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Structures, energies and bonding in the water heptamer		
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Cartesian coordinates of the structural motifs for the water heptamer. Optimized geometries at the MP2/6-311++G(d,p) level.		
S1		
O	-0.95226200	-1.44623800
H	-0.68010800	-1.73124900
H	-1.73367900	-0.85923100
O	0.17150200	-1.60748600
H	0.26603800	-2.31952900
H	1.09052000	-1.30435300
O	-1.09879000	0.97563800
H	-0.36761400	1.45914100
H	-0.73275100	0.08337000
O	1.09349700	2.02806500
H	1.01382900	1.53664600
H	1.12111400	2.97123300
O	2.47483400	-0.50962600
H	2.40807700	0.42970100
H	2.25713100	-0.49230200
O	-2.81892200	0.45354500
H	-2.31475600	0.73515100
H	-3.74063800	0.32950500
O	1.10768200	0.06303900
H	0.29319900	-0.51180900
H	1.29930100	0.01822600
S2		
O	1.12294100	-0.48206500
H	0.63484500	-1.09801900
H	1.08934100	-0.88890500
O	-2.78496300	-1.31124600
H	-2.88167900	-0.32555000
H	-3.37953500	-1.60866300
O	1.25887700	0.27447200
H	2.12408000	0.20723400
H	1.46024000	0.38178600
O	-2.76147900	1.41564100
H	-1.79713300	1.62560800
H	-3.24156300	1.90933100
O	-0.07483600	-1.81572200
H	0.24060300	-1.24514100
H	-1.05702900	-1.70296400
O	-0.07295600	1.77606300
H	0.26620500	1.14212400
H	0.32267500	1.46547700
O	3.29095600	0.06918100
H	2.67071300	-0.16787500
H	3.71991200	0.89495700
S3		
O	1.61811500	-0.14626100
H	0.89108000	-0.80178500
H	2.13545400	-0.29837700
O	0.84689800	2.15566700
H	1.03907100	1.49009300
H	1.32483800	1.77755400
O	-1.78628900	2.12971100
H	-0.79842000	2.20795700
H	-2.21414800	2.71622600
O	0.10011600	-1.63763000

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H	-0.73484200	-1.14527100
H	0.15300200	-2.20462900
O	2.18518800	0.09292400
H	1.46068800	-0.53285000
H	2.88234000	0.01478000
O	-2.23173600	-0.48720900
H	-3.11255600	-0.65515800
H	-2.14665400	0.50725600
O	-0.56438700	-1.99055600
H	-0.89440700	-2.52510900
H	-1.32869600	-1.48384600
S4		
O	0.63755600	-1.45794700
H	0.34949800	-1.70374000
H	-0.00103500	-0.76754700
O	2.90655700	-0.08923900
H	2.18863900	-0.64305600
H	3.72647500	-0.59998700
O	-0.22232400	-1.42587700
H	-0.04816300	-2.00819700
H	0.36708100	-0.60658400
O	1.32899800	0.69220900
H	2.04568500	0.50265800
H	0.81778200	1.43935200
O	-2.69911500	-0.67177000
H	-3.27614600	-1.44365800
H	-1.87668900	-0.99152100
O	-0.32039100	2.51405900
H	-1.05585600	2.90255200
H	-0.72802600	1.93358700
O	-1.44357400	0.57326800
H	-1.95134100	0.79501200
H	-2.05956300	0.11350400
S5		
O	1.98849500	0.66219700
H	2.13541800	0.00262800
H	1.48785500	0.17290200
O	-2.03977500	-0.96509100
H	-2.10379800	-0.11289000
H	-2.85791500	-1.05392100
O	0.33826700	-0.80017800
H	0.68604900	-1.69052300
H	-0.50660200	-0.91806600
O	-1.75869100	1.15246600
H	-0.99770800	1.76743200
H	-2.38564300	1.66878700
O	2.00794900	-1.32793300
H	1.05637100	-1.36794700
H	2.52758400	-1.32532000
O	0.38391400	2.58795200
H	1.04736100	1.90230100
H	0.37633900	3.29233500
O	-0.70944500	-1.32627100
H	-1.02242400	-0.40415900
H	-1.12859900	-1.79869400
S6		
O	-2.13334400	-1.35110500
H	-1.42114300	-1.31516400
H	-2.73679300	-2.06963500
O	0.01385200	-0.64208900
H	-0.76600900	-1.11078800
H	0.79262100	-1.09088100
O	-0.05660700	-0.87677600
H	0.75817400	-1.26262100
H	-0.01057300	0.06156500
O	-2.78150100	1.40248900

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H	-3.36086600	1.70541600	0.61726800
H	-2.74914500	0.42059200	-0.03397900
O	2.71977600	1.38639300	-0.21257000
H	1.77703800	1.67887600	-0.20878300
H	3.17093800	1.92083400	0.45732900
O	0.00509900	1.45841300	-0.00492200
H	-0.92135100	1.77654400	-0.08735000
H	-0.02034700	0.82631100	0.75896800
O	2.22382400	-1.28960600	0.07227000
