

Interaction of Oxalic Acid with Dimethylamine and Its Atmospheric Implication

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Sensitivity analysis of the applied DFT methods and single-point energy calculation based on the DFT methods

In order to investigate the sensitivity of the applied DFT methods and single-point energy calculation based on the DFT methods, the binding energy (ΔE), the Gibbs free energy (ΔG) have been calculated for six typical reactions employing DFT method with 6-311+G(2d,p) and 6-311++G(3df,3pd) basis sets. The DFT and DF-LMP2-F12/VDZ-F12//DFT results are compared with a high level calculation of CCSD(T)-F12a/VDZ-F12 as a benchmark of the energies.

Table S1 shown the mean absolute error (MAE), mean signed error (MSE) and Maximum error (MaxE) in the DFT binding energies (ΔE) and single-point energy calculation based on the DFT compared against CCSD(T)-F12a/VDZ-F12 results using both 6-311+G(2d,p) and 6-311++G(3df,3pd) basis sets. Our results show that there is a smallest error in the binding energy with 0.71 kcal/mol of MAE and 1.53

kcal/mol of MaxE for M06-2X, using the small 6-311+G(2d,p) basis set. PW91PW91 show the largest MAE, MSE and MaxE of 1.55, 1.37, 2.94 kcal/mol, respectively. The error of MAE is the lowest for ω B97X-D with a value of 0.97 kcal/mol. The value of M06-2X is close to ω B97X-D. Compared the DF-LMP2-F12/VDZ-F12 binding energy with CCSD(T)-F12a/VDZ-F12. The MAE and MSE drop obviously with the value within 0.4 kcal/mol for DF-LMP2-F12/VDZ-F12//DFT. And the maximum errors are also reduced, around 1 kcal/mol. Extending the basis set to 6-311++G(3df,3pd) improves the results slightly for M06-2X, PW91PW91 and ω B97X-D with a difference value of 0.07, 0.40, 0.52 kcal/mol for MAE, and 0.26, 0.29, 0.74 kcal/mol for MaxE, respectively.

Table S2 show that changing the basis set from 6-311+G(2d,p) to 6-311++G(3df,3pd) obtain a small effect on the Gibbs free energy. There is a very small difference with MAE of 0.6 kcal/mol or less, and the maximum errors are below 0.9 kcal/mol. The MAE difference between the different DFT methods is also very small, below 0.05 kcal/mol. Our comparison results imply that increasing the basis set from 6-311++G(3df,3pd) to 6-311+G(2d,p) does not improve the ΔG significantly.

The MAE, MSE and MaxE in the CCSD(T)-F12a/VDZ-F12 and DF-LMP2-F12/VDZ-F12 Gibbs free energy can be seen when changing from a 6-31++G(d,p) to a 6-311++G(3df,3pd) basis set in Table S3. In all cases there is a minute difference in the CCSD(T)-F12a/VDZ-F12 and DF-LMP2-F12/VDZ-F12 whether the geometries have been optimized with the 6-31++G(d,p) or 6-311++G(3df,3pd) basis set. The value of MAE, MSE and MaxE using DF-LMP2-F12/VDZ-F12 almost equal to the

CCSD(T)-F12a/VDZ-F12. In conclusion, our results indicate that DF-LMP2-F12/VDZ-F12// M06-2X /6-311+G(2d,p) basis set can be used as a good compromise between accuracy and computational efficient.

Table S1 Mean absolute error (MAE), mean signed error (MSE) and Maximum error

(MaxE) in the DFT binding energies (ΔE) and single-point energy calculation based on the DFT of all six reactions^a compared against CCSD(T)-F12a/VDZ-F12 results.

All energies are in kcal/mol.

Method	MAE	MES	MaxE
6-311+G(2d,p)			
M06-2x	1.05	0.71	1.53
DF-LMP2-F12/VDZ-F12//M06-2x	0.34	0.20	1.07
PW91PW91	1.55	1.37	2.94
DF-LMP2-F12/VDZ-F12//PW91PW91	0.37	0.25	1.27
ω B97X-D	0.97	0.97	1.55
DF-LMP2-F12/VDZ-F12// ω B97X-D	0.34	0.19	0.92
6-311++G(3df,3pd)			
M06-2x	0.98	0.25	1.27
DF-LMP2-F12/VDZ-F12//M06-2x	0.37	0.21	0.99
PW91PW91	1.15	0.93	2.65
DF-LMP2-F12/VDZ-F12//PW91PW91	0.38	0.25	1.20
ω B97X-D	0.45	0.43	0.76
DF-LMP2-F12/VDZ-F12// ω B97X-D	0.34	0.19	0.87

^aReactions are refer to $OA + W \rightleftharpoons (OA)(W)$, $(OA)(W) + W \rightleftharpoons (OA)(W)_2$, $OA + OA \rightleftharpoons (OA)_2$, $OA + DMA \rightleftharpoons (OA)(DMA)$, $(OA)(DMA) + W \rightleftharpoons (OA)(DMA)(W)$, $OA + (DMA)(OA) \rightleftharpoons (OA)_2(DMA)$.

Table S2 Mean absolute error (MAE), mean signed error (MSE) and Maximum error

(MaxE) in the DFT Gibbs free energy (ΔG) when changing the basis from 6-311+G(2d,p) to 6-311++G(3df,3pd). All energies are in kcal/mol.

Method	MAE	MES	MaxE
6-311+G(2d,p) $\rightarrow$ 6-311++G(3df,3pd)			
M06-2x	0.50	0.50	0.88
PW91PW91	0.46	0.46	0.74
ω B97X-D	0.53	0.53	0.72

Table S3 Mean absolute error (MAE), mean signed error (MSE) and Maximum error

(MaxE) in the CCSD(T)-F12a/VDZ-F12 and DF-LMP2-F12/VDZ-F12 Gibbs free energy (ΔG) when changing the basis from 6-311+G(2d,p) to 6-311++G(3df,3pd).

All energies are in kcal/mol.

Method	MAE	MES	MaxE
6-311+G(2d,p) $\rightarrow$ 6-311++G(3df,3pd)			
CCSD(T)-F12a/VDZ-F12//M06-2x	0.13	0.04	0.20
DF-LMP2-F12/VDZ-F12//M06-2x	0.12	0.03	0.21
CCSD(T)-F12a/VDZ-F12//PW91PW91	0.09	0.03	0.17
DF-LMP2-F12/VDZ-F12//PW91PW91	0.06	0.03	0.12
CCSD(T)-F12a/VDZ-F12// ω B97X-D	0.15	-0.01	0.30
DF-LMP2-F12/VDZ-F12// ω B97X-D	0.17	-0.01	0.31

Figure Caption

Figure S1 The local minima for $(\text{C}_2\text{H}_2\text{O}_4)(\text{CH}_3\text{NHCH}_3)(\text{H}_2\text{O})_n$ ($n = 1-2$) optimized at the M06-2x/6-311+G(2d,p) level.

Figure S2 The local minima for $(\text{C}_2\text{H}_2\text{O}_4)(\text{CH}_3\text{NHCH}_3)(\text{H}_2\text{O})_n$ ($n = 3-4$) optimized at the M06-2x/6-311+G(2d,p) level.

Figure S3 The local minima for $(\text{C}_2\text{H}_2\text{O}_4)_2(\text{CH}_3\text{NHCH}_3)(\text{H}_2\text{O})_n$ ($n = 1-2$) optimized at the M06-2x/6-311+G(2d,p) level.

Figure S4 The local minima for $(\text{C}_2\text{H}_2\text{O}_4)_2(\text{CH}_3\text{NHCH}_3)(\text{H}_2\text{O})_n$ ($n = 3-4$) optimized at the M06-2x/6-311+G(2d,p) level.

Figure S1

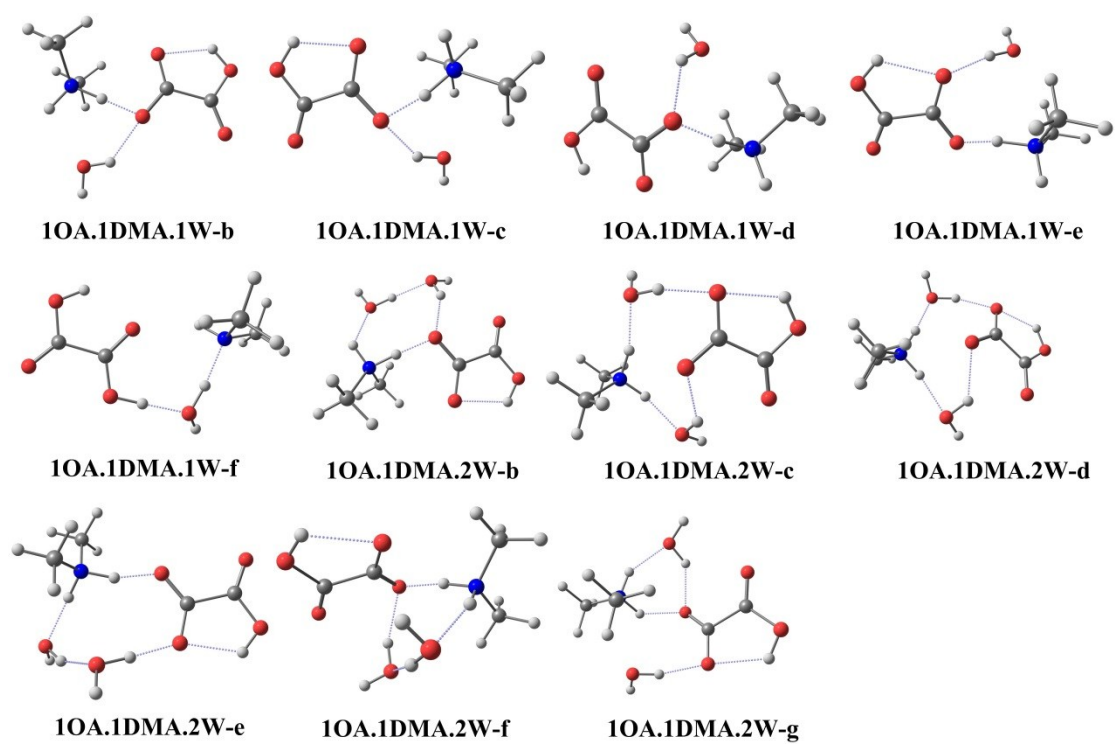


Figure S2

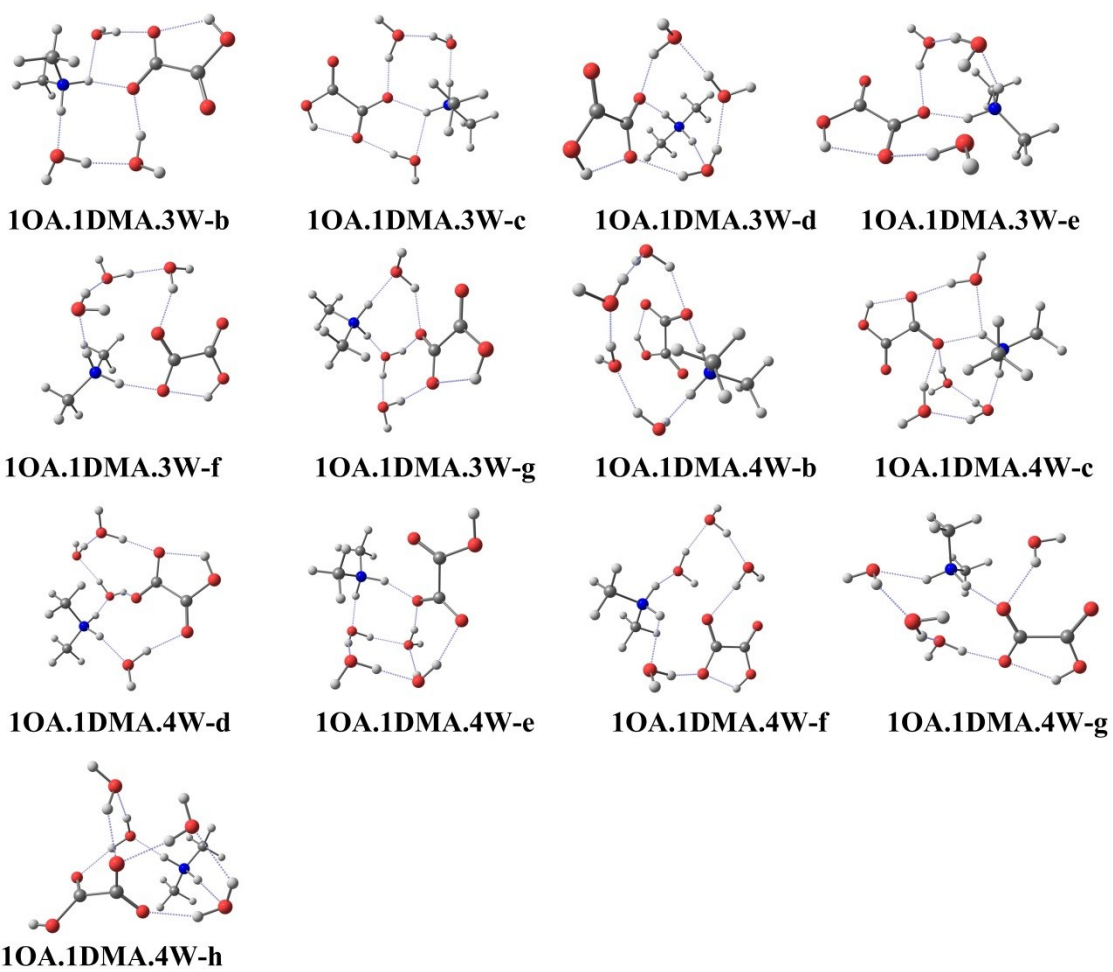


Figure S3

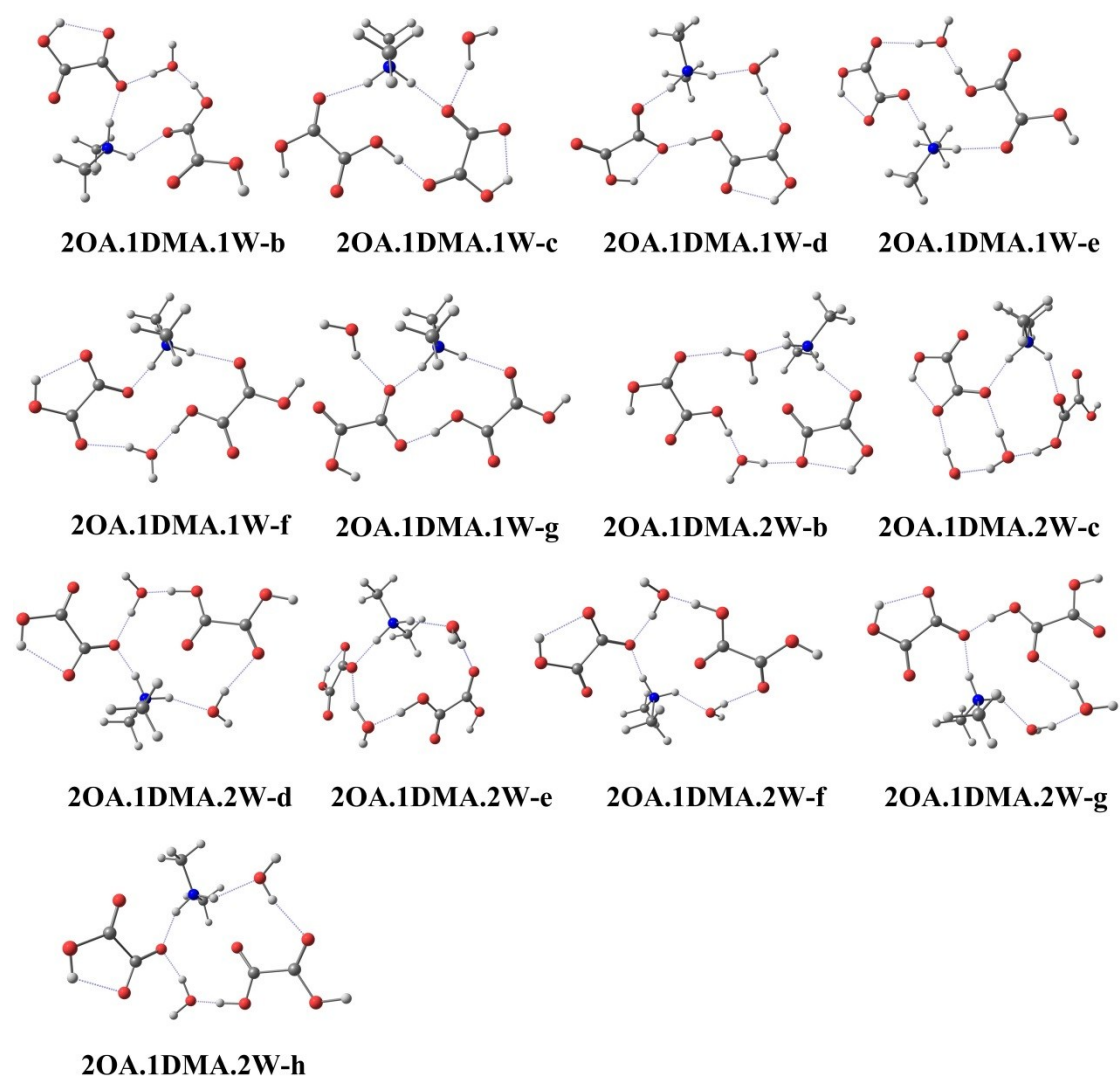
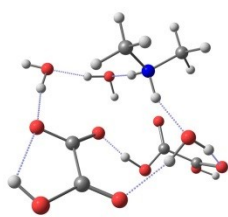
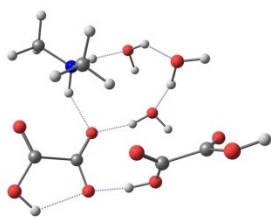


