

Supplemental information

Experiment-Theory Hybrid Method for Studying Atmospheric New Particle Formation Mechanism

Yi-Rong Liu,^{*‡a} Shuai Jiang,^{‡a} Teng Huang,^b Fan Zhang^a

^aSchool of Information Science and Technology, University of Science and Technology of China, Hefei, Anhui 230026, China

^bLaboratory of Atmospheric Physico-Chemistry, Anhui Institute of Optics & Fine Mechanics, Chinese Academy of Sciences, Hefei, Anhui 230031, China

[‡]The two authors contributed equally to this work

^{*}Corresponding authors

E-mail: yrliu@ustc.edu.cn

Cluster concentration and formation rate simulation

The Atmospheric Cluster Dynamic Code (ACDC) is a general model for the simulation of the concentration and formation rate of cluster molecules without empirical parameters.¹ Input parameters come from quantum chemical calculations or experimental/field measurements. For example, the evaporation rate calculation for Gibbs free energy comes from ab initio calculations, while the monomer concentration, temperature, and condensation sink (CS) coefficients come from experimental/field measurements. To compare with the experimental or field measurements of the nucleation cluster concentration and formation rate at 1.7 nm, we extended the simulation box to eight sulfuric acid molecules-eight dimethylamine ((SA)₈(DMA)₈, the maximum size of the SA-DMA system)) and tetrasulfuric acid-tetramalic acid-tetradimethylamine ((SA)₄(MA)₄(DMA)₄, the maximum size of the SA-MA-DMA system). The boxes of these two sizes can reach 1.7 nm, which can give the nucleation rate of the critical nucleus size, which is exactly the size of the nucleation cluster that can be observed in experiments or field measurements. In this way, we give a perfect one-to-one correspondence between the experimental and theoretical results, and thus provide a very powerful tool and method for atmospheric nucleation.

For comparison with experimental data, all parameters including temperature, monomer concentration and condensation sink (CS) are the same as CLOUD measurements and field observations. To reduce the computational cost, the simulation box of the SA-DMA system does not contain some clusters with extremely high evaporation rates. In addition, clusters larger than 1.7 nm are not included in the simulation box. For the SA-MA-DMA system, all clusters with up to four sulfuric acid molecules, four malic acid molecules, and four dimethylamine molecules were simulated except for some clusters with high evaporation rates and sizes greater than 1.7 nm.

Previous studies have shown that the SA-DMA system has a strong acid-base mechanism², so the influence of water molecules on the formation rate and concentration of simulated SA-DMA clusters is relatively small. Therefore, water molecules are not considered in the model. The simulated cluster concentration labelled from N1 (monomer) to N8 (octamer) refers to the number of sulfuric acid molecules with different dimethylamine contents in the cluster, which can be directly compared with the CLOUD measurement and field observation results. The rate

of formation of dimer (N2) is simulated by considering condensation and evaporation outside the dimer "box".

Boundary conditions are very important for ACDC simulation. This requires that the cluster leaving the simulation framework be stable enough to grow. For the binary system of $(SA)_n(DMA)_m$ ($n=1-8$ and $m=1-8$), the most stable clusters have roughly the same number of acids as base molecules or one or two more because these clusters have a high concentration and low evaporation rate. Therefore, assuming that $(SA)_9(DMA)_9$ and $(SA)_9(DMA)_8$ are stable enough to leave the simulation box, other clusters with high evaporation rates are brought back to the simulation box by monomer evaporation, and this boundary condition is consistent with the previous study.³ For the $(SA)_n(MA)_m(DMA)_k$ ($n=1-4$, $m=1-4$ and $k=1-4$) ternary system, the main growth path is the SA-MA-DMA ternary system and pure MA system judged based on cluster stability. We consider clusters with evaporation rate lower than $10^{-2} s^{-1}$ to be stable, and these low evaporation rate cluster information is displayed in Fig. S4. The $(SA)_4(DMA)_4$, $(SA)_4(MA)_4$ and $(MA)_4(DMA)_4$ binary systems are not large enough to leave the simulation box. Therefore, only the SA-MA-DMA ternary system needs to be considered. The boundary conditions of the SA-DMA and SA-MA-DMA system simulation frames can be expressed as:

Two bodies: $(SA)_a(DMA)_c$ with $a=9-16$ and $c=8-16$ and $|a-c|=0$ or 1

Three bodies: $(SA)_a(MA)_b(DMA)_c$ with $a=b$ and $a+b=c$ and $c>4$

Supplementary figures

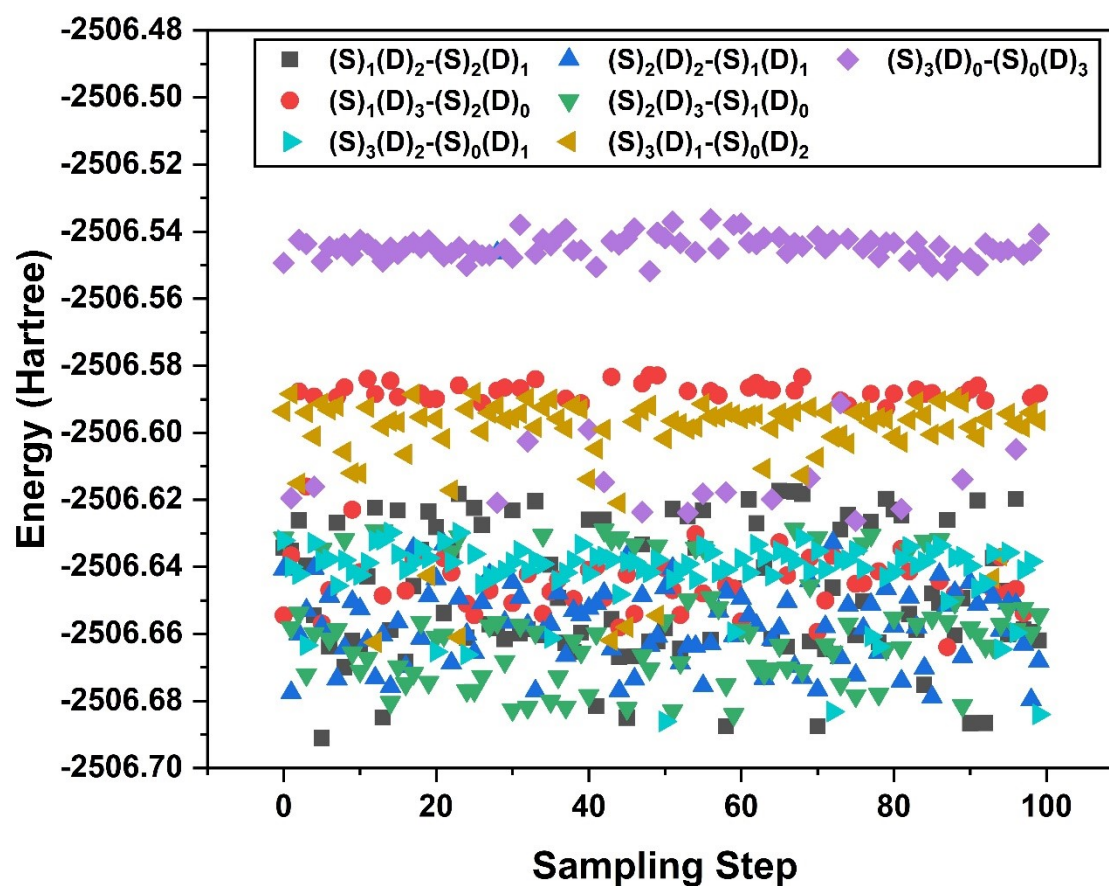


Fig. S1 The energy distribution of products produced by different collision reactions for the $(SA)_i(DMA)_j + (SA)_m(DMA)_n \rightarrow (SA)_3(DMA)_3$ ($i+m=3, j+n=3$) system. The S represents the sulfuric acid molecule, and D represents the dimethylamine molecule.

