297600				
O	4.76469900	1.93083800	1.87064400				
N	-4.38841500	-0.60568900	0.12580000				

P_Int2 Structure

C	0.65991600	-1.04730200	0.15839400	C	-4.37534200	-1.33644000	-1.51240700
C	1.97152900	-1.23513300	0.95206100	H	-4.83359900	0.58028000	-2.06254800
C	3.19228200	-1.41938900	0.02898700	O	-3.61727700	-2.11580100	-0.89762900
C	2.10946600	-0.38870900	-1.83053800	C	-5.61582700	-1.83878800	-2.20108200
C	0.80924600	-0.12589500	-1.05885400	H	-5.33153400	-2.62626500	-2.90192100
H	2.14557300	-0.33920500	1.54717600	H	-6.27148100	-2.28564500	-1.45012400
H	0.34515700	-2.02785900	-0.19798200	H	-6.15084400	-1.05030800	-2.72749600
H	2.09507000	-1.38846900	-2.28297700	C	1.70495600	-3.56755400	3.96574100
H	0.84906300	0.90584200	-0.70330400	H	2.61805100	-3.84784700	4.49532100
H	3.12879800	-2.35086300	-0.54412500	H	0.93685300	-3.36870000	4.71570300
O	4.40148300	-1.43555700	0.70392300	H	1.38736500	-4.39611200	3.33303700
H	4.41762800	-0.74270000	1.41234700	O	-2.24951400	-2.26343000	1.65203600
O	3.19495600	-0.32314200	-0.89605500	H	-2.05226500	-3.22132300	1.63576200
O	-0.35525400	-0.51904700	1.01387700	H	-2.87857600	-2.13302400	0.92440600
H	-0.99003800	-1.23307500	1.28438500	O	4.30531900	0.32182300	2.74125000
O	-0.32491200	-0.22345000	-1.91964600	H	5.10913600	0.38982400	3.26818100
C	-2.13459400	1.30284000	-1.88808300	H	3.66317700	-0.17764900	3.28591700
C	-3.04358000	0.63442900	-0.90730900	O	-1.84049300	-4.98428500	1.20069600
C	-3.52231000	1.60683800	0.18503800	H	-2.62391700	-5.09130600	0.60419700
C	-2.31105600	2.37789900	0.73285300	H	-1.91520800	-5.65096000	1.89203600
C	-1.57342100	3.15121200	-0.37428700	O	-3.95808200	-4.87972200	-0.46656900
H	-2.08468800	0.95678500	-2.91392300	H	-4.79580200	-5.06266900	-0.02649500
H	-4.23511700	2.32088200	-0.24974200	H	-3.97695300	-3.92338400	-0.66654000
H	-1.63661500	1.64461100	1.18390900	O	4.63105400	-2.26667900	-3.19763000
H	-2.12868000	4.05267900	-0.63237700	H	5.30636200	-1.95170800	-2.56820300
H	-2.43825400	-0.13852500	-0.42099300	H	4.21417700	-1.44240300	-3.49626000
O	-4.13117200	0.81949200	1.17548600	O	5.22162800	1.40642200	-1.65745700
H	-4.66401100	1.41213400	1.74906900	H	5.00734900	2.35962400	-1.56140200
O	-2.74800600	3.31196900	1.70317000	H	4.56111300	0.94252900	-1.11499200
H	-2.04318900	3.37220800	2.40191300	O	6.45429200	-1.16148100	-1.27805900
C	-0.10151500	3.49447800	-0.12853200	H	6.35855900	-0.21330500	-1.46250000
H	0.34449600	3.75705400	-1.09216500	H	5.86060100	-1.30287500	-0.51873900
H	0.41753300	2.61569700	0.26798900	O	0.44495800	-4.32851900	-0.10879000
O	-0.01244000	4.58185000	0.78033000	H	0.94626900	-5.08198800	-0.44071300
H	0.89856800	4.93041300	0.70087900	H	-0.32243300	-4.70492600	0.37896200
O	-1.53684300	2.39075500	-1.67631100	O	-6.11170900	1.58270900	-2.84237900
O	-1.04672900	-2.84799700	-2.10006200	H	-6.71686400	2.04564400	-2.25157000
H	-0.55271800	-1.17919600	-2.05316700	H	-5.83624600	2.24225400	-3.48934100
H	-1.91581300	-2.78438000	-1.67242300	O	-5.31612600	2.79125600	2.66373300
O	0.58060700	1.03142900	3.13758700	H	-5.29260500	2.59895000	3.60812700
H	0.17753900	0.48521500	2.43489100	H	-4.46305500	3.22488000	2.47467900
H	1.15400200	0.41545600	3.61834900	O	-0.63717200	3.48962400	3.30221300
H	-0.51734300	-3.43739100	-1.52758500	H	-0.19096800	3.96674800	2.57905200
C	2.35500100	0.64868800	-2.92314800	H	-0.17309800	2.62830300	3.36736600
H	1.52483000	0.60729200	-3.62856200	O	2.67432000	5.27394900	0.48158500
H	2.37487800	1.64868900	-2.47268100	H	3.10725100	5.13224500	1.33381600
O	3.55969200	0.40830000	-3.64471300	H	2.81128900	6.21016500	0.28550100
H	4.28461700	0.77950900	-3.10082400	O	4.31376500	4.00370200	-1.53444000
N	1.81280500	-2.36216000	1.86132000	H	3.87959900	4.23432000	-2.36261100
C	1.96636000	-2.29580400	3.19608900	H	3.72545400	4.34342400	-0.83643900
H	1.48940300	-3.22980500	1.43850300				
O	2.30190200	-1.25568400	3.79326600				
N	-4.13287500	-0.01725400	-1.60354700				

P.Int1 (Applied Force = 0.0 nN, Pulling Direction A) Structure

C	1.74739600	-0.25707400	0.81824000	C	-4.50224000	-2.08010600	0.30969300
C	3.25151300	-0.06116100	0.52491800	H	-4.80469500	-0.15590600	-0.34191900
C	3.88350100	-1.17651900	-0.36116000	O	-3.68579500	-2.89970300	0.75973300
C	1.65533000	-1.79858000	-1.14660400	C	-5.92611000	-2.45014500	-0.01571900
C	0.95570800	-0.61497400	-0.45011500	H	-6.36187000	-1.77444800	-0.75214300
H	3.32439600	0.85816200	-0.05529700	H	-5.94959400	-3.47512100	-0.38541600
H	1.63029000	-1.08254200	1.53117000	H	-6.51776000	-2.40772000	0.90328100
H	1.70714400	-2.64386900	-0.45917500	C	5.22632700	1.40946500	3.43986900
H	0.88984400	0.24197800	-1.12074700	H	5.20906800	0.46940100	3.99054300
H	4.12654800	-2.13863700	0.14932400	H	6.25154500	1.77323400	3.36303300
O	5.10230300	-0.77839800	-0.90022100	H	4.64774300	2.15561300	3.99069600
H	5.03503300	0.13443900	-1.25254500	O	-1.59951200	-3.25146900	3.47144100
O	2.98503300	-1.37459800	-1.46645400	H	-2.30845900	-3.91284100	3.28353100
O	1.23892000	0.94411300	1.38608700	H	-1.08644600	-3.60666900	4.20547000
H	0.26547300	0.90466300	1.41843700	O	4.96543800	1.99928400	-1.42396200
O	-0.39931400	-0.89380300	0.03407700	H	5.74299600	2.39937300	-1.83054300
C	-1.88477500	-0.58021200	-0.73290000	H	5.00282900	2.21072900	-0.46286800
C	-2.83247800	-0.26773300	0.43555200	O	-3.55428300	-4.91856500	2.61022100
C	-2.91123200	1.23979800	0.74267800	H	-3.77985100	-4.31057700	1.87794200
C	-3.24419700	2.05070900	-0.53731100	H	-3.16137700	-5.68800800	2.18310400
C	-2.25473600	1.72624800	-1.65531700	O	-1.73857400	-4.06567200	-1.02045300
H	-2.01095900	-1.57788800	-1.14483800	H	-1.15422600	-3.94687700	-0.25416700
H	-3.72388600	1.38540500	1.46184100	H	-2.60443300	-3.87672100	-0.63133700
H	-3.26326200	3.14297200	-0.36876800	O	3.20510000	-4.90277000	-0.88335300
H	-2.77067000	1.81842600	-2.61067800	H	3.99053200	-4.45984700	-1.26120300
H	-2.47434600	-0.78649700	1.32349400	H	2.52013800	-4.67785600	-1.53489100
O	-1.66558200	1.62158800	1.30729800	O	2.43787000	2.96424200	-2.08037900
H	-1.78895100	2.54036700	1.64134700	H	3.36962000	2.71785400	-1.90740000
O	-4.59893200	1.74953700	-0.93383100	H	2.23413800	2.59855700	-2.94765100
H	-5.13210100	2.38861000	-0.42495300	O	4.88201900	-3.31115500	-2.51083700
C	-1.02511800	2.62645400	-1.67537800	H	4.00421900	-3.02554500	-2.80893500
H	-0.34384400	2.23977400	-2.44228700	H	5.24290100	-2.50456600	-2.11146000
H	-0.51609800	2.59306000	-0.70775700	O	2.26117300	-3.86075600	1.44996300
O	-1.47255200	3.93494100	-1.98569000	H	2.65046200	-4.33385600	0.67494700
H	-0.68945000	4.51324800	-1.90876000	H	2.54782000	-4.33207100	2.23936000
O	-1.75742300	0.31979900	-1.69808500	O	-6.48787800	0.11811200	-2.32902900
O	-0.28166900	-3.03791800	1.22916800	H	-5.78322100	0.75100800	-2.12249600
H	-0.39473200	-1.84199300	0.59294900	H	-7.24742800	0.45446400	-1.84069100
H	-0.77239900	-3.11315100	2.10524000	O	-2.29681400	4.19181700	1.92649400
O	2.12761400	3.50906400	2.12034800	H	-2.34101300	4.40259200	2.86648600
H	1.84077800	2.60606700	1.89359300	H	-1.46523000	4.63061700	1.59443300
H	3.00550700	3.57036800	1.72012900	O	-5.05749900	3.94251200	0.88667800
H	0.63720800	-3.39489200	1.36020700	H	-4.18492500	4.15725800	1.26447700
C	1.01977300	-2.26938900	-2.44053900	H	-5.35490400	4.76244300	0.47701000
H	-0.01298500	-2.57716300	-2.25436000	O	0.95041400	5.15739300	-1.50389800
H	1.03838100	-1.46473500	-3.18255400	H	1.26993800	5.94842300	-1.95060100
O	1.79315800	-3.39143600	-2.89581900	H	1.59281700	4.43625200	-1.70472800
H	1.39146100	-3.73610800	-3.70107300	O	0.08408600	5.15449000	1.17254700
N	3.99246500	0.15883900	1.75580100	H	0.33774900	5.23768100	0.23418800
C	4.63861400	1.30639800	2.05558000	H	0.80445400	4.61732500	1.56477300
H	3.95964700	-0.56352700	2.46164200				
O	4.72484000	2.25777800	1.26236000				
N	-4.15301100	-0.79399300	0.10103600				