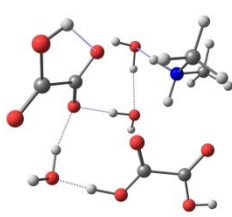
Figure S4



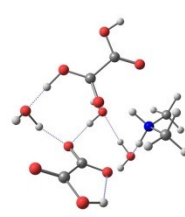
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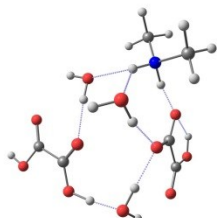
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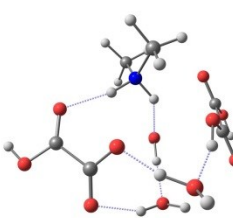
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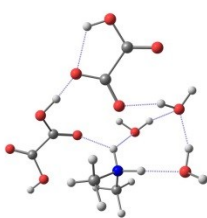
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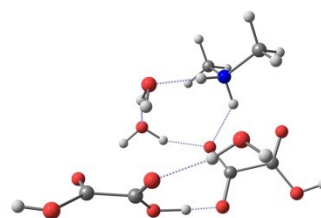
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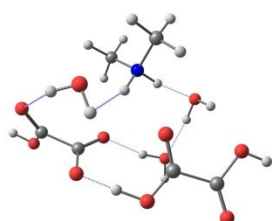
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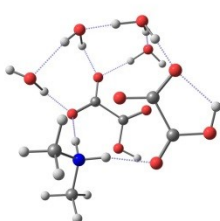
2OA.1DMA.3W-h



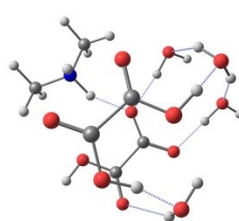
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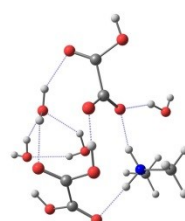
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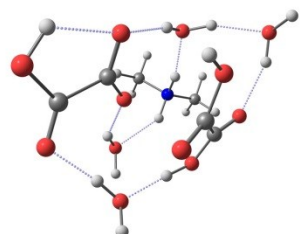
2OA.1DMA.4W-b



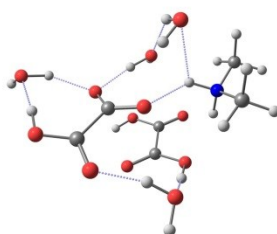
2OA.1DMA.4W-c



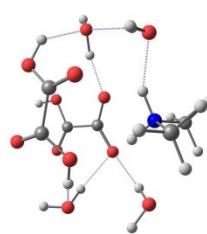
2OA.1DMA.4W-d



2OA.1DMA.4W-e



2OA.1DMA.4W-f



2OA.1DMA.4W-g

Cartesian Coordinates of optimized Structures

OA.1W

C	-0.593947000	-0.746777000	0.004092000
C	-0.588983000	0.803053000	0.002894000
O	-1.815156000	-1.238731000	-0.011054000
O	0.398894000	-1.416888000	0.022389000
O	-1.650131000	1.368555000	0.007940000
O	0.570125000	1.395620000	0.002582000
H	-2.428117000	-0.480138000	-0.017890000
H	1.353571000	0.782590000	-0.018705000
O	2.778065000	-0.073565000	-0.093086000
H	3.503463000	0.038747000	0.526676000
H	2.414281000	-0.958783000	0.037838000

OA.2W

C	1.426491000	0.602981000	0.028381000
C	0.784426000	-0.803264000	-0.039483000
O	0.621577000	1.618052000	0.023771000
O	2.628466000	0.663432000	0.085226000
O	-0.399481000	-0.983567000	-0.079382000
O	1.682161000	-1.765411000	-0.043040000
H	-0.363164000	1.406425000	-0.043295000
H	2.555657000	-1.331836000	0.001622000
O	-1.944036000	1.514712000	-0.164496000
H	-2.378142000	2.189763000	0.363148000
H	-2.448895000	0.685492000	-0.041523000
O	-3.159104000	-0.926077000	0.193314000
H	-2.317219000	-1.395393000	0.115470000
H	-3.750401000	-1.321883000	-0.451958000

OA.3W

O	3.061240000	-0.049996000	0.475350000
C	1.911763000	0.365888000	-0.027322000
O	1.682510000	1.497982000	-0.336888000
C	0.869473000	-0.764682000	-0.140391000
O	-0.206151000	-0.388300000	-0.757035000
O	1.110122000	-1.844624000	0.344481000
H	2.962620000	-0.995912000	0.682223000
H	-0.953658000	-1.088290000	-0.663863000
O	-3.095909000	0.483037000	0.641922000
H	-3.916691000	0.876325000	0.335301000
H	-2.394373000	1.134441000	0.431390000
O	-1.144914000	2.291161000	-0.071581000
H	-0.338659000	1.880415000	-0.420354000
H	-0.843471000	3.047801000	0.437628000

O	-2.211766000	-1.844861000	-0.326175000
H	-2.067535000	-2.518608000	0.345094000
H	-2.696702000	-1.098600000	0.098257000

OA.4W

C	0.770717000	-0.044732000	-0.012572000
C	-0.770718000	0.044783000	-0.012488000
O	1.186539000	-1.277308000	-0.051832000
O	1.454044000	0.950012000	0.022796000
O	-1.454041000	-0.949956000	0.023109000
O	-1.186541000	1.277359000	-0.051891000
H	2.193117000	-1.315138000	-0.044730000
H	-2.193098000	1.315205000	-0.044667000
O	3.788908000	-1.383319000	-0.036473000
H	4.201441000	-1.851716000	0.693984000
H	4.138432000	-0.465958000	-0.020320000
O	-4.227553000	-1.269971000	0.068036000
H	-3.261776000	-1.388376000	0.061735000
H	-4.575585000	-1.820024000	-0.637743000
O	4.227583000	1.269802000	0.068197000
H	4.576181000	1.819778000	-0.637364000
H	3.261861000	1.388593000	0.061467000
O	-3.788968000	1.383324000	-0.036383000
H	-4.138598000	0.466022000	-0.020393000
H	-4.201739000	1.851756000	0.693916000

2OA

C	-2.445943000	-0.470825000	0.104734000
C	-1.641502000	0.840087000	-0.052127000
O	-1.746511000	-1.565142000	0.267417000
O	-3.643655000	-0.423329000	0.072486000
O	-0.444492000	0.872207000	-0.031895000
O	-2.414628000	1.892683000	-0.206517000
H	-0.782264000	-1.402414000	0.267811000
H	-3.338230000	1.581972000	-0.183631000
C	1.641624000	-0.775561000	-0.288307000
C	2.481435000	0.401597000	0.237128000
O	1.584689000	-0.840428000	-1.594108000
O	1.097219000	-1.543202000	0.461948000
O	3.048538000	1.125327000	-0.525868000
O	2.501818000	0.500296000	1.549133000
H	2.094397000	-0.089659000	-1.950507000
H	1.948584000	-0.208981000	1.916989000

20A.1W

O	-4.583712000	0.364192000	-0.178300000
C	-3.698540000	-0.614230000	-0.018670000
O	-3.972064000	-1.762430000	0.100370000
C	-2.246411000	-0.090669000	-0.004870000
O	-1.363223000	-1.022206000	0.157901000
O	-2.036465000	1.098677000	-0.141824000
H	-4.106286000	1.205747000	-0.248473000
H	-0.443817000	-0.663113000	0.145117000
O	3.427233000	-1.969516000	-0.054539000
C	3.628481000	-0.655799000	-0.061538000
O	4.693206000	-0.136163000	-0.131073000
C	2.309175000	0.143617000	0.029052000
O	2.468345000	1.417748000	0.031515000
O	1.252652000	-0.465357000	0.088088000
H	2.473755000	-2.136842000	0.009420000
H	1.577193000	1.901248000	0.091244000
O	0.237288000	2.650357000	0.198401000
H	-0.567830000	2.118833000	0.058044000
H	0.124680000	3.474189000	-0.283503000

20A.2W

O	4.496493000	-0.120752000	-0.761879000
C	3.321927000	-0.458214000	-0.268941000
O	2.987710000	-1.589372000	-0.055151000
C	2.410852000	0.761300000	-0.014948000
O	1.286553000	0.428254000	0.528050000
O	2.794354000	1.859998000	-0.338747000
H	4.502127000	0.848607000	-0.858766000
H	0.644054000	1.225676000	0.625785000
O	-4.496312000	0.120587000	-0.762317000
C	-3.322024000	0.458146000	-0.268808000
O	-2.987943000	1.589326000	-0.054923000
C	-2.410831000	-0.761242000	-0.014718000
O	-1.286747000	-0.428068000	0.528700000
O	-2.793990000	-1.859948000	-0.338888000
H	-4.501798000	-0.848769000	-0.859277000
H	-0.644099000	-1.225305000	0.626265000
O	0.373074000	-2.319937000	0.766773000
H	1.273795000	-2.026509000	0.531394000
H	0.202919000	-3.137960000	0.291060000
O	-0.373119000	2.319805000	0.766502000
H	-0.203048000	3.138327000	0.291622000
H	-1.274059000	2.026840000	0.531439000

20A.3W

O	3.061240000	-0.049996000	0.475350000
C	1.911763000	0.365888000	-0.027322000
O	1.682510000	1.497982000	-0.336888000
C	0.869473000	-0.764682000	-0.140391000
O	-0.206151000	-0.388300000	-0.757035000
O	1.110122000	-1.844624000	0.344481000
H	2.962620000	-0.995912000	0.682223000
H	-0.953658000	-1.088290000	-0.663863000
O	-3.095909000	0.483037000	0.641922000
H	-3.916691000	0.876325000	0.335301000
H	-2.394373000	1.134441000	0.431390000
O	-1.144914000	2.291161000	-0.071581000
H	-0.338659000	1.880415000	-0.420354000
H	-0.843471000	3.047801000	0.437628000
O	-2.211766000	-1.844861000	-0.326175000
H	-2.067535000	-2.518608000	0.345094000
H	-2.696702000	-1.098600000	0.098257000

20A.4W

O	0.653989000	-1.170087000	1.125890000
C	0.715439000	-1.193936000	-0.163987000
O	-0.184048000	-1.021901000	-0.954663000
C	2.164456000	-1.392259000	-0.648402000
O	2.222081000	-1.743703000	-1.923114000
O	3.116053000	-1.213853000	0.059785000
H	-0.319582000	-0.889981000	1.479600000
H	3.156024000	-1.826348000	-2.166020000
O	-0.906571000	1.853633000	-1.985858000
C	-0.971690000	1.787867000	-0.672041000
O	-2.000418000	1.718422000	-0.059709000
C	0.415027000	1.758810000	-0.000970000
O	0.354195000	1.739213000	1.293399000
O	1.406022000	1.705407000	-0.693451000
H	0.032099000	1.806575000	-2.240743000
H	1.272510000	1.478018000	1.663391000
O	-3.065818000	-0.724312000	-1.336834000
H	-3.107096000	0.227507000	-1.180901000
H	-2.116699000	-0.914190000	-1.381521000
O	-1.532317000	-0.421367000	1.972353000
H	-2.309941000	-0.977171000	1.718370000
H	-1.698522000	0.469487000	1.629335000
O	-3.529134000	-1.914171000	1.046037000

H	-3.544578000	-1.564663000	0.129123000
H	-4.435691000	-1.952843000	1.358258000
O	2.623188000	0.849149000	2.039058000
H	3.317990000	1.210011000	1.476855000
H	2.556318000	-0.080726000	1.763509000

1OA.1DMA

C	2.677105000	0.243677000	-1.217438000
N	2.416196000	-0.531759000	0.000463000
C	2.680454000	0.247460000	1.215248000
H	2.499045000	-0.381073000	-2.092003000
H	3.702104000	0.625133000	-1.248257000
H	1.982805000	1.083866000	-1.240144000
H	2.994166000	-1.366636000	0.000985000
H	2.506229000	-0.374997000	2.092218000
H	1.985290000	1.086921000	1.238006000
H	3.705168000	0.630039000	1.241346000
O	-2.899239000	1.046555000	-0.001089000
C	-2.286567000	-0.136121000	0.000165000
O	-2.849139000	-1.183301000	0.000703000
C	-0.747885000	0.020977000	0.000734000
O	-0.096526000	-1.090542000	0.001920000
O	-0.276534000	1.143807000	-0.000041000
H	-2.203936000	1.726344000	-0.001476000
H	0.948619000	-0.895399000	0.001885000

1OA.1DMA.1W-a

C	-3.065920000	-1.442539000	-0.501004000
N	-2.158940000	-0.374509000	-0.052163000
C	-2.234676000	-0.095011000	1.395573000
H	-2.950069000	-1.582642000	-1.573513000
H	-4.098897000	-1.183249000	-0.270194000
H	-2.797994000	-2.365552000	0.010497000
H	-2.319646000	0.507451000	-0.554502000
H	-1.512184000	0.685341000	1.626337000
H	-1.979338000	-1.003956000	1.938359000
H	-3.238635000	0.231431000	1.663553000
O	3.257178000	0.730511000	0.305788000
C	2.552040000	-0.356468000	-0.016621000
O	3.037511000	-1.422074000	-0.228591000
C	1.025699000	-0.064762000	-0.080217000
O	0.279369000	-1.022740000	-0.366121000
O	0.696949000	1.113753000	0.174033000
H	2.607181000	1.445461000	0.422283000

H	-1.092547000	-0.656056000	-0.261772000
O	-1.633049000	2.262598000	-0.616157000
H	-0.724510000	1.983859000	-0.370141000
H	-1.547305000	3.015765000	-1.203778000