H	2.56913200	-0.36155100	-0.01064800
H	2.98952200	-1.88125000	0.02797700
S7			
O	2.84730200	-1.36513100	-0.60663400
H	2.78384400	-1.81095900	-1.46386800
H	2.00331200	-1.54880600	-0.13039300
O	2.94498600	1.39628700	-0.48816300
H	3.75589500	1.68940900	-0.04712400
H	3.03339900	0.41970900	-0.60597700
O	0.50240200	-1.55400200	0.88095200
H	-0.38609900	-1.79580400	0.49181600
H	0.56106600	-2.01942800	1.72932600
O	-1.92757000	-2.12139900	-0.10966600
H	-2.01261800	-2.63168100	-0.92828900
H	-2.46212100	-1.29005700	-0.24626000
O	0.58681900	1.33489500	1.02365400
H	1.41824300	1.49705500	0.51972600
H	0.51690400	0.35931800	1.07517600
O	-3.30249100	0.16347700	-0.51370600
H	-4.07402800	0.31641200	0.05158500
H	-2.71794400	0.96350800	-0.40006500
O	-1.67388700	2.27911300	-0.11917100
H	-1.41884300	2.80112800	-0.89386700
H	-0.82150900	1.98427200	0.31009900
S8			
O	0.86284300	-1.41995900	-1.04245800
H	0.35754100	-1.86043500	-0.33210300
H	0.52879400	-0.49979700	-0.98549000
O	-2.49329900	1.73662600	-0.71779000
H	-2.84539700	2.54000200	-0.30775100
H	-1.54946400	1.66241100	-0.42987100
O	2.61064300	1.66409700	0.55143300
H	3.02038000	1.89646200	1.39726600
H	3.03581800	0.81820200	0.25480900
O	3.42252900	-0.80444100	-0.31071200
H	2.54313200	-1.16194400	-0.60565000
H	4.02022100	-0.89717300	-1.06717800
O	-3.35926100	-0.74178500	0.02512600
H	-3.62957500	-1.22661100	-0.76886300
H	-3.16836300	0.18640500	-0.27238700
O	-0.03065500	1.01115100	0.19233000
H	0.86896400	1.36566300	0.40466200
H	-0.23928100	0.31810300	0.85284900
O	-1.00065500	-1.44300000	1.18036700
H	-1.13384600	-1.87065800	2.03925600
H	-1.90606900	-1.29214900	0.79408200
S9			
O	-1.04378400	2.46829700	-0.14710200
H	-1.19274200	2.80750600	-0.04247500
H	-1.71602900	1.74184600	-0.02560000
O	-1.91930200	-2.01209700	-0.10799900
H	-0.92316200	-2.07260500	-0.19087900
H	-2.28364500	-2.61924800	-0.76831200
O	1.46953300	1.68465900	0.33229800
H	0.52981100	1.99108400	0.16310000
H	1.97382800	2.47510100	0.57769300
O	-2.87670000	0.50209300	0.08388700

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H	-2.53473900	-0.42832600	-0.02258600
H	-3.43609300	0.49258000	0.87420600
O	1.89946800	-0.05525400	-1.84564400
H	1.88919200	0.64232100	-1.15339500
H	2.82959400	-0.20285500	-2.07197600
O	0.75845000	-2.11847600	-0.27509800
H	1.11686100	-1.77330000	0.57274300
H	1.12034100	-1.50431400	-0.95203100
O	1.69810100	-0.61969300	1.93480000
H	1.15183100	-0.60355200	2.73429200
H	1.58882600	0.25753400	1.50408000
S10			
O	-3.89671400	-0.09163900	-0.01578600
H	-4.48330100	0.28909500	-0.68597300
H	-3.27508400	-0.69290800	-0.50250300
O	1.98517500	1.25012800	-1.47348300
H	1.92192100	2.21660900	-1.47323000
H	1.17204200	0.91433200	-1.01641600
O	-2.02594600	1.52495200	1.15228000
H	-2.79753000	1.02119500	0.78356800
H	-2.18545900	1.60826400	2.10369200
O	-0.00128700	0.05612500	0.00678600
H	-0.62282200	0.62987400	0.52191500
H	0.58702100	-0.40827900	0.65370800
O	-1.90258600	-1.50101100	-1.23613300
H	-1.12034300	-1.02815200	-0.85259700
H	-1.76526800	-2.44324500	-1.05941100
O	1.94124900	-1.20788900	1.48981400
H	2.10688400	-1.08402500	2.43580700
H	2.73977600	-0.85526700	1.01740400
O	3.89829200	-0.03825900	-0.01387300
H	3.30994400	0.49744200	-0.60692000
H	4.42675600	-0.60419000	-0.59587600
S11			
O	0.70703300	1.39167100	1.05768400
H	0.00554400	1.90439000	0.56012000
H	0.62277400	1.64862000	1.98854800
O	-1.32947900	2.50143100	-0.27539600
H	-1.24496200	3.14405100	-0.99489200
H	-1.77498000	1.69359500	-0.66309800
O	3.20683300	0.67141200	0.06482400
H	3.55245400	1.29004100	-0.59521600
H	2.36650200	1.06070300	0.40243900
O	-2.22222600	0.15243300	-1.23072600
H	-1.39518300	-0.35940900	-1.09551200