P.Int1 (Applied Force = 0.5 nN, Pulling Direction A) Structure

C	1.61480200	-0.15335800	0.82844300	C	-4.64534000	-1.86625800	0.12629800
C	3.09623300	0.05133900	0.47435500	H	-4.72128800	0.10391700	-0.39668700
C	3.62852600	-1.10900400	-0.39463500	O	-3.94763800	-2.79284600	0.58819500
C	1.43188500	-1.72512600	-1.11616900	C	-6.06417700	-2.08334700	-0.32803300
C	0.76201800	-0.54776200	-0.38897200	H	-6.40449300	-1.28722100	-0.99030000
H	3.17745900	0.97454400	-0.09986900	H	-6.12963800	-3.04682600	-0.83420200
H	1.54048300	-0.97415400	1.55635700	H	-6.71176500	-2.12225800	0.55260900
H	1.53087900	-2.57180600	-0.43060300	C	5.32767700	1.28198600	3.32822000
H	0.68972500	0.29334500	-1.07779200	H	5.25836400	0.33042400	3.85510900
H	3.68479800	-2.04355600	0.18025800	H	6.37476300	1.56354200	3.21298000
O	4.90363500	-0.88618500	-0.89763800	H	4.83631800	2.05477000	3.92510500
H	4.97420600	0.02581200	-1.25376100	O	-1.91572900	-4.23070200	3.24301200
O	2.73886000	-1.27981000	-1.50063900	H	-2.84317900	-4.56632300	2.79639800
O	1.12502400	1.04516000	1.40820600	H	-1.51832000	-4.93225100	3.77693000
H	0.14750400	1.00442200	1.47367800	O	5.16167000	1.83881700	-1.46042300
O	-0.52164200	-0.83493800	0.18291200	H	6.00198400	2.13173000	-1.83175300
C	-1.76166600	-0.63735900	-0.56058400	H	5.16798200	2.07982700	-0.50441700
C	-2.81675300	-0.26544700	0.50054300	O	-4.03948700	-4.87070000	2.19423500
C	-2.78549500	1.22694200	0.85545500	H	-4.20005400	-4.14821900	1.53406500
C	-2.89853200	2.10462200	-0.40860400	H	-4.01057000	-5.69890300	1.69979100
C	-1.98587500	1.66556300	-1.55513200	O	-1.91548300	-4.18545700	-0.96355700
H	-2.00891400	-1.60151500	-1.00497000	H	-1.29189600	-4.12179900	-0.22298100
H	-3.65990500	1.43780900	1.48086800	H	-2.71999400	-3.79658100	-0.58927800
H	-2.62279500	3.13017600	-0.16294600	O	2.93792800	-4.95365800	-1.00268000
H	-2.52270600	1.86195900	-2.48488800	H	3.71294200	-4.49754300	-1.38932200
H	-2.60492800	-0.85210700	1.39367700	H	2.22618600	-4.66255800	-1.59744800
O	-1.59645000	1.51248400	1.58366700	O	2.77983400	3.04244300	-2.17461500
H	-1.66400300	2.45281300	1.86780500	H	3.67858900	2.69517600	-2.00089400
O	-4.27438900	2.14232600	-0.82841200	H	2.52257600	2.69036500	-3.03272600
H	-4.65725000	2.88883800	-0.32160900	O	4.57380900	-3.29920500	-2.56477300
C	-0.69519800	2.48301800	-1.60003500	H	3.69820800	-2.98935800	-2.84526000
H	-0.04387300	2.04915900	-2.36874000	H	4.93480700	-2.52375600	-2.10510100
H	-0.17424600	2.43639500	-0.63745000	O	2.20654100	-3.99607700	1.41714000
O	-1.06438400	3.81451500	-1.92339600	H	2.52740000	-4.42948600	0.58665500
H	-0.27511900	4.37501200	-1.79517300	H	2.62711000	-4.45091000	2.15439400
O	-1.66489500	0.24713300	-1.62717000	O	-6.30167200	0.80359600	-2.25045700
O	-0.38952000	-3.47432400	1.41013400	H	-5.53940500	1.34558200	-1.98765500
H	-0.44578200	-2.52886500	1.17503300	H	-7.02187400	1.14850200	-1.71114600
H	-1.24237000	-3.91498600	2.50768200	O	-1.97297500	4.18719200	2.07077000
O	2.30979000	3.42913900	2.26164900	H	-2.03527900	4.44650800	2.99750800
H	1.91293400	2.57280700	2.01145200	H	-1.12917600	4.60130700	1.73100600
H	3.15320200	3.43800600	1.78758700	O	-4.54764500	4.38883000	0.80283500
H	0.57721200	-3.71470100	1.46999800	H	-3.68926000	4.42198700	1.26943700
C	0.73307200	-2.20664200	-2.37183800	H	-4.56763600	5.19356700	0.27277600
H	-0.27852800	-2.53890400	-2.12611000	O	1.29229900	5.13654300	-1.36886900
H	0.69120100	-1.40301700	-3.11358900	H	1.53799400	5.94398200	-1.83277100
O	1.49760400	-3.31577500	-2.87961500	H	1.94534700	4.44622900	-1.63369700
H	1.06378300	-3.64794200	-3.67344200	O	0.38383900	5.15842200	1.29687400
N	3.88974900	0.20931300	1.68736400	H	0.64312300	5.21708500	0.35835900
C	4.67339500	1.26748000	1.96971000	H	1.08830200	4.60706600	1.70114700
H	3.82093100	-0.52055400	2.38282000				
O	4.82744600	2.22027300	1.18528300				
N	-4.15558200	-0.62153400	0.02974000				

P.Int1 (Applied Force = 1.0 nN, Pulling Direction A) Structure

C	1.63308800	-0.14730000	0.82685900	C	-4.60674000	-1.89576100	0.18673100
C	3.11627300	0.04895600	0.47144400	H	-4.71489200	0.05977900	-0.39100000
C	3.66272300	-1.11719400	-0.38554700	O	-3.89214500	-2.79799200	0.67115900
C	1.45253200	-1.75072800	-1.08243700	C	-6.02449700	-2.14679000	-0.25378300
C	0.78213300	-0.55302500	-0.38769700	H	-6.37460200	-1.38209800	-0.94747700
H	3.19251600	0.96226800	-0.11900900	H	-6.08134300	-3.13044200	-0.72050500
H	1.55485900	-0.95811700	1.56516100	H	-6.67002700	-2.15573500	0.62915200
H	1.54850500	-2.57789500	-0.37355400	C	5.31647000	1.36977400	3.30664500
H	0.71976100	0.27583400	-1.09321800	H	5.26079800	0.42712900	3.85080800
H	3.76708000	-2.04791900	0.19414700	H	6.35925600	1.66600900	3.18882200
O	4.92244600	-0.86343900	-0.91465900	H	4.81117100	2.14563000	3.88766100
H	4.96048400	0.04555300	-1.28255800	O	-1.85469300	-4.19209900	3.33370200
O	2.76152000	-1.31935200	-1.47783900	H	-2.78300000	-4.54105500	2.89329100
O	1.14344300	1.05999800	1.39085100	H	-1.44631300	-4.88549700	3.86997100
H	0.16617000	1.02339300	1.44563500	O	5.10746400	1.86894900	-1.50181200
O	-0.50695600	-0.81597000	0.18543100	H	5.94102900	2.17088200	-1.88116600
C	-1.74794700	-0.62271400	-0.55919200	H	5.11964700	2.11404000	-0.54692700
C	-2.80446400	-0.25066700	0.50191400	O	-3.97336500	-4.85833200	2.29667300
C	-2.80601400	1.25086500	0.82425800	H	-4.13622300	-4.14329600	1.62806200
C	-2.96613000	2.09380200	-0.45889900	H	-3.93843500	-5.69185300	1.81162500
C	-2.01567800	1.67077300	-1.57948900	O	-1.87199800	-4.20799800	-0.87805500
H	-1.99226900	-1.58979800	-0.99952100	H	-1.24458400	-4.12955800	-0.14235000
H	-3.67173800	1.45197900	1.46500900	H	-2.67402200	-3.81143300	-0.50659700
H	-2.77106600	3.14671900	-0.24508300	O	3.00020000	-4.94626700	-0.89178000
H	-2.53461700	1.84216700	-2.52435500	H	3.76969600	-4.49807700	-1.29754400
H	-2.57160100	-0.81128200	1.40638300	H	2.28258800	-4.67926100	-1.49096500
O	-1.60645800	1.57805600	1.51613000	O	2.72053300	3.06150800	-2.23165300
H	-1.69338500	2.51941300	1.79088000	H	3.61788300	2.71512400	-2.04900800
O	-4.34129400	2.03259300	-0.88763700	H	2.47794200	2.72083600	-3.09860800
H	-4.77054500	2.76458400	-0.39986100	O	4.60973000	-3.32720800	-2.52472300
C	-0.74267300	2.51550800	-1.60188300	H	3.72662300	-3.03497600	-2.80047500
H	-0.06948900	2.09261800	-2.35738400	H	4.96863300	-2.53498700	-2.09328100
H	-0.23852500	2.47917800	-0.63027300	O	2.25685800	-3.93763800	1.50516200
O	-1.13066900	3.83957800	-1.93557100	H	2.58417100	-4.38750900	0.68621400
H	-0.34191900	4.40597900	-1.83412500	H	2.67416200	-4.37566900	2.25437300
O	-1.65457200	0.25915800	-1.62929600	O	-6.31793100	0.64185200	-2.35853100
O	-0.34603800	-3.43990100	1.48052600	H	-5.56545700	1.19006500	-2.08269600
H	-0.41807900	-2.50056500	1.22783800	H	-7.05206100	0.98706600	-1.83861800
H	-1.19044300	-3.87678300	2.59215500	O	-2.05719000	4.24317800	1.97234300
O	2.27072900	3.48742700	2.19584200	H	-2.12524900	4.51089100	2.89626400
H	1.89446000	2.61749500	1.96221300	H	-1.21163100	4.65438800	1.63585500
H	3.11667600	3.50230600	1.72673000	O	-4.68320700	4.30397200	0.73872000
H	0.62389000	-3.66492000	1.54566600	H	-3.81955000	4.38858500	1.18696200
C	0.75642100	-2.26616500	-2.32587700	H	-4.76224300	5.10661200	0.21104500
H	-0.25485700	-2.59303500	-2.07165500	O	1.23844900	5.16739400	-1.44405600
H	0.71447700	-1.48272700	-3.08909500	H	1.48517000	5.96965300	-1.91620300
O	1.52339600	-3.38712500	-2.80319900	H	1.88824200	4.47216300	-1.70427200
H	1.08395900	-3.74955500	-3.58046700	O	0.32015300	5.19318100	1.21777300
N	3.90924200	0.23705100	1.67962600	H	0.58682600	5.25363000	0.28152100
C	4.66578000	1.31907700	1.94729100	H	1.02352000	4.64462000	1.62707700
H	3.85448700	-0.48323500	2.38622100				
O	4.79921900	2.26263500	1.14852000				
N	-4.13818500	-0.64737200	0.05134100				