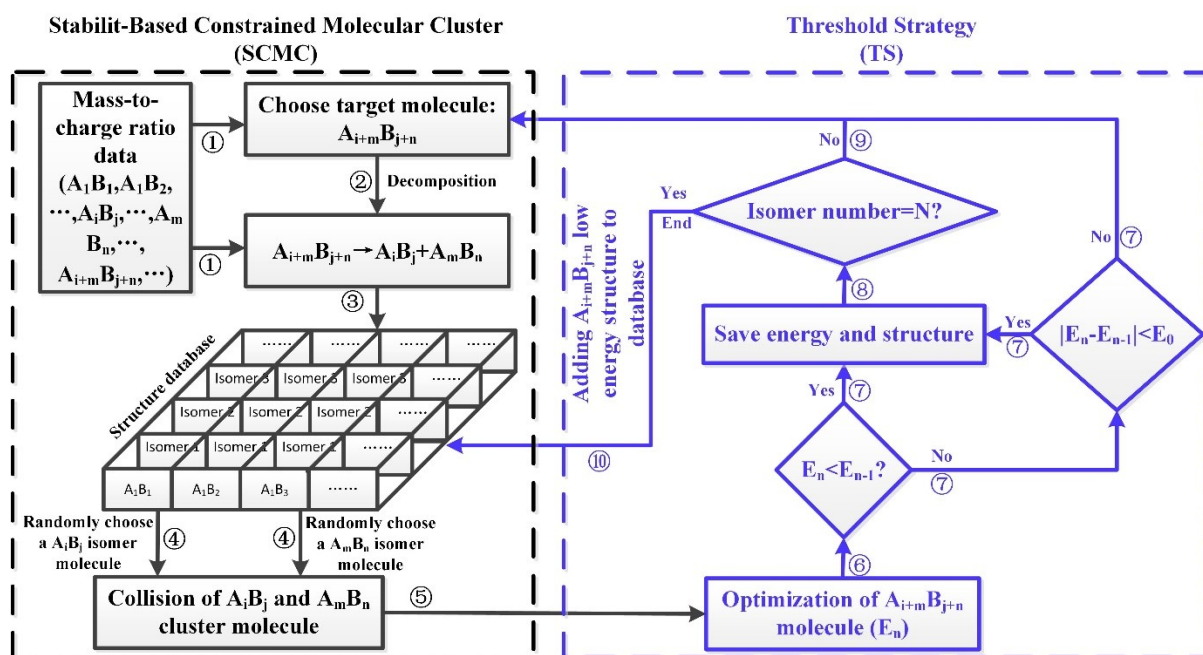


Fig. S2 Flow chart of the Stability-based Constrained Molecular Cluster (SCMC) model for the nucleation system. As shown in the figure on the left (black dotted line), the target molecule is selected through the mass spectrum database, and then the target molecule is decomposed into two small molecules. These two small molecules can also be found in the mass spectrometry database, and then they are randomly selected from the structural database. The right side of the figure (blue dotted line) shows the threshold strategy, which represents a constraint that the new structure is rejected or accepted by a threshold. E_n and E_{n-1} represent the energy of this cycle and last cycle, respectively; E_0 represents the empirical threshold, which is set from 0.2 to 0.5 Hartree; the total isomer value (N) is typically set to 1000.

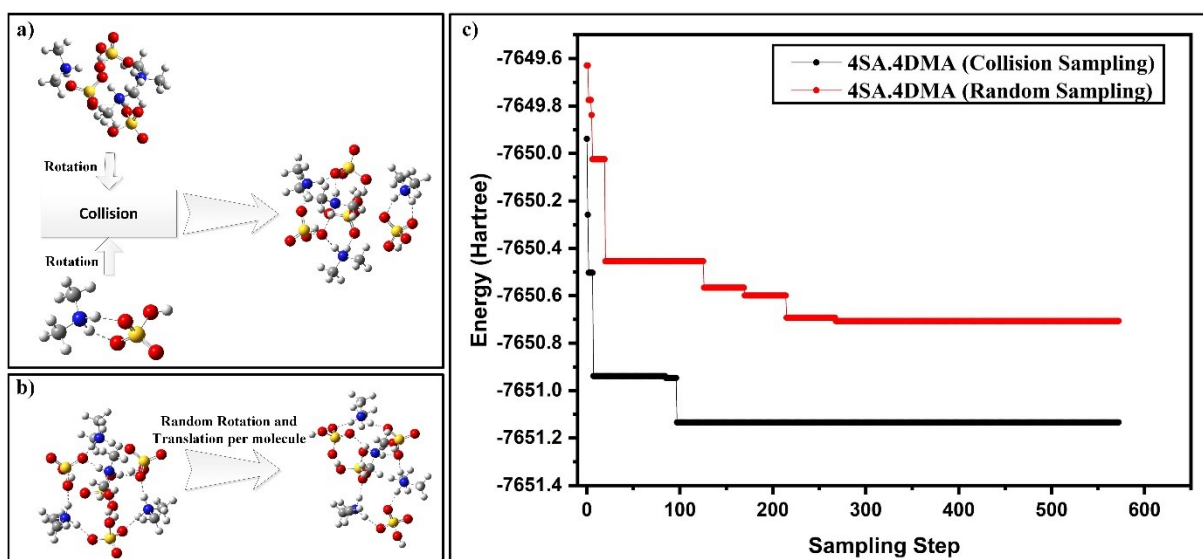


Fig. S3 Collision sampling based on experimental data ($3\text{SA.3DMA} + 1\text{SA.1DMA} \rightarrow 4\text{SA.4DMA}$, upper left) and random sampling (randomly moving each molecule when sampling, under left) for the 4SA.4DMA system, and the cluster energy convergence comparison between the two sampling techniques (right). The test is based on the taboo accept strategy that only lower energy structure accepted when compared with the previous save structure.

Tables

Table S1. The temperatures (T , K) and concentrations of DMA (molecules cm^{-3}) in the studied cities.

Cities	Month	DMA concentration (cm^{-3})	T (K)
Shanghai	1	1.44×10^8	275
	2	1.50×10^8	277
	3	1.33×10^8	282
	4	2.35×10^8	288
	5	1.24×10^8	294
	6	3.21×10^8	298
	7	1.40×10^8	301
	8	2.18×10^8	301
	9	1.40×10^8	296
	10	2.08×10^8	291
	11	1.78×10^8	284
	12	3.57×10^8	278
Beijing	1	4.68×10^8	265
	2	4.31×10^8	269
	3	3.74×10^8	275
	4	3.13×10^8	284
	5	2.12×10^8	291
	6	2.22×10^8	296
	7	1.55×10^8	298
	8	2.56×10^8	296
	9	3.00×10^8	291
	10	3.63×10^8	283
	11	7.60×10^8	274
	12	5.18×10^8	267

Table S2. The Gibbs free energies (ΔG) of formation from monomers at 254 K, 262 K and 278 K for all clusters used in ACDC simulations. The SA and DMA represent the sulfuric acid and dimethylamine in the cluster, respectively.

Cluster	$\Delta G_{254\text{ K}}$ (kcal/mol)	$\Delta G_{262\text{ K}}$ (kcal/mol)	$\Delta G_{278\text{ K}}$ (kcal/mol)
(SA) ₁ (DMA) ₁	-13.73	-13.48	-12.98
(SA) ₁ (DMA) ₂	-21.04	-20.53	-19.49
(SA) ₁ (DMA) ₃	-26.60	-25.76	-24.08
(SA) ₁ (DMA) ₄	-29.52	-28.33	-25.96
(SA) ₁ (DMA) ₅	-30.81	-29.43	-26.68
(SA) ₁ (DMA) ₆	-27.09	-25.46	-22.21
(SA) ₁ (DMA) ₇	-31.21	-29.35	-25.63
(SA) ₁ (DMA) ₈	-31.04	-28.93	-24.71
(DMA) ₂	2.31	2.53	2.96
(SA) ₂	-8.64	-8.34	-7.74
(SA) ₂ (DMA) ₁	-35.00	-34.41	-33.21
(SA) ₂ (DMA) ₂	-53.21	-52.31	-50.52
(SA) ₂ (DMA) ₃	-61.79	-60.54	-58.04
(SA) ₂ (DMA) ₄	-67.49	-65.96	-62.90
(SA) ₂ (DMA) ₅	-66.81	-64.97	-61.29
(SA) ₂ (DMA) ₆	-67.09	-65.07	-61.04
(SA) ₂ (DMA) ₇	-62.08	-59.84	-55.34
(SA) ₂ (DMA) ₈	-61.18	-58.65	-53.59
(DMA) ₃	1.91	2.38	3.33
(SA) ₃	-17.14	-16.54	-15.32
(SA) ₃ (DMA) ₁	-48.52	-47.62	-45.81
(SA) ₃ (DMA) ₂	-67.57	-66.35	-63.91
(SA) ₃ (DMA) ₃	-90.16	-88.57	-85.37
(SA) ₃ (DMA) ₄	-102.69	-100.82	-97.08
(SA) ₃ (DMA) ₅	-94.51	-92.38	-88.12
(SA) ₃ (DMA) ₆	-95.49	-93.13	-88.42
(SA) ₃ (DMA) ₇	-91.59	-89.10	-84.12
(SA) ₃ (DMA) ₈	-91.51	-88.77	-83.31
(DMA) ₄	1.62	2.35	3.81
(SA) ₄	-25.23	-24.29	-22.41
(SA) ₄ (DMA) ₁	-58.82	-57.59	-55.14
(SA) ₄ (DMA) ₂	-83.89	-82.38	-79.36
(SA) ₄ (DMA) ₃	-107.16	-105.28	-101.54
(SA) ₄ (DMA) ₄	-124.34	-122.14	-116.09
(SA) ₄ (DMA) ₅	-133.34	-130.86	-125.92
(SA) ₄ (DMA) ₆	-132.01	-129.24	-123.71