H	-2.83666900	-0.30845200	-0.62327300
O	-0.13433800	-1.19129000	0.12801400
H	0.70431500	-1.60843100	-0.18515400
H	0.15299900	-0.38406400	0.60620000
O	-2.78115200	-1.67086300	0.86779900
H	-1.80913200	-1.76757300	0.76043400
H	-3.15206700	-2.56487700	0.86179300
O	2.43022400	-1.87983000	-0.65988900
H	2.95461200	-2.54380900	-0.18893000
H	2.83863300	-1.00450500	-0.45193400
S12			
O	2.29604100	-1.19510500	-1.30169200
H	2.34081300	-2.13983700	-1.50935000
H	2.45507500	-1.11572100	-0.32889000
O	-2.40801500	-0.69641800	1.51786500
H	-1.56762500	-0.18852600	1.62827800
H	-2.35964100	-1.44081600	2.13566200
O	0.02698900	0.61451500	1.30528600
H	0.02157600	1.59086000	1.33333200
H	0.01110300	0.44467000	0.32172900
O	-2.36279800	-1.15895300	-1.20540700

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H	-3.17567000	-0.83625700	-1.62132600
H	-2.49358700	-1.06102300	-0.22926800
O	2.43770500	-0.76030900	1.43115900
H	3.18137900	-0.24339900	1.77450400
H	1.62848000	-0.21007400	1.56730600
O	-0.02818300	0.28838500	-1.39593100
H	-0.84411500	-0.25611800	-1.52003800
H	0.75525000	-0.29015500	-1.56308800
O	0.00967300	2.89304700	-0.36735900
H	0.26018700	3.70109900	-0.83668300
H	0.01547300	2.16399900	-1.02353100
S13			
O	0.99995400	1.76110700	1.16920600
H	1.33029400	2.38329800	1.83427800
H	1.11284300	0.83886300	1.54095600
O	-3.49273200	-0.15572300	-0.10424100
H	-2.90394300	-0.93280600	-0.00969600
H	-4.23227200	-0.28637700	0.50631400
O	1.83907400	-1.60109200	-0.85000200
H	2.53431900	-2.07997800	-1.32531400
H	1.83523200	-0.67132200	-1.20628500
O	1.60079300	1.03382600	-1.52054300
H	1.65231400	1.45779500	-0.63758100
H	0.66572600	1.16492600	-1.76420700
O	-0.98842100	-1.43282600	0.03278600
H	-0.88199900	-0.50608200	-0.29480100
H	-0.33846300	-1.94847200	-0.47883700
O	1.16584300	-0.85357100	1.80919200
H	1.71083600	-1.21134800	1.07687300
H	0.26755900	-1.14939300	1.54827900
O	-1.12181000	1.25835100	-0.60392400
H	-0.69223600	1.67280800	0.17236400
H	-2.08182000	1.18750900	-0.42213600
S14			
O	1.33818500	0.78083000	-1.71981900
H	0.41132800	0.89753100	-1.41778000
H	1.83841800	1.28895900	-1.05615700
O	1.95033400	-1.80665900	-1.03486500
H	2.80166800	-2.11654300	-1.37554900
H	1.77822800	-0.92057800	-1.44367700
O	1.16435300	-1.04574700	1.50133200
H	1.39870700	-0.09620300	1.46030700
H	1.55228700	-1.44474300	0.68556200
O	-3.32391300	-0.26011900	-0.84082300
H	-3.64392200	-0.83140100	-1.55381100
H	-2.79339900	-0.82840500	-0.24750200
O	-1.03270700	1.38470400	-0.19615700
H	-1.23541100	0.59377500	0.36027800
H	-1.85061700	1.49697600	-0.71280300
O	-1.48340000	-0.96279700	1.21523300
H	-1.88847100	-0.96050400	2.09556900
H	-0.50238700	-1.13382800	1.35609300
O	1.39099400	1.84560400	1.01181200
H	1.63515400	2.54870600	1.63180800
H	0.46764800	2.01971300	0.72396300
S15			
O	-0.61937100	-1.98550300	-0.66143400
H	-0.00231100	-1.25707500	-0.44601400
H	-0.07603300	-2.77585800	-0.66988500
O	-3.13894300	-1.44804600	0.27781900
H	-3.22668700	-1.80034800	1.16575100
H	-2.26296700	-1.75419800	-0.02433800
O	-3.28409300	1.23485800	-0.26425200
H	-3.31023000	0.28255500	-0.04687200
H	-3.63869500	1.28203300	-1.15530500
O	3.47089500	0.64349600	-1.19907900

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H	3.79079100	0.18721100	-0.40470300
H	3.97504700	0.26638600	-1.92280800
O	0.98608400	0.14387700	0.00440400
H	0.40154700	0.90664100	0.18875700
H	1.62673800	0.46388500	-0.65011000
O	3.32951600	-0.67024100	1.26362100
H	2.39583700	-0.42976600	1.13419200
H	3.51732400	-0.45068600	2.17839100
O	-0.82851900	2.09942400	0.56074000
H	-1.72371100	1.87892700	0.23342300
H	-0.79120300	3.05738300	0.56496000
S16			
O	-1.91370700	1.21336600	-0.76962900