P.Int1 (Applied Force = 1.5 nN, Pulling Direction A) Structure

C	1.64753900	-0.14568300	0.82691300	C	-4.55504800	-1.93576900	0.23445100
C	3.13289800	0.04608600	0.47419900	H	-4.71692700	0.00164000	-0.39011900
C	3.69474900	-1.11706900	-0.38188100	O	-3.81329900	-2.80759200	0.73483000
C	1.47143600	-1.75955900	-1.06536800	C	-5.96848900	-2.23466800	-0.18957800
C	0.79997100	-0.55027900	-0.38971700	H	-6.34301200	-1.49663600	-0.89916400
H	3.20471100	0.95451800	-0.12397100	H	-6.00262300	-3.23050600	-0.63209300
H	1.56379100	-0.95360800	1.56743700	H	-6.60781900	-2.23897300	0.69787600
H	1.56159600	-2.57626100	-0.34433600	C	5.29507500	1.43894600	3.30123400
H	0.74859500	0.27416300	-1.10226100	H	5.25418000	0.50214500	3.85657600
H	3.84644200	-2.04859000	0.19205400	H	6.33269800	1.75340200	3.18477700
O	4.93814500	-0.82656000	-0.93350700	H	4.77242200	2.21231000	3.87009500
H	4.94051400	0.08069500	-1.30679300	O	-1.75457600	-4.30801600	3.35545200
O	2.78391900	-1.33909700	-1.46347000	H	-2.70000000	-4.62143300	2.91031300
O	1.15661600	1.06472400	1.38611500	H	-1.33665300	-5.04174400	3.82685000
H	0.17966800	1.02934200	1.42966200	O	5.03693600	1.91920600	-1.52754700
O	-0.49466400	-0.79570600	0.17989100	H	5.86366400	2.23287100	-1.91245800
C	-1.73477900	-0.59750000	-0.56554600	H	5.05653100	2.15912800	-0.57152000
C	-2.79492300	-0.23775100	0.49764000	O	-3.89283900	-4.89229100	2.32150700
C	-2.83200800	1.26768200	0.80487700	H	-4.04833500	-4.15890700	1.66884100
C	-3.02736400	2.09381400	-0.48488300	H	-3.88065200	-5.71625300	1.81908600
C	-2.04660800	1.69653700	-1.58873300	O	-1.81290800	-4.22847500	-0.83858300
H	-1.97606600	-1.56180500	-1.01422600	H	-1.17610800	-4.14694200	-0.11135800
H	-3.69317700	1.45267500	1.45663800	H	-2.60674500	-3.82112600	-0.46162700
H	-2.90091800	3.16289900	-0.28732500	O	3.07547500	-4.92330800	-0.85810900
H	-2.55419600	1.84932100	-2.54304900	H	3.83674100	-4.47448800	-1.27801000
H	-2.53908000	-0.77880200	1.40751800	H	2.34876700	-4.66995100	-1.45248400
O	-1.62837300	1.62328600	1.47589200	O	2.65163800	3.12086700	-2.27163300
H	-1.73281000	2.56217000	1.75182900	H	3.54394000	2.76789500	-2.07744100
O	-4.39625900	1.95646700	-0.92194600	H	2.42411000	2.79516500	-3.14833000
H	-4.86488100	2.66495400	-0.43812700	O	4.65002600	-3.30675100	-2.53197900
C	-0.79443800	2.57130900	-1.59247700	H	3.75831000	-3.02749000	-2.79301900
H	-0.10270200	2.16573600	-2.34029000	H	5.00523300	-2.50733100	-2.11111000
H	-0.30166800	2.54162700	-0.61501900	O	2.33499800	-3.90015600	1.53363100
O	-1.20673900	3.88822000	-1.92741000	H	2.66455900	-4.35383100	0.71765900
H	-0.42234400	4.46328000	-1.84454300	H	2.75432000	-4.33145700	2.28565200
O	-1.64178300	0.29459200	-1.62851600	O	-6.33641200	0.48591000	-2.37350200
O	-0.27867300	-3.45209600	1.50956400	H	-5.59742600	1.05945600	-2.11419300
H	-0.37875600	-2.51301700	1.27153400	H	-7.07917200	0.82933100	-1.86478900
H	-1.10991800	-3.94729700	2.62295700	O	-2.14119700	4.27605500	1.93252500
O	2.22576000	3.52869800	2.15530600	H	-2.20892600	4.54392800	2.85638200
H	1.87051000	2.64762000	1.93153500	H	-1.29664600	4.68786000	1.59661600
H	3.07482600	3.55349000	1.69257400	O	-4.80517300	4.22337500	0.73603100
H	0.69702400	-3.65097800	1.57256300	H	-3.93855700	4.34929900	1.16720500
C	0.77933900	-2.29044400	-2.30423300	H	-4.93959200	5.02795600	0.22281100
H	-0.23114500	-2.61695500	-2.04639200	O	1.16713700	5.22380900	-1.47549500
H	0.73640000	-1.51552800	-3.07622700	H	1.41256900	6.02760100	-1.94559800
O	1.55004100	-3.41427200	-2.76866500	H	1.81567100	4.52904100	-1.73995500
H	1.10513500	-3.79481800	-3.53403400	O	0.24748400	5.21714800	1.18611500
N	3.92385000	0.25532900	1.67935600	H	0.51650300	5.29159200	0.25162600
C	4.65156100	1.35927700	1.93991900	H	0.95386200	4.66937300	1.59065200
H	3.88135200	-0.45882400	2.39293800				
O	4.76522100	2.29808000	1.13295700				
N	-4.12060800	-0.67963100	0.06650300				

P.Int1 (Applied Force = 2.0 nN, Pulling Direction A) Structure

C	1.66241200	-0.14373300	0.82189100	C	-4.50489200	-1.96953600	0.26538500
C	3.15071800	0.03862000	0.47229900	H	-4.71760200	-0.04982200	-0.39670100
C	3.72415600	-1.12515500	-0.38062600	O	-3.73945200	-2.81287600	0.77990100
C	1.48572100	-1.77137400	-1.05009200	C	-5.91107600	-2.31391600	-0.14808600
C	0.81710800	-0.54712400	-0.39621300	H	-6.30776500	-1.60001700	-0.87010800
H	3.22061700	0.94105500	-0.13498100	H	-5.91973600	-3.31845600	-0.57189000
H	1.57029700	-0.94678500	1.56631800	H	-6.54732000	-2.31903400	0.74156600
H	1.56702200	-2.57640300	-0.31560200	C	5.27683100	1.49688100	3.29122500
H	0.77951300	0.27143100	-1.11723700	H	5.24506100	0.56725800	3.85895200
H	3.91930800	-2.05545300	0.18875500	H	6.31078800	1.82404500	3.17684200
O	4.95137100	-0.80483700	-0.95471600	H	4.74009800	2.27076100	3.84609000
H	4.92299900	0.09935200	-1.33343200	O	-1.67443700	-4.39816600	3.37067100
O	2.80329000	-1.36666600	-1.45085600	H	-2.62821800	-4.68924400	2.91621600
O	1.17343100	1.07241200	1.37337200	H	-1.24636100	-5.15787300	3.78906900
H	0.19701100	1.03788200	1.40992800	O	4.97798100	1.95109200	-1.55627100
O	-0.48392700	-0.76864300	0.17068200	H	5.79664800	2.27543300	-1.94955300
C	-1.72253400	-0.56549400	-0.57610100	H	5.00730900	2.18763600	-0.59971600
C	-2.78801300	-0.22245200	0.48895600	O	-3.81425000	-4.92909700	2.32054700
C	-2.86004600	1.28473600	0.78829300	H	-3.96376000	-4.17768200	1.68514300
C	-3.08582900	2.09985000	-0.50459600	H	-3.80732200	-5.74091000	1.79841800
C	-2.07860300	1.73115000	-1.59501000	O	-1.75742800	-4.25333900	-0.79999800
H	-1.95931800	-1.52570500	-1.03659400	H	-1.11252600	-4.16647700	-0.08071400
H	-3.71845000	1.45159300	1.44869600	H	-2.54059400	-3.82531800	-0.42384700
H	-3.02328900	3.17980700	-0.31879300	O	3.13572600	-4.90341800	-0.81682400
H	-2.57642900	1.86838600	-2.55694100	H	3.89074200	-4.45813700	-1.25112200
H	-2.51218000	-0.74750400	1.40214700	H	2.40174300	-4.66284900	-1.40787600
O	-1.65562200	1.66389700	1.44524100	O	2.58714600	3.15775700	-2.29395000
H	-1.77638100	2.59948700	1.72446700	H	3.47737200	2.80138800	-2.09664800
O	-4.44523500	1.89364600	-0.94963900	H	2.37083800	2.85042400	-3.18007800
H	-4.94960000	2.57716400	-0.46867400	O	4.68383600	-3.30191900	-2.53396600
C	-0.84773200	2.63461600	-1.58122100	H	3.78575500	-3.03264700	-2.78317300
H	-0.13783900	2.24486700	-2.31999100	H	5.03746800	-2.49545500	-2.12551500
H	-0.36748000	2.61264300	-0.59764200	O	2.39970400	-3.85671900	1.56683300
O	-1.28210400	3.94413600	-1.91944400	H	2.73086900	-4.31706100	0.75527000
H	-0.50136300	4.52567800	-1.85223400	H	2.82121700	-4.27897700	2.32279500
O	-1.63008500	0.34046400	-1.62864500	O	-6.33913200	0.34891400	-2.39230800
O	-0.22260700	-3.45564800	1.54017000	H	-5.61690700	0.94819100	-2.14516500
H	-0.34845500	-2.51834500	1.31250300	H	-7.09433400	0.68817200	-1.89934300
H	-1.04402700	-3.99794000	2.65032700	O	-2.21950500	4.30390300	1.91012500
O	2.19262000	3.56229700	2.12050400	H	-2.28574300	4.56997500	2.83456800
H	1.85744100	2.67225700	1.90183500	H	-1.37501400	4.71451400	1.57511400
H	3.04244900	3.60084800	1.66054500	O	-4.91238900	4.15944700	0.74209400
H	0.75764700	-3.63011000	1.60413700	H	-4.04590700	4.31788600	1.16140400
C	0.79666900	-2.31835700	-2.28330200	H	-5.08698800	4.96203600	0.23794600
H	-0.21421200	-2.64064300	-2.02162700	O	1.10568000	5.26719000	-1.49381600
H	0.75587300	-1.55404600	-3.06606600	H	1.36108100	6.07299200	-1.95499400
O	1.56752200	-3.44877100	-2.73113900	H	1.75030500	4.56952000	-1.75967200
H	1.11642400	-3.84790800	-3.48326100	O	0.18180000	5.23149700	1.16783000
N	3.93914400	0.26779700	1.67475600	H	0.45174900	5.31809300	0.23474000
C	4.64232300	1.39000800	1.92758400	H	0.89223500	4.68572200	1.56725800
H	3.90441400	-0.43836500	2.39662400				
O	4.74165200	2.32231800	1.11178000				
N	-4.10363700	-0.70643100	0.07242800				