(SA) ₄ (DMA) ₇	-133.94	-130.99	-125.09
(SA) ₄ (DMA) ₈	-132.46	-129.24	-122.79
(DMA) ₅	2.65	3.63	5.59
(SA) ₅	-35.28	-34.02	-31.51
(SA) ₅ (DMA) ₁	-66.72	-65.13	-61.98
(SA) ₅ (DMA) ₂	-96.34	-94.49	-90.79
(SA) ₅ (DMA) ₃	-118.38	-116.22	-111.88
(SA) ₅ (DMA) ₄	-140.98	-138.53	-133.65
(SA) ₅ (DMA) ₅	-160.22	-157.47	-151.97
(SA) ₅ (DMA) ₆	-162.19	-159.16	-153.10
(SA) ₅ (DMA) ₇	-164.49	-161.26	-154.78
(SA) ₅ (DMA) ₈	-164.87	-161.38	-154.40
(DMA) ₆	4.53	5.77	8.25
(SA) ₆	-47.29	-45.71	-42.54
(SA) ₆ (DMA) ₁	-77.89	-76.03	-72.32
(SA) ₆ (DMA) ₂	-104.82	-102.61	-98.19
(SA) ₆ (DMA) ₃	-133.97	-131.46	-126.45
(SA) ₆ (DMA) ₄	-155.08	-152.28	-146.67
(SA) ₆ (DMA) ₅	-174.69	-171.57	-165.34
(SA) ₆ (DMA) ₆	-193.58	-190.15	-183.28
(SA) ₆ (DMA) ₇	-195.66	-192.03	-184.77
(SA) ₆ (DMA) ₈	-197.24	-193.29	-185.39
(DMA) ₇	5.262	6.73	9.67
(SA) ₇	-54.33	-52.42	-48.58
(SA) ₇ (DMA) ₁	-85.85	-83.61	-79.14
(SA) ₇ (DMA) ₂	-116.88	-114.40	-109.43
(SA) ₇ (DMA) ₃	-148.99	-146.17	-140.52
(SA) ₇ (DMA) ₄	-171.67	-168.53	-162.27
(SA) ₇ (DMA) ₅	-191.28	-187.95	-181.29
(SA) ₇ (DMA) ₆	-206.77	-203.11	-195.79
(SA) ₇ (DMA) ₇	-228.79	-224.70	-216.52
(SA) ₇ (DMA) ₈	-227.19	-222.89	-214.28
(DMA) ₈	7.22	8.95	12.41
(SA) ₈	-59.31	-57.17	-52.91
(SA) ₈ (DMA) ₁	-98.45	-95.91	-90.83
(SA) ₈ (DMA) ₂	-126.03	-123.19	-117.51
(SA) ₈ (DMA) ₃	-155.11	-151.97	-145.69
(SA) ₈ (DMA) ₄	-186.29	-182.87	-176.03
(SA) ₈ (DMA) ₅	-205.93	-202.21	-194.77
(SA) ₈ (DMA) ₆	-224.67	-220.58	-212.41
(SA) ₈ (DMA) ₇	-242.19	-237.81	-229.03
(SA) ₈ (DMA) ₈	-261.21	-256.52	-247.17

Table S3. Gibbs free energies (ΔG) of formation from monomers at 276 K and 278 K for all clusters used in ACDC simulations. SA, MA and DMA represent sulfuric acid, malic acid and dimethylamine in the cluster, respectively.

Cluster	$\Delta G_{276\text{ K}}$ (kcal/mol)	$\Delta G_{278\text{ K}}$ (kcal/mol)
(MA) ₁ .(DMA) ₁	-5.98	-5.91
(MA) ₁ .(DMA) ₂	-10.56	-10.42
(MA) ₁ .(DMA) ₃	-10.11	-9.91
(MA) ₁ .(DMA) ₄	-9.72	-9.45
(SA) ₁ .(DMA) ₁	-13.05	-12.98
(SA) ₁ .(MA) ₁	-10.68	-10.60
(SA) ₁ .(MA) ₁ .(DMA) ₁	-24.03	-23.87
(SA) ₁ .(MA) ₁ .(DMA) ₂	-38.42	-38.17
(SA) ₁ .(MA) ₁ .(DMA) ₃	-47.38	-47.05
(SA) ₁ .(MA) ₁ .(DMA) ₄	-49.84	-49.42
(SA) ₁ .(DMA) ₂	-19.62	-19.49
(SA) ₁ .(MA) ₂	-18.47	-18.28
(SA) ₁ .(MA) ₂ .(DMA) ₁	-41.85	-41.58
(SA) ₁ .(MA) ₂ .(DMA) ₂	-44.57	-44.24
(SA) ₁ .(MA) ₂ .(DMA) ₃	-42.71	-42.31
(SA) ₁ .(MA) ₂ .(DMA) ₄	-42.17	-41.69
(SA) ₁ .(DMA) ₃	-24.29	-24.08
(SA) ₁ .(MA) ₃	-29.61	-29.33
(SA) ₁ .(MA) ₃ .(DMA) ₁	-47.26	-46.91
(SA) ₁ .(MA) ₃ .(DMA) ₂	-59.96	-59.53
(SA) ₁ .(MA) ₃ .(DMA) ₃	-60.47	-59.98
(SA) ₁ .(MA) ₃ .(DMA) ₄	-55.25	-54.68
(SA) ₁ .(DMA) ₄	-26.26	-25.96
(SA) ₁ .(MA) ₄	-33.16	-32.79
(SA) ₁ .(MA) ₄ .(DMA) ₁	-56.69	-56.24
(SA) ₁ .(MA) ₄ .(DMA) ₂	-68.85	-68.31
(SA) ₁ .(MA) ₄ .(DMA) ₃	-78.55	-77.94
(SA) ₁ .(MA) ₄ .(DMA) ₄	-77.71	-77.03
(DMA) ₂	2.91	2.96
(MA) ₂	-8.88	-8.77
(MA) ₂ .(DMA) ₁	-18.63	-18.45
(MA) ₂ .(DMA) ₂	-27.41	-27.14
(MA) ₂ .(DMA) ₃	-25.63	-25.29
(MA) ₂ .(DMA) ₄	-24.89	-24.51
(SA) ₂	-7.82	-7.74
(SA) ₂ .(DMA) ₁	-33.36	-33.22