H	-1.15948100	1.78528400	-0.45242900
H	-2.27511100	1.65969500	-1.55002900
O	2.59236100	1.65326100	0.05080400
H	2.69947100	0.67289500	0.17799100
H	3.20365200	1.89973400	-0.65844600
O	0.95271900	-2.72407600	-0.15202400
H	0.05937000	-2.31572400	-0.31597700
H	1.08472400	-3.36823900	-0.86272300
O	0.12626100	2.77240000	0.03818200
H	1.02374400	2.34418300	0.01768900
H	0.04724200	3.17515000	0.91552400
O	2.97929600	-1.00956200	0.39939400
H	3.27884700	-1.24984400	1.28848200
H	2.24316900	-1.64181900	0.18153300
O	-3.21651900	-0.37284600	1.15581900
H	-4.18247400	-0.37071700	1.21898800
H	-2.96818700	0.37780300	0.57462100
O	-1.46259900	-1.61988700	-0.67929500
H	-1.41850300	-0.67890200	-0.94613100
H	-2.09896900	-1.59074500	0.06490100
S17			
O	1.33763600	2.56423900	0.57573000
H	0.36809400	2.57152700	0.36358800
H	1.41806900	2.86577200	1.49180300
O	-3.05886300	0.66008100	-0.27467400
H	-2.75545200	-0.28452400	-0.30729500
H	-3.79452300	0.67403100	0.35498800
O	3.05532600	0.70195400	-0.42350600
H	2.43487000	1.38075100	-0.05187000
H	3.33997400	1.04822200	-1.28195100
O	2.29959800	-1.91610700	-0.41565100
H	2.53675700	-0.95233900	-0.41930800
H	3.11759800	-2.39256300	-0.21285800
O	-1.31646800	2.73249300	0.00128300
H	-1.90992200	1.94075600	-0.08052100
H	-1.50713800	3.28395400	-0.77159600
O	0.01439800	-2.80754100	0.77551900
H	0.84135500	-2.46469600	0.34805000
H	0.12094700	-2.65823300	1.72616700
O	-2.36016500	-1.96768700	-0.26457900
H	-2.49277800	-2.49406000	-1.06620700
H	-1.48954400	-2.25804300	0.11405600
S18			
O	-1.45261500	1.39324600	0.52073100
H	-0.68483400	1.93003100	0.17203200
H	-1.45549800	1.53179700	1.48041400
O	1.33401900	-1.42237900	-1.81388400
H	0.49011000	-1.44695900	-1.30603400
H	1.10358300	-1.15796100	-2.71646200
O	1.23541000	-1.22619300	1.95988000
H	1.69736800	-2.03715500	2.21839900
H	0.47516000	-1.50349100	1.40231400
O	2.45321000	0.42370800	-0.00958700

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H	2.17439300	-0.07668400	0.78917100
H	2.25811200	-0.19303800	-0.75125500
O	0.79859900	2.49009900	-0.41146500
H	1.21634500	3.33724000	-0.20067400
H	1.48284100	1.77406100	-0.25269200
O	-0.77001300	-1.26980100	0.01987600
H	-1.68534200	-1.57604800	-0.12891700
H	-0.90262100	-0.30350400	0.17956500
O	-3.46255200	-0.44080300	-0.25749800
H	-3.02561200	0.42492900	-0.12707600
H	-4.23247400	-0.28623700	-0.82321200
S19			
O	0.37271200	2.60194500	0.22490000
H	-0.51215000	2.17614000	0.03858700
H	0.30093300	3.51671200	-0.08397000
O	1.09818000	-1.61812400	-1.01269600
H	1.48282200	-0.72430400	-1.12739200
H	1.49042000	-1.89757300	-0.15903700
O	-3.00690300	-0.68415000	1.26158300
H	-2.77868400	-1.08897000	2.11060000
H	-2.52270800	-1.18424000	0.56890000
O	2.64640000	-1.28684700	1.31719900
H	2.48192600	-1.17819500	2.26494000
H	2.68099800	-0.38476000	0.93132700
O	-1.96976700	1.39658700	-0.33753100
H	-2.42950000	1.02639800	0.44466500
H	-1.80591200	0.59210900	-0.87229300
O	2.34739700	0.88655200	-0.42995400
H	3.07746100	1.32983600	-0.88680200
H	1.66938700	1.58675400	-0.21522600
O	-1.56750100	-1.34575900	-1.04801500
H	-0.57966900	-1.50905300	-1.03005100
H	-1.91946100	-1.86250200	-1.78812700
S20			
O	-1.93533000	1.03282700	-0.93078500
H	-1.23096500	1.67855500	-0.66868200
H	-2.54910200	0.94787700	-0.17552800
O	3.52154100	-0.70268000	-0.51667000
H	3.66549500	-0.68457900	-1.47386500
H	2.73891700	-1.27186000	-0.35999900
O	-3.32102600	-0.55496400	0.98189600
H	-4.23212900	-0.87400200	1.05594100
H	-2.82653500	-1.22958400	0.47558900
O	1.91347700	1.00924500	1.06386100
H	2.68327700	0.76220400	0.50995800
H	1.45080200	0.15358600	1.15900200
O	1.09009700	-1.72585400	0.49177900
H	0.22278000	-1.71165100	0.00945300