1OA.1DMA.1W-b

C	-2.374592000	-1.519438000	-0.958191000
N	-2.176930000	-0.288260000	-0.172715000
C	-2.248641000	-0.502867000	1.287229000
H	-2.325423000	-1.277164000	-2.017770000
H	-3.339908000	-1.966716000	-0.722679000
H	-1.564218000	-2.200793000	-0.704334000
H	-2.823289000	0.453587000	-0.440308000
H	-2.117633000	0.460834000	1.774430000
H	-1.437428000	-1.176048000	1.559304000
H	-3.211435000	-0.937233000	1.554967000
O	3.216493000	-0.874212000	0.331200000
C	2.456886000	0.163189000	-0.024016000
O	2.880755000	1.256097000	-0.235585000
C	0.956529000	-0.227365000	-0.117854000
O	0.158251000	0.677138000	-0.483955000
O	0.671521000	-1.393462000	0.178172000
H	2.603915000	-1.622679000	0.447193000
H	-1.155665000	0.125649000	-0.379898000
O	-1.841491000	2.460253000	0.084485000
H	-1.903965000	3.416978000	0.123003000
H	-0.911755000	2.253780000	-0.102450000

1OA.1DMA.1W-c

C	3.132956000	-0.400010000	-0.967608000
N	1.918952000	-0.799527000	-0.232569000
C	2.111910000	-0.901161000	1.230383000
H	2.901536000	-0.341072000	-2.028994000
H	3.925903000	-1.128182000	-0.799672000
H	3.429767000	0.581565000	-0.605421000
H	1.537116000	-1.681656000	-0.576396000
H	1.165921000	-1.213319000	1.668453000
H	2.390868000	0.084543000	1.595960000
H	2.890556000	-1.630645000	1.450684000
O	-3.347775000	-0.787076000	0.195614000
C	-2.520218000	0.230157000	-0.049280000
O	-2.870412000	1.364681000	-0.141685000
C	-1.047857000	-0.244872000	-0.188853000
O	-0.187177000	0.636877000	-0.447074000

O	-0.844577000	-1.457138000	-0.028482000
H	-2.787254000	-1.583101000	0.226212000
H	1.079259000	-0.093820000	-0.398758000
O	1.881509000	2.164752000	0.439453000
H	1.963857000	3.103847000	0.619102000
H	0.956510000	2.017085000	0.186353000

1OA.1DMA.1W-d

C	-1.949311000	-0.820990000	1.257246000
N	-2.194021000	-0.757337000	-0.201347000
C	-3.189271000	0.269440000	-0.573867000
H	-1.192940000	-1.580147000	1.444833000
H	-2.874588000	-1.056478000	1.782603000
H	-1.577866000	0.156540000	1.564560000
H	-2.467009000	-1.673229000	-0.549927000
H	-3.314745000	0.267707000	-1.654588000
H	-2.798415000	1.234102000	-0.251297000
H	-4.142408000	0.065312000	-0.086397000
O	3.171736000	-0.561166000	0.409342000
C	2.199050000	0.212005000	-0.064194000
O	2.275249000	1.400452000	-0.159419000
C	0.926014000	-0.594249000	-0.429675000
O	0.020450000	0.067088000	-1.017736000
O	0.892127000	-1.771080000	-0.076143000
H	2.805686000	-1.463707000	0.432281000
H	-1.194975000	-0.471121000	-0.681024000
O	-0.778237000	2.204212000	0.530310000
H	-0.270864000	2.938834000	0.884045000
H	-0.183225000	1.770276000	-0.103553000

1OA.1DMA.1W-e

C	2.988604000	-0.764122000	-0.900856000
N	2.128631000	-1.002561000	0.277166000
C	2.414730000	-0.089375000	1.404307000
H	2.720049000	-1.474159000	-1.680654000
H	4.038122000	-0.886954000	-0.631431000
H	2.803503000	0.251671000	-1.244198000
H	2.243563000	-1.964658000	0.590479000
H	1.673134000	-0.250704000	2.184358000
H	2.342128000	0.932875000	1.040383000
H	3.416397000	-0.275461000	1.792795000
O	-3.245601000	0.789195000	0.317324000
C	-2.560729000	-0.290222000	-0.066058000
O	-3.067213000	-1.300239000	-0.439098000

C	-1.025676000	-0.069070000	0.035115000
O	-0.301222000	-1.035030000	-0.305180000
O	-0.663766000	1.043482000	0.450430000
H	-2.581156000	1.453062000	0.572232000
H	0.993637000	-0.927130000	-0.021951000
O	1.580723000	2.093293000	-0.748162000
H	0.738433000	1.817311000	-0.338067000
H	1.386831000	2.893190000	-1.241679000

1OA.1DMA.1W-f

C	-2.555517000	-0.757130000	1.243139000
N	-2.529838000	-0.357639000	-0.164209000
C	-3.807061000	-0.589879000	-0.831371000
H	-1.558912000	-0.635493000	1.665391000
H	-2.875999000	-1.796584000	1.376128000
H	-3.245789000	-0.109005000	1.785833000
H	-1.784210000	-0.869494000	-0.627299000
H	-3.726763000	-0.329600000	-1.886409000
H	-4.568598000	0.046727000	-0.377726000
H	-4.139928000	-1.630941000	-0.748783000
O	2.899984000	-1.598428000	-0.159800000
C	2.782236000	-0.276141000	-0.047395000
O	3.699127000	0.474308000	0.038915000
C	1.300671000	0.166914000	-0.044627000
O	1.133476000	1.438879000	0.071129000
O	0.435094000	-0.683433000	-0.147867000
H	2.001388000	-1.964075000	-0.213221000
H	0.133070000	1.678509000	0.059126000
O	-1.335283000	1.996850000	0.056170000
H	-1.874449000	1.150813000	-0.114172000
H	-1.632099000	2.674624000	-0.556248000

1OA.1DMA.2W-a

C	3.063051000	1.057225000	-0.502175000
N	2.165492000	-0.011941000	-0.020824000
C	1.855892000	0.082837000	1.424821000
H	3.241420000	0.916791000	-1.565914000
H	4.005333000	1.013049000	0.042080000
H	2.566369000	2.011030000	-0.332434000
H	2.514662000	-0.955082000	-0.222707000
H	1.204121000	-0.748625000	1.686113000
H	1.353670000	1.033943000	1.593682000
H	2.780722000	0.025163000	1.996777000
O	-3.304535000	-0.647689000	0.491958000

C	-2.413669000	0.192162000	-0.027760000
O	-2.608235000	1.360889000	-0.179562000
C	-1.067077000	-0.495989000	-0.381123000
O	-0.237940000	0.211796000	-0.989913000
O	-0.944125000	-1.669613000	0.013690000
H	-2.857713000	-1.511086000	0.546793000
H	1.225242000	0.039493000	-0.536302000
O	0.311596000	2.653287000	0.152345000
H	-0.298950000	3.345459000	0.417684000
H	-0.231393000	2.023968000	-0.352700000
O	1.587150000	-2.674170000	-0.178597000
H	0.633974000	-2.432369000	-0.177040000
H	1.643627000	-3.571552000	-0.512208000

1OA.1DMA.2W-b

C	1.994409000	-0.925371000	1.332201000
N	2.121335000	-0.639924000	-0.112547000
C	2.526623000	-1.809831000	-0.909981000
H	1.715114000	-0.001278000	1.832851000
H	2.946370000	-1.285653000	1.720780000
H	1.219148000	-1.678541000	1.459387000
H	2.729992000	0.174356000	-0.233452000
H	2.616302000	-1.516684000	-1.953654000
H	1.745155000	-2.562076000	-0.810259000
H	3.476853000	-2.200494000	-0.547914000
O	-3.282992000	-1.037054000	0.460584000
C	-2.441823000	-0.097655000	0.041510000
O	-2.725255000	1.059785000	-0.053820000
C	-1.030996000	-0.660703000	-0.273891000
O	-0.219090000	0.164919000	-0.770205000
O	-0.825604000	-1.840907000	0.020375000
H	-2.766026000	-1.863269000	0.479154000
H	1.138747000	-0.299349000	-0.466862000
O	-0.177307000	2.854702000	-0.292190000
H	-0.496608000	1.977508000	-0.576567000
H	-0.904512000	3.219633000	0.218603000
O	2.362004000	2.074727000	0.376383000
H	1.458757000	2.417926000	0.195341000
H	2.928046000	2.849381000	0.402374000

1OA.1DMA.2W-c

C	2.664971000	-0.327102000	-1.234876000
N	2.202361000	-0.168834000	0.162909000
C	3.300052000	-0.102804000	1.144257000

H	1.784481000	-0.345255000	-1.870532000
H	3.219948000	-1.259573000	-1.318133000
H	3.299000000	0.520197000	-1.489523000
H	1.562956000	-0.960730000	0.372038000
H	2.880135000	0.016514000	2.140417000
H	3.932088000	0.751262000	0.907918000
H	3.883717000	-1.020252000	1.096965000
O	-3.547630000	0.257704000	0.465912000
C	-2.461197000	-0.406054000	0.089722000
O	-2.364181000	-1.600153000	0.127766000
C	-1.305551000	0.528565000	-0.367387000
O	-0.295980000	-0.025062000	-0.822981000
O	-1.511507000	1.747700000	-0.181571000
H	-3.313391000	1.200586000	0.372070000
H	0.141004000	2.283560000	-0.055046000
O	1.094471000	2.379359000	0.188980000
H	1.639166000	0.705428000	0.213485000
H	1.129686000	3.087860000	0.835620000
O	0.540653000	-2.396709000	0.149585000
H	0.060529000	-3.008414000	0.713583000
H	-0.152095000	-1.847676000	-0.271054000

10A.1DMA.2W-d

C	-2.649920000	-0.555471000	1.211127000
N	-2.181238000	-0.135853000	-0.128348000
C	-3.256962000	-0.022234000	-1.130242000
H	-1.784791000	-0.576845000	1.867911000
H	-3.092306000	-1.546524000	1.132814000
H	-3.386939000	0.161847000	1.568318000
H	-1.476324000	-0.834946000	-0.426722000
H	-2.829622000	0.323964000	-2.068245000
H	-3.993168000	0.698464000	-0.779192000
H	-3.725935000	-0.995045000	-1.266437000
O	3.512129000	0.284942000	-0.480189000
C	2.448373000	-0.392670000	-0.067720000
O	2.376302000	-1.589402000	-0.079246000
C	1.280388000	0.526358000	0.392237000
O	0.298291000	-0.037062000	0.889551000
O	1.456572000	1.744359000	0.160446000
H	3.256205000	1.224490000	-0.411080000
H	-1.687649000	0.779876000	-0.045162000
O	-0.497944000	-2.353410000	-0.294303000
H	0.201311000	-1.880106000	0.198082000
H	-0.022357000	-2.929823000	-0.898093000

O	-1.097050000	2.410066000	-0.262713000
H	-1.374857000	3.214079000	0.181570000
H	-0.132565000	2.299702000	-0.056112000

1OA.1DMA.2W-e

C	2.466655000	-0.850953000	1.380755000
N	1.940052000	-0.881494000	0.001797000
C	2.098630000	-2.192270000	-0.656965000
H	2.310998000	0.148573000	1.778274000
H	3.527680000	-1.097015000	1.373609000
H	1.917986000	-1.579385000	1.975878000
H	2.399966000	-0.141009000	-0.550676000
H	1.691062000	-2.131693000	-1.663354000
H	1.537038000	-2.933603000	-0.091599000
H	3.152548000	-2.464703000	-0.693014000
O	-3.732946000	0.782028000	-0.154629000
C	-2.940900000	-0.291078000	-0.089693000
O	-3.344017000	-1.411276000	-0.106208000
C	-1.435646000	0.093945000	0.009145000
O	-0.620563000	-0.840399000	0.088712000
O	-1.208279000	1.324255000	-0.003756000
H	-3.139630000	1.552929000	-0.124426000
H	0.871897000	-0.681321000	0.037499000
O	1.222109000	2.054036000	0.636673000
H	0.291138000	1.803806000	0.373534000
H	1.138585000	2.808237000	1.224911000
O	3.168588000	1.415382000	-1.086252000
H	3.202720000	1.828860000	-1.951617000
H	2.506083000	1.906707000	-0.557359000

1OA.1DMA.2W-f

C	-3.097612000	0.844582000	-0.586928000
N	-2.196969000	-0.224804000	-0.120584000
C	-2.785058000	-1.575575000	-0.117893000
H	-2.561261000	1.790942000	-0.538209000
H	-3.981930000	0.885480000	0.047333000
H	-3.390661000	0.641580000	-1.615575000
H	-1.829247000	0.025824000	0.818798000
H	-2.018606000	-2.272227000	0.214962000
H	-3.098761000	-1.827408000	-1.129780000
H	-3.645322000	-1.601515000	0.549590000
O	3.046431000	-1.123667000	0.456271000
C	2.341469000	-0.267233000	-0.278654000
O	2.798172000	0.725740000	-0.761616000

C	0.843648000	-0.669985000	-0.390969000
O	0.155554000	-0.019187000	-1.213625000
O	0.465139000	-1.558706000	0.387553000
H	2.409924000	-1.791842000	0.768376000
H	-1.292780000	-0.214921000	-0.708781000
O	0.428274000	2.435722000	0.074267000
H	1.280244000	2.873928000	0.160753000
H	0.563273000	1.780944000	-0.633401000
O	-0.711415000	0.765761000	2.005232000
H	-0.081050000	0.040693000	2.094485000
H	-0.246966000	1.446119000	1.477548000

1OA.1DMA.2W-g

C	3.485021000	-0.232941000	-0.216771000
N	2.069115000	-0.513789000	0.081505000
C	1.693378000	-0.240347000	1.487884000
H	3.676380000	-0.447023000	-1.265518000
H	4.116574000	-0.858354000	0.411744000
H	3.665030000	0.819902000	-0.013664000
H	1.793961000	-1.485573000	-0.131458000
H	0.643244000	-0.497164000	1.608580000
H	1.853749000	0.817481000	1.681404000
H	2.304460000	-0.858007000	2.143733000
O	-3.336801000	0.578010000	0.586499000
C	-2.396461000	-0.194357000	0.054668000
O	-2.478649000	-1.386654000	-0.023936000
C	-1.146401000	0.604261000	-0.412689000
O	-0.284128000	-0.046773000	-1.026997000
O	-1.129551000	1.804118000	-0.076302000
H	-2.969365000	1.481407000	0.567697000
H	1.801867000	2.999035000	-0.814407000
O	1.575795000	2.279377000	-0.220964000
H	0.592840000	2.249251000	-0.214758000
H	1.439743000	0.061096000	-0.516122000
O	0.318228000	-2.614293000	-0.347677000
H	-0.241927000	-3.299980000	0.023130000
H	-0.292737000	-1.915530000	-0.654439000

1OA.1DMA.3W-a

C	-2.285708000	-2.162814000	0.772843000
N	-1.857131000	-0.977505000	0.007108000
C	-1.763590000	-1.216762000	-1.448816000
H	-2.335973000	-1.902459000	1.827729000
H	-1.548209000	-2.947852000	0.625023000

H	-3.265174000	-2.485734000	0.423105000
H	-0.909330000	-0.643607000	0.343496000
H	-1.413683000	-0.300850000	-1.920456000
H	-2.749044000	-1.472957000	-1.834330000
H	-1.057899000	-2.025540000	-1.621890000
O	2.931946000	-1.868257000	-0.236106000
C	1.681535000	-1.539941000	0.038302000
O	0.769463000	-2.322406000	0.029144000
C	1.504123000	-0.025342000	0.346805000
O	0.351855000	0.325006000	0.680277000
O	2.524143000	0.659975000	0.207460000
H	3.433751000	-1.031463000	-0.181708000
H	-0.392682000	1.996108000	0.787712000
O	-3.110223000	1.473923000	-0.174278000
H	-2.493535000	-0.170552000	0.147525000
H	-3.887519000	1.916908000	0.172768000
O	-0.927823000	2.773951000	0.545985000
H	-2.340383000	2.070951000	0.019946000
H	-0.301415000	3.285029000	0.011723000
O	1.615033000	3.240087000	-0.515586000
H	2.199122000	3.557490000	-1.206816000
H	2.008591000	2.407993000	-0.193544000