(SA) ₂ .(MA) ₁	-18.88	-18.71
(SA) ₂ .(MA) ₁ .(DMA) ₁	-41.25	-40.99
(SA) ₂ .(MA) ₁ .(DMA) ₂	-62.08	-61.76
(SA) ₂ .(MA) ₁ .(DMA) ₃	-66.28	-65.88
(SA) ₂ .(MA) ₁ .(DMA) ₄	-69.55	-69.08
(SA) ₂ .(DMA) ₂	-50.74	-50.52
(SA) ₂ .(MA) ₂	-33.21	-32.94
(SA) ₂ .(MA) ₂ .(DMA) ₁	-50.97	-50.63
(SA) ₂ .(MA) ₂ .(DMA) ₂	-75.15	-74.72
(SA) ₂ .(MA) ₂ .(DMA) ₃	-83.33	-82.82
(SA) ₂ .(MA) ₂ .(DMA) ₄	-99.25	-98.66
(SA) ₂ .(DMA) ₃	-58.35	-58.04
(SA) ₂ .(MA) ₃	-41.73	-41.37
(SA) ₂ .(MA) ₃ .(DMA) ₁	-56.53	-56.11
(SA) ₂ .(MA) ₃ .(DMA) ₂	-78.17	-77.65
(SA) ₂ .(MA) ₃ .(DMA) ₃	-88.59	-88.02
(SA) ₂ .(MA) ₃ .(DMA) ₄	-95.89	-95.22
(SA) ₂ .(DMA) ₄	-63.28	-62.91
(SA) ₂ .(MA) ₄	-44.93	-44.47
(SA) ₂ .(MA) ₄ .(DMA) ₁	-67.25	-66.72
(SA) ₂ .(MA) ₄ .(DMA) ₂	-87.65	-87.03
(SA) ₂ .(MA) ₄ .(DMA) ₃	-97.71	-97.01
(SA) ₂ .(MA) ₄ .(DMA) ₄	-99.47	-98.68
(DMA) ₃	3.22	3.34
(MA) ₃	-22.87	-22.67
(MA) ₃ .(DMA) ₁	-27.15	-26.87
(MA) ₃ .(DMA) ₂	-29.75	-29.41
(MA) ₃ .(DMA) ₃	-27.25	-26.84
(MA) ₃ .(DMA) ₄	-32.22	-31.72
(SA) ₃	-15.48	-15.33
(SA) ₃ .(DMA) ₁	-46.04	-45.81
(SA) ₃ .(MA) ₁	-25.67	-25.42
(SA) ₃ .(MA) ₁ .(DMA) ₁	-53.35	-53.02
(SA) ₃ .(MA) ₁ .(DMA) ₂	-70.34	-69.93
(SA) ₃ .(MA) ₁ .(DMA) ₃	-88.19	-87.71
(SA) ₃ .(MA) ₁ .(DMA) ₄	-94.92	-94.36
(SA) ₃ .(DMA) ₂	-64.21	-63.91
(SA) ₃ .(MA) ₂	-33.13	-32.78
(SA) ₃ .(MA) ₂ .(DMA) ₁	-63.53	-63.11
(SA) ₃ .(MA) ₂ .(DMA) ₂	-82.82	-82.33
(SA) ₃ .(MA) ₂ .(DMA) ₃	-100.72	-100.13
(SA) ₃ .(MA) ₂ .(DMA) ₄	-115.12	-114.45
(SA) ₃ .(DMA) ₃	-85.77	-85.37

(SA) ₃ .(MA) ₃	-44.56	-44.13
(SA) ₃ .(MA) ₃ .(DMA) ₁	-65.72	-65.18
(SA) ₃ .(MA) ₃ .(DMA) ₂	-86.92	-86.31
(SA) ₃ .(MA) ₃ .(DMA) ₃	-102.34	-101.69
(SA) ₃ .(MA) ₃ .(DMA) ₄	-104.86	-104.11
(SA) ₃ .(DMA) ₄	-97.54	-97.07
(SA) ₃ .(MA) ₄	-55.88	-55.33
(SA) ₃ .(MA) ₄ .(DMA) ₁	-76.93	-76.31
(SA) ₃ .(MA) ₄ .(DMA) ₂	-96.95	-96.25
(SA) ₃ .(MA) ₄ .(DMA) ₃	-115.25	-114.48
(SA) ₃ .(MA) ₄ .(DMA) ₄	-113.53	-112.68
(DMA) ₄	3.63	3.81
(MA) ₄	-25.62	-25.34
(MA) ₄ .(DMA) ₁	-32.18	-31.82
(MA) ₄ .(DMA) ₂	-36.45	-36.01
(MA) ₄ .(DMA) ₃	-41.73	-41.21
(MA) ₄ .(DMA) ₄	-41.41	-40.82
(SA) ₄	-22.64	-22.41
(SA) ₄ .(DMA) ₁	-55.45	-55.14
(SA) ₄ .(MA) ₁	-34.09	-33.76
(SA) ₄ .(MA) ₁ .(DMA) ₁	-65.63	-65.21
(SA) ₄ .(MA) ₁ .(DMA) ₂	-89.78	-89.31
(SA) ₄ .(MA) ₁ .(DMA) ₃	-108.35	-107.79
(SA) ₄ .(MA) ₁ .(DMA) ₄	-116.96	-116.31
(SA) ₄ .(DMA) ₂	-79.74	-79.36
(SA) ₄ .(MA) ₂	-41.73	-41.28
(SA) ₄ .(MA) ₂ .(DMA) ₁	-70.88	-70.38
(SA) ₄ .(MA) ₂ .(DMA) ₂	-95.08	-94.51
(SA) ₄ .(MA) ₂ .(DMA) ₃	-116.24	-115.59
(SA) ₄ .(MA) ₂ .(DMA) ₄	-120.91	-120.19
(SA) ₄ .(DMA) ₃	-102.01	-101.54
(SA) ₄ .(MA) ₃	-51.14	-50.63
(SA) ₄ .(MA) ₃ .(DMA) ₁	-79.44	-78.84
(SA) ₄ .(MA) ₃ .(DMA) ₂	-97.23	-96.55
(SA) ₄ .(MA) ₃ .(DMA) ₃	-113.19	-112.44
(SA) ₄ .(MA) ₃ .(DMA) ₄	-148.96	-148.12
(SA) ₄ .(DMA) ₄	-118.28	-117.73
(SA) ₄ .(MA) ₄	-64.64	-64.02
(SA) ₄ .(MA) ₄ .(DMA) ₁	-89.05	-88.35
(SA) ₄ .(MA) ₄ .(DMA) ₂	-111.86	-111.07
(SA) ₄ .(MA) ₄ .(DMA) ₃	-138.98	-138.12
(SA) ₄ .(MA) ₄ .(DMA) ₄	-142.18	-141.25

Table S4. Low evaporation rate cluster information for SA-MA-DMA system at 276 K. SA, MA and DMA represent sulfuric acid, malic acid and dimethylamine in the cluster, respectively

Cluster	Evaporation rate (s ⁻¹)
(SA) ₃ (DMA) ₃	2.16×10 ⁻⁷
(SA) ₂ (DMA) ₁	8.64×10 ⁻⁷
(SA) ₁ (MA) ₂ (DMA) ₁	9.62×10 ⁻⁵
(SA) ₂ (DMA) ₂	2.76×10 ⁻⁴
(SA) ₄ (DMA) ₃	2.05×10 ⁻³
(SA) ₄ (DMA) ₄	3.52×10 ⁻³
(SA) ₂ (MA) ₂ (DMA) ₄	5.74×10 ⁻³
(SA) ₁ (MA) ₁ (DMA) ₂	6.95×10 ⁻²
(MA) ₃	9.50×10 ⁻²

Coordinate information for SA-DMA system

1DMA

C	-1.215409	-0.222460	0.020279
N	-0.000001	0.563873	-0.148568
C	1.215399	-0.222459	0.020275
H	-1.281702	-0.967127	-0.779310
H	-2.089737	0.427627	-0.062971
H	-1.276324	-0.763900	0.982026
H	-0.000006	1.329153	0.517117
H	1.282043	-0.966764	-0.779628
H	1.276085	-0.764314	0.981807
H	2.089706	0.427733	-0.062391

1SA

S	0.000000	0.000000	0.165250
O	0.000000	1.262810	0.826070
O	0.000000	-1.262810	0.826070
O	1.247360	-0.047260	-0.851640
O	-1.247360	0.047260	-0.851640
H	-1.456140	-0.860950	-1.117450
H	1.456140	0.860950	-1.117450

1SA1DMA

S	-1.285695	-0.159856	0.012831
O	-2.469759	-0.978144	-0.010158
O	-0.456470	-0.216358	1.230023
O	-0.439366	-0.260000	-1.202805
O	-1.798478	1.405750	0.038194
H	1.159509	-0.130108	-0.760661
H	-2.597751	1.440414	-0.504032
C	2.856127	-1.140608	-0.007352
N	1.882379	-0.026852	0.007616
C	2.459777	1.337215	-0.016000
H	2.305239	-2.079844	0.010481
H	3.502744	-1.077887	0.868351
H	3.459671	-1.087947	-0.913816
H	1.202156	-0.116481	0.805054
H	1.639083	2.052892	-0.000362
H	3.047537	1.470524	-0.924437
H	3.093436	1.484477	0.858901