H	1.03173400	-2.43739000	1.14684900
O	0.15788400	2.65111000	-0.21069500
H	0.83929100	2.10913300	0.26992500
H	0.05443300	3.47166200	0.29234400
O	-1.30341400	-1.51413500	-0.82507700
H	-1.39269400	-1.95321400	-1.68448600
H	-1.44112300	-0.52512900	-0.99096600
S21			
O	3.80147200	0.07979600	0.39806400
H	4.20348100	-0.10622300	1.25873200
H	3.29013200	-0.71633900	0.14484900
O	-0.62720400	1.53740300	0.86537200
H	-1.49648500	1.54523800	0.37415300
H	-0.71668000	2.17173200	1.59245700
O	-2.97985700	1.26223600	-0.42603200
H	-3.02758700	1.52541300	-1.35710200
H	-3.08530300	0.27298900	-0.40959400
O	1.68186900	-1.37966800	-0.77080100

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H	1.68678700	-1.89598400	-1.59056800
H	1.54429700	-0.42223300	-1.02352400
O	1.57940300	1.29672500	-0.89269700
H	2.40668600	1.32273000	-0.37123200
H	0.85629300	1.54332700	-0.27587000
O	-2.90995300	-1.44403400	-0.25128600
H	-2.03728700	-1.53587700	0.22244700
H	-3.56123300	-1.93183900	0.27388300
O	-0.52375400	-1.33597800	1.02237200
H	0.23625900	-1.53708500	0.43359000
H	-0.47517500	-0.36767800	1.16784200
S22			
O	2.65434300	-0.27191500	-0.16449600
H	2.49702700	-0.36916100	0.79137000
H	2.03803300	-0.92556900	-0.55596000
O	-3.32285300	0.40649200	0.37368000
H	-2.54164700	0.97237500	0.55096800
H	-4.09538100	0.98959300	0.38399300
O	1.72475800	2.31458800	-0.43256600
H	2.17015000	1.43142600	-0.46898600
H	1.90875600	2.75929900	-1.27244400
O	0.50350700	-2.15705100	-0.60568300
H	-0.27476000	-1.69155700	-1.03735300
H	0.57202000	-3.03930500	-0.99964400
O	-0.65794800	1.26192900	0.47200000
H	0.08338300	1.83809100	0.16567700
H	-0.24204800	0.60981300	1.07817000
O	-1.40309100	-0.55040900	-1.52222600
H	-2.31390500	-0.62285800	-1.17680200
H	-1.05882300	0.21237000	-0.99905700
O	0.57910800	-0.91665400	1.84549700
H	0.43611500	-1.59480400	1.14530000
H	0.19847900	-1.26554700	2.66510200
S23			
O	3.21531300	1.39597200	-0.01364500
H	3.72815800	1.65318500	-0.79401400
H	3.27339900	0.40546900	0.03673000
O	3.26401800	-1.32614300	0.07629000
H	2.33875700	-1.67838500	-0.00544800
H	3.63492300	-1.73200300	0.87363800
O	-0.98373400	-0.04502200	-0.05526100
H	-0.43638500	0.78203400	0.00091300
H	-1.59165800	-0.04467200	0.71913200
O	0.60446400	2.17843100	0.01205800
H	0.50640800	2.80155500	0.74698300
H	1.56492100	1.92498700	-0.00571700
O	0.69165700	-2.20355800	-0.11321300
H	0.46533900	-2.71120700	-0.90645200
H	0.05639600	-1.44024500	-0.08463800
O	-3.33331600	-0.00716100	1.43351600
H	-3.71753900	-0.00886400	0.52722300
H	-3.72901400	-0.75467700	1.90497200
O	-3.44991300	0.00631500	-1.33106200
H	-2.47604800	0.05498000	-1.18744000
H	-3.68558100	0.75717600	-1.89535100
S24			
O	-1.32624200	-0.47882600	2.14569100
H	-2.16296500	-0.46161000	2.63316500
H	-1.46952300	-1.06740500	1.37327500
O	-2.40960700	0.74042200	-1.22543200
H	-1.81883800	1.26472900	-0.60831200
H	-2.32714200	1.13662900	-2.10457100
O	1.85081100	1.53616100	-0.47589200
H	2.45633600	0.93944000	0.03278300
H	2.34952900	2.34241300	-0.67430300
O	1.15808000	-1.28080800	-1.18924000

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H	1.13471600	-0.33038100	-1.40278300
H	0.24420100	-1.51028000	-0.91168800
O	-0.76042200	1.80356100	0.60707000
H	0.17770200	1.77161000	0.32177800
H	-0.86337000	1.11063800	1.29954700
O	3.03888500	-0.63112600	0.67379100
H	3.91327900	-1.02139900	0.53359100
H	2.40538200	-1.12911400	0.09815100
O	-1.55546300	-1.65869700	-0.41344800
H	-2.04335700	-2.43514200	-0.72611800
H	-1.96429000	-0.85563200	-0.84482500
S25			
O	3.91690200	0.34666900	-0.02186500
H	4.32048200	-0.13246600	-0.76227400
H	4.04518600	-0.21934700	0.75587700
O	1.11019000	0.61716800	-0.22169900
H	2.09096600	0.65193200	-0.21946000