P.Int1 (Applied Force = 2.5 nN, Pulling Direction A) Structure

C	1.67439800	-0.09868800	0.82053900	C	-4.40569900	-2.10493600	0.26918000
C	3.16351700	0.10034700	0.47959700	H	-4.70853400	-0.21541300	-0.44223900
C	3.77556900	-1.05970900	-0.35776400	O	-3.60290300	-2.89682400	0.80890600
C	1.53993700	-1.76304300	-1.01516500	C	-5.78795400	-2.53151100	-0.14862700
C	0.84595600	-0.53239900	-0.39843600	H	-6.20903500	-1.86154200	-0.89820100
H	3.21619100	0.99197000	-0.14494400	H	-5.74202900	-3.54805500	-0.54013000
H	1.58636100	-0.88858400	1.57886200	H	-6.43518900	-2.53947900	0.73301700
H	1.62647200	-2.54695400	-0.25924400	C	5.19495600	1.69576200	3.29098900
H	0.80748400	0.27179400	-1.13603300	H	5.19891900	0.77558500	3.87463300
H	4.02920000	-1.97898400	0.21377800	H	6.21350500	2.07069200	3.18561000
O	4.98062400	-0.68965500	-0.95199200	H	4.61298000	2.45233200	3.82382200
H	4.90310100	0.20562000	-1.34361900	O	-1.52993100	-4.43276900	3.42872600
O	2.85515100	-1.34950300	-1.41749200	H	-2.46856100	-4.75344600	2.95562200
O	1.15981000	1.12003600	1.34572800	H	-1.07711400	-5.18205200	3.83998800
H	0.18530800	1.06225300	1.37879500	O	4.87041600	2.07360800	-1.58178500
O	-0.45998500	-0.75201200	0.16106100	H	5.67394200	2.42304700	-1.98478900
C	-1.69584600	-0.56935100	-0.59546900	H	4.90401500	2.31394500	-0.62637600
C	-2.78178800	-0.26796900	0.46320700	O	-3.62824900	-5.02486700	2.33417200
C	-2.92813100	1.23727400	0.75340700	H	-3.78974300	-4.27187400	1.70223300
C	-3.19032700	2.03501900	-0.54502700	H	-3.58159800	-5.83078000	1.80489700
C	-2.14206800	1.71931600	-1.61426400	O	-1.58757100	-4.33284900	-0.72569900
H	-1.90433500	-1.52899200	-1.07143300	H	-0.94801500	-4.21406000	-0.00645400
H	-3.79408400	1.36508300	1.41286300	H	-2.37498200	-3.89479600	-0.37066700
H	-3.21610300	3.12279600	-0.37132100	O	3.30274500	-4.81132900	-0.70683300
H	-2.62626900	1.82681600	-2.58704400	H	4.04443700	-4.36118500	-1.15832200
H	-2.48124300	-0.76769100	1.38260200	H	2.56033800	-4.60906900	-1.30203300
O	-1.74098800	1.66806300	1.40992200	O	2.45949200	3.26431100	-2.31490300
H	-1.90336400	2.59632600	1.69107100	H	3.34973900	2.91243300	-2.11047400
O	-4.52536200	1.72672500	-1.00956600	H	2.26305000	2.97605400	-3.21202900
H	-5.08779600	2.36602100	-0.53424700	O	4.80072200	-3.22150000	-2.48372200
C	-0.95835300	2.68210400	-1.57777700	H	3.89274800	-2.98589600	-2.73075600
H	-0.21702600	2.32718500	-2.30265000	H	5.13137900	-2.39504400	-2.09655500
H	-0.49613700	2.68076200	-0.58559300	O	2.53334200	-3.72660200	1.65194200
O	-1.44631300	3.97118400	-1.92362400	H	2.88092900	-4.19669900	0.85316700
H	-0.68528300	4.57885600	-1.86704800	H	2.96663700	-4.11557400	2.41905900
O	-1.61346800	0.35472900	-1.63462700	O	-6.21634100	0.02467600	-2.52628700
O	-0.10355900	-3.42866000	1.60665100	H	-5.56470400	0.68817000	-2.24856100
H	-0.27498300	-2.50264200	1.36576300	H	-7.03466500	0.32263200	-2.11400300
H	-0.91026200	-4.00391400	2.71804800	O	-2.42043800	4.27964700	1.87625700
O	2.06284200	3.65254000	2.09315600	H	-2.49810700	4.54276000	2.80061900
H	1.77449400	2.74653400	1.87385700	H	-1.58352900	4.70831800	1.54788800
H	2.90909700	3.73459700	1.63304300	O	-5.12471500	3.96203400	0.72582200
H	0.88309300	-3.55566400	1.68045300	H	-4.26669000	4.18161500	1.13349700
C	0.87191100	-2.35421200	-2.23921500	H	-5.37084400	4.75626900	0.23865000
H	-0.13314700	-2.69253700	-1.97523600	O	0.92040600	5.33738000	-1.50615800
H	0.82050000	-1.61029400	-3.04088100	H	1.16878200	6.15274300	-1.95412700
O	1.67041400	-3.47808900	-2.65344400	H	1.58057800	4.65434700	-1.77074700
H	1.22487000	-3.91617400	-3.38693100	O	-0.02285800	5.24888500	1.15079000
N	3.93772900	0.37648000	1.68059700	H	0.24995800	5.35374100	0.22052800
C	4.58592500	1.53494200	1.92109500	H	0.70340800	4.72407500	1.54887500
H	3.91931400	-0.31453400	2.41759300				
O	4.65557400	2.45515400	1.08944100				
N	-4.06881300	-0.82732700	0.05211900				

P.Int1 (Applied Force = 3.0 nN, Pulling Direction A) Structure

C	1.69672400	-0.09581400	0.80035100	C	-4.30696700	-2.17523500	0.25033000
C	3.18655800	0.09280800	0.45445900	H	-4.69650000	-0.31665200	-0.49537000
C	3.80939900	-1.07408600	-0.37141100	O	-3.47138100	-2.91879700	0.81006900
C	1.55313900	-1.79756900	-0.98688700	C	-5.66028400	-2.67903100	-0.17627200
C	0.86864400	-0.53871500	-0.41511700	H	-6.11098800	-2.03773000	-0.93340900
H	3.23146500	0.97075800	-0.18897100	H	-5.55535600	-3.69366500	-0.56163700
H	1.60358100	-0.87436400	1.56930600	H	-6.31340100	-2.71844600	0.70015900
H	1.63027200	-2.55385000	-0.20252600	C	5.17417100	1.79611700	3.23032400
H	0.85360000	0.24756800	-1.17323400	H	5.22953000	0.88289000	3.82223300
H	4.12113400	-1.97839700	0.20313700	H	6.17005800	2.22597500	3.11967000
O	4.98416300	-0.67113700	-1.00801500	H	4.55152600	2.52405700	3.75737000
H	4.85725300	0.21034100	-1.41569000	O	-1.45618600	-4.53145200	3.47966400
O	2.87281200	-1.40982400	-1.40436400	H	-2.37004500	-4.84920500	2.93810900
O	1.18423500	1.13217600	1.30887400	H	-1.00410400	-5.29032700	3.87385800
H	0.21121100	1.06830800	1.33982600	O	4.73414900	2.11001200	-1.66674800
O	-0.44688200	-0.71418600	0.13888000	H	5.52268700	2.46549200	-2.09369500
C	-1.67170600	-0.51650100	-0.62759200	H	4.79914500	2.34963900	-0.71303100
C	-2.77592200	-0.26042200	0.42663800	O	-3.47117300	-5.10918300	2.24439200
C	-2.98379800	1.23756100	0.72397600	H	-3.63055300	-4.32248400	1.65109100
C	-3.26765900	2.03676000	-0.57039100	H	-3.36004100	-5.87562300	1.66765700
C	-2.18015600	1.78145100	-1.61723500	O	-1.43800000	-4.46192600	-0.58967800
H	-1.86893800	-1.45976800	-1.14116800	H	-0.80601900	-4.28359900	0.12388500
H	-3.85676400	1.32720300	1.38074900	H	-2.21070200	-3.95033000	-0.30923400
H	-3.37125600	3.12419000	-0.39417300	O	3.38478200	-4.76527500	-0.59663700
H	-2.64612900	1.87185100	-2.60088200	H	4.11389000	-4.32949600	-1.08085000
H	-2.45304900	-0.74335000	1.34724200	H	2.63000100	-4.59898200	-1.18776900
O	-1.81248400	1.69689700	1.38901800	O	2.35395700	3.43020400	-2.36547800
H	-2.00264700	2.61579100	1.68154900	H	3.21911800	3.02416900	-2.15612100
O	-4.57219500	1.64960100	-1.06554500	H	2.17961000	3.21441100	-3.28719300
H	-5.18448600	2.23802200	-0.58927100	O	4.83909300	-3.24236700	-2.47599200
C	-1.04192000	2.79459600	-1.54438000	H	3.92210000	-3.02787000	-2.70787500
H	-0.26986400	2.48176100	-2.25579000	H	5.16418300	-2.39907400	-2.12194800
H	-0.60230100	2.79749700	-0.54232400	O	2.63873000	-3.62300600	1.74611100
O	-1.57429500	4.06869200	-1.88378100	H	2.98029900	-4.10942900	0.95478700
H	-0.82939100	4.69571000	-1.83221900	H	3.09121600	-3.98444600	2.51568300
O	-1.57576000	0.44681700	-1.63224100	O	-6.16733600	-0.15570400	-2.56224400
O	-0.00729500	-3.42066800	1.72375400	H	-5.54981400	0.54635000	-2.30225900
H	-0.22299100	-2.50259800	1.49625900	H	-7.00249900	0.11699000	-2.16650100
H	-0.82087800	-4.06206400	2.81777400	O	-2.55074300	4.28506000	1.89177900
O	2.00580700	3.68952900	2.06389700	H	-2.63404600	4.53237000	2.81995300
H	1.75228900	2.77467700	1.83941300	H	-1.71317400	4.71968500	1.57634700
H	2.84145000	3.80992500	1.59369500	O	-5.26729400	3.83753800	0.76216500
H	0.98418000	-3.50284100	1.79662300	H	-4.41787100	4.10330800	1.15850700
C	0.88441000	-2.42994700	-2.18922400	H	-5.58115800	4.62906200	0.31096600
H	-0.11765200	-2.76332200	-1.90853000	O	0.78731900	5.45349000	-1.46556300
H	0.82739100	-1.71333700	-3.01509000	H	1.03008100	6.28688700	-1.88231200
O	1.68494100	-3.56434200	-2.56826800	H	1.45462200	4.78733100	-1.75251900
H	1.22619400	-4.04227400	-3.26795900	O	-0.14040500	5.26325800	1.19278800
N	3.96391900	0.40452300	1.64375900	H	0.12691000	5.40439600	0.26569800
C	4.57194100	1.58988700	1.86343100	H	0.59616100	4.73768200	1.56926000
H	3.96439200	-0.27235700	2.39400000				
O	4.60972800	2.49683600	1.01624400				
N	-4.03351300	-0.88513700	0.01947300				

P-TS2 (Applied Force = 0.0 nN, Pulling Direction A) Structure

C	1.55027800	-0.38114500	1.01513300	C	-4.83880400	-1.84046300	0.43966600
C	3.03949000	-0.06999200	0.78022300	H	-5.05629700	0.05634500	-0.28394700
C	3.63050500	-1.05642100	-0.24861500	O	-4.07336000	-2.70773400	0.89029400
C	1.52566000	-1.49603300	-1.26431600	C	-6.30746200	-2.10103400	0.22708600
C	0.77448500	-0.55745600	-0.30630500	H	-6.78459700	-1.32539000	-0.36929400
H	3.11402100	0.93874900	0.37477700	H	-6.42571200	-3.07175700	-0.25591700
H	1.47488100	-1.33111100	1.56248900	H	-6.79419300	-2.15351700	1.20475000
H	1.60441000	-2.48832700	-0.81057600	C	5.22413600	0.64701600	3.83693700
H	0.64663700	0.41702300	-0.77481300	H	5.02944100	-0.34043800	4.25415200
H	3.57853100	-2.08285600	0.13209200	H	6.30052300	0.79195100	3.73047700
O	4.95290300	-0.81621500	-0.58345300	H	4.85416600	1.40825000	4.52763200
H	5.08765800	0.13633100	-0.78401800	O	-1.47279900	-3.86877400	3.25125900
O	2.83729000	-0.95838700	-1.43811700	H	-2.35404900	-4.28043100	3.08709700
O	0.99468900	0.66468000	1.79629100	H	-0.99223300	-4.49471800	3.80359000
H	0.02357600	0.68456700	1.68736900	O	5.26594600	1.92687700	-0.78133000
O	-0.53695100	-1.03558100	0.05681200	H	6.09938500	2.30460700	-1.08428300
C	-2.17823500	-0.68843300	-0.80113300	H	5.21086800	2.07068900	0.19059900
C	-3.00198900	-0.22559300	0.38997700	O	-3.92818400	-4.85218200	2.59646900
C	-2.84790500	1.27306500	0.67188300	H	-4.17201900	-4.14372800	1.96832300
C	-2.86208300	2.16622300	-0.59601100	H	-3.84552700	-5.64587200	2.05643900
C	-2.20996300	1.55381500	-1.84095100	O	-2.33734500	-3.97118700	-1.06055400
H	-2.26652000	-1.73522400	-1.08395400	H	-1.57723000	-3.97501600	-0.45142000
H	-3.69533200	1.58190500	1.29208600	H	-3.07615000	-3.76842800	-0.46805700
H	-2.27980600	3.05579900	-0.35656000	O	2.98259700	-4.76457400	-1.84516700
H	-2.90270000	1.66374900	-2.67382900	H	3.77204400	-4.22413900	-2.05498800
H	-2.66735600	-0.78289300	1.26271300	H	2.30204500	-4.33393400	-2.38754100
O	-1.62584100	1.45124000	1.37840400	O	2.75037300	2.51236700	-1.71017800
H	-1.58991900	2.39722800	1.65502200	H	3.69413600	2.44647900	-1.45642500
O	-4.17927500	2.60259800	-0.92481100	H	2.62012700	1.82976600	-2.37735500
H	-4.29652200	3.46058900	-0.45153300	O	4.72774000	-2.78604800	-2.77474200
C	-0.88284100	2.21188100	-2.20820100	H	3.89000300	-2.38367100	-3.05184100
H	-0.43446200	1.66604300	-3.04725200	H	5.05176700	-2.16328400	-2.10364100
H	-0.20022900	2.16389400	-1.35289700	O	2.20939700	-4.25077600	0.70309900
O	-1.16769800	3.55370200	-2.54658600	H	2.52323900	-4.54248400	-0.18803900
H	-0.37237400	4.07645800	-2.32029300	H	2.59970700	-4.85200200	1.34594200
O	-1.96494700	0.08876200	-1.81382900	O	-6.41798300	1.04745700	-1.11217500
O	-0.35748500	-3.43839000	0.87687300	H	-5.71666800	1.72122000	-1.20821600
H	-0.48498300	-2.00723300	0.40602400	H	-6.99286400	1.39459600	-0.42039900
H	-0.74129600	-3.61294100	1.78029400	O	-1.71232900	4.13550900	1.90995100
O	2.17912100	3.19807800	2.26760500	H	-1.74715400	4.36731900	2.84542500
H	1.75227900	2.33284700	2.12734900	H	-0.85593700	4.52621500	1.55641800
H	3.11479400	3.03771800	2.07249400	O	-3.99419800	4.90660000	0.48390500
H	0.55314400	-3.82369400	0.85291200	H	-3.20909700	4.73554600	1.04612900
C	0.91258200	-1.65057000	-2.64227200	H	-3.73281100	5.63329400	-0.09290100
H	-0.12742600	-1.97408400	-2.55337300	O	1.18023500	4.69322700	-1.69215900
H	0.94888200	-0.69751500	-3.17910700	H	1.56296800	5.43454400	-2.17424000
O	1.68622600	-2.64224500	-3.33333900	H	1.83509800	3.95524200	-1.74241200
H	1.33756800	-2.73713600	-4.22689800	O	0.59349500	5.03807900	1.03171900
N	3.76984600	-0.10751000	2.04050800	H	0.76052600	4.97883900	0.07120500
C	4.57413700	0.87100700	2.49582500	H	1.24723400	4.43205100	1.44644500
H	3.66929900	-0.93420200	2.61297600				
O	4.76469900	1.93083800	1.87064400				
N	-4.38841500	-0.60568900	0.12580000				