1SA2DMA

C	2.927949	-1.496911	1.086988
N	3.032429	-0.427463	0.085205
C	4.192494	-0.558135	-0.802986
H	2.771776	-2.452110	0.579774
H	2.066055	-1.301894	1.726259

H	3.827299	-1.578738	1.711332
H	3.055067	0.472533	0.560350
H	4.095913	-1.472730	-1.392975
H	5.142557	-0.601233	-0.253859
H	4.220051	0.289623	-1.489369
S	-0.000082	1.011879	-0.000636
O	1.007895	1.725579	0.742500
O	-1.007679	1.724488	-0.745341
O	0.713128	0.035753	-1.009507
O	-0.713814	0.038360	1.010390
H	1.657901	-0.215288	-0.625801
H	-1.658280	-0.213726	0.626741
C	-2.926785	-1.501527	-1.082857
N	-3.032104	-0.428212	-0.085317
C	-4.193410	-0.554941	0.801806
H	-2.063721	-1.309592	-1.721489
H	-3.825195	-1.585111	-1.708323
H	-2.772113	-2.454897	-0.571750
H	-3.053685	0.470009	-0.563869
H	-4.221481	0.295460	1.484892
H	-4.098065	-1.467310	1.395434
H	-5.142770	-0.599693	0.251589

1SA3DMA

C	1.778445	2.389059	1.140982
N	2.396783	1.572592	0.090142
C	3.567028	2.211659	-0.514627
H	2.445940	2.454006	2.006377
H	0.837788	1.927216	1.442269
H	1.560877	3.412760	0.803324
H	1.698065	1.382262	-0.632203
H	4.370167	2.298913	0.223804
H	3.350693	3.220294	-0.896414
H	3.930287	1.603881	-1.346201
C	2.738618	-1.677755	1.900130
N	2.314496	-1.220363	0.560602
C	2.974016	-1.916612	-0.570182
H	2.520594	-2.740541	2.011271
H	2.185830	-1.119457	2.655214
H	3.808747	-1.510276	2.033520
H	2.463570	-0.169303	0.459190
H	2.757221	-2.983835	-0.513214
H	4.052999	-1.757027	-0.529911
H	2.558214	-1.510456	-1.490417
S	-0.622342	-0.439468	-0.917149

O	0.580722	-0.001557	-1.629474
O	-1.754127	-0.847484	-1.728624
O	-0.276994	-1.447460	0.132886
O	-1.074599	0.878772	-0.097318
H	1.253473	-1.347186	0.445158
H	-2.048253	0.755406	0.155643
C	-3.780858	-0.689531	1.473407
N	-3.661968	0.227367	0.337379
C	-4.752069	1.197323	0.243789
H	-2.954305	-1.401087	1.442403
H	-4.731012	-1.244258	1.480399
H	-3.712445	-0.123033	2.406785
H	-3.592735	-0.310778	-0.524792
H	-4.619518	1.807275	-0.651739
H	-4.729176	1.860492	1.113291
H	-5.745819	0.726036	0.203025

1SA4DMA

C	3.297109	2.148105	1.572041
N	2.901414	1.412050	0.372916
C	3.468472	1.974998	-0.856642
H	4.374459	2.046648	1.740222
H	2.777169	1.742812	2.443860
H	3.071436	3.224688	1.509976
H	1.878978	1.424497	0.282633
H	4.553485	1.824484	-0.876427
H	3.278098	3.055421	-0.951182
H	3.014020	1.465824	-1.706390
C	-2.853111	-1.938295	1.456898
N	-3.378007	-1.165867	0.326855
C	-4.708229	-1.598691	-0.095814
H	-3.411749	-1.701419	2.369247
H	-1.800182	-1.688497	1.593099
H	-2.923323	-3.024259	1.290865
H	-2.714825	-1.240048	-0.451230
H	-5.440413	-1.390923	0.691619
H	-4.756851	-2.675448	-0.320852
H	-5.008069	-1.050982	-0.992410
C	-2.792617	2.359298	1.500552
N	-2.535732	1.561720	0.287222
C	-3.003273	2.182397	-0.972833
H	-2.284608	3.321869	1.422557
H	-2.403613	1.821971	2.365515
H	-3.864147	2.526666	1.629594
H	-2.965400	0.597238	0.380234

H	-2.500928	3.141022	-1.110703
H	-4.084365	2.335935	-0.942782
H	-2.728231	1.510195	-1.783860
S	0.015464	-0.262618	-0.909864
O	-1.298174	-0.430507	-1.565849
O	1.151464	-0.170372	-1.837438
O	-0.035485	1.021690	-0.065798
O	0.247645	-1.408729	0.060061
H	-1.458113	1.363362	0.178847
H	1.724982	-1.511760	0.256617
C	3.238840	-2.042925	1.644839
N	2.817720	-1.452996	0.360369
C	3.440215	-2.065052	-0.835351
H	2.716235	-1.534542	2.455138
H	4.316820	-1.933379	1.782029
H	2.978671	-3.102311	1.665158
H	2.990876	-0.406271	0.368127
H	2.998079	-1.588079	-1.708119
H	3.215569	-3.132799	-0.850493
H	4.522725	-1.920055	-0.814546
1SA5DMA			
C	-0.660373	4.223989	-1.356044
N	-0.692428	3.468658	-0.106318
C	-0.000174	4.160780	0.975859
H	-1.246140	5.143561	-1.251318
H	-1.104983	3.630569	-2.158229
H	0.356795	4.511696	-1.671278
H	-0.261683	2.557033	-0.252741
H	-0.538232	5.078340	1.237290
H	1.036998	4.445752	0.728090
H	0.029056	3.524740	1.864205
C	3.399251	1.543695	1.901789
N	3.006680	0.930318	0.638232
C	3.530058	1.637368	-0.530082
H	4.483081	1.462939	2.035078
H	2.920788	1.019713	2.733290
H	3.137170	2.613415	1.973054
H	1.990409	0.891853	0.566790
H	4.618953	1.528622	-0.575650
H	3.304410	2.717367	-0.518875
H	3.094126	1.201589	-1.429599
C	-2.517423	-2.991737	1.362792
N	-3.126329	-2.152926	0.324619
C	-4.421499	-2.661126	-0.130959

H	-3.100593	-2.925680	2.287030
H	-1.501142	-2.644013	1.549853
H	-2.465417	-4.050658	1.069927
H	-2.482612	-2.091721	-0.467550
H	-5.152176	-2.605861	0.682037
H	-4.373904	-3.706985	-0.469050
H	-4.785972	-2.051424	-0.960622
C	-2.896854	1.293452	1.865712
N	-2.662073	0.641664	0.557956
C	-3.345931	1.311105	-0.578668
H	-2.547758	2.324000	1.807489
H	-2.339566	0.757749	2.634045
H	-3.961113	1.272020	2.105080
H	-2.942580	-0.383681	0.581250
H	-2.993395	2.340824	-0.626454
H	-4.425946	1.280484	-0.424457
H	-3.070517	0.776805	-1.485910
S	0.063824	-0.648338	-1.058142
O	-1.263176	-0.903258	-1.625250
O	1.149611	-0.432259	-1.996304
O	-0.022882	0.467896	-0.042288
O	0.389130	-1.955894	-0.211664
H	-1.623172	0.625435	0.355274
H	1.423350	-2.026989	-0.027807
C	3.353289	-2.879009	1.387056
N	2.961260	-2.097273	0.213547
C	3.607135	-2.543265	-1.026179
H	2.876473	-2.464159	2.277812
H	4.441220	-2.889435	1.547313
H	3.018412	-3.914082	1.272877
H	3.169182	-1.101092	0.375850
H	3.267355	-1.908786	-1.844617
H	3.307512	-3.572415	-1.244235
H	4.704315	-2.510597	-0.964823
1SA6DMA			
C	4.546330	-1.975829	-1.607954
N	4.949161	-1.162256	-0.455048
C	4.996106	0.268032	-0.779142
H	3.527583	-1.702969	-1.887957
H	4.562215	-3.034181	-1.334269
H	5.198688	-1.835070	-2.485367
H	5.867485	-1.461796	-0.141350
H	3.989024	0.598663	-1.038794
H	5.667174	0.498646	-1.622894