10A.1DMA.3W-b

C	1.891071000	-0.458550000	1.479717000
N	2.210315000	-0.118108000	0.074215000
C	3.484005000	-0.696986000	-0.391700000
H	0.939609000	0.005706000	1.727385000
H	2.676497000	-0.067248000	2.123557000
H	1.817379000	-1.540673000	1.560217000
H	2.222088000	0.921282000	-0.001216000
H	3.635366000	-0.429170000	-1.434894000
H	3.421964000	-1.777202000	-0.292536000
H	4.295539000	-0.298031000	0.214670000
O	-3.648205000	-0.764487000	0.468033000
C	-2.685385000	0.076400000	0.110369000
O	-2.829557000	1.263233000	0.054090000
C	-1.343368000	-0.647386000	-0.205215000
O	-0.399595000	0.062682000	-0.597622000
O	-1.356830000	-1.877480000	-0.006346000
H	-3.240225000	-1.650414000	0.448906000
H	1.181158000	-3.409703000	-1.171383000
O	-0.447287000	2.793847000	-0.626044000
H	-1.251372000	3.106428000	-0.200161000

H	-0.608275000	1.830857000	-0.718738000
O	2.015623000	2.619089000	0.276811000
H	2.546782000	3.329756000	-0.089524000
H	1.077777000	2.807884000	0.007610000
O	1.177810000	-2.684825000	-0.542528000
H	1.412132000	-0.445435000	-0.497834000
H	0.227757000	-2.494635000	-0.365742000

1OA.1DMA.3W-c

C	2.135258000	-0.091387000	1.406535000
N	2.246551000	-0.284103000	-0.058766000
C	3.354511000	-1.173265000	-0.451864000
H	1.347044000	0.635298000	1.592254000
H	3.086466000	0.277804000	1.785881000
H	1.879841000	-1.051318000	1.850517000
H	2.351421000	0.653821000	-0.493010000
H	3.329025000	-1.318337000	-1.529275000
H	3.217997000	-2.128773000	0.046409000
H	4.296755000	-0.713470000	-0.158645000
O	-3.899781000	-0.353072000	-0.003420000
C	-2.763923000	0.332341000	-0.048932000
O	-2.703957000	1.525864000	0.022006000
C	-1.515212000	-0.583934000	-0.193597000
O	-1.752155000	-1.804372000	-0.200607000
O	-0.412762000	-0.008905000	-0.276360000
H	-3.638727000	-1.291098000	-0.065074000
H	-0.133035000	-2.492493000	-0.050451000
O	0.814706000	-2.737235000	0.044315000
H	1.333462000	-0.658819000	-0.369696000
H	0.845964000	-3.686818000	-0.091489000
O	2.422708000	2.406081000	-0.703862000
H	1.551526000	2.658890000	-0.315800000
H	2.482605000	2.855016000	-1.550280000
O	0.044873000	2.537751000	0.467727000
H	-0.709416000	3.130163000	0.529891000
H	-0.339644000	1.687437000	0.158897000

1OA.1DMA.3W-d

C	2.523761000	-1.679351000	-0.950758000
N	2.195264000	-0.344676000	-0.412979000
C	3.150202000	0.715418000	-0.782029000
H	1.736742000	-2.365031000	-0.642844000
H	3.487865000	-2.003676000	-0.562167000
H	2.562177000	-1.623614000	-2.037499000

H	2.092225000	-0.414057000	0.620975000
H	2.808675000	1.646933000	-0.337361000
H	3.178279000	0.805717000	-1.866700000
H	4.141302000	0.458546000	-0.410629000
O	-3.119901000	-1.414528000	0.456048000
C	-2.499060000	-0.444835000	-0.205505000
O	-3.047860000	0.533181000	-0.620455000
C	-0.972423000	-0.706945000	-0.352541000
O	-0.333657000	0.102076000	-1.061020000
O	-0.537192000	-1.690192000	0.273035000
H	-2.424534000	-2.051871000	0.702455000
H	1.209980000	-0.094411000	-0.739176000
O	0.891421000	1.953158000	1.272364000
H	0.133051000	2.244980000	0.715262000
H	1.117251000	2.716663000	1.810690000
O	1.326571000	-0.654052000	2.201754000
H	0.982602000	0.254523000	2.166358000
H	0.602715000	-1.202554000	1.862831000
O	-1.076446000	2.687884000	-0.455801000
H	-1.024583000	1.848846000	-0.949221000
H	-2.008955000	2.745805000	-0.224522000

10A.1DMA.3W-e

C	-2.544195000	-1.333360000	-1.100641000
N	-2.298422000	-0.015281000	-0.477537000
C	-3.234835000	1.042605000	-0.893924000
H	-1.825428000	-2.042658000	-0.693198000
H	-2.413031000	-1.246136000	-2.177728000
H	-3.560118000	-1.652606000	-0.873370000
H	-1.301307000	0.247342000	-0.674620000
H	-2.948624000	1.963184000	-0.392915000
H	-4.248071000	0.756071000	-0.617092000
H	-3.173047000	1.166735000	-1.973927000
O	3.722849000	0.608141000	-0.113182000
C	2.674708000	-0.185164000	-0.299041000
O	2.737901000	-1.379802000	-0.321484000
C	1.341238000	0.600163000	-0.445323000
O	1.415894000	1.821310000	-0.221240000
O	0.337940000	-0.080582000	-0.734591000
H	3.364376000	1.514281000	-0.086265000
H	-0.111544000	2.112982000	0.592677000
O	-1.510947000	-0.602552000	2.070763000
H	-0.874254000	-1.287169000	1.792348000
H	-2.280002000	-0.141062000	0.558162000

O	-0.951287000	2.044175000	1.100519000
H	-1.023193000	0.234421000	2.079321000
H	-0.987928000	2.831261000	1.650231000
O	0.090326000	-2.442214000	0.670233000
H	0.504194000	-1.814014000	0.049360000
H	0.804028000	-3.028947000	0.935206000

1OA.1DMA.3W-f

C	3.055141000	-2.112348000	-0.063480000
N	1.963053000	-1.129301000	0.040359000
C	1.800782000	-0.555243000	1.394906000
H	3.096823000	-2.493928000	-1.080905000
H	2.867664000	-2.931831000	0.628271000
H	3.998668000	-1.629926000	0.185654000
H	1.037862000	-1.557929000	-0.223064000
H	1.014621000	0.195582000	1.351664000
H	2.731825000	-0.077547000	1.695364000
H	1.538196000	-1.350398000	2.090256000
O	-3.123489000	-1.702460000	0.393519000
C	-2.545460000	-0.562675000	0.028575000
O	-3.091969000	0.499879000	0.064871000
C	-1.068463000	-0.749224000	-0.420464000
O	-0.474847000	0.245050000	-0.856826000
O	-0.609149000	-1.906347000	-0.252350000
H	-2.438064000	-2.388375000	0.298811000
H	1.240217000	1.077730000	-1.699028000
O	-1.165764000	2.762379000	-0.010323000
H	-2.011761000	2.793161000	0.445391000
H	-1.162382000	1.878097000	-0.426600000
O	2.145004000	1.192943000	-1.373281000
H	2.031074000	1.837623000	-0.646429000
H	2.115342000	-0.316211000	-0.607992000
O	1.394500000	2.702754000	0.835194000
H	0.434423000	2.805117000	0.639414000
H	1.717830000	3.587294000	1.023020000

1OA.1DMA.3W-g

C	3.362058000	-1.393648000	0.433701000
N	2.046583000	-0.735725000	0.321483000
C	1.651897000	0.014882000	1.533788000
H	3.567898000	-1.927827000	-0.490713000
H	3.346715000	-2.093244000	1.267632000
H	4.125981000	-0.636409000	0.600413000
H	1.320379000	-1.448489000	0.100224000

H	0.678468000	0.467370000	1.360978000
H	2.379056000	0.804841000	1.712207000
H	1.612920000	-0.665723000	2.382732000
O	-3.539299000	0.180044000	0.688438000
C	-2.557431000	-0.449391000	0.055264000
O	-2.569105000	-1.622195000	-0.187722000
C	-1.365539000	0.486256000	-0.303633000
O	-0.456483000	-0.016279000	-0.983083000
O	-1.447241000	1.635416000	0.178034000
H	-3.235155000	1.101461000	0.787598000
H	1.042580000	0.912620000	-1.776090000
O	1.957877000	1.184122000	-1.583873000
H	2.058568000	-0.043562000	-0.478482000
H	1.820601000	1.988073000	-1.049064000
O	0.937369000	2.944366000	0.282937000
H	0.034603000	2.554949000	0.221557000
H	0.816726000	3.896823000	0.277800000
O	0.168029000	-2.626260000	-0.473328000
H	-0.411199000	-1.927700000	-0.836251000
H	-0.439312000	-3.215428000	-0.016857000

1OA.1DMA.4W-a

O	-3.828916000	-0.856791000	0.279505000
C	-2.871945000	-0.072455000	-0.200231000
O	-3.057033000	1.049295000	-0.572014000
C	-1.478236000	-0.764427000	-0.211098000
O	-1.451511000	-1.903768000	0.283465000
O	-0.536772000	-0.105846000	-0.699848000
H	-3.389328000	-1.690985000	0.526401000
H	0.174965000	-2.277984000	0.710288000
C	2.308682000	1.137192000	-1.322717000
N	2.131239000	-0.233746000	-0.798580000
C	2.786581000	-1.280464000	-1.601879000
H	1.805965000	1.219795000	-2.284735000
H	3.372113000	1.342816000	-1.435208000
H	1.865615000	1.838384000	-0.618071000
H	1.098978000	-0.413554000	-0.737861000
H	2.576765000	-2.241629000	-1.140224000
H	3.859358000	-1.096491000	-1.626525000
H	2.386843000	-1.253986000	-2.614413000
O	1.127147000	-2.362227000	0.952890000
H	2.450434000	-0.255033000	0.198447000
H	1.219397000	-3.237999000	1.336636000
O	2.445260000	-0.050072000	1.897474000

H	1.862563000	-0.816189000	2.010179000
H	1.893835000	0.744563000	2.017936000
O	-0.599119000	2.625079000	-0.480728000
H	-0.733163000	1.681885000	-0.705475000
H	-1.498707000	2.966844000	-0.456017000
O	0.941792000	2.284140000	1.734327000
H	1.034506000	3.087943000	2.249678000
H	0.303910000	2.480295000	1.014003000

1OA.1DMA.4W-b

O	-0.639256000	0.218893000	-1.326285000
C	-1.134624000	-0.809198000	-0.807660000
O	-2.320653000	-1.072399000	-0.573794000
C	-0.131399000	-1.912086000	-0.358598000
O	-0.737440000	-2.937208000	0.217341000
O	1.061733000	-1.842436000	-0.495165000
H	0.843434000	0.536448000	-0.853583000
H	-1.690925000	-2.721358000	0.158992000
C	2.810734000	0.642330000	-1.519654000
N	1.777628000	0.904134000	-0.500582000
C	1.622719000	2.328453000	-0.147839000
H	2.831638000	-0.427588000	-1.711903000
H	3.777879000	0.982312000	-1.152060000
H	2.552307000	1.177653000	-2.431703000
H	2.004290000	0.349108000	0.349117000
H	0.805248000	2.425927000	0.564984000
H	1.381090000	2.889282000	-1.049631000
H	2.552338000	2.700847000	0.280401000
O	-2.911047000	1.704305000	-0.742994000
H	-3.277486000	0.820241000	-0.590301000
H	-2.125945000	1.470137000	-1.267970000
O	2.395247000	-0.663064000	1.759610000
H	2.348230000	-1.509451000	1.296462000
H	1.496976000	-0.555167000	2.119596000
O	-0.335905000	-0.211748000	1.988908000
H	-1.019608000	-0.811827000	2.298623000
H	-0.771841000	0.657494000	1.860667000
O	-1.418889000	2.217208000	1.414305000
H	-1.863599000	2.787554000	2.045847000
H	-2.042317000	2.094050000	0.653636000

1OA.1DMA.4W-c

O	3.769811000	-0.891656000	0.149275000
C	2.706149000	-0.108736000	0.067359000

O	2.748266000	1.088763000	0.124056000
C	1.376119000	-0.895885000	-0.103380000
O	0.345328000	-0.191857000	-0.204078000
O	1.477486000	-2.128807000	-0.113016000
H	3.431696000	-1.804268000	0.083714000
H	-1.503041000	-0.651227000	-0.361188000
C	-3.544822000	-0.743194000	-0.707835000
N	-2.362578000	-0.191353000	-0.024205000
C	-2.391297000	-0.369329000	1.445299000
H	-4.434729000	-0.226139000	-0.353488000
H	-3.604658000	-1.805916000	-0.485690000
H	-3.435481000	-0.596954000	-1.779948000
H	-2.237308000	0.834173000	-0.221997000
H	-1.510801000	0.113799000	1.865554000
H	-2.376676000	-1.435715000	1.659226000
H	-3.294513000	0.095064000	1.838002000
O	0.478846000	2.156498000	-1.767507000
H	1.287317000	2.642440000	-1.579448000
H	0.593368000	1.314824000	-1.292724000
O	-1.825105000	2.475866000	-0.240162000
H	-1.290073000	2.559451000	0.568792000
H	-1.150102000	2.576311000	-0.938075000
O	0.151467000	1.916222000	1.655194000
H	0.463518000	1.270089000	0.996091000
H	0.935166000	2.420003000	1.892741000
O	-1.222557000	-2.789756000	-0.247883000
H	-1.348842000	-3.683220000	-0.574862000
H	-0.252034000	-2.662576000	-0.202941000

10A.1DMA.4W-d

O	3.967072000	0.563588000	0.096814000
C	2.896737000	-0.191407000	-0.084945000
O	2.940396000	-1.390619000	-0.150196000
C	1.579153000	0.631205000	-0.186738000
O	0.544592000	-0.003892000	-0.422230000
O	1.731219000	1.858294000	-0.000361000
H	3.626601000	1.478598000	0.136059000
H	-0.859184000	0.491146000	-1.702442000
C	-2.011808000	-0.433021000	1.334833000
N	-1.773795000	-1.381027000	0.223949000
C	-2.750852000	-2.481464000	0.154442000
H	-1.240986000	0.334177000	1.299703000
H	-1.975159000	-0.972861000	2.279969000
H	-2.988255000	0.029539000	1.197890000

H	-0.820703000	-1.782757000	0.289204000
H	-2.491032000	-3.126572000	-0.681408000
H	-3.746579000	-2.065819000	0.010520000
H	-2.719771000	-3.051312000	1.081629000
O	0.570377000	-2.873295000	0.113989000
H	1.286288000	-2.249471000	-0.120953000
H	1.001202000	-3.583471000	0.595284000
O	-0.622336000	2.708813000	0.962323000
H	0.229748000	2.449611000	0.531488000
H	-0.409860000	3.435898000	1.551763000
O	-1.794252000	0.308217000	-1.893943000
H	-2.279667000	1.065829000	-1.518246000
H	-1.796474000	-0.821245000	-0.668663000
O	-2.979115000	2.243589000	-0.294667000
H	-2.158578000	2.515018000	0.170355000
H	-3.384033000	3.051443000	-0.619176000

10A.1DMA.4W-e

O	-0.304403000	-0.431296000	0.917124000
C	-1.196040000	-1.128619000	0.353155000
O	-1.181115000	-2.314173000	0.061665000
C	-2.447040000	-0.294292000	-0.037213000
O	-3.516390000	-1.032453000	-0.305369000
O	-2.437647000	0.909838000	-0.107075000
H	-0.171848000	1.141222000	0.418462000
H	-4.233405000	-0.427954000	-0.545581000
C	0.134910000	2.207000000	-1.338410000
N	0.282512000	2.044549000	0.123837000
C	-0.282138000	3.158667000	0.903109000
H	0.667457000	3.105086000	-1.649552000
H	-0.923672000	2.292367000	-1.572308000
H	0.567007000	1.332498000	-1.823594000
H	1.292878000	1.875763000	0.331531000
H	-0.124619000	2.967019000	1.962195000
H	-1.349058000	3.215394000	0.696371000
H	0.209266000	4.087894000	0.618700000
O	2.068575000	-1.245387000	1.790034000
H	1.132386000	-1.022972000	1.558804000
H	2.067875000	-1.567091000	2.694589000
O	2.832410000	1.063326000	0.332411000
H	2.807798000	0.356424000	0.998960000
H	2.783463000	0.580153000	-0.515064000
O	2.128250000	-0.396611000	-1.925474000
H	1.860029000	-1.254039000	-1.505532000