H	0.85151400	-0.10226000	-0.86138600
O	-0.96755300	2.40635000	-0.12663400
H	-0.13594000	1.87614800	-0.19867500
H	-0.92423800	3.07608100	-0.82471600
O	-3.02047100	0.54413200	-0.21051300
H	-3.74009900	0.82475200	0.37316900
H	-2.34413900	1.26447800	-0.18509100
O	0.23379300	-1.47884200	-1.68978900
H	-0.49013400	-1.73976900	-1.04747100
H	-0.19598200	-1.37527900	-2.55147000
O	0.24803500	-0.72795100	2.07414000
H	-0.09086300	-0.12235300	2.74987700
H	0.59752100	-0.16051800	1.34636400
O	-1.60977200	-1.84988600	0.23311200
H	-2.20860100	-1.07784000	0.11271400
H	-1.06465800	-1.62468200	1.01852600
S26			
O	-3.38279700	0.49772800	0.10560700
H	-2.70328200	1.22137000	0.11522300
H	-4.01056900	0.72897500	-0.59478800
O	3.66962700	0.51476800	-0.59661500
H	2.80628200	0.96937000	-0.69835200
H	4.35767700	1.18872400	-0.69488900
O	0.90721000	1.00531100	-0.20082300
H	0.62116300	0.19789400	-0.68606200
H	1.21832800	0.60011900	0.64603100
O	0.35294500	-1.68275500	-0.71318700
H	0.53474400	-2.21749800	-1.50051500
H	-0.59986900	-1.85021900	-0.47458600
O	-1.43666600	2.41153700	0.06383300
H	-0.54756100	1.97768900	-0.01309200
H	-1.37646500	3.03317400	0.80391700
O	2.16555600	-0.80746000	1.45591800
H	2.98080900	-0.57898200	0.96582800
H	1.71203200	-1.46271800	0.89163300
O	-2.25622500	-1.97651300	-0.05676600
H	-2.45648000	-2.42305700	0.77913700
H	-2.69400600	-1.08576600	-0.00322200
S27			
O	1.30887600	-1.94867600	1.65769200
H	0.95430300	-1.92578400	2.55823100
H	1.36853100	-1.01293500	1.35776900
O	3.80863700	0.93825300	-0.96905800
H	3.89249600	0.44101800	-1.79762700
H	4.50115600	0.59219200	-0.38478400
O	-3.01026800	1.29795700	0.10516400
H	-3.60697500	1.24977000	0.86660200
H	-2.94336500	0.36876600	-0.24341500
O	1.26458600	0.39195800	0.15613400

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H	2.11013800	0.71296900	-0.22031400
H	0.67975100	1.17444200	0.32400900
O	-2.76113900	-1.26802400	-0.75904800
H	-1.80083000	-1.53869300	-0.78145100
H	-3.12775700	-1.50663900	-1.62299300
O	-0.12111100	-1.85102000	-0.81536400
H	0.18781400	-2.31507600	-0.01083500
H	0.33612900	-0.98483500	-0.73036200
O	-0.56074000	2.38046600	0.63522100
H	-1.46115400	2.00200300	0.45273400
H	-0.52096000	3.21549500	0.14650700
S28			
O	0.78414000	2.17033100	-0.09361100
H	-0.08471600	1.69740600	-0.09939500
H	0.59295500	3.11541600	-0.18900000
O	0.10958100	-1.44325700	1.40599800
H	0.94864800	-0.90413600	1.54570400
H	-0.01486600	-2.00228300	2.18775400
O	0.11499600	-1.65362200	-1.34448800
H	-0.08072300	-2.44925000	-1.86186800
H	0.15721300	-1.92020000	-0.39656300
O	-4.23851900	0.23618700	0.01365800
H	-3.27502200	0.40476800	-0.02081900
H	-4.66085100	1.10724100	0.01017400
O	2.42110300	0.10264100	-1.33567600
H	1.95287400	0.95806300	-1.27562200
H	1.72705500	-0.54734100	-1.56480300
O	2.24765100	0.13578600	1.42967100
H	2.56128600	-0.01222000	0.50312800
H	1.87452200	1.03578500	1.37338800
O	-1.37264100	0.42589500	-0.08118000
H	-1.13544300	-0.14057300	-0.84439800
H	-1.09341800	-0.13435400	0.67734100
S29			
O	2.15932500	-0.28067100	1.68231900
H	2.71496800	-0.47016700	2.45254200
H	2.75706100	-0.15907500	0.91359700
O	0.90422600	1.90164200	0.12574100
H	-0.04107100	1.79469300	-0.13526400
H	1.00030800	1.44841800	0.98333900
O	2.66584100	0.21369600	-0.97966200
H	3.30626900	0.54776100	-1.62459500
H	2.02150000	0.95004800	-0.78075600
O	-1.72641700	1.39969200	-0.66612700
H	-1.66981100	0.44116300	-0.97155000
H	-2.05858900	1.91690100	-1.41526700
O	-1.71781100	-1.22028900	-1.03164800
H	-2.29456900	-1.35470300	-0.25464600
H	-0.82859700	-1.58132000	-0.79024500
O	-3.20314800	-0.19336400	1.17947100
H	-4.11792300	-0.04777700	1.46051000
H	-2.90756900	0.62894000	0.73817500