H	5.335850	0.831272	0.094160
C	-3.330912	-2.166191	-2.571791
N	-3.433120	-2.768501	-1.237598
C	-2.262152	-3.595059	-0.917119
H	-2.460647	-1.508977	-2.590990
H	-4.226290	-1.572591	-2.777093
H	-3.219878	-2.912938	-3.375108
H	-4.264634	-3.351018	-1.203405
H	-1.382353	-2.954758	-0.839437
H	-2.063786	-4.371690	-1.673665
H	-2.414293	-4.086435	0.047436
C	0.721351	4.533041	-1.549904
N	0.379066	4.021486	-0.226397
C	1.098889	4.713800	0.836903
H	0.357041	5.560379	-1.660336
H	0.242709	3.921373	-2.318207
H	1.806036	4.541316	-1.752883
H	0.595614	3.026079	-0.181929
H	0.770638	5.757509	0.895145
H	2.194224	4.719295	0.698855
H	0.883565	4.239946	1.797933
C	-2.710661	-1.247606	2.113154
N	-3.563474	-0.690099	1.054315
C	-4.974604	-0.642442	1.442207
H	-2.722324	-0.588441	2.988019
H	-1.685314	-1.327758	1.748019
H	-3.046146	-2.242475	2.443100
H	-3.478982	-1.300150	0.227719
H	-5.113621	0.049644	2.279009
H	-5.366144	-1.623209	1.753620
H	-5.577268	-0.286798	0.602936
C	-2.467508	2.758039	1.370994
N	-2.281406	1.734070	0.316703
C	-2.675184	2.198712	-1.036136
H	-1.849673	3.620931	1.120449
H	-2.149596	2.341739	2.326887
H	-3.519201	3.043864	1.428856
H	-2.812712	0.842531	0.563561
H	-2.112405	3.102541	-1.267396
H	-3.746189	2.409311	-1.054067
H	-2.421561	1.411973	-1.742972
S	0.440198	-0.164300	-0.662570
O	-0.781813	-0.331232	-1.446304
O	1.691873	-0.146265	-1.403132

O	0.318664	1.018707	0.256401
O	0.462566	-1.443550	0.303375
H	-1.258809	1.456045	0.290974
H	1.367155	-1.490372	0.805573
C	2.732322	-0.409792	2.578197
N	2.742417	-1.543183	1.648937
C	2.955763	-2.827906	2.316134
H	2.558366	0.510236	2.019039
H	3.668890	-0.318349	3.148463
H	1.910517	-0.526875	3.290854
H	3.486222	-1.401501	0.949681
H	2.997971	-3.623307	1.569164
H	2.120593	-3.040934	2.990111
H	3.883833	-2.854599	2.907296

1SA7DMA

C	-5.431698	1.727936	-1.483582
N	-4.322768	1.797468	-0.537966
C	-4.035060	3.160041	-0.097908
H	-6.363789	2.021039	-0.989077
H	-5.548286	0.701538	-1.838797
H	-5.300531	2.382415	-2.361877
H	-3.481228	1.402712	-0.958090
H	-4.874332	3.549490	0.488235
H	-3.856557	3.859755	-0.931509
H	-3.147229	3.154744	0.537898
C	0.377781	-4.087536	2.069626
N	0.840729	-2.715625	2.235626
C	0.605373	-2.206802	3.581298
H	0.979348	-4.764475	2.686172
H	0.492310	-4.392489	1.026652
H	-0.679725	-4.236457	2.352600
H	0.371800	-2.119345	1.555469
H	1.240777	-2.736495	4.299684
H	-0.440291	-2.319456	3.919651
H	0.857785	-1.145804	3.622830
C	2.493719	3.676228	-1.762900
N	2.815389	3.829330	-0.340778
C	1.655457	4.278357	0.438398
H	1.725551	2.907747	-1.864528
H	3.385213	3.358497	-2.310689
H	2.116355	4.602786	-2.225901
H	3.563434	4.509311	-0.242313
H	0.889471	3.501935	0.401221
H	1.219240	5.218163	0.062256

H	1.948702	4.428345	1.480513
C	-0.509906	-1.848466	-4.054005
N	0.202502	-2.557162	-2.994606
C	-0.015744	-3.997234	-3.040850
H	-0.077509	-2.099859	-5.028905
H	-0.414705	-0.771974	-3.901969
H	-1.586525	-2.086743	-4.093570
H	-0.100834	-2.191105	-2.093853
H	0.432537	-4.414555	-3.949134
H	-1.081689	-4.286913	-3.036446
H	0.466494	-4.474630	-2.183542
C	2.777848	1.062249	2.217129
N	3.595302	1.125942	0.998588
C	5.028649	1.193206	1.290166
H	2.974428	0.126318	2.749075
H	1.723074	1.090891	1.941563
H	2.986951	1.892950	2.907978
H	3.327355	1.974941	0.482211
H	5.357674	0.269635	1.776703
H	5.291574	2.030735	1.954827
H	5.591512	1.307232	0.360333
C	3.246715	-2.291805	-0.217675
N	2.667201	-0.993714	-0.642741
C	2.905132	-0.652240	-2.068532
H	2.923242	-3.069150	-0.910546
H	2.875464	-2.520393	0.783514
H	4.335993	-2.227066	-0.226343
H	3.039047	-0.206224	-0.025113
H	2.376854	-1.377370	-2.690947
H	3.977312	-0.663368	-2.272200
H	2.497932	0.341964	-2.243274
S	-0.581938	0.257304	-0.284574
O	0.496014	1.209911	-0.545386
O	-1.744744	0.346736	-1.166107
O	-0.040274	-1.142930	-0.242584
O	-1.069051	0.574417	1.195090
H	1.629875	-1.026710	-0.483791
H	-2.044249	0.219640	1.354361
C	-3.709523	-1.593430	1.041495
N	-3.531484	-0.236017	1.568169
C	-4.004742	-0.082218	2.944762
H	-3.382643	-1.612933	0.001507
H	-4.753248	-1.934101	1.099152
H	-3.088851	-2.293624	1.607636

H	-4.016252	0.431121	0.950709
H	-3.889066	0.957935	3.256025
H	-3.406518	-0.705952	3.615236
H	-5.059900	-0.367844	3.064909
1SA8DMA			
C	4.752162	-1.577720	-2.986817
N	4.535875	-1.308361	-1.570578
C	5.733513	-1.544301	-0.774747
H	5.470013	-0.861497	-3.402744
H	3.811843	-1.462723	-3.531742
H	5.142208	-2.590621	-3.192137
H	3.776394	-1.907324	-1.226529
H	6.512936	-0.820787	-1.039718
H	6.164516	-2.553225	-0.905642
H	5.505004	-1.413978	0.286451
C	-4.511939	-3.259395	-1.959497
N	-4.080572	-1.948382	-1.485609
C	-4.547663	-0.856809	-2.335330
H	-5.601081	-3.344984	-1.883339
H	-4.069022	-4.040137	-1.336972
H	-4.235016	-3.458976	-3.008435
H	-3.062725	-1.915861	-1.426442
H	-5.637312	-0.768731	-2.268159
H	-4.288405	-0.990606	-3.399021
H	-4.106687	0.082651	-1.996354
C	2.281489	-0.771154	3.950823
N	1.402776	0.264520	3.422037
C	0.390100	0.680362	4.384823
H	2.879006	-0.370181	4.777014
H	2.970192	-1.104598	3.170654
H	1.743973	-1.657750	4.331493
H	0.948048	-0.082780	2.579327
H	0.862957	1.200273	5.225544
H	-0.194293	-0.159532	4.800972
H	-0.308297	1.369333	3.907046
C	-1.052574	3.255909	-3.213174
N	-1.557160	4.002830	-2.056941
C	-2.790836	3.418831	-1.520413
H	-0.806516	2.242506	-2.891930
H	-0.146456	3.734544	-3.594349
H	-1.780499	3.188376	-4.038583
H	-1.737938	4.962752	-2.334906
H	-2.564930	2.421118	-1.139665
H	-3.592880	3.333453	-2.272273