P-TS2 (Applied Force = 0.5 nN, Pulling Direction A) Structure

C	1.61318100	-0.39174000	0.92676800	C	-4.81644300	-1.77021700	0.43250500
C	3.11094500	-0.13788400	0.67751800	H	-4.93850400	0.12646800	-0.32692600
C	3.68764100	-1.17119900	-0.31456400	O	-4.07980100	-2.65207400	0.89878100
C	1.54779500	-1.59785000	-1.29709200	C	-6.28815400	-1.98718400	0.20002700
C	0.83141000	-0.58678600	-0.38661900	H	-6.69822800	-1.26993800	-0.50941900
H	3.20845600	0.85019500	0.22835500	H	-6.44296400	-3.00592200	-0.15523500
H	1.50561200	-1.31720500	1.50904200	H	-6.80847800	-1.88095600	1.15640400
H	1.58714400	-2.57038600	-0.79898500	C	5.24132400	0.71912100	3.73387200
H	0.73917500	0.36874500	-0.90066500	H	5.08953400	-0.26897600	4.16727700
H	3.66898900	-2.18666100	0.10412000	H	6.30982600	0.92649500	3.66033300
O	5.00106400	-0.92450600	-0.68407000	H	4.80145000	1.47069000	4.39403000
H	5.11563600	0.02252300	-0.91900900	O	-1.52924300	-3.66728100	3.27658800
O	2.87864100	-1.12059500	-1.49626600	H	-2.39169500	-4.12232100	3.12781300
O	1.09618600	0.70206500	1.66714900	H	-1.03998900	-4.22636000	3.88963000
H	0.12182800	0.72713400	1.59662200	O	5.28540700	1.82804900	-0.94930600
O	-0.50020600	-1.00049900	0.00223500	H	6.11843200	2.19514200	-1.26648800
C	-2.10950900	-0.61232800	-0.80403000	H	5.24385100	1.98789100	0.02147400
C	-2.93600800	-0.19110200	0.40575500	O	-3.93714700	-4.76965100	2.63978700
C	-2.79352800	1.30043800	0.72367600	H	-4.18883800	-4.07973300	1.99492100
C	-2.94796300	2.17696700	-0.53864600	H	-3.81421400	-5.56800600	2.11445600
C	-2.14573700	1.67808000	-1.73615600	O	-2.34094900	-3.90340500	-1.06844600
H	-2.23435800	-1.64092000	-1.13524300	H	-1.59140200	-3.91315200	-0.44717300
H	-3.59842800	1.56795900	1.41515500	H	-3.08667700	-3.69844800	-0.48570200
H	-2.57765700	3.17941100	-0.32023700	O	2.94022700	-4.87860700	-1.73085400
H	-2.72647600	1.85825600	-2.63957100	H	3.74380100	-4.37242900	-1.96877600
H	-2.60973500	-0.77837000	1.26179300	H	2.27134200	-4.46234800	-2.29874000
O	-1.52736100	1.51371300	1.33034300	O	2.78603700	2.62928000	-1.77076100
H	-1.53043400	2.44708400	1.65034800	H	3.72844500	2.46342700	-1.56029700
O	-4.33123900	2.30858400	-0.87381200	H	2.61005800	2.12467600	-2.57190400
H	-4.62971800	3.08555200	-0.35323800	O	4.72990400	-2.99630100	-2.78416700
C	-0.79075600	2.36373900	-1.88581000	H	3.89513400	-2.59093300	-3.06551800
H	-0.23166400	1.85475400	-2.68065800	H	5.07802500	-2.34647900	-2.15223100
H	-0.22810900	2.28817500	-0.94933600	O	2.14757200	-4.27005800	0.79185800
O	-1.06148000	3.71189000	-2.21513900	H	2.46683900	-4.59526400	-0.08547500
H	-0.25015500	4.22411600	-2.02301100	H	2.49243800	-4.87679600	1.45525600
O	-1.91399200	0.21028100	-1.79217700	O	-6.51901800	0.80762300	-1.70963800
O	-0.38996600	-3.36328700	0.90257800	H	-5.77418700	1.43140600	-1.70897700
H	-0.48053100	-1.96714900	0.38783100	H	-7.16786800	1.22444800	-1.13127200
H	-0.78654600	-3.49348100	1.80928800	O	-1.81798100	4.14943400	1.95444800
O	2.24303700	3.20373200	2.30934000	H	-1.86386900	4.34273900	2.89826000
H	1.84060300	2.34019300	2.10280400	H	-0.96148900	4.56067400	1.63343800
H	3.16373700	3.10487700	2.02615600	O	-4.37950700	4.55267300	0.74231400
H	0.50935900	-3.77696200	0.90117600	H	-3.51525700	4.52475500	1.19937700
C	0.92752200	-1.78376100	-2.66801000	H	-4.35633300	5.36381000	0.22224300
H	-0.12269700	-2.06954800	-2.56562800	O	1.31820200	4.86122300	-1.47966500
H	0.99548700	-0.85210900	-3.23829200	H	1.67923500	5.61687800	-1.95566900
O	1.66611200	-2.82566300	-3.32219700	H	1.95705200	4.11696500	-1.59771700
H	1.30422000	-2.95169800	-4.20653900	O	0.54628400	5.06392400	1.20790200
N	3.84103800	-0.13099500	1.93739500	H	0.77618500	5.06877700	0.25899200
C	4.62275200	0.87746700	2.36851500	H	1.20078500	4.45594200	1.61680400
H	3.73779700	-0.93456100	2.54140200				
O	4.81276600	1.91301000	1.70530100				
N	-4.32580400	-0.54695300	0.12521900				

P-TS2 (Applied Force = 1.0 nN, Pulling Direction A) Structure

C	1.65838400	-0.38111400	0.88774800	C	-4.78489300	-1.76438700	0.33979800
C	3.15847900	-0.16159000	0.61547800	H	-4.88925900	0.18930100	-0.28231600
C	3.72502700	-1.22404900	-0.35571900	O	-4.05027900	-2.67692900	0.74648400
C	1.55034300	-1.67704900	-1.27348700	C	-6.25533800	-1.95847100	0.08040000
C	0.86220300	-0.60736700	-0.40968400	H	-6.64317100	-1.21760100	-0.61859400
H	3.26160200	0.81188200	0.13649000	H	-6.41757600	-2.96542300	-0.30331600
H	1.53936700	-1.28202400	1.50496100	H	-6.79073800	-1.86707400	1.03004700
H	1.58666900	-2.62086900	-0.72370500	C	5.29493400	0.79650500	3.63626100
H	0.78846600	0.32645800	-0.96663900	H	5.17459200	-0.18753000	4.08851600
H	3.75770400	-2.22916500	0.09334100	H	6.35582800	1.03865800	3.56170400
O	5.02057700	-0.95635400	-0.77345100	H	4.82682500	1.54504400	4.28051000
H	5.10616800	-0.01361400	-1.03489000	O	-1.66450000	-3.60952800	3.26654900
O	2.88408600	-1.22677600	-1.51758700	H	-2.49709500	-4.10156300	3.07231400
O	1.16357800	0.74942300	1.58810400	H	-1.19176000	-4.13799800	3.91848000
H	0.18731900	0.76514800	1.55506100	O	5.26105400	1.80251300	-1.08846200
O	-0.47796200	-0.96760300	0.01314700	H	6.08541500	2.16768100	-1.42974200
C	-2.06762200	-0.56739400	-0.77976900	H	5.24464500	1.97135600	-0.11832800
C	-2.90678600	-0.17627900	0.43346000	O	-3.97902300	-4.80695300	2.47855100
C	-2.78292300	1.31283400	0.77688700	H	-4.20024800	-4.12044400	1.81889800
C	-2.98594400	2.19307500	-0.47669600	H	-3.78628200	-5.59629900	1.96056600
C	-2.14101700	1.74468900	-1.66386600	O	-2.21318700	-3.86619200	-1.16117600
H	-2.19731000	-1.58474200	-1.14045100	H	-1.52354500	-3.87434500	-0.47425600
H	-3.57946000	1.55323100	1.48796300	H	-3.01175100	-3.68097600	-0.64579700
H	-2.70392500	3.22610600	-0.26075800	O	2.93501400	-4.94879200	-1.54999400
H	-2.69841000	1.93765400	-2.57946000	H	3.73584900	-4.46122500	-1.83125000
H	-2.58724000	-0.77629800	1.28342900	H	2.25986500	-4.57223400	-2.13774200
O	-1.50997400	1.53883900	1.36245700	O	2.75471500	2.67315500	-1.82263000
H	-1.52702100	2.46522500	1.70180300	H	3.69756500	2.47547900	-1.64372200
O	-4.37849700	2.22218500	-0.81465000	H	2.55402000	2.23319600	-2.65551300
H	-4.73192600	2.96375100	-0.27997900	O	4.70498400	-3.14155200	-2.76535600
C	-0.79373600	2.45468100	-1.75681100	H	3.86021000	-2.75343300	-3.04182200
H	-0.21149600	1.97779400	-2.55510000	H	5.07468400	-2.45422600	-2.18829600
H	-0.24940800	2.35426400	-0.81213800	O	2.12638600	-4.22816500	0.94185100
O	-1.07605100	3.80928800	-2.05051500	H	2.45552900	-4.59305200	0.08440200
H	-0.25548300	4.31533300	-1.88405600	H	2.45011800	-4.81290600	1.63501000
O	-1.88128700	0.28212500	-1.75088200	O	-6.55185100	0.81550200	-1.93151000
O	-0.41084700	-3.30825900	0.95502900	H	-5.77759200	1.39140200	-1.82976100
H	-0.47953500	-1.92770600	0.42651200	H	-7.22134500	1.23196500	-1.37727300
H	-0.85241600	-3.43624200	1.84174500	O	-1.85066900	4.15312000	2.02980800
O	2.30269100	3.22149200	2.32213900	H	-1.88944200	4.33385200	2.97642800
H	1.90880100	2.36076200	2.08939400	H	-0.99708100	4.56796600	1.71047400
H	3.20694600	3.15904300	1.98245000	O	-4.49465200	4.42580000	0.89559200
H	0.48695300	-3.72354700	0.99746700	H	-3.61518600	4.44921600	1.32061400
C	0.90396800	-1.92905900	-2.62171300	H	-4.56068200	5.26253200	0.42191900
H	-0.13973200	-2.22390500	-2.48193300	O	1.34140900	4.92390900	-1.38707700
H	0.94646100	-1.02266900	-3.23380400	H	1.69697900	5.68688600	-1.85529100
O	1.64000200	-2.99163500	-3.24527900	H	1.96280900	4.17356300	-1.54900900
H	1.25521400	-3.16568300	-4.11161600	O	0.52838100	5.06837500	1.29653300
N	3.90227100	-0.12007100	1.86617600	H	0.77025200	5.09771900	0.35139400
C	4.67413700	0.90910000	2.26728600	H	1.19359800	4.46696400	1.69671800
H	3.80947600	-0.90827600	2.49170200				
O	4.85083000	1.92780900	1.57596100				
N	-4.29299800	-0.52280300	0.12617600				