O	0.86464200	-1.95145900	-0.34218500
H	1.07265600	-1.65800900	0.56546300
H	1.47210700	-1.41085200	-0.88457900
S30			
O	-0.69731300	1.61917400	-1.20576800
H	0.11314500	1.06823700	-1.13942700
H	-0.69106900	2.09878300	-0.35532800
O	-0.02842900	-0.93985700	1.67821000
H	-0.85887000	-1.32981700	1.30871800
H	-0.27182300	-0.06047900	2.01791400
O	-2.90326000	0.02985800	-1.32826900
H	-2.11661100	0.64000500	-1.32718800
H	-3.08885100	-0.17237500	-2.25672800
O	1.53764400	0.24765000	-0.17074000

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H	2.39265300	-0.15285300	-0.42922200
H	1.06211600	-0.39890500	0.41636100
O	3.96014900	-1.05785900	-0.93405400
H	4.33279100	-1.65553600	-0.26752700
H	3.87867000	-1.58250100	-1.74540000
O	-2.32402600	-1.92350300	0.48971300
H	-3.10942600	-2.06943500	1.03685300
H	-2.58954200	-1.26708400	-0.20513900
O	0.34685600	2.07806400	1.47005400
H	1.08436500	1.63571700	0.98953900
H	0.72948400	2.81802300	1.96340500
S31			
O	3.40097800	0.32300200	-0.23459500
H	3.56300500	0.67344900	-1.12345600
H	3.09617100	-0.61742500	-0.36321000
O	-1.90126100	-0.12748300	-0.96921400
H	-1.59682000	0.80638800	-0.95350100
H	-2.76906300	-0.15152900	-0.51918400
O	2.24948900	-2.10632600	-0.49088200
H	1.35763500	-1.89127500	-0.09282200
H	2.57912400	-2.88508100	-0.01926900
O	-0.63323900	2.37457300	-0.64112500
H	0.06431900	2.15342300	0.01688100
H	-1.03626700	3.20541900	-0.35110100
O	1.30464800	1.35187500	1.10733800
H	2.12174900	1.05817400	0.61130100
H	1.61202000	1.71923500	1.94951900
O	-4.36529700	-0.63823400	0.38981300
H	-4.11491300	-1.25331500	1.09693900
H	-4.93766300	-1.14412300	-0.20756900
O	-0.00252400	-1.22162300	0.69512800
H	-0.70486300	-0.94082900	0.05236800
H	0.34321600	-0.37878100	1.05140600
S32			
O	0.85223900	-0.02838900	0.06875600
H	1.49014600	-0.77214300	-0.02239000
H	0.25724000	-0.02697600	-0.73533900
O	3.26131700	1.36335800	0.10446900
H	2.29255100	1.19036000	0.06545000
H	3.45555000	2.00674900	-0.59287200
O	3.26909000	-1.38798000	-0.12549400
H	3.60413400	-0.46399500	-0.06289200
H	3.75074300	-1.90448000	0.53661800
O	-2.61860900	-1.74120900	-0.15731400
H	-2.23082000	-1.35804700	0.65866500
H	-2.52657400	-2.70231800	-0.08555900
O	-1.11842200	0.07164000	-1.77018900
H	-1.58379800	0.85595800	-1.40454100
H	-1.67505500	-0.67972900	-1.47376300
O	-1.27635100	-0.10089700	1.69973600
H	-1.11282200	-0.03656700	2.65244600
H	-0.38585500	-0.10011500	1.24421200
O	-2.35721200	1.91203700	-0.00900800
H	-3.32493200	1.95385300	-0.00754000
H	-2.10692300	1.32897400	0.73985900
S33			
O	0.68123900	-2.17183800	-0.57246800
H	-0.04274800	-1.67150900	-0.98988200
H	1.50584600	-1.69957300	-0.82466300
O	1.95306500	1.25033400	0.97091200
H	2.38234700	1.94287700	1.49505500
H	1.31193600	1.70785400	0.35505100
O	-1.44280500	0.01737500	-0.38961500
H	-1.10014300	-0.23887600	0.50697300
H	-2.42011400	0.04381500	-0.33275100
O	0.11020900	2.19996800	-0.74965900

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H	0.41663500	2.22459500	-1.66859700
H	-0.56149300	1.46492900	-0.70357400
O	2.97843400	-0.56110000	-0.89483600
H	3.83221100	-0.97200300	-0.69499800
H	2.80654700	0.09530400	-0.18160200
O	-4.28754200	-0.03182000	-0.17093400
H	-4.64689200	-0.93246300	-0.16948400
H	-4.67502300	0.41067300	0.59990200
O	0.02104800	-0.79937500	1.76739600
H	0.36411000	-1.49084700	1.15331100
H	0.71759600	-0.11313300	1.76889000
S34			
O	1.20445900	-2.05379200	0.98854900
H	2.04664400	-1.64154000	0.65898900
H	1.17231600	-1.86141300	1.93740500
O	3.29389200	-0.64436000	-0.03278800
H	3.90679700	-1.02228700	-0.68019400
H	2.75186400	0.03574100	-0.51696500
O	-0.64015600	-0.88006900	-0.63449700
H	-0.03979800	-1.35098800	0.00507900