H	-3.158695	4.032002	-0.693821
C	1.443698	-3.751387	-1.614387
N	2.158050	-3.084252	-0.528284
C	2.485890	-3.995877	0.562767
H	2.105905	-4.470166	-2.109511
H	1.126502	-3.011888	-2.351658
H	0.545467	-4.291722	-1.275390
H	1.577992	-2.327791	-0.166997
H	3.214861	-4.739979	0.223948
H	1.611368	-4.541876	0.956282
H	2.935429	-3.438029	1.387819
C	-0.355664	3.560595	1.522310
N	0.443958	3.872952	0.330578
C	1.073959	5.192140	0.412582
H	0.296649	3.482877	2.397415
H	-0.856732	2.601767	1.382517
H	-1.113467	4.330700	1.733901
H	-0.180037	3.862850	-0.487061
H	1.802300	5.211402	1.229301
H	0.350340	6.002215	0.593929
H	1.601673	5.409986	-0.519335
C	3.295457	1.733993	0.920942
N	2.183581	1.652368	-0.059434
C	2.621204	1.602570	-1.478282
H	4.005019	0.932192	0.716863
H	2.876460	1.611963	1.922102
H	3.797797	2.697735	0.822423
H	1.528767	2.481517	0.076858
H	3.291895	0.749246	-1.611487
H	3.134869	2.532525	-1.730037
H	1.730829	1.488125	-2.094358
S	-0.680147	-0.383621	-0.033234
O	-0.696411	0.742678	-0.969923
O	-1.234399	-1.635374	-0.552928
O	0.694061	-0.570792	0.529835
O	-1.564549	0.040606	1.217032
H	1.618277	0.792356	0.145670
H	-2.441286	-0.555815	1.306770
C	-3.259182	-2.679563	2.098419
N	-3.685517	-1.413653	1.491287
C	-4.745532	-0.736865	2.242131
H	-2.496623	-3.130729	1.462954
H	-4.090719	-3.386424	2.226206
H	-2.818290	-2.486422	3.080316

H	-3.998850	-1.596032	0.526436
H	-5.045041	0.168950	1.711353
H	-4.373358	-0.445980	3.228484
H	-5.633013	-1.369431	2.383873

2DMA

C	-2.148635	1.164459	0.020895
N	-1.668550	-0.117380	0.530752
C	-1.851764	-1.210418	-0.422970
H	-1.539164	1.461000	-0.837539
H	-2.039666	1.932364	0.790300
H	-3.201940	1.146017	-0.306710
H	-2.148591	-0.337072	1.396853
H	-1.175089	-1.060198	-1.268232
H	-2.881221	-1.292940	-0.809957
H	-1.585050	-2.157902	0.051003
C	2.243450	-1.112792	0.231257
N	1.399318	-0.023976	-0.235913
C	2.056130	1.271438	-0.154517
H	3.104824	-1.230114	-0.435717
H	1.682688	-2.050844	0.211186
H	2.638460	-0.972121	1.255078
H	0.525660	-0.008816	0.289620
H	2.904100	1.304683	-0.847783
H	2.445257	1.519684	0.850999
H	1.359268	2.059630	-0.450961

2SA

S	1.769793	0.023050	-0.081256
O	1.273918	1.278519	-0.568001
O	1.280545	-1.197772	-0.679657
O	3.343903	0.077463	-0.194602
O	1.628745	-0.061620	1.486392
H	3.707601	-0.819103	-0.119457
H	0.655946	-0.094496	1.674825
S	-1.947474	-0.013423	0.104614
O	-1.049244	-0.086017	1.243375
O	-3.352225	-0.038109	0.272861
O	-1.594459	1.299804	-0.715394
O	-1.567797	-1.191539	-0.890023
H	-0.628022	1.464940	-0.696936
H	-0.599718	-1.351201	-0.871779

2SA1DMA

S	-2.277531	0.022843	0.005944
O	-1.376427	1.092759	-0.408666
O	-3.665923	0.291648	0.130548

O	-2.107588	-1.179725	-0.995579
O	-1.757477	-0.544133	1.381528
H	-1.152647	-1.463491	-1.050198
H	-0.760531	-0.655452	1.352915
S	1.450802	-1.261293	-0.092366
O	2.276391	-0.270205	-0.775200
O	0.462035	-1.952409	-0.921982
O	2.526700	-2.380001	0.350567
O	0.856408	-0.721198	1.150520
H	2.041275	-3.176252	0.609749
H	0.169204	1.763061	-0.046412
C	1.238878	3.185203	-1.100836
N	1.144769	2.123103	-0.065920
C	1.554792	2.534023	1.303449
H	0.912107	2.768572	-2.052033
H	2.271478	3.523908	-1.179296
H	0.592316	4.017561	-0.824908
H	1.707830	1.289637	-0.357209
H	1.464830	1.664302	1.951197
H	0.904285	3.336441	1.650396
H	2.589141	2.875950	1.280430
2SA2DMA			
S	1.311844	-1.750213	-0.533975
O	1.179412	-1.046971	0.779173
O	2.576625	-2.393360	-0.745511
O	0.101629	-2.556645	-0.777637
O	1.277045	-0.546960	-1.632662
H	-1.137313	-1.942420	0.099440
H	0.365440	-0.174590	-1.668408
C	-3.218497	-1.832304	0.091441
N	-1.904751	-1.597669	0.739380
C	-1.720550	-2.250593	2.059039
H	-3.220888	-1.301534	-0.858850
H	-4.015517	-1.451377	0.730032
H	-3.351716	-2.900534	-0.078318
H	-1.767563	-0.571570	0.841394
H	-0.709424	-2.030051	2.395811
H	-1.840640	-3.327760	1.945671
H	-2.454149	-1.864180	2.766969
S	-1.323787	1.697252	-0.399284
O	-0.167893	2.602311	-0.390794
O	-1.708125	1.193010	0.918666
O	-2.600310	2.614348	-0.815646
O	-1.225477	0.641388	-1.415858

H	-2.399888	3.020094	-1.670938
H	1.773189	0.448200	0.781010
C	2.145427	2.029665	2.093848
N	2.089819	1.461249	0.725202
C	3.362541	1.522243	-0.038659
H	1.151616	1.956666	2.533102
H	2.446525	3.076185	2.045245
H	2.859352	1.464038	2.692301
H	1.329079	1.943282	0.202113
H	3.189427	1.070094	-1.013256
H	4.126547	0.955658	0.493156
H	3.674767	2.561080	-0.148257

2SA3DMA

C	-0.536177	3.600811	-0.307406
N	0.141914	2.480478	-0.998523
C	0.943412	2.872868	-2.182679
H	0.216020	4.282676	0.089986
H	-1.131664	3.186408	0.504262
H	-1.184035	4.134360	-1.005104
H	-0.567232	1.777432	-1.261219
H	1.700935	3.592596	-1.871648
H	0.298300	3.319315	-2.941582
H	1.433721	1.976350	-2.556534
S	2.297443	0.013589	0.061598
O	1.699166	-1.167931	0.805359
O	3.742438	0.022148	0.110286
O	1.766120	-0.059119	-1.360773
O	1.691093	1.263314	0.680094
H	0.865427	-1.248239	-1.541361
H	0.801209	1.967051	-0.292510
C	-0.460355	-2.049049	-2.978714
N	0.201583	-2.106757	-1.655218
C	0.985831	-3.338443	-1.399660
H	-1.049879	-1.134718	-3.022780
H	-1.115109	-2.912409	-3.107453
H	0.300650	-2.043872	-3.759488
H	-0.515606	-1.978743	-0.923993
H	1.457551	-3.228185	-0.425257
H	1.756814	-3.431149	-2.164937
H	0.331913	-4.211948	-1.425883
S	-2.354571	-0.014355	-0.049304
O	-2.042233	0.865475	1.085088
O	-1.907794	-1.393285	0.127349
O	-3.977956	-0.182199	-0.068178

O -1.993552 0.583145 -1.342330
H -4.359923 0.695537 -0.205645
H 0.730677 -0.714555 1.868439
C -0.638592 -1.553488 3.240597
N 0.039887 -0.379902 2.642889
C 0.797504 0.457294 3.604310
H -1.199643 -2.056242 2.455060
H -1.320317 -1.229201 4.028496
H 0.112294 -2.225545 3.656666
H -0.663656 0.191073 2.148258
H 1.292218 1.241861 3.035354
H 1.550569 -0.161852 4.092159
H 0.121125 0.875184 4.352118