H	2.682566000	-0.637297000	-2.672058000
O	1.531887000	-2.656192000	-0.631357000
H	1.943504000	-2.467674000	0.224860000
H	0.580088000	-2.721582000	-0.427154000

10A.1DMA.4W-f

O	-3.716261000	-0.972136000	0.447037000
C	-2.750815000	-0.095465000	0.204258000
O	-2.918300000	1.089871000	0.204366000
C	-1.377883000	-0.777887000	-0.074928000
O	-0.409410000	-0.032705000	-0.313455000
O	-1.395218000	-2.023398000	-0.018480000
H	-3.294904000	-1.849669000	0.383283000
H	2.082189000	0.230358000	0.456131000
C	3.497255000	-1.082610000	-0.413636000
N	2.181382000	-0.774684000	0.172723000
C	1.855151000	-1.601769000	1.356231000
H	3.682275000	-0.409609000	-1.247672000
H	3.479687000	-2.113102000	-0.762353000
H	4.267009000	-0.949918000	0.344333000
H	1.437535000	-0.939209000	-0.519375000
H	0.837893000	-1.365667000	1.660043000
H	2.553299000	-1.360743000	2.155515000
H	1.922645000	-2.650355000	1.076276000
O	-0.782482000	2.653905000	-0.973340000
H	-1.659136000	2.790937000	-0.597260000
H	-0.678574000	1.686914000	-0.898474000
O	1.550852000	3.898293000	-0.318494000
H	0.671055000	3.621071000	-0.648693000
H	1.466836000	4.815817000	-0.050547000
O	1.452304000	1.619586000	1.194306000
H	0.521446000	1.463232000	0.978010000
H	1.645040000	2.495515000	0.803814000
O	0.926291000	-2.839573000	-1.207525000
H	0.744599000	-3.174776000	-2.088297000
H	0.046974000	-2.672368000	-0.800665000

10A.1DMA.4W-g

O	-3.940016000	-0.826267000	0.243343000
C	-2.983198000	-0.063163000	-0.272681000
O	-3.184458000	0.990304000	-0.800465000
C	-1.562006000	-0.668420000	-0.093432000
O	-0.624383000	-0.055990000	-0.644034000
O	-1.512265000	-1.698991000	0.603370000

H	-3.487662000	-1.593059000	0.638377000
H	0.872804000	0.304501000	0.071934000
C	2.187277000	1.841476000	-0.377210000
N	1.710918000	0.750965000	0.506448000
C	1.328582000	1.206492000	1.861153000
H	2.379195000	1.419441000	-1.360737000
H	3.113978000	2.240376000	0.029762000
H	1.410932000	2.601711000	-0.428249000
H	2.436735000	0.025783000	0.555425000
H	1.000519000	0.337815000	2.427635000
H	0.520205000	1.927574000	1.753228000
H	2.192112000	1.666391000	2.338575000
O	1.757745000	-1.510152000	-1.614460000
H	0.955783000	-1.058147000	-1.904268000
H	1.505400000	-1.891358000	-0.754148000
O	1.093243000	-2.013671000	1.063883000
H	1.307693000	-2.818021000	1.543033000
H	0.107717000	-2.002752000	0.959810000
O	4.041064000	-0.508253000	-0.485846000
H	3.423541000	-0.916059000	-1.120902000
H	4.792618000	-1.099860000	-0.410609000
O	-0.832769000	2.702827000	-0.106926000
H	-1.061960000	1.862631000	-0.538104000
H	-1.655251000	3.199506000	-0.123799000

10A.1DMA.4W-h

O	0.418997000	1.273910000	0.855695000
C	1.260848000	0.376878000	0.717948000
O	1.266836000	-0.777476000	1.194991000
C	2.424639000	0.708574000	-0.223763000
O	3.449105000	1.300931000	0.381741000
O	2.414333000	0.464146000	-1.407181000
H	-1.212790000	0.006591000	-0.796652000
H	4.124666000	1.478310000	-0.290746000
C	-1.871318000	1.910760000	-1.201987000
N	-2.039739000	0.593114000	-0.558073000
C	-3.249612000	-0.132532000	-0.986990000
H	-2.728346000	2.537998000	-0.962564000
H	-1.801024000	1.767369000	-2.279167000
H	-0.956515000	2.355506000	-0.817910000
H	-2.049044000	0.706024000	0.478327000
H	-3.287685000	-1.071522000	-0.441217000
H	-3.186102000	-0.321197000	-2.057261000
H	-4.128353000	0.470000000	-0.763095000

O	-1.980163000	0.941472000	2.216571000
H	-2.012773000	0.004332000	2.449845000
H	-1.031449000	1.127980000	2.087478000
O	-1.362435000	-1.617780000	1.161144000
H	-0.452538000	-1.289109000	1.318087000
H	-1.215375000	-2.530304000	0.888316000
O	-0.082457000	-0.854759000	-1.831777000
H	0.775775000	-0.403937000	-1.901639000
H	0.128078000	-1.716559000	-1.432729000
O	0.782956000	-3.030974000	-0.230991000
H	1.439289000	-3.700477000	-0.437253000
H	1.227635000	-2.350644000	0.311894000

2OA.1DMA

C	0.682411000	2.151240000	1.470527000
N	0.710933000	1.976386000	0.001721000
C	0.704263000	3.245463000	-0.749991000
H	0.687280000	1.161553000	1.920528000
H	-0.223248000	2.687769000	1.746633000
H	1.564522000	2.710409000	1.776612000
H	-0.106034000	1.391515000	-0.249312000
H	0.721881000	3.027313000	-1.814954000
H	1.585453000	3.823568000	-0.478667000
H	-0.197133000	3.802714000	-0.501831000
O	4.254532000	-1.255503000	-0.248300000
C	3.159835000	-0.535803000	-0.173059000
O	3.155265000	0.670381000	-0.258052000
C	1.880555000	-1.399429000	0.030960000
O	0.820936000	-0.715118000	0.137909000
O	2.060076000	-2.604297000	0.060571000
H	3.954880000	-2.184095000	-0.159557000
H	1.556089000	1.411391000	-0.221670000
O	-4.404456000	0.496880000	-0.309460000
C	-3.731971000	-0.630458000	-0.072975000
O	-4.240882000	-1.689274000	0.097663000
C	-2.201478000	-0.397448000	-0.042295000
O	-1.506079000	-1.440987000	0.158298000
O	-1.799720000	0.756388000	-0.208834000
H	-3.749081000	1.206142000	-0.408738000
H	-0.450196000	-1.222133000	0.161551000

2OA.1DMA.1W-a

C	-0.056202000	2.115090000	1.427349000
N	-0.277735000	1.957914000	-0.024566000

C	0.156769000	3.129518000	-0.808536000
H	-0.396674000	1.207936000	1.921905000
H	-0.612962000	2.975878000	1.794854000
H	1.012211000	2.251151000	1.589972000
H	-1.265387000	1.731357000	-0.185683000
H	-0.059520000	2.951589000	-1.859657000
H	1.231386000	3.240319000	-0.670208000
H	-0.370168000	4.019649000	-0.467619000
O	-4.747577000	-0.308647000	-0.196889000
C	-3.494637000	0.081130000	-0.079519000
O	-3.151932000	1.231022000	-0.063211000
C	-2.511505000	-1.107246000	0.021431000
O	-1.291286000	-0.725177000	0.193083000
O	-2.947326000	-2.230603000	-0.074753000
H	-4.743831000	-1.283568000	-0.202019000
H	-0.610352000	-1.521672000	0.210199000
O	4.684161000	-0.511273000	0.100699000
C	3.438210000	-0.902903000	-0.098853000
O	3.105875000	-2.056093000	-0.167256000
C	2.440018000	0.279413000	-0.216542000
O	1.267068000	-0.056028000	-0.497137000
O	2.904432000	1.405409000	-0.005329000
H	4.641662000	0.463579000	0.145091000
H	0.313863000	1.093899000	-0.322078000
O	0.368873000	-2.583224000	0.314438000
H	0.174288000	-3.431923000	-0.091987000
H	1.255405000	-2.296694000	0.008045000

2OA.1DMA.1W-b

C	-0.574398000	2.179285000	1.833589000
N	-0.027740000	1.802656000	0.513379000
C	-0.177241000	2.848356000	-0.517887000
H	-0.389878000	1.356786000	2.521067000
H	-1.644041000	2.341529000	1.718983000
H	-0.084052000	3.085225000	2.185999000
H	-0.514959000	0.902568000	0.241855000
H	0.223861000	2.470774000	-1.455202000
H	0.383695000	3.730166000	-0.212174000
H	-1.233832000	3.075862000	-0.627008000
O	1.749297000	-0.244591000	1.274534000
C	2.325762000	-0.695200000	0.314184000
O	2.337900000	-1.918114000	-0.105498000
C	3.088133000	0.287817000	-0.589851000
O	4.099075000	-0.251166000	-1.252543000

O	2.754168000	1.439902000	-0.666390000
H	0.961416000	1.546851000	0.611381000
H	4.508337000	0.442271000	-1.791854000
O	-4.274824000	-0.256124000	-0.944790000
C	-3.101990000	0.159245000	-0.500758000
O	-2.812719000	1.317603000	-0.361136000
C	-2.135719000	-1.012008000	-0.170683000
O	-0.998190000	-0.667976000	0.249542000
O	-2.583740000	-2.141955000	-0.344576000
H	-4.215384000	-1.232357000	-0.941561000
H	-0.232006000	-2.056461000	0.806724000
O	0.294661000	-2.888296000	0.939346000
H	-0.206999000	-3.558393000	0.462001000
H	1.565720000	-2.442641000	0.366672000

2OA.1DMA.1W-c

C	-0.407187000	2.241800000	1.301587000
N	-0.437519000	2.035085000	-0.166880000
C	-0.458260000	3.296171000	-0.940455000
H	-0.340324000	1.263049000	1.770255000
H	-1.322531000	2.750306000	1.598827000
H	0.472592000	2.834311000	1.542039000
H	-1.269555000	1.468876000	-0.379854000
H	-0.482934000	3.057773000	-2.001225000
H	0.444959000	3.851670000	-0.701883000
H	-1.351410000	3.854886000	-0.667084000
O	-4.443583000	-0.865221000	-0.008085000
C	-3.256796000	-0.303306000	-0.084409000
O	-3.083328000	0.876920000	-0.228497000
C	-2.104348000	-1.327257000	0.029725000
O	-0.944009000	-0.752297000	-0.023039000
O	-2.376196000	-2.493840000	0.151987000
H	-4.298872000	-1.823724000	0.100860000
H	-0.136077000	-1.402535000	0.010626000
O	3.151773000	-2.817203000	-0.132749000
C	2.149622000	-1.979628000	-0.060335000
O	0.996198000	-2.354373000	-0.015075000
C	2.605279000	-0.489343000	-0.038267000
O	1.688033000	0.353547000	0.055923000
O	3.824014000	-0.339412000	-0.106763000
H	3.946788000	-2.240788000	-0.158391000
H	2.463346000	2.012606000	0.165326000
O	2.440680000	2.988738000	0.176665000
H	0.385101000	1.452242000	-0.399682000

H	3.353027000	3.270232000	0.078343000
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2OA.1DMA.1W-d

C	0.296654000	2.264524000	1.501821000
N	0.222698000	2.329705000	0.026678000
C	0.591037000	3.653344000	-0.512445000
H	0.031685000	1.258372000	1.817801000
H	-0.403741000	2.982496000	1.924330000
H	1.315134000	2.494186000	1.810747000
H	-0.748511000	2.119359000	-0.252233000
H	0.512605000	3.626820000	-1.596803000
H	1.618046000	3.876050000	-0.229081000
H	-0.084710000	4.405146000	-0.107766000
O	-3.961559000	-2.261957000	-0.238160000
C	-3.262690000	-1.150025000	-0.147519000
O	-3.754927000	-0.056769000	-0.198197000
C	-1.750852000	-1.424823000	0.032450000
O	-1.020576000	-0.362688000	0.124644000
O	-1.397733000	-2.580782000	0.072372000
H	-3.325999000	-2.998911000	-0.165214000
H	0.031452000	-0.635653000	0.262277000
O	3.534792000	-2.315470000	0.395887000
C	3.603143000	-1.101159000	-0.150800000
O	4.600497000	-0.628498000	-0.594392000
C	2.240713000	-0.355662000	-0.145700000
O	2.170788000	0.738772000	-0.704027000
O	1.315126000	-0.974243000	0.461489000
H	2.616113000	-2.451681000	0.681860000
H	0.898712000	1.604872000	-0.365117000
O	-2.519953000	2.398191000	-0.153471000
H	-2.916804000	1.506117000	-0.114144000
H	-3.142541000	2.935263000	-0.649397000

2OA.1DMA.1W-e

C	0.206335000	3.145302000	0.982848000
N	-0.276846000	1.931036000	0.300597000
C	-0.251730000	2.041036000	-1.172080000
H	0.134877000	2.999470000	2.058505000
H	-0.392035000	4.004737000	0.683299000
H	1.249271000	3.288063000	0.702970000
H	-1.226641000	1.674147000	0.582255000
H	-0.601004000	1.097420000	-1.585233000
H	0.777186000	2.225327000	-1.476853000
H	-0.903196000	2.853173000	-1.491561000

O	4.556247000	-0.478384000	-0.705148000
C	3.402465000	-0.863935000	-0.186745000
O	3.111805000	-2.013221000	0.007693000
C	2.447415000	0.320741000	0.116435000
O	1.380303000	0.000451000	0.687740000
O	2.829240000	1.435162000	-0.260193000
H	4.490893000	0.493212000	-0.780385000
H	0.380470000	1.096903000	0.560264000
O	-4.675805000	-0.392558000	-0.431186000
C	-3.451807000	0.007658000	-0.134293000
O	-3.135520000	1.158851000	0.021541000
C	-2.463272000	-1.174055000	-0.017098000
O	-1.278829000	-0.732891000	0.305931000
O	-2.806006000	-2.303089000	-0.218787000
H	-5.239616000	0.392856000	-0.489155000
H	-0.599394000	-1.507780000	0.424150000
O	0.384573000	-2.590573000	0.653002000
H	0.303526000	-3.403835000	0.147433000
H	1.299102000	-2.261407000	0.541006000

2OA.1DMA.1W-f

C	0.186170000	3.183482000	-0.870182000
N	0.465381000	1.936534000	-0.124653000
C	0.270866000	2.074447000	1.337980000
H	0.348088000	3.003235000	-1.930356000
H	0.857061000	3.966003000	-0.519937000
H	-0.852515000	3.455296000	-0.688920000
H	1.417576000	1.589357000	-0.294203000
H	0.468177000	1.106726000	1.793796000
H	-0.761150000	2.375942000	1.510680000
H	0.966221000	2.819565000	1.720628000
O	-3.505011000	-2.549387000	0.250368000
C	-3.278940000	-1.266587000	-0.010423000
O	-4.128471000	-0.427638000	-0.026736000
C	-1.785707000	-0.941276000	-0.269745000
O	-1.525725000	0.220760000	-0.605826000
O	-0.988688000	-1.895168000	-0.087638000
H	-2.640601000	-2.995555000	0.235874000
H	-0.188008000	1.179808000	-0.441698000
O	4.678054000	-0.776802000	0.105676000
C	3.471749000	-0.250952000	0.003762000
O	3.255674000	0.933429000	-0.066105000
C	2.360075000	-1.326604000	-0.021892000
O	1.194162000	-0.742915000	-0.023571000

O	2.618714000	-2.493133000	-0.042560000
H	5.321257000	-0.052628000	0.108494000
H	0.350020000	-1.374628000	-0.076077000
O	-2.779272000	2.514884000	0.252960000
H	-2.743723000	1.608898000	-0.098755000
H	-3.700838000	2.654938000	0.483507000