H	-1.43859200	-1.43505300	-0.73460000
O	-2.08404000	1.22097500	0.26277700
H	-2.39969700	1.65323800	-0.54685500
H	-1.47225700	0.49560100	-0.04792100
O	1.50167800	1.01710400	-1.22430000
H	1.19200400	1.65820600	-0.54608300
H	0.75634100	0.39655300	-1.33933800
O	0.31048200	2.56584700	0.82978600
H	-0.62877900	2.27404700	0.81289400
H	0.31209600	3.52211700	0.98009100
O	-3.42874100	-1.28297700	-0.24642500
H	-3.35143800	-0.43781500	0.23803400
H	-4.06810200	-1.82823600	0.23464300
S35			
O	-1.81277800	0.09491500	-0.54904000
H	-1.39228400	0.97269500	-0.37989300
H	-2.75962000	0.16819400	-0.31686900
O	-0.54527600	-1.86002800	0.79471400
H	-0.41799200	-1.47374700	1.67406600
H	-1.02035200	-1.15518600	0.26761100
O	1.85996600	-2.39929900	-0.35753400
H	2.15489000	-3.25449800	-0.01302200
H	0.96191000	-2.23284900	0.03763300
O	2.18703000	2.09563600	0.41738200
H	2.56289600	2.34577300	1.27367000
H	2.63274800	1.24708400	0.15745000
O	-0.49535300	2.47212500	-0.02224900
H	-0.52042900	3.13090300	-0.73168900
H	0.46592100	2.31592600	0.15731900
O	3.46824500	-0.20505100	-0.29961300
H	2.90285200	-1.02165300	-0.30014800
H	3.83787400	-0.14291900	-1.19287600
O	-4.61630300	-0.14886600	-0.02065100
H	-4.73366800	-0.93789500	0.53084600
H	-5.03899800	-0.35728400	-0.86817000
S36			
O	-0.19292500	2.59382200	-0.84269300
H	-1.10700600	2.43264900	-0.49023100
H	-0.30028600	2.85181200	-1.76962700
O	3.03109200	-1.25265300	-1.16535500
H	3.44026300	-0.98127200	-0.31128800
H	3.66488200	-1.02181700	-1.85975200
O	-2.90219400	-2.70160200	-0.41615100
H	-3.17777300	-3.42363600	0.16914500
H	-3.70929700	-2.39013700	-0.85403100
O	0.95679500	0.23140800	-0.01035200

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H	1.45495800	-0.25894300	-0.70064200
H	0.67295300	1.09675500	-0.39849900
O	3.36674900	-0.06406400	1.30857500
H	3.33281000	-0.51598600	2.16428700
H	2.44343400	0.21631400	1.10304700
O	-2.58437100	1.82990600	0.24003500
H	-2.29658800	0.92175200	0.53887400
H	-2.85858300	2.30175300	1.04032400
O	-1.55008700	-0.56812600	0.92678200
H	-1.93371500	-1.32549300	0.44083100
H	-0.62652800	-0.45327600	0.60085400
S37			
O	-0.75352500	-0.51934200	1.13989800
H	0.06707500	-0.81244300	0.65640200
H	-1.38977000	-1.26415300	1.11409800
O	-2.22177300	0.52833600	-0.97354300
H	-1.67184000	0.32835900	-0.17498400
H	-2.78667900	1.27580000	-0.72289400
O	-0.29822400	2.18776300	1.32022500
H	0.14664000	2.60512200	2.07175400
H	-0.45478800	1.24835600	1.56417100
O	1.38507400	-0.87729100	-0.45666200
H	2.31607300	-0.90241900	-0.15940700
H	1.24754700	-0.00148100	-0.89256300
O	4.19431800	-0.95354200	0.19206000
H	4.60600900	-1.68956100	-0.28671300
H	4.66227400	-0.15588100	-0.09976200
O	0.54579000	1.62337100	-1.34986000
H	-0.34150600	1.38460200	-1.67772000
H	0.36955900	2.02037800	-0.46935700
O	-2.95910400	-1.98608800	0.12626900
H	-2.95546800	-2.80877900	-0.38444800
H	-2.95557300	-1.25355300	-0.52566100
S38			
O	-0.08619200	2.75703900	-0.25532200
H	0.00742900	3.50704100	0.34952200
H	0.70876500	2.18974900	-0.13385900
O	-3.25443900	-1.05671800	-1.37207600
H	-3.93535800	-0.72765200	-1.97668100
H	-3.67100100	-1.11729000	-0.48215600
O	-1.35573500	0.32231900	0.11418100
H	-1.84615600	-0.02478300	-0.66594200
H	-1.22528100	1.28797000	-0.02575400
O	3.46341600	-0.88585100	-1.33472600
H	3.25477500	-1.61665800	-1.93469300
H	2.62352300	-0.39433800	-1.18404400
O	-3.61796300	-0.71696300	1.34893500
H	-2.74932600	-0.26855300	1.22857100
H	-3.48888400	-1.39463700	2.02853700
O	3.42076500	-0.87587400	1.42634700
H	4.18099600	-0.48728100	1.88300500
H	3.71383300	-1.06878200	0.50615900
O	1.42509600	0.44591900	0.01403200
H	1.95635800	0.10447100	0.76887200
H	0.51075500	0.09177200	0.10749100