P-TS2 (Applied Force = 1.5 nN, Pulling Direction A) Structure

C	1.68127500	-0.39361700	0.87571400	C	-4.74643100	-1.76175800	0.31549000
C	3.18530800	-0.19937600	0.59891900	H	-4.85169300	0.20666900	-0.26638200
C	3.75005700	-1.26898800	-0.36972000	O	-4.01118000	-2.67978300	0.70958100
C	1.54922600	-1.70635300	-1.26829300	C	-6.21410400	-1.95519400	0.03846600
C	0.88154400	-0.61048700	-0.42017300	H	-6.59196600	-1.21378100	-0.66603900
H	3.29577700	0.76890300	0.11124600	H	-6.37281200	-2.96140900	-0.34841500
H	1.54821600	-1.28849800	1.49815800	H	-6.76220600	-1.86285900	0.98071700
H	1.56481400	-2.64269000	-0.70564600	C	5.32189200	0.79126600	3.60744600
H	0.82396500	0.31993400	-0.98495000	H	5.21415900	-0.19203000	4.06452500
H	3.82296200	-2.27398000	0.08235600	H	6.37958200	1.04613500	3.53035700
O	5.03296600	-0.97902000	-0.81348400	H	4.84527100	1.53696200	4.24878700
H	5.09544300	-0.03709500	-1.08309400	O	-1.70379400	-3.56040000	3.26407000
O	2.89241200	-1.28795700	-1.52039500	H	-2.51997400	-4.07568400	3.05968800
O	1.20381100	0.74936900	1.56957300	H	-1.22720100	-4.07088000	3.92747900
H	0.22785300	0.77231700	1.54705900	O	5.22772800	1.78849100	-1.13392900
O	-0.46828500	-0.93949100	0.01385100	H	6.04359500	2.16027700	-1.48834700
C	-2.02122600	-0.53586200	-0.75934800	H	5.22890500	1.95249600	-0.16287700
C	-2.87917000	-0.15863200	0.44870300	O	-3.96853800	-4.81630500	2.43126000
C	-2.77718000	1.33310300	0.79513500	H	-4.17882800	-4.13112700	1.76636400
C	-3.01631400	2.20729500	-0.45795800	H	-3.74223300	-5.59963100	1.91765500
C	-2.14232600	1.78640700	-1.63466300	O	-2.16735100	-3.85848800	-1.19029400
H	-2.16985000	-1.54307000	-1.14027100	H	-1.49841100	-3.85841300	-0.48386700
H	-3.56655400	1.55728300	1.51954200	H	-2.97934000	-3.66928100	-0.69792800
H	-2.80276400	3.26036800	-0.25032800	O	2.90793100	-4.96843300	-1.47385500
H	-2.68993700	1.97169900	-2.55790700	H	3.71105700	-4.49738200	-1.77543700
H	-2.55953200	-0.75350700	1.30243300	H	2.23254500	-4.60864000	-2.07167600
O	-1.49819300	1.57462500	1.36107800	O	2.71418100	2.68179800	-1.82972300
H	-1.52501000	2.49712500	1.70985300	H	3.65649200	2.47325900	-1.66034500
O	-4.41106300	2.16356600	-0.80119100	H	2.50788900	2.26551200	-2.67338300
H	-4.80158300	2.88367900	-0.26557700	O	4.68589600	-3.21659100	-2.76526800
C	-0.80900400	2.52441900	-1.70246300	H	3.83909200	-2.82978100	-3.03748800
H	-0.21366600	2.07177500	-2.50504700	H	5.07183900	-2.51553800	-2.21654800
H	-0.26929200	2.41476400	-0.75650800	O	2.09843000	-4.19650600	1.00367500
O	-1.10965100	3.88042000	-1.97411200	H	2.42870400	-4.58015400	0.15499100
H	-0.28479700	4.38569500	-1.83056400	H	2.39865800	-4.78041900	1.70808600
O	-1.84584200	0.33053600	-1.72632000	O	-6.54629100	0.78549700	-2.06975100
O	-0.42627300	-3.25540700	0.97468400	H	-5.76945000	1.34277700	-1.90664700
H	-0.48444300	-1.90402200	0.44177300	H	-7.23438000	1.18827600	-1.52852500
H	-0.88351400	-3.38113900	1.85553200	O	-1.87103900	4.17572900	2.05217300
O	2.32837300	3.22305700	2.31456500	H	-1.90434900	4.34992600	3.00020100
H	1.94087800	2.36074400	2.07778700	H	-1.01674200	4.58706200	1.73351300
H	3.22933000	3.17089500	1.96515600	O	-4.56415800	4.35914300	0.95962500
H	0.47007000	-3.67433000	1.03254900	H	-3.67917600	4.41557500	1.36812200
C	0.90132700	-1.96369400	-2.61482200	H	-4.68044900	5.20376000	0.51031300
H	-0.14926500	-2.23246900	-2.47486300	O	1.34145200	4.95694100	-1.36067700
H	0.96783600	-1.06758100	-3.23983700	H	1.70913600	5.71788900	-1.82265500
O	1.61558700	-3.05201600	-3.21898300	H	1.94660800	4.19637000	-1.53480100
H	1.22523400	-3.23615500	-4.08071900	O	0.52429600	5.07058500	1.32388500
N	3.93294400	-0.14846000	1.84615400	H	0.76926300	5.11470700	0.38022300
C	4.69770600	0.88999700	2.23892600	H	1.19190100	4.46732700	1.71639400
H	3.84690400	-0.93361700	2.47635600				
O	4.86547200	1.90492200	1.54051600				
N	-4.25972800	-0.51492800	0.13070300				

P-TS2 (Applied Force = 2.0 nN, Pulling Direction A) Structure

C	1.69787400	-0.40631900	0.86756200	C	-4.70948600	-1.76579300	0.30036800
C	3.20560500	-0.23517000	0.58760000	H	-4.82593600	0.20532000	-0.26890700
C	3.76883200	-1.31031300	-0.37994200	O	-3.97139200	-2.68128700	0.69607300
C	1.54454800	-1.73122300	-1.26287500	C	-6.17256100	-1.96900700	0.00450800
C	0.89469200	-0.61397900	-0.42713100	H	-6.54352800	-1.23480700	-0.71141900
H	3.32325700	0.72859400	0.09283600	H	-6.32109400	-2.97844700	-0.37783300
H	1.55231300	-1.29566400	1.49451600	H	-6.73532600	-1.87205800	0.93756200
H	1.54201900	-2.66155900	-0.69105800	C	5.34501500	0.78163800	3.58388800
H	0.85082400	0.31350000	-0.99803500	H	5.24652200	-0.20036200	4.04585800
H	3.87848000	-2.31555700	0.07241200	H	6.40031900	1.04501600	3.50310000
O	5.03960400	-1.00037100	-0.84688100	H	4.86356300	1.52631000	4.22282300
H	5.08130600	-0.05948300	-1.12310200	O	-1.72588700	-3.51383200	3.26407100
O	2.89595300	-1.34126300	-1.52015200	H	-2.52842000	-4.04997600	3.05776700
O	1.23660400	0.74758800	1.55612100	H	-1.24023500	-4.00770600	3.93351900
H	0.26112100	0.77659000	1.54456400	O	5.19762800	1.77425600	-1.17102700
O	-0.46345400	-0.91524600	0.01721100	H	6.00761300	2.14885800	-1.53593200
C	-1.97732900	-0.50545800	-0.74111200	H	5.21447600	1.93294000	-0.19931500
C	-2.85943100	-0.14148100	0.45758100	O	-3.94864100	-4.82159600	2.40904100
C	-2.78131500	1.35269100	0.80694800	H	-4.15140600	-4.13838900	1.73943200
C	-3.04112400	2.22456700	-0.44556500	H	-3.69653400	-5.60055500	1.90077300
C	-2.13734800	1.82759000	-1.60892700	O	-2.13946300	-3.85622600	-1.21212800
H	-2.14670400	-1.50093000	-1.14374100	H	-1.48664900	-3.84750100	-0.49162100
H	-3.56951200	1.56198200	1.53719400	H	-2.96034200	-3.66174400	-0.73710900
H	-2.88705200	3.29109500	-0.24094600	O	2.87817300	-4.98616200	-1.41946100
H	-2.67410100	2.00428400	-2.54038500	H	3.68452600	-4.53061900	-1.73531900
H	-2.54014400	-0.72936200	1.31651600	H	2.20409700	-4.63678300	-2.02489400
O	-1.50124500	1.60631200	1.36592900	O	2.68360700	2.70029200	-1.83590100
H	-1.53661700	2.52578400	1.72126500	H	3.62390200	2.47746700	-1.67383200
O	-4.43195500	2.12446500	-0.80446800	H	2.46952800	2.30092000	-2.68578600
H	-4.85641800	2.82483700	-0.27112700	O	4.66506600	-3.28034300	-2.76827300
C	-0.81839100	2.59185900	-1.65292500	H	3.81676000	-2.89428700	-3.03702900
H	-0.20912300	2.15983300	-2.45628900	H	5.06372000	-2.56932300	-2.24241200
H	-0.28448600	2.47668500	-0.70461900	O	2.06199700	-4.17290000	1.04375200
O	-1.13648900	3.94753200	-1.90894600	H	2.39570800	-4.57105200	0.20312100
H	-0.30961300	4.45390100	-1.78533800	H	2.34286800	-4.75445000	1.75808400
O	-1.80480900	0.37903000	-1.70182100	O	-6.50949200	0.73830700	-2.18150200
O	-0.44657700	-3.20646300	0.98730000	H	-5.74138600	1.29283600	-1.97462400
H	-0.49238100	-1.88904400	0.45857700	H	-7.21892900	1.12635300	-1.65744000
H	-0.91247100	-3.32926400	1.86650600	O	-1.89204100	4.19993000	2.07090300
O	2.34959800	3.22275200	2.30874500	H	-1.92185400	4.37171300	3.01945700
H	1.96985100	2.35799300	2.06908500	H	-1.03524800	4.60432200	1.75293300
H	3.24788800	3.18126100	1.95172600	O	-4.61910400	4.31690600	1.00345000
H	0.44835800	-3.63021400	1.05350900	H	-3.73214300	4.39934700	1.40167700
C	0.89578300	-1.99019000	-2.60878300	H	-4.77463000	5.16666300	0.57630900
H	-0.15970600	-2.23903400	-2.46952300	O	1.34184400	4.99292300	-1.33708900
H	0.98067500	-1.10131600	-3.24189400	H	1.72012400	5.75371600	-1.79055700
O	1.59245100	-3.09699200	-3.19978200	H	1.93450500	4.22537800	-1.52199900
H	1.19572600	-3.28865000	-4.05695300	O	0.52000400	5.06981200	1.34758900
N	3.95646100	-0.17666300	1.83178900	H	0.76853800	5.12929800	0.40577400
C	4.71668000	0.86894300	2.21648200	H	1.18918500	4.46423000	1.73298200
H	3.87620100	-0.95919900	2.46589800				
O	4.87722700	1.88019000	1.51173600				
N	-4.23245700	-0.51458400	0.12863300				