2OA.1DMA.1W-g

C	0.020375000	2.134080000	1.468003000
N	0.290309000	1.948907000	0.027987000
C	-0.107420000	3.108529000	-0.791512000
H	0.337345000	1.234153000	1.990411000
H	-1.052100000	2.279877000	1.590663000
H	0.567604000	2.999414000	1.839837000
H	1.278448000	1.707895000	-0.102352000
H	0.144615000	2.910224000	-1.831109000
H	0.411633000	4.002643000	-0.448278000
H	-1.185682000	3.228065000	-0.694576000
O	-4.675430000	-0.480383000	-0.001118000
C	-3.425127000	-0.884776000	-0.148883000
O	-3.099289000	-2.040310000	-0.186525000
C	-2.415979000	0.289699000	-0.247719000
O	-1.235386000	-0.054228000	-0.485929000
O	-2.878845000	1.421366000	-0.064088000
H	-4.627014000	0.494447000	0.031567000
H	-0.301435000	1.079543000	-0.277209000
O	4.724533000	-0.433854000	-0.235603000
C	3.483109000	0.000121000	-0.113786000
O	3.169735000	1.163412000	-0.126116000
C	2.468551000	-1.154706000	0.018509000
O	1.315234000	-0.700707000	0.422505000
O	2.764420000	-2.282382000	-0.258229000
H	5.301694000	0.337725000	-0.334511000
H	0.606161000	-1.460942000	0.426051000
O	-0.375375000	-2.561881000	0.481331000
H	-1.239563000	-2.298214000	0.104539000
H	-0.091695000	-3.363114000	0.031565000

2OA.1DMA.2W-a

C	-4.286187000	-1.210355000	-0.716792000
N	-3.057515000	-1.295379000	0.095838000
C	-3.298404000	-1.139611000	1.546259000
H	-4.024700000	-1.332681000	-1.765431000
H	-4.735206000	-0.232233000	-0.561895000

H	-4.972236000	-1.999291000	-0.412440000
H	-2.374565000	-0.553214000	-0.193852000
H	-2.340998000	-1.202878000	2.058787000
H	-3.951152000	-1.940765000	1.888425000
H	-3.756090000	-0.168263000	1.718556000
O	-3.225262000	1.645533000	0.052994000
C	-2.171608000	2.216721000	-0.022735000
O	-2.036185000	3.524145000	0.103870000
C	-0.832505000	1.469487000	-0.264522000
O	-0.905579000	0.242668000	-0.424806000
O	0.182273000	2.199209000	-0.256382000
H	-1.082376000	3.710388000	0.020052000
H	0.403794000	-1.178492000	-0.665184000
O	2.001646000	0.456146000	-0.250978000
C	3.245734000	0.658286000	0.036298000
O	3.816603000	1.702185000	0.240252000
C	4.044559000	-0.662810000	0.119788000
O	5.323953000	-0.455363000	0.383753000
O	3.560695000	-1.746629000	-0.028268000
H	1.398291000	1.288340000	-0.267660000
H	5.444015000	0.507704000	0.466907000
O	-1.405055000	-3.480241000	0.093221000
H	-1.412214000	-4.350322000	-0.311608000
H	-2.562647000	-2.200287000	-0.052563000
O	0.694957000	-2.104063000	-0.687831000
H	1.630869000	-2.074680000	-0.438536000
H	-0.536087000	-3.064706000	-0.150795000

2OA.1DMA.2W-b

C	2.844883000	3.279239000	0.326764000
N	2.010335000	2.173624000	-0.176690000
C	1.859703000	2.153282000	-1.646875000
H	2.891734000	3.219938000	1.411412000
H	2.406838000	4.229223000	0.025920000
H	3.846859000	3.181705000	-0.087294000
H	1.049444000	2.178835000	0.246260000
H	1.230041000	1.304787000	-1.903351000
H	2.842862000	2.042993000	-2.101623000
H	1.398075000	3.083960000	-1.972010000
O	-5.179474000	0.663118000	0.365911000
C	-3.874205000	0.783394000	0.198696000
O	-3.287872000	1.824462000	0.272355000
C	-3.197162000	-0.575612000	-0.094933000
O	-1.933554000	-0.478619000	-0.329681000

O	-3.880726000	-1.575946000	-0.078330000
H	-5.391069000	-0.283375000	0.271851000
H	-1.501182000	-1.423988000	-0.505752000
O	1.065956000	-0.451799000	-0.100855000
C	1.807871000	-1.418315000	0.091780000
O	1.546897000	-2.641920000	0.106765000
C	3.310836000	-1.096903000	0.345192000
O	4.054496000	-2.165618000	0.537734000
O	3.753123000	0.026023000	0.358676000
H	2.432030000	1.267456000	0.100378000
H	3.437621000	-2.921339000	0.464450000
O	-0.448539000	1.721299000	0.798939000
H	-1.366130000	1.931275000	0.565516000
H	-0.356857000	0.780078000	0.579711000
O	-0.943831000	-2.716473000	-0.738394000
H	-0.009795000	-2.778088000	-0.392695000
H	-1.466165000	-3.415560000	-0.334652000

2OA.1DMA.2W-c

C	0.059578000	-2.455038000	1.805776000
N	-0.371443000	-2.051791000	0.450072000
C	-0.415723000	-3.160319000	-0.523451000
H	0.046561000	-1.569074000	2.436439000
H	1.067921000	-2.856167000	1.734923000
H	-0.628178000	-3.204679000	2.192844000
H	0.284919000	-1.295003000	0.150875000
H	-0.754875000	-2.768959000	-1.479257000
H	-1.121463000	-3.909404000	-0.168503000
H	0.582407000	-3.578785000	-0.617464000
O	-2.292613000	1.982907000	0.029912000
C	-2.395382000	0.738902000	0.329791000
O	-1.838713000	0.142178000	1.227348000
C	-3.269649000	-0.089539000	-0.627613000
O	-4.226425000	0.599566000	-1.229186000
O	-3.059607000	-1.261292000	-0.796861000
H	-1.290792000	-1.596229000	0.515861000
H	-4.710984000	-0.005444000	-1.810675000
O	1.055526000	0.293521000	0.228631000
C	2.240040000	0.371637000	-0.153205000
O	2.950016000	1.371017000	-0.346269000
C	2.952677000	-0.984197000	-0.431915000
O	4.207951000	-0.842565000	-0.815835000
O	2.411622000	-2.050705000	-0.308336000
H	0.254577000	1.763294000	0.990721000

H	4.366814000	0.121708000	-0.824175000
O	-0.205593000	2.619004000	1.126220000
H	-1.423312000	2.375803000	0.547163000
H	0.374075000	3.264135000	0.666907000
O	1.804812000	3.873024000	-0.184463000
H	2.292760000	3.027330000	-0.266216000
H	1.774618000	4.252090000	-1.065522000

2OA.1DMA.2W-d

C	-0.277723000	2.214367000	-1.208328000
N	-0.258337000	2.149494000	0.269808000
C	-1.001097000	3.256765000	0.903147000
H	0.242055000	1.337885000	-1.587288000
H	0.239094000	3.117609000	-1.526476000
H	-1.316141000	2.214979000	-1.533067000
H	0.725918000	2.157126000	0.563931000
H	-0.921380000	3.163382000	1.984061000
H	-2.043679000	3.175058000	0.601538000
H	-0.575387000	4.205164000	0.578778000
O	1.865645000	-2.260877000	0.248081000
C	2.173848000	-1.029572000	0.054659000
O	1.457661000	-0.055392000	0.121184000
C	3.659441000	-0.794697000	-0.294027000
O	4.347543000	-1.904403000	-0.510300000
O	4.122830000	0.312104000	-0.357684000
H	0.839639000	-2.358571000	0.546062000
H	5.258870000	-1.651563000	-0.721210000
O	-1.621401000	-0.092385000	0.733124000
C	-2.695602000	0.071411000	0.102076000
O	-3.193773000	1.134275000	-0.282905000
C	-3.486421000	-1.216353000	-0.269681000
O	-4.639912000	-0.942747000	-0.862587000
O	-3.094896000	-2.329885000	-0.065356000
H	-0.699504000	1.230571000	0.555453000
H	-4.675852000	0.031098000	-0.920908000
O	-0.457296000	-2.429010000	1.022683000
H	-1.098068000	-3.018181000	0.605753000
H	-0.904731000	-1.542065000	0.963338000
O	2.509513000	2.672820000	0.175836000
H	2.920717000	1.811724000	-0.011700000
H	3.214810000	3.231791000	0.509402000

2OA.1DMA.2W-e

C	-0.138744000	1.954064000	1.205457000
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N	0.319614000	2.322152000	-0.152167000
C	1.193068000	3.513346000	-0.166686000
H	-0.771678000	1.073424000	1.120466000
H	-0.712410000	2.777836000	1.627694000
H	0.737010000	1.738992000	1.814454000
H	-0.523194000	2.451972000	-0.739374000
H	1.460987000	3.742847000	-1.195660000
H	2.089459000	3.275628000	0.403041000
H	0.664038000	4.355937000	0.275497000
O	4.121242000	-1.363238000	1.201189000
C	3.193878000	-1.328726000	0.254685000
O	2.852987000	-2.283642000	-0.382183000
C	2.569435000	0.082324000	0.080144000
O	1.737092000	0.200064000	-0.857487000
O	2.924212000	0.941384000	0.891695000
H	4.160394000	-0.459438000	1.565389000
H	0.868649000	1.495058000	-0.538243000
O	-4.061107000	-1.330975000	1.416140000
C	-3.302716000	-0.559621000	0.664820000
O	-3.435251000	0.630597000	0.587658000
C	-2.214559000	-1.357344000	-0.089875000
O	-1.463302000	-0.621492000	-0.838013000
O	-2.157080000	-2.552516000	0.087794000
H	-3.736496000	-2.243867000	1.304209000
H	-0.693144000	-1.206697000	-1.300324000
O	0.400749000	-1.821454000	-1.902020000
H	1.129808000	-1.217244000	-1.618399000
H	0.640596000	-2.680108000	-1.534654000
O	-2.220756000	2.348060000	-1.323931000
H	-2.664575000	1.755513000	-0.691115000
H	-2.279191000	1.886521000	-2.165819000

2OA.1DMA.2W-f

C	-0.567622000	1.956799000	-1.154652000
N	-0.638750000	1.850729000	0.319550000
C	-1.317429000	3.001687000	0.945641000
H	-0.119844000	1.041833000	-1.535292000
H	0.058273000	2.809805000	-1.408783000
H	-1.577479000	2.075862000	-1.538613000
H	0.325996000	1.798419000	0.664192000
H	-1.342680000	2.853080000	2.022782000
H	-2.330995000	3.054299000	0.556714000
H	-0.759135000	3.905652000	0.707584000
O	2.246247000	-2.144998000	0.138161000

C	2.333085000	-0.869694000	0.001404000
O	1.461072000	-0.041964000	0.140666000
C	3.741910000	-0.363027000	-0.372418000
O	4.600912000	-1.324648000	-0.671367000
O	4.004657000	0.809002000	-0.381192000
H	1.268684000	-2.416473000	0.467776000
H	5.448529000	-0.908947000	-0.889303000
O	-4.551438000	-0.754511000	-1.006734000
C	-3.552611000	-0.138236000	-0.397098000
O	-3.439791000	1.056136000	-0.341830000
C	-2.523347000	-1.128499000	0.214884000
O	-1.581684000	-0.604398000	0.863072000
O	-2.728731000	-2.321193000	-0.018003000
H	-4.355396000	-1.707798000	-0.913673000
H	-1.118945000	0.946107000	0.570519000
O	0.006703000	-2.683289000	1.009784000
H	-0.613927000	-3.255961000	0.540485000
H	-0.505511000	-1.831171000	1.080759000
O	2.011297000	2.811944000	0.401333000
H	2.605811000	3.445284000	0.809733000
H	2.569991000	2.064070000	0.130590000

2OA.1DMA.2W-g

C	-1.492106000	2.830594000	0.953625000
N	-0.694149000	1.825434000	0.221588000
C	-0.607210000	2.105176000	-1.228646000
H	-1.549947000	2.538682000	2.000078000
H	-2.490000000	2.860091000	0.525662000
H	-0.989686000	3.791516000	0.862955000
H	-1.081539000	0.866570000	0.344425000
H	-0.004632000	1.325631000	-1.687932000
H	-0.132538000	3.075298000	-1.364883000
H	-1.615957000	2.100905000	-1.635534000
O	0.843275000	-2.048365000	0.440586000
C	1.706697000	-1.160831000	0.121609000
O	1.514301000	0.022510000	-0.092161000
C	3.157584000	-1.672241000	-0.005492000
O	3.293880000	-2.961452000	0.274747000
O	4.050845000	-0.942756000	-0.329594000
H	2.952571000	1.092206000	-0.699733000
H	4.228530000	-3.189972000	0.164217000
O	-1.302053000	-0.877079000	0.401517000
C	-2.419577000	-1.418423000	0.127509000
O	-2.722239000	-2.598104000	0.089598000

C	-3.545629000	-0.406038000	-0.217898000
O	-4.700610000	-0.998069000	-0.462087000
O	-3.380707000	0.782854000	-0.267894000
H	-0.144423000	-1.613178000	0.455575000
H	-4.526085000	-1.954697000	-0.362502000
O	1.639365000	3.224279000	0.822893000
H	0.263243000	1.835522000	0.594264000
H	2.060332000	3.484143000	1.645422000
O	3.321196000	1.970223000	-0.901217000
H	2.361357000	2.909570000	0.239842000
H	4.271239000	1.837917000	-0.948311000

2OA.1DMA.2W-h

C	1.391712000	3.144569000	-0.014969000
N	0.696398000	1.956748000	0.516638000
C	0.305592000	2.087548000	1.936598000
H	1.627717000	2.973669000	-1.061019000
H	2.318303000	3.286395000	0.536441000
H	0.735198000	4.005383000	0.099769000
H	1.279104000	1.092378000	0.434678000
H	-0.133292000	1.145174000	2.251728000
H	-0.419905000	2.893839000	2.025160000
H	1.196595000	2.302028000	2.523520000
O	4.071314000	-0.970465000	-1.612476000
C	3.249764000	-0.267565000	-0.851128000
O	3.138609000	0.927004000	-0.911152000
C	2.415214000	-1.153585000	0.114185000
O	1.664179000	-0.527937000	0.902795000
O	2.561188000	-2.371807000	-0.019346000
H	3.914463000	-1.901962000	-1.360778000
H	0.585243000	-1.691390000	1.405665000
O	-1.453862000	0.055658000	0.420958000
C	-2.220245000	-0.832433000	0.121406000
O	-2.094297000	-2.094177000	0.329152000
C	-3.524217000	-0.435334000	-0.603876000
O	-4.326201000	-1.454011000	-0.869654000
O	-3.761927000	0.707023000	-0.889082000
H	-2.388663000	2.038494000	-0.460879000
H	-5.110141000	-1.104953000	-1.319406000
O	-1.785293000	2.800400000	-0.482353000
H	-2.115018000	3.366267000	-1.184453000
H	-0.164357000	1.813619000	-0.024489000
O	0.060756000	-2.536279000	1.444239000
H	-1.162164000	-2.309053000	0.805299000

H	0.659484000	-3.149594000	0.994342000
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2OA.1DMA.3W-a

C	0.211217000	2.698261000	-1.021155000
N	0.581225000	2.196792000	0.321004000
C	1.564866000	3.047855000	1.023676000
H	-0.498063000	2.002696000	-1.460949000
H	1.113486000	2.746955000	-1.625266000
H	-0.239950000	3.683602000	-0.916850000
H	1.007211000	1.253659000	0.259730000
H	1.783811000	2.594409000	1.987492000
H	1.153013000	4.047117000	1.152183000
H	2.469549000	3.076636000	0.420610000
O	3.249765000	-1.043533000	-1.920294000
C	2.747190000	-0.209485000	-1.027379000
O	2.738546000	0.984415000	-1.164333000
C	2.127481000	-0.921422000	0.208297000
O	1.751845000	-0.178235000	1.128615000
O	2.061548000	-2.162590000	0.107302000
H	3.066685000	-1.938028000	-1.576019000
H	0.444750000	-0.621720000	2.197416000
O	-3.135225000	1.224829000	-0.456924000
C	-2.993644000	0.075223000	-1.106528000
O	-3.657551000	-0.249537000	-2.041151000
C	-1.822225000	-0.780575000	-0.599844000
O	-2.118929000	-2.041293000	-0.461519000
O	-0.745510000	-0.273087000	-0.374405000
H	-2.582534000	1.248725000	0.358985000
H	-1.352209000	-2.518468000	-0.025792000
O	-0.424475000	-0.757865000	2.636865000
H	-1.275618000	0.475114000	2.158985000
H	-0.680732000	-1.640856000	2.335757000
O	-0.216192000	-3.110917000	0.981787000
H	-0.157084000	-4.055885000	1.147483000
H	0.694147000	-2.804685000	0.707471000
O	-1.702019000	1.338690000	1.847857000
H	-0.264573000	2.064403000	0.896557000
H	-2.174198000	1.702624000	2.602373000

2OA.1DMA.3W-b

C	-0.796855000	2.608468000	-1.837909000
N	0.202055000	1.774444000	-1.143222000
C	1.536951000	1.789044000	-1.773629000
H	-1.734166000	2.539965000	-1.290219000

H	-0.926093000	2.236620000	-2.852997000
H	-0.449770000	3.639951000	-1.853865000
H	-0.154874000	0.804797000	-1.128902000
H	2.218806000	1.204349000	-1.160059000
H	1.893373000	2.816431000	-1.822620000
H	1.462669000	1.365839000	-2.774232000
O	2.905923000	-3.067737000	-0.308309000
C	1.808754000	-2.335631000	-0.223658000
O	0.741627000	-2.692267000	-0.639948000
C	2.050635000	-0.951102000	0.440999000
O	1.043594000	-0.258970000	0.712896000
O	3.242323000	-0.653604000	0.601897000
H	3.625821000	-2.514062000	0.047089000
H	-0.031160000	2.087154000	1.800872000
O	-1.274684000	-1.145245000	1.027886000
C	-2.057434000	-0.138441000	0.815447000
O	-1.776579000	1.039124000	0.833609000
C	-3.457309000	-0.567850000	0.383745000
O	-4.367116000	-0.459393000	1.342174000
O	-3.685816000	-0.920122000	-0.741745000
H	-0.282225000	-0.839419000	0.950786000
H	-5.224546000	-0.720756000	0.972158000
O	0.539595000	2.733084000	1.366998000
H	0.295670000	2.100304000	-0.145037000
H	1.460282000	2.451285000	1.538298000
O	3.181724000	2.003988000	1.310842000
H	3.284854000	1.042234000	1.158447000
H	3.895489000	2.269285000	1.894983000
O	-0.915450000	-0.701842000	-1.869925000
H	-1.862837000	-0.883429000	-1.796048000
H	-0.475262000	-1.464725000	-1.457061000

2OA.1DMA.3W-c

C	1.101470000	-1.536256000	1.491095000
N	1.876959000	-1.898623000	0.280172000
C	3.181340000	-2.521488000	0.575714000
H	0.181059000	-1.043245000	1.185382000
H	1.702849000	-0.857415000	2.092710000
H	0.870956000	-2.442735000	2.047944000
H	2.001977000	-1.024064000	-0.260826000
H	3.684131000	-2.754332000	-0.359956000
H	3.016882000	-3.434489000	1.145040000
H	3.779067000	-1.814829000	1.146104000
O	3.079917000	2.779932000	0.406215000

C	2.734036000	1.547703000	0.083035000
O	3.363891000	0.574046000	0.398143000
C	1.409639000	1.464361000	-0.720902000
O	1.059908000	0.331848000	-1.084145000
O	0.827253000	2.557389000	-0.884916000
H	2.371560000	3.356174000	0.062363000
H	-0.484053000	-0.298446000	-1.639356000
O	-1.636209000	1.925482000	-0.813021000
C	-1.776555000	1.280422000	0.314676000
O	-0.949097000	1.098695000	1.167245000
C	-3.180947000	0.673790000	0.442516000
O	-3.661662000	0.797759000	1.674250000
O	-3.747070000	0.117430000	-0.457425000
H	-0.669788000	2.256061000	-0.902199000
H	-4.535183000	0.380299000	1.692502000
O	-2.005995000	-2.336927000	0.437322000
H	-2.952790000	-2.487502000	0.499663000
H	-0.718449000	-3.407499000	-0.524416000
O	0.019544000	-3.381890000	-1.157469000
H	1.283061000	-2.521912000	-0.307470000
H	-0.307127000	-2.767613000	-1.831543000
O	-1.263107000	-0.876009000	-1.784269000
H	-1.887984000	-1.711852000	-0.305433000
H	-1.987765000	-0.289478000	-2.033960000

2OA.1DMA.3W-d

C	-2.239695000	2.672664000	-0.087768000
N	-1.019805000	1.943899000	-0.489961000
C	-0.665192000	2.084483000	-1.916141000
H	-2.448453000	2.428463000	0.950381000
H	-3.061789000	2.354104000	-0.723313000
H	-2.054868000	3.740092000	-0.185953000
H	-1.137586000	0.941884000	-0.297217000
H	0.251119000	1.527690000	-2.092101000
H	-0.523414000	3.139110000	-2.144518000
H	-1.475134000	1.667963000	-2.511511000
O	3.379471000	0.562797000	-1.586074000
C	2.969413000	-0.284403000	-0.649831000
O	3.284051000	-1.439066000	-0.627785000
C	2.029729000	0.396810000	0.391605000
O	1.647665000	-0.285737000	1.359955000
O	1.751338000	1.583897000	0.126174000
H	2.976693000	1.419150000	-1.349390000
H	0.031191000	0.115017000	1.807011000

O	-0.874866000	-2.702382000	0.306492000
C	-1.111345000	-1.619603000	-0.345576000
O	-0.320773000	-0.848909000	-0.843306000
C	-2.611879000	-1.278535000	-0.464221000
O	-3.420165000	-2.278346000	-0.144886000
O	-2.982161000	-0.191919000	-0.817572000
H	0.165516000	-2.832833000	0.498000000
H	-4.331649000	-1.969404000	-0.255611000
O	-0.908897000	0.393246000	1.928140000
H	-0.269004000	2.328546000	2.315621000
H	-1.251692000	-0.149630000	2.643480000
O	0.121455000	3.106267000	1.892204000
H	-0.239978000	2.252486000	0.110429000
H	1.007844000	2.806028000	1.645027000
O	1.503494000	-2.920901000	0.915614000
H	2.128291000	-3.044210000	0.188797000
H	1.700450000	-1.991826000	1.190540000

2OA.1DMA.3W-e

C	0.662929000	2.081523000	-1.917378000
N	1.017712000	1.944062000	-0.490913000
C	2.235186000	2.677234000	-0.089449000
H	-0.251343000	1.521245000	-2.092884000
H	1.474500000	1.667174000	-2.512035000
H	0.517466000	3.135366000	-2.147061000
H	1.139039000	0.942802000	-0.296582000
H	2.444155000	2.435563000	0.949240000
H	2.047338000	3.743951000	-0.189542000
H	3.058473000	2.359907000	-0.724089000
O	-3.379348000	0.561620000	-1.585436000
C	-2.968635000	-0.285931000	-0.649769000
O	-3.282300000	-1.440868000	-0.628651000
C	-2.029724000	0.395400000	0.392268000
O	-1.647460000	-0.287060000	1.360513000
O	-1.752166000	1.582881000	0.127363000
H	-2.977182000	1.418117000	-1.348203000
H	-0.030370000	0.114805000	1.807083000
O	0.877084000	-2.701969000	0.307382000
C	1.112575000	-1.619270000	-0.345244000
O	0.321277000	-0.849681000	-0.843463000
C	2.612760000	-1.276707000	-0.463676000
O	3.421953000	-2.276014000	-0.145138000
O	2.982060000	-0.189461000	-0.816160000
H	-0.163242000	-2.833216000	0.498491000

H	4.333161000	-1.966193000	-0.255657000
O	0.909506000	0.393845000	1.927376000
H	1.253474000	-0.148725000	2.642373000
H	0.267709000	2.328916000	2.315875000
O	-1.501405000	-2.922430000	0.915282000
H	-2.125705000	-3.045437000	0.187993000
H	-1.699105000	-1.993796000	1.190951000
O	-0.123006000	3.106760000	1.892995000
H	-1.008932000	2.805977000	1.644863000
H	0.236473000	2.250634000	0.108554000

2OA.1DMA.3W-f

C	-2.803313000	2.883659000	1.067137000
N	-2.478810000	1.910507000	0.008595000
C	-3.504459000	1.799643000	-1.048610000
H	-1.976873000	2.903927000	1.770963000
H	-3.722930000	2.574148000	1.560783000
H	-2.935336000	3.868277000	0.621614000
H	-2.370031000	0.945183000	0.426179000
H	-3.180484000	1.041736000	-1.757328000
H	-3.605369000	2.756938000	-1.556229000
H	-4.448751000	1.509610000	-0.591213000
O	-1.074245000	-0.944676000	-0.857791000
C	-1.676428000	-1.302974000	0.161712000
O	-2.454567000	-0.630907000	0.880722000
C	-1.471835000	-2.768842000	0.653777000
O	-2.202850000	-3.055816000	1.721587000
O	-0.734503000	-3.556387000	0.133772000
H	-0.700922000	0.638264000	-1.784698000
H	-2.685746000	-2.236858000	1.937997000
O	3.007781000	-1.201681000	-0.466933000
C	2.624009000	0.015885000	-0.309341000
O	1.629804000	0.531401000	-0.774542000
C	3.534797000	0.868991000	0.595640000
O	4.727774000	0.324582000	0.805063000
O	3.170407000	1.915140000	1.049413000
H	2.251596000	-1.736450000	-0.980014000
H	5.226744000	0.923657000	1.379867000
O	0.216454000	2.521761000	0.696116000
H	0.890745000	2.956173000	1.226703000
H	0.729087000	1.870669000	0.188564000
O	-0.702197000	1.562827000	-2.090629000
H	-1.574536000	2.140733000	-0.431619000
H	0.230842000	1.783870000	-2.167193000

O	1.139848000	-2.377486000	-1.598500000
H	0.351637000	-1.806534000	-1.452922000
H	0.865730000	-3.195123000	-1.159719000

2OA.1DMA.3W-g

C	-0.223935000	2.168293000	-1.847074000
N	0.142009000	1.866231000	-0.448910000
C	-0.024772000	3.000647000	0.481255000
H	0.037348000	1.306869000	-2.455426000
H	0.336150000	3.043693000	-2.171436000
H	-1.294810000	2.351232000	-1.889888000
H	1.118943000	1.533619000	-0.411051000
H	0.236666000	2.657475000	1.479003000
H	-1.062047000	3.325421000	0.453852000
H	0.645284000	3.802352000	0.177276000
O	-1.666685000	-0.423084000	-1.270241000
C	-2.482259000	-0.736217000	-0.306033000
O	-2.789057000	-1.840516000	0.070150000
C	-3.067503000	0.500247000	0.401406000
O	-3.874324000	0.172079000	1.396275000
O	-2.809564000	1.626381000	0.089174000
H	-1.131716000	-1.242580000	-1.589580000
H	-3.893128000	-0.801003000	1.438227000
O	4.456835000	0.087151000	0.867455000
C	3.288400000	0.422868000	0.343689000
O	2.898310000	1.565876000	0.282804000
C	2.449144000	-0.782796000	-0.155459000
O	2.666588000	-1.873317000	0.356102000
O	1.592444000	-0.457186000	-1.021805000
H	4.890083000	0.901659000	1.162170000
H	1.012060000	-2.565533000	0.814812000
O	-0.562512000	-0.028029000	1.541928000
H	-0.790955000	0.066733000	2.470171000
H	-0.414681000	1.074316000	-0.103317000
O	-0.045029000	-2.246405000	-1.804472000
H	0.721506000	-1.635039000	-1.536228000
H	0.154343000	-2.637294000	-2.658501000
O	0.073421000	-2.561889000	1.083652000
H	-0.304706000	-0.979485000	1.417786000
H	-0.412271000	-2.872800000	0.309618000

2OA.1DMA.3W-h

C	-1.083491000	1.424251000	-1.757938000
N	-0.533391000	1.973779000	-0.503545000

C	-1.477250000	2.845828000	0.230543000
H	-0.394215000	0.672186000	-2.133837000
H	-1.204654000	2.231723000	-2.478074000
H	-2.054039000	0.979204000	-1.546382000
H	0.335721000	2.506481000	-0.697061000
H	-0.975459000	3.202245000	1.125217000
H	-2.346645000	2.249884000	0.501188000
H	-1.761353000	3.676315000	-0.413671000
O	3.239224000	-3.103697000	-0.011538000
C	3.062519000	-1.792953000	-0.088977000
O	3.949228000	-0.997422000	0.028744000
C	1.582765000	-1.379008000	-0.340542000
O	1.339013000	-0.177066000	-0.466721000
O	0.789512000	-2.354972000	-0.381715000
H	2.359314000	-3.506240000	-0.123684000
H	1.510340000	1.470622000	1.898543000
O	-4.035260000	0.317406000	0.136306000
C	-3.648304000	-0.969808000	0.174215000
O	-4.396071000	-1.896242000	0.171688000
C	-2.115631000	-1.075876000	0.245334000
O	-1.661519000	-2.048756000	-0.461055000
O	-1.491540000	-0.283011000	0.919899000
H	-5.003691000	0.321734000	0.116079000
H	-0.606071000	-2.125575000	-0.414406000
O	3.042591000	1.635833000	0.656298000
H	2.648034000	0.890571000	0.153168000
H	3.949053000	1.353598000	0.813721000
O	0.557447000	1.501008000	2.068485000
H	0.265835000	0.586242000	2.153548000
H	-0.250925000	1.201173000	0.115695000
O	1.756806000	3.563987000	-0.734095000
H	2.228018000	3.876615000	-1.510010000
H	2.395381000	3.025632000	-0.221372000

2OA.1DMA.3W-i

C	-1.923662000	-2.622050000	-1.187768000
N	-1.928089000	-1.877252000	0.087778000
C	-3.040807000	-2.216415000	0.991105000
H	-1.048607000	-2.317158000	-1.758816000
H	-2.830773000	-2.381469000	-1.739106000
H	-1.879774000	-3.688941000	-0.976116000
H	-1.963173000	-0.872862000	-0.136754000
H	-2.943559000	-1.606960000	1.885386000
H	-2.988117000	-3.274410000	1.242194000

H	-3.980388000	-1.992308000	0.490022000
O	1.607257000	0.364158000	1.260185000
C	2.266388000	0.753099000	0.307489000
O	1.948546000	1.607848000	-0.582339000
C	3.647772000	0.126985000	0.064721000
O	4.396743000	0.116754000	1.163434000
O	3.987375000	-0.330865000	-0.990423000
H	-0.179958000	0.368391000	1.669560000
H	5.236794000	-0.311256000	0.940367000
O	-0.334373000	2.374204000	-0.338553000
C	-1.108324000	1.431975000	-0.631046000
O	-0.836843000	0.349802000	-1.158116000
C	-2.595080000	1.613792000	-0.245724000
O	-2.917044000	2.857078000	0.088225000
O	-3.373814000	0.696729000	-0.245000000
H	0.894987000	1.991471000	-0.469532000
H	-3.859585000	2.862739000	0.310084000
O	1.302839000	-1.291461000	-1.702892000
H	0.711943000	-0.517836000	-1.661154000
H	2.188546000	-0.953005000	-1.889625000
O	0.683374000	-2.347101000	0.760123000
H	1.031633000	-2.081827000	-0.117608000
H	-1.000008000	-2.023057000	0.549228000
O	-1.104358000	0.155705000	1.896589000
H	-1.286484000	0.664073000	2.691278000
H	1.037807000	-1.671952000	1.353636000