P-TS2 (Applied Force = 2.5 nN, Pulling Direction A) Structure

C	1.72499700	-0.23619300	0.82580700	C	-4.54830300	-2.07695100	0.32447100
C	3.22445500	-0.01759900	0.53126600	H	-4.82468700	-0.15035300	-0.33253600
C	3.85904800	-1.12873300	-0.35340000	O	-3.74236500	-2.90644700	0.77415700
C	1.65440800	-1.77511800	-1.14911800	C	-5.97944300	-2.42542500	0.00836400
C	0.93804000	-0.61067200	-0.44083100	H	-6.41003300	-1.74236200	-0.72421400
H	3.28932500	0.90581200	-0.04358900	H	-6.02047300	-3.44968900	-0.36171300
H	1.62112400	-1.06327800	1.53953000	H	-6.56380300	-2.37500900	0.93163000
H	1.72456500	-2.62510800	-0.46832800	C	5.21431500	1.42949200	3.44951200
H	0.85181500	0.24722700	-1.10779900	H	5.19167600	0.48703600	3.99591100
H	4.07091400	-2.08981200	0.16385100	H	6.24216300	1.78527100	3.37036000
O	5.09003100	-0.74546000	-0.87250500	H	4.64393700	2.17759400	4.00616000
H	5.04089400	0.16986600	-1.22240000	O	-1.57561700	-3.31661100	3.48387500
O	2.97353500	-1.32220800	-1.46864200	H	-2.30276000	-3.95549400	3.28977500
O	1.19981500	0.95764700	1.39144600	H	-1.07040000	-3.69752000	4.21032700
H	0.22592400	0.90971000	1.42218500	O	4.99131700	2.02153000	-1.40116000
O	-0.40763800	-0.92090300	0.04074700	H	5.77448600	2.41875100	-1.79963800
C	-1.91717800	-0.62234600	-0.73520100	H	5.01419600	2.23959000	-0.44099000
C	-2.84871800	-0.29305900	0.43835700	O	-3.58569000	-4.92533200	2.62702400
C	-2.90087100	1.21435800	0.74210700	H	-3.82259300	-4.31083700	1.90420000
C	-3.21251700	2.02727700	-0.53960200	H	-3.21930100	-5.69948700	2.18514700
C	-2.24519800	1.67676800	-1.66762700	O	-1.77151600	-4.05589400	-0.99640900
H	-2.02947800	-1.63019000	-1.12553000	H	-1.17356200	-3.94719000	-0.23817500
H	-3.71517300	1.37655000	1.45562900	H	-2.63281600	-3.87836200	-0.59169300
H	-3.17862300	3.11488900	-0.36768800	O	3.23418400	-4.89305500	-0.93606900
H	-2.76987900	1.77831100	-2.61706300	H	4.01324500	-4.43202500	-1.30601700
H	-2.49509100	-0.82086900	1.32272100	H	2.54420200	-4.65954400	-1.57907600
O	-1.65428400	1.58331600	1.31364900	O	2.46226500	2.94495300	-2.08256500
H	-1.76945700	2.50592300	1.64101600	H	3.39748600	2.71278300	-1.90788000
O	-4.57778800	1.77667200	-0.92605900	H	2.26128300	2.56715600	-2.94527000
H	-5.08364300	2.44064700	-0.41872400	O	4.89290900	-3.24477400	-2.51543000
C	-0.99750600	2.55177300	-1.70632600	H	4.01559300	-2.95999500	-2.81559800
H	-0.32466400	2.14049800	-2.46836300	H	5.24239200	-2.44460800	-2.09307200
H	-0.48674700	2.52779700	-0.73908100	O	2.30329300	-3.88285600	1.41423500
O	-1.42643600	3.86064800	-2.03743900	H	2.68794500	-4.34505400	0.63039400
H	-0.64536700	4.43951700	-1.94003600	H	2.61424800	-4.35143800	2.19595100
O	-1.78586700	0.25873700	-1.70994100	O	-6.51124800	0.16729400	-2.27237900
O	-0.25912500	-3.08908400	1.22890800	H	-5.79394700	0.79223300	-2.08541800
H	-0.39057900	-1.85432800	0.58190900	H	-7.25692100	0.51991500	-1.77419100
H	-0.73946800	-3.17330400	2.10662600	O	-2.27437900	4.16205600	1.91225300
O	2.11160800	3.51221500	2.13644700	H	-2.32457300	4.37838600	2.85071800
H	1.81356200	2.61246800	1.91050700	H	-1.44623000	4.60858600	1.57951000
H	2.98999500	3.56362700	1.73534700	O	-5.01075600	3.98332800	0.83465100
H	0.66136600	-3.44117800	1.34868300	H	-4.13876600	4.17015800	1.22951300
C	1.01933600	-2.24497700	-2.44379800	H	-5.25986700	4.80301300	0.39333800
H	-0.00750600	-2.57080200	-2.25512100	O	0.96201200	5.12356900	-1.51667900
H	1.02010400	-1.43336500	-3.17839700	H	1.26595800	5.91400300	-1.97524800
O	1.80806800	-3.34962500	-2.91409400	H	1.61320800	4.40909000	-1.71460200
H	1.41468600	-3.68480600	-3.72744500	O	0.08852900	5.15346200	1.15663000
N	3.96464500	0.19716800	1.76414600	H	0.34341300	5.22210300	0.21740500
C	4.62090900	1.33743900	2.06692800	H	0.80837800	4.62225800	1.55858500
H	3.93168100	-0.52940400	2.46569600				
O	4.71124500	2.29210400	1.27753500				
N	-4.17944100	-0.79665600	0.10817000				

P-TS2 (Applied Force = 3.0 nN, Pulling Direction A) Structure

C	1.74739600	-0.25707400	0.81824000	C	-4.50224000	-2.08010600	0.30969300
C	3.25151300	-0.06116100	0.52491800	H	-4.80469500	-0.15590600	-0.34191900
C	3.88350100	-1.17651900	-0.36116000	O	-3.68579500	-2.89970300	0.75973300
C	1.65533000	-1.79858000	-1.14660400	C	-5.92611000	-2.45014500	-0.01571900
C	0.95570800	-0.61497400	-0.45011500	H	-6.36187000	-1.77444800	-0.75214300
H	3.32439600	0.85816200	-0.05529700	H	-5.94959400	-3.47512100	-0.38541600
H	1.63029000	-1.08254200	1.53117000	H	-6.51776000	-2.40772000	0.90328100
H	1.70714400	-2.64386900	-0.45917500	C	5.22632700	1.40946500	3.43986900
H	0.88984400	0.24197800	-1.12074700	H	5.20906800	0.46940100	3.99054300
H	4.12654800	-2.13863700	0.14932400	H	6.25154500	1.77323400	3.36303300
O	5.10230300	-0.77839800	-0.90022100	H	4.64774300	2.15561300	3.99069600
H	5.03503300	0.13443900	-1.25254500	O	-1.59951200	-3.25146900	3.47144100
O	2.98503300	-1.37459800	-1.46645400	H	-2.30845900	-3.91284100	3.28353100
O	1.23892000	0.94411300	1.38608700	H	-1.08644600	-3.60666900	4.20547000
H	0.26547300	0.90466300	1.41843700	O	4.96543800	1.99928400	-1.42396200
O	-0.39931400	-0.89380300	0.03407700	H	5.74299600	2.39937300	-1.83054300
C	-1.88477500	-0.58021200	-0.73290000	H	5.00282900	2.21072900	-0.46286800
C	-2.83247800	-0.26773300	0.43555200	O	-3.55428300	-4.91856500	2.61022100
C	-2.91123200	1.23979800	0.74267800	H	-3.77985100	-4.31057700	1.87794200
C	-3.24419700	2.05070900	-0.53731100	H	-3.16137700	-5.68800800	2.18310400
C	-2.25473600	1.72624800	-1.65531700	O	-1.73857400	-4.06567200	-1.02045300
H	-2.01095900	-1.57788800	-1.14483800	H	-1.15422600	-3.94687700	-0.25416700
H	-3.72388600	1.38540500	1.46184100	H	-2.60443300	-3.87672100	-0.63133700
H	-3.26326200	3.14297200	-0.36876800	O	3.20510000	-4.90277000	-0.88335300
H	-2.77067000	1.81842600	-2.61067800	H	3.99053200	-4.45984700	-1.26120300
H	-2.47434600	-0.78649700	1.32349400	H	2.52013800	-4.67785600	-1.53489100
O	-1.66558200	1.62158800	1.30729800	O	2.43787000	2.96424200	-2.08037900
H	-1.78895100	2.54036700	1.64134700	H	3.36962000	2.71785400	-1.90740000
O	-4.59893200	1.74953700	-0.93383100	H	2.23413800	2.59855700	-2.94765100
H	-5.13210100	2.38861000	-0.42495300	O	4.88201900	-3.31115500	-2.51083700
C	-1.02511800	2.62645400	-1.67537800	H	4.00421900	-3.02554500	-2.80893500
H	-0.34384400	2.23977400	-2.44228700	H	5.24290100	-2.50456600	-2.11146000
H	-0.51609800	2.59306000	-0.70775700	O	2.26117300	-3.86075600	1.44996300
O	-1.47255200	3.93494100	-1.98569000	H	2.65046200	-4.33385600	0.67494700
H	-0.68945000	4.51324800	-1.90876000	H	2.54782000	-4.33207100	2.23936000
O	-1.75742300	0.31979900	-1.69808500	O	-6.48787800	0.11811200	-2.32902900
O	-0.28166900	-3.03791800	1.22916800	H	-5.78322100	0.75100800	-2.12249600
H	-0.39473200	-1.84199300	0.59294900	H	-7.24742800	0.45446400	-1.84069100
H	-0.77239900	-3.11315100	2.10524000	O	-2.29681400	4.19181700	1.92649400
O	2.12761400	3.50906400	2.12034800	H	-2.34101300	4.40259200	2.86648600
H	1.84077800	2.60606700	1.89359300	H	-1.46523000	4.63061700	1.59443300
H	3.00550700	3.57036800	1.72012900	O	-5.05749900	3.94251200	0.88667800
H	0.63720800	-3.39489200	1.36020700	H	-4.18492500	4.15725800	1.26447700
C	1.01977300	-2.26938900	-2.44053900	H	-5.35490400	4.76244300	0.47701000
H	-0.01298500	-2.57716300	-2.25436000	O	0.95041400	5.15739300	-1.50389800
H	1.03838100	-1.46473500	-3.18255400	H	1.26993800	5.94842300	-1.95060100
O	1.79315800	-3.39143600	-2.89581900	H	1.59281700	4.43625200	-1.70472800
H	1.39146100	-3.73610800	-3.70107300	O	0.08408600	5.15449000	1.17254700
N	3.99246500	0.15883900	1.75580100	H	0.33774900	5.23768100	0.23418800
C	4.63861400	1.30639800	2.05558000	H	0.80445400	4.61732500	1.56477300
H	3.95964700	-0.56352700	2.46164200				
O	4.72484000	2.25777800	1.26236000				
N	-4.15301100	-0.79399300	0.10103600				

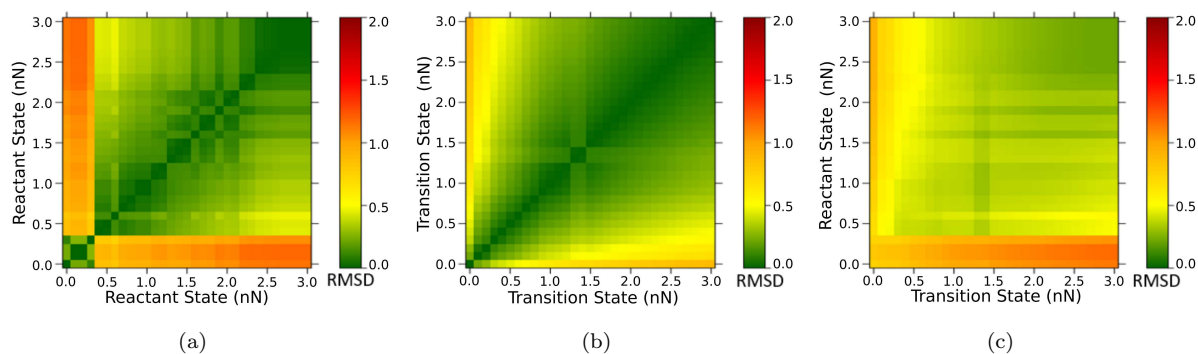


Fig. S4 Depolymerization RMSD Matrices for Pulling Direction B for (a)Reactant-Reactant (b)Transition State-Transition State and (c)Reactant-Transition State Comparisons

Structure progression in Pulling Direction B is similar to Pulling Direction A. It can be seen that the diagonal of the reactant - transition state matrix decreases in value. This shows that the reactant and transition state structures converges together. It can be seen in Figures 4(a) and 4(b), that the reactant structure is more susceptible to the applied force. Same conclusion can be drawn that the reactant structure approaches that of the transition state.