2OA.1DMA.3W-j

C	-0.026553000	3.139307000	-0.894665000
N	0.406472000	2.164408000	0.128109000
C	1.636957000	2.552266000	0.843340000
H	-0.905393000	2.732644000	-1.389974000
H	0.776237000	3.263800000	-1.616943000
H	-0.265291000	4.081551000	-0.404620000
H	0.576306000	1.269847000	-0.348962000
H	1.856821000	1.786286000	1.582909000
H	1.483773000	3.518217000	1.321282000
H	2.447807000	2.613920000	0.118946000
O	1.065199000	-0.558425000	1.046652000
C	1.695233000	-1.171599000	0.172940000
O	1.269258000	-1.872478000	-0.770685000
C	3.219928000	-0.995081000	0.200192000
O	3.798709000	-1.617974000	1.222685000
O	3.829716000	-0.338354000	-0.605909000

H	-0.580413000	-0.789698000	1.687392000
H	4.752548000	-1.455654000	1.163269000
O	-1.206583000	-2.033541000	-0.739756000
C	-1.726273000	-0.857860000	-0.765041000
O	-1.177201000	0.189993000	-1.039395000
C	-3.218654000	-0.879567000	-0.387693000
O	-3.720771000	0.368611000	-0.305937000
O	-3.859337000	-1.863153000	-0.192684000
H	-0.155095000	-1.974554000	-0.802265000
H	-4.650611000	0.277077000	-0.052188000
O	-1.503990000	-0.709395000	2.004593000
H	-1.914409000	1.087180000	1.985883000
H	-1.740896000	-1.556578000	2.389828000
O	-1.974179000	1.934779000	1.509384000
H	-2.528596000	1.703115000	0.751085000
H	-0.392762000	2.013395000	0.780854000
O	1.649882000	0.870618000	-2.008609000
H	1.045296000	0.147046000	-2.214838000
H	2.499933000	0.441323000	-1.825566000

2OA.1DMA.4W-a

O	-4.465101000	-1.507236000	-0.285943000
C	-3.630897000	-0.621899000	0.235034000
O	-3.907479000	0.533269000	0.403271000
C	-2.229274000	-1.205637000	0.560016000
O	-2.024095000	-2.350974000	0.105982000
O	-1.455079000	-0.462297000	1.183217000
H	-3.958766000	-2.335286000	-0.377194000
H	-0.523467000	-2.405718000	-0.267944000
O	3.026627000	-1.719939000	-0.307163000
C	2.287603000	-0.839731000	-0.922089000
O	2.691753000	0.182633000	-1.424845000
C	0.775994000	-1.144767000	-0.918242000
O	0.010601000	-0.297034000	-1.311418000
O	0.479241000	-2.314966000	-0.433358000
H	3.930814000	-1.301406000	-0.128512000
H	-1.441832000	1.029587000	0.315103000
C	-1.964629000	2.136208000	-1.381850000
N	-1.297868000	1.989117000	-0.067604000
C	-1.779753000	2.950841000	0.946888000
H	-3.037950000	2.043096000	-1.239145000
H	-1.594110000	1.352514000	-2.037720000
H	-1.715511000	3.115576000	-1.787668000
H	-0.282652000	2.101996000	-0.221599000

H	-1.236569000	2.781771000	1.873750000
H	-2.840896000	2.770346000	1.103059000
H	-1.608012000	3.964802000	0.589891000
O	1.412647000	2.461434000	-0.798227000
H	1.734662000	3.177868000	-1.352243000
H	1.708892000	1.629463000	-1.228141000
O	5.058726000	-0.314848000	0.407692000
H	4.482799000	0.404934000	0.760268000
H	5.627160000	-0.588744000	1.132366000
O	3.181917000	1.380997000	1.395986000
H	2.480407000	0.764837000	1.676882000
H	2.764095000	1.924876000	0.714975000
O	1.241092000	-0.580617000	1.867323000
H	0.274777000	-0.619608000	1.738635000
H	1.560163000	-1.468194000	1.669782000

2OA.1DMA.4W-b

O	-0.798064000	-1.848019000	1.118351000
C	0.225455000	-1.208229000	1.445335000
O	1.399860000	-1.594820000	1.459250000
C	0.005083000	0.275092000	1.850270000
O	-1.280217000	0.567846000	2.082741000
O	0.878972000	1.094827000	1.912847000
H	-1.970578000	-0.961374000	0.296732000
H	-1.334333000	1.528946000	2.206301000
O	0.072743000	3.696733000	-0.698197000
C	-0.481927000	2.506569000	-0.618687000
O	-1.606330000	2.330563000	-0.215265000
C	0.442438000	1.342851000	-1.078917000
O	1.570271000	1.736217000	-1.483143000
O	0.000040000	0.202475000	-0.987589000
H	0.973739000	3.545098000	-1.044206000
H	2.496697000	0.603372000	-1.509518000
C	-2.771105000	-0.980992000	-1.627068000
N	-2.632780000	-0.384881000	-0.280087000
C	-3.914193000	-0.224322000	0.432154000
H	-3.208088000	-1.972563000	-1.530241000
H	-1.780985000	-1.064985000	-2.064217000
H	-3.412635000	-0.341014000	-2.231206000
H	-2.156632000	0.529480000	-0.356101000
H	-3.717425000	0.200537000	1.412569000
H	-4.384376000	-1.199881000	0.541204000
H	-4.561714000	0.436561000	-0.141485000
O	3.169343000	-0.170443000	-1.325257000

H	3.415944000	-0.041369000	-0.339033000
H	2.668463000	-1.076805000	-1.353247000
O	2.052438000	-2.413264000	-1.111221000
H	1.163580000	-2.561722000	-1.479503000
H	1.887551000	-2.391861000	-0.148866000
O	3.503535000	0.110449000	1.184450000
H	2.781470000	-0.490937000	1.474246000
H	3.169039000	0.977313000	1.442582000
O	-0.634621000	-3.236338000	-1.211528000
H	-0.667991000	-2.905994000	-0.289719000
H	-0.590542000	-4.194263000	-1.147719000

2OA.1DMA.4W-c

O	-1.815988000	-0.879946000	1.384590000
C	-0.606786000	-0.650790000	1.335982000
O	-0.019498000	0.447222000	1.193233000
C	0.316109000	-1.900177000	1.429415000
O	1.618518000	-1.577155000	1.385785000
O	-0.079863000	-3.026367000	1.500094000
H	-1.608049000	-3.106535000	0.041733000
H	2.111896000	-2.409646000	1.334069000
O	2.248681000	-0.652311000	-1.627114000
C	1.071811000	-0.915455000	-1.639145000
O	0.615096000	-2.131903000	-1.528717000
C	0.049360000	0.247341000	-1.748013000
O	-1.187458000	-0.139533000	-1.820565000
O	0.447257000	1.388190000	-1.731841000
H	2.247266000	1.232902000	-0.717101000
H	-1.820391000	0.700709000	-1.712154000
C	3.669909000	0.852012000	0.737348000
N	2.357789000	1.363881000	0.297671000
C	2.093777000	2.777009000	0.651616000
H	3.787345000	-0.155419000	0.347562000
H	3.699360000	0.846404000	1.824979000
H	4.453674000	1.498631000	0.346829000
H	1.583220000	0.789227000	0.705243000
H	1.115529000	3.055110000	0.265083000
H	2.869591000	3.403157000	0.214888000
H	2.100693000	2.872705000	1.735756000
O	-2.603058000	1.847765000	-1.379614000
H	-3.190671000	1.603549000	-0.638260000
H	-1.961979000	2.441126000	-0.941033000
O	-1.800871000	-2.757607000	-0.841927000
H	-2.280233000	-1.940090000	-0.659893000

H	-0.381566000	-2.239611000	-1.414074000
O	-3.544404000	1.194218000	1.132134000
H	-2.932837000	0.438643000	1.295816000
H	-4.384611000	0.954102000	1.530150000
O	-1.202146000	2.918132000	0.775054000
H	-0.845351000	2.030622000	0.975674000
H	-2.042617000	2.931966000	1.248912000

2OA.1DMA.4W-d

O	1.642289000	0.576790000	0.093299000
C	1.985919000	-0.390709000	-0.602445000
O	1.409198000	-0.880185000	-1.597552000
C	3.247962000	-1.135326000	-0.145401000
O	4.345360000	-0.383822000	-0.220372000
O	3.243224000	-2.263477000	0.271148000
H	-0.159020000	-0.607089000	1.299293000
H	5.089015000	-0.920039000	0.094247000
O	-3.683208000	-0.850387000	0.148553000
C	-2.912311000	-0.039403000	-0.536637000
O	-3.131564000	1.137105000	-0.664108000
C	-1.673584000	-0.719703000	-1.154317000
O	-0.839140000	0.118294000	-1.681598000
O	-1.558534000	-1.922723000	-1.081202000
H	-3.232313000	-1.711563000	0.276950000
H	0.126960000	-0.326927000	-1.762934000
C	-1.021362000	3.120410000	1.213548000
N	-0.594986000	2.382935000	0.003732000
C	0.057491000	3.226149000	-1.021509000
H	-1.458014000	2.402139000	1.902026000
H	-1.758854000	3.865737000	0.921158000
H	-0.143287000	3.586441000	1.653043000
H	-1.413197000	1.913079000	-0.410069000
H	0.332551000	2.588148000	-1.858052000
H	0.942709000	3.676602000	-0.578923000
H	-0.646318000	3.989486000	-1.348349000
O	-0.940306000	-0.056265000	1.463929000
H	-1.553754000	-0.667712000	1.895774000
H	0.053783000	1.619885000	0.254960000
O	2.166762000	2.964108000	1.326167000
H	2.887052000	3.129417000	1.937979000
H	2.279685000	2.052074000	1.011880000
O	-2.187881000	-2.640223000	1.720968000
H	-1.292387000	-2.891858000	1.431211000
H	-2.483839000	-3.319125000	2.331934000

O	0.409904000	-2.565772000	0.712056000
H	1.352769000	-2.785648000	0.686292000
H	0.127848000	-2.509656000	-0.214263000

2OA.1DMA.4W-e

O	3.751891000	1.028998000	1.445672000
C	2.992986000	0.153459000	0.814580000
O	3.437594000	-0.699756000	0.091546000
C	1.474481000	0.348689000	1.085152000
O	1.191483000	1.404206000	1.684520000
O	0.711144000	-0.530086000	0.651527000
H	3.130252000	1.617941000	1.915118000
H	-0.738316000	1.213941000	1.826281000
O	-0.529587000	-0.735912000	-2.079277000
C	-0.915445000	0.433973000	-1.666089000
O	-2.076165000	0.744055000	-1.547669000
C	0.205919000	1.429749000	-1.326137000
O	-0.252352000	2.414332000	-0.566207000
O	1.334567000	1.305622000	-1.703699000
H	0.468920000	-0.916570000	-2.015448000
H	0.511040000	2.882606000	-0.191621000
C	-1.706492000	-2.220299000	1.967251000
N	-1.935765000	-1.505140000	0.692350000
C	-3.308052000	-1.656664000	0.168187000
H	-0.688931000	-2.010844000	2.287128000
H	-1.836013000	-3.288058000	1.805834000
H	-2.412925000	-1.842327000	2.703447000
H	-1.244485000	-1.856354000	0.014641000
H	-3.377314000	-1.133386000	-0.782007000
H	-4.001581000	-1.218741000	0.884084000
H	-3.524839000	-2.715728000	0.039323000
O	1.886839000	-1.593519000	-1.976337000
H	2.426021000	-1.289535000	-2.713545000
H	2.370315000	-1.296397000	-1.172216000
O	0.255665000	-3.115283000	-0.125043000
H	0.760135000	-2.352414000	0.207044000
H	0.655364000	-3.299021000	-0.981769000
O	-1.671656000	0.935631000	1.808829000
H	-2.178258000	1.660077000	1.401378000
H	-1.736687000	-0.492606000	0.894493000
O	-3.239324000	2.617856000	0.218093000
H	-2.831652000	2.176366000	-0.544345000
H	-3.061853000	3.554418000	0.102428000

2OA.1DMA.4W-f

O	0.102859000	1.359531000	-2.581299000
C	0.996780000	0.478177000	-2.173038000
O	2.170252000	0.706450000	-2.089902000
C	0.365066000	-0.876921000	-1.787503000
O	1.213943000	-1.698138000	-1.241192000
O	-0.810472000	-1.056109000	-1.985320000
H	-0.778146000	0.953964000	-2.475554000
H	0.694015000	-2.418602000	-0.690294000
O	-3.725127000	-0.395296000	0.618674000
C	-2.512806000	-0.879355000	0.701940000
O	-2.315918000	-2.058940000	0.875028000
C	-1.312014000	0.105081000	0.567606000
O	-0.221102000	-0.337087000	0.960099000
O	-1.536732000	1.224771000	0.052315000
H	-3.766507000	0.583170000	0.490835000
H	1.686603000	0.429161000	0.773728000
C	3.677027000	0.949455000	0.824711000
N	2.597642000	-0.047111000	0.669130000
C	2.657965000	-1.164965000	1.638652000
H	3.580637000	1.392157000	1.813015000
H	3.551943000	1.704721000	0.053576000
H	4.638046000	0.450168000	0.716204000
H	2.593941000	-0.416809000	-0.287086000
H	1.807003000	-1.818799000	1.460790000
H	2.605032000	-0.740644000	2.638380000
H	3.594218000	-1.701541000	1.495736000
O	-0.002902000	-3.234831000	0.287933000
H	-0.394562000	-4.042340000	-0.059558000
H	-0.769214000	-2.695225000	0.617888000
O	-4.011142000	2.278141000	0.301947000
H	-4.510116000	2.613948000	-0.446599000
H	-3.071057000	2.312676000	0.060838000
O	1.248859000	1.359307000	2.848554000
H	0.516387000	0.768544000	2.626715000
H	1.127062000	2.103181000	2.242630000
O	0.931240000	2.380449000	0.217293000
H	1.123637000	2.892030000	-0.574126000
H	0.005419000	2.065196000	0.111730000

2OA.1DMA.4W-g

O	0.600635000	-2.447604000	1.399035000
C	-0.105550000	-1.358431000	1.599922000
O	-1.306281000	-1.288122000	1.636183000

C	0.803998000	-0.126116000	1.734243000
O	0.115463000	0.996649000	1.642938000
O	1.994408000	-0.214179000	1.836949000
H	0.032102000	-3.111442000	0.961133000
H	0.775799000	1.734420000	1.454535000
O	0.697369000	1.409832000	-1.352633000
C	0.873824000	0.182540000	-1.274902000
O	0.006354000	-0.708338000	-1.209379000
C	2.359507000	-0.255135000	-1.170439000
O	2.519243000	-1.575178000	-1.294197000
O	3.255157000	0.514746000	-0.972206000
H	-2.135395000	-0.193891000	-0.325962000
H	3.455872000	-1.765123000	-1.139139000
C	-2.525957000	1.308329000	-1.654437000
N	-2.152634000	0.838864000	-0.303463000
C	-3.063520000	1.297644000	0.763663000
H	-1.764906000	0.959393000	-2.347786000
H	-2.565984000	2.395219000	-1.645834000
H	-3.496161000	0.883142000	-1.904571000
H	-1.200984000	1.152168000	-0.086525000
H	-2.695764000	0.906731000	1.709050000
H	-4.061028000	0.914633000	0.554466000
H	-3.056546000	2.385079000	0.771127000
O	-0.572157000	-3.284865000	-0.909754000
H	-0.128999000	-2.437168000	-1.144162000
H	-0.218035000	-3.956076000	-1.498509000
O	-3.022998000	-1.854369000	-0.546128000
H	-2.941676000	-2.061769000	0.392729000
H	-2.334771000	-2.412922000	-0.942299000
O	1.943925000	2.651698000	0.774348000
H	1.904519000	2.292118000	-0.134117000
H	2.779751000	2.317973000	1.122106000
O	-0.836789000	3.423273000	-0.166061000
H	-0.258931000	2.940027000	-0.777353000
H	-0.228873000	3.904108000	0.404298000