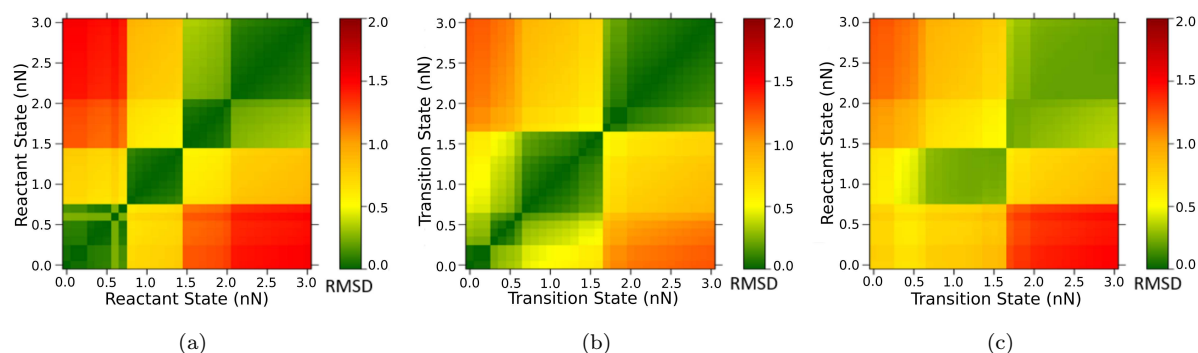


Fig. S5 Depolymerization RMSD Matrices for Pulling Direction C for (a)Reactant-Reactant (b)Transition State-Transition State and (c)Reactant-Transition State Comparisons

In the Pulling Direction C, multiple sections can be seen that does not correlate to changes in total energy. These can be attributed to the changes in water environment which drives the changes calculated RMSD. At the 0.7 nN boundary, it can clearly be seen that reactant and transition state structure converges as well. Similar to the other directions, it can be attributed to the reactant structure approaching that of the transition state structure.

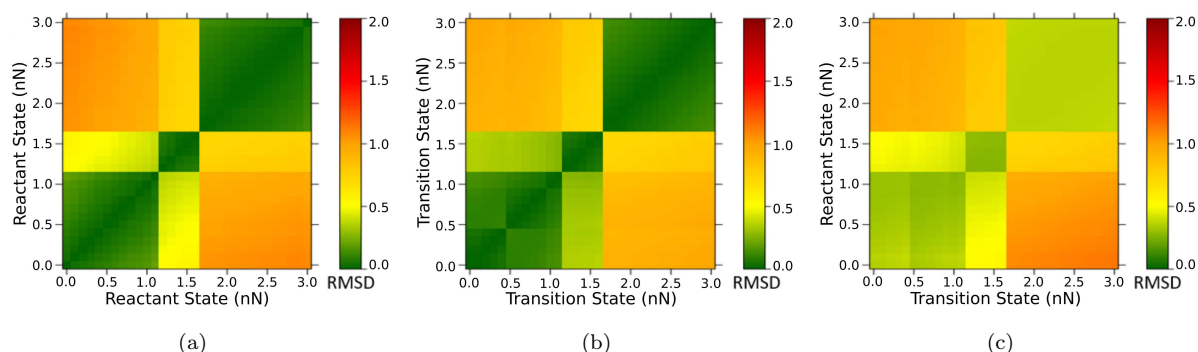


Fig. S6 Deacetylation RMSD Matrices for Pulling Direction B for (a)Reactant-Reactant (b)Transition State-Transition State and (c)Reactant-Transition State Comparisons

In this representative RMSD matrices for the deacetylation, it can be seen that though the reactant and transition state structure changes with the application of force, the structural difference of the reactant and transition state remains the same. This can be seen in the diagonal of the Figure 6(c). This conserved structural difference was expected to the energy trend previously calculated.

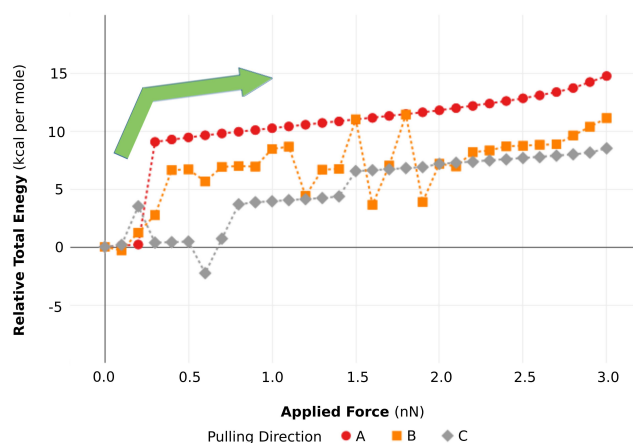


Fig. S7 Calculated GlcNAc dimer - solvent interaction energy of the depolymerization reactant state as a function of external force

As discussed in the main text, the activation of the depolymerization is mainly attributed to the change in the conformation of the reactant. In Figure S7, it can be seen that the destabilization in the reactant state can be anchored to GlcNAc Dimer - Solvent Interaction. This was concluded since the force required to increase the energy of the reactant is also the same energy in which the GlcNAc Dimer - Solvent interaction decreased.

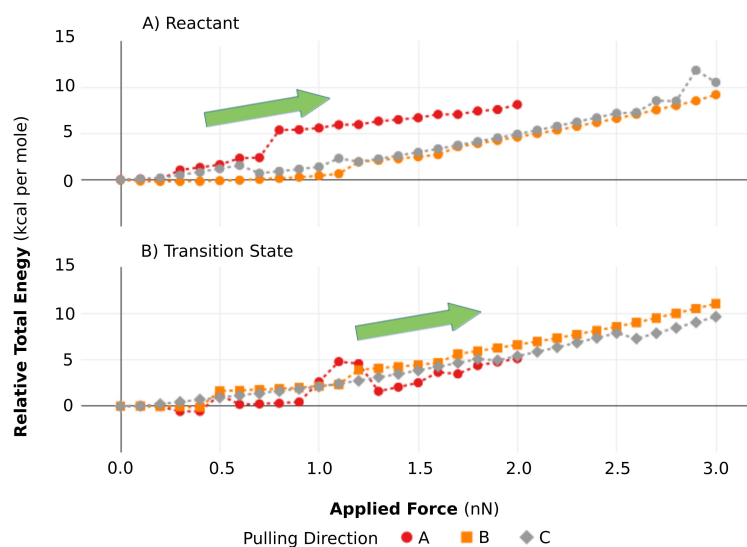


Fig. S8 Selected energies in the decomposition analysis. GlcNAc dimer of (a)reactant and (b)transition state single point energy of the deacetylation reactant as a function of external force

GlcNAc dimer contribution to total energies both follow a monotonic increase as function of the applied force. It can be seen that the destabilization brought by force to reactant state is very similar in magnitude to its effect in the transition state. This trend corresponded to calculated activation energy in FMPES using the chemical model described in main text (See Figure 5).

Table S1 Stabilizing interaction E(2) (kcal mol⁻¹) for deacetylation reactant state at different directions and forces

Pulling	Interaction		Applied Force (nN)						
Direction	Donor	Acceptor	0.00	0.50	1.00	1.50	2.00	2.50	3.00
A	<i>n</i> _{O3-1}	σ_{O7H}^*	1.97	1.99	2.07	2.13	2.15		
	<i>n</i> _{O3-2}	σ_{O7H}^*	49.73	51.68	55.17	55.93	56.08		
B	<i>n</i> _{O3-1}	σ_{O7H}^*	1.97	1.96	1.97	2.06	2.19	2.21	2.23
	<i>n</i> _{O3-2}	σ_{O7H}^*	49.73	51.40	51.96	54.89	59.91	60.62	61.27
C	<i>n</i> _{O3-1}	σ_{O7H}^*	1.97	1.96	1.99	2.00	2.03	2.03	2.06
	<i>n</i> _{O3-2}	σ_{O7H}^*	49.73	51.06	53.41	54.26	54.54	55.00	57.99

Table S2 Selected orbital occupancies for deacetylation reactant state at different directions and forces

Pulling	Orbital	Applied Force (nN)						
Direction		0.00	0.50	1.00	1.50	2.00	2.50	3.00
A	σ_{N2C7-1}^*	0.043	0.043	0.043	0.044	0.043		
	σ_{N2C7-2}^*	0.330	0.334	0.333	0.334	0.332		
	σ_{O7C7}^*	0.027	0.027	0.027	0.028	0.027		
	σ_{C7C8}^*	0.021	0.021	0.022	0.022	0.022		
	σ_{C7H}^*	0.111	0.114	0.119	0.119	0.120		
B	σ_{N2C7-1}^*	0.043	0.043	0.044	0.046	0.044	0.044	0.044
	σ_{N2C7-2}^*	0.330	0.331	0.332	0.335	0.335	0.335	0.336
	σ_{O7C7}^*	0.027	0.031	0.042	0.052	0.036	0.038	0.041
	σ_{C7C8}^*	0.021	0.021	0.021	0.021	0.022	0.022	0.022
	σ_{C7H}^*	0.111	0.113	0.114	0.118	0.125	0.126	0.126
C	σ_{N2C7-1}^*	0.043	0.041	0.043	0.043	0.044	0.044	0.044
	σ_{N2C7-2}^*	0.330	0.338	0.333	0.334	0.335	0.335	0.343
	σ_{O7C7}^*	0.027	0.027	0.026	0.026	0.039	0.029	0.082
	σ_{C7C8}^*	0.021	0.021	0.021	0.021	0.021	0.021	0.021
	σ_{C7H}^*	0.111	0.113	0.116	0.118	0.118	0.119	0.124

Table S3 Selected orbital occupancy for depolymerization reactant state at different directions and forces

Pulling	Orbital	Applied Force (nN)						
Direction		0.00	0.50	1.00	1.50	2.00	2.50	3.00
A	σ_{C1O1}^*	0.048	0.085	0.085	0.085	0.084	0.083	0.081
	σ_{C1O5}^*	0.036	0.037	0.041	0.048	0.042	0.042	0.043
B	σ_{C1O1}^*	0.048	0.077	0.078	0.075	0.075	0.082	0.079
	σ_{C1O5}^*	0.036	0.036	0.036	0.039	0.040	0.038	0.041
C	σ_{C1O1}^*	0.048	0.050	0.075	0.089	0.092	0.095	0.096
	σ_{C1O5}^*	0.036	0.036	0.035	0.034	0.033	0.033	0.033