2SA4DMA

C 5.610510 1.025543 -0.640313
N 4.703507 -0.059481 -0.253600
C 5.387449 -1.323688 0.032998
H 6.272164 1.260604 0.196901
H 5.026788 1.917671 -0.872465
H 6.232732 0.771649 -1.509851
H 4.002251 -0.197564 -0.977751
H 6.041139 -1.193501 0.898786
H 5.998620 -1.678948 -0.808583
H 4.648580 -2.087950 0.280007
C 0.071654 2.870126 -2.014611
N -0.949130 2.437221 -1.034768
C -2.023360 3.423691 -0.773650
H -0.397633 3.000545 -2.990292
H 0.837990 2.098181 -2.065325
H 0.522402 3.810779 -1.693507
H -0.465995 2.183422 -0.154850
H -2.524634 3.657685 -1.713329
H -1.600818 4.333561 -0.343395
H -2.734128 2.958624 -0.093459
S -2.947489 -0.352649 -0.750810
O -2.276996 -1.623373 -0.249532
O -4.283696 -0.598513 -1.246130
O -2.927164 0.630776 0.403477
O -2.030106 0.217154 -1.821669
H -2.202682 0.051834 1.618000
H -1.410524 1.508562 -1.374887
C -1.536930 0.670281 3.520488
N -1.693269 -0.369595 2.477388
C -2.440276 -1.575214 2.908681

H	-0.924392	1.470540	3.109433
H	-1.043409	0.246305	4.396423
H	-2.520554	1.049809	3.798708
H	-0.751853	-0.634962	2.134014
H	-2.541251	-2.224489	2.041410
H	-3.431394	-1.273790	3.248826
H	-1.907034	-2.074990	3.719331
S	1.459554	0.388245	0.861652
O	1.690492	0.150015	-0.587351
O	0.944067	-0.818577	1.532294
O	2.873927	0.716732	1.487495
O	0.627900	1.569210	1.128570
H	3.627273	0.391640	0.864003
H	-0.964586	-1.838940	-0.907195
C	0.642743	-3.200555	-0.774254
N	-0.004033	-2.027216	-1.403226
C	-0.260275	-2.165943	-2.856187
H	0.846717	-2.954855	0.266301
H	1.576860	-3.434676	-1.288890
H	-0.031626	-4.055201	-0.835287
H	0.574694	-1.190346	-1.216583
H	-0.796875	-1.276664	-3.180195
H	-0.889550	-3.041041	-3.020400
H	0.681676	-2.282370	-3.396084
2SA5DMA			
C	-0.054955	3.979384	0.292350
N	-0.212877	2.899931	-0.706473
C	-0.513188	3.355853	-2.081759
H	0.812453	4.589749	0.036703
H	0.077407	3.513843	1.267315
H	-0.949549	4.604585	0.307361
H	-0.950315	2.236645	-0.371464
H	0.275950	4.029618	-2.418017
H	-1.473123	3.875188	-2.104608
H	-0.530218	2.474559	-2.720382
S	1.418733	-0.008127	-1.471104
O	0.146444	0.164667	-2.212612
O	2.491010	-0.632730	-2.247905
O	1.872432	1.334159	-0.932154
O	1.140409	-0.880122	-0.233266
H	0.676450	2.288293	-0.753045
H	-0.162089	-0.926618	0.587581
C	5.931930	-1.029180	-0.273223
N	4.507285	-1.316643	-0.099195

C	4.221736	-2.754395	-0.029809
H	6.076785	0.045779	-0.401027
H	6.367360	-1.540369	-1.145051
H	6.489994	-1.346842	0.613524
H	3.983810	-0.950954	-0.902311
H	3.139858	-2.893679	-0.020658
H	4.648462	-3.181098	0.884304
H	4.633014	-3.307496	-0.886777
C	-4.466678	-2.405448	1.175743
N	-4.832776	-1.547468	0.032779
C	-5.366271	-0.245822	0.476748
H	-3.677532	-1.915967	1.747090
H	-4.096076	-3.365835	0.809642
H	-5.316977	-2.590787	1.847207
H	-5.549535	-2.022652	-0.509551
H	-4.586827	0.285867	1.022943
H	-6.241196	-0.355752	1.133057
H	-5.656487	0.347113	-0.394158
C	-2.835077	-0.405355	-2.832797
N	-2.484434	-1.058318	-1.547518
C	-1.713771	-2.318955	-1.716397
H	-1.911123	-0.182189	-3.362120
H	-3.373680	0.516911	-2.617143
H	-3.467765	-1.073698	-3.418457
H	-3.362485	-1.247446	-0.982323
H	-0.792302	-2.086851	-2.244305
H	-2.321700	-3.031928	-2.275927
H	-1.482264	-2.709531	-0.728451
S	-1.497140	0.465277	1.587719
O	-2.576001	0.232124	2.523409
O	-0.991317	-1.009240	1.175079
O	-1.980206	1.055497	0.291198
O	-0.327707	1.191188	2.090039
H	-1.942008	-0.379565	-0.985421
H	1.994026	-0.117342	1.020162
C	3.047632	1.416339	1.987033
N	2.762881	-0.013983	1.729697
C	2.382001	-0.784728	2.936593
H	3.256000	1.888600	1.029685
H	3.902360	1.503709	2.660702
H	2.163712	1.868426	2.434327
H	3.567488	-0.473031	1.207704
H	2.175075	-1.812664	2.642282
H	1.480159	-0.343252	3.359020

H	3.196193	-0.762883	3.662525
2SA6DMA			
C	-4.808973	0.856824	-0.594507
N	-4.795878	-0.600112	-0.575992
C	-6.133951	-1.178412	-0.585918
H	-5.212653	1.216583	-1.547965
H	-3.785125	1.222277	-0.494782
H	-5.416971	1.304290	0.212130
H	-4.298235	-0.915624	0.254951
H	-6.629717	-0.962600	-1.539030
H	-6.786588	-0.799638	0.220216
H	-6.065180	-2.263741	-0.481490
C	-0.153544	-2.911369	-2.706555
N	-1.139975	-2.003728	-2.065890
C	-2.502328	-2.053920	-2.656524
H	-0.438919	-3.947705	-2.523222
H	0.830212	-2.694609	-2.292157
H	-0.135627	-2.716213	-3.779030
H	-0.734989	-1.027291	-2.113254
H	-2.844109	-3.090094	-2.672771
H	-2.462869	-1.668240	-3.676101
H	-3.190215	-1.460954	-2.045461
S	-1.683580	-1.441494	1.566711
O	-3.094410	-1.531577	1.867617
O	-0.793598	-1.303258	2.731384
O	-1.171433	-2.477049	0.634020
O	-1.556507	-0.046410	0.729739
H	-1.201168	-2.218951	-1.042254
H	-0.594488	0.072489	0.449159
C	2.047882	-2.995209	1.287512
N	1.803841	-1.647460	1.859956
C	2.908001	-1.140662	2.714522
H	1.153261	-3.291100	0.744551
H	2.237610	-3.700350	2.097920
H	2.907771	-2.942842	0.622819
H	0.890743	-1.640428	2.366736
H	2.618416	-0.168481	3.112063
H	3.800188	-1.042304	2.090902
H	3.076840	-1.835470	3.538199
C	0.066986	2.594506	2.525975
N	-0.981107	2.850282	1.525118
C	-2.037039	3.735083	2.031970
H	0.558484	3.535367	2.793327
H	0.803365	1.917629	2.091159

H	-0.331594	2.141025	3.442979
H	-1.400046	1.947799	1.295930
H	-1.627903	4.731761	2.223620
H	-2.484764	3.368562	2.966252
H	-2.830324	3.827672	1.286925
C	1.085292	4.846414	-0.660560
N	0.393784	3.557829	-0.886442
C	-0.541738	3.562514	-2.039704
H	1.672961	5.103319	-1.542239
H	1.752111	4.744500	0.195046
H	0.356114	5.634066	-0.464319
H	-0.137489	3.286480	-0.003227
H	-0.002103	3.869420	-2.935905
H	-1.364930	4.252416	-1.847100
H	-0.903980	2.545546	-2.179874
S	1.409657	0.343888	-1.288558
O	0.166859	0.347374	-2.124646
O	2.259873	-0.823946	-1.566979
O	2.130750	1.636784	-1.471317
O	0.960351	0.280376	0.177311
H	1.124258	2.793917	-1.071127
H	1.630379	-0.953470	1.084973
C	5.435673	0.597899	-0.069537
N	4.924664	-0.770350	-0.047263
C	5.928458	-1.746471	-0.453373
H	4.610235	1.294404	0.085709
H	5.923232	0.865162	-1.022673
H	6.171076	0.739440	0.730816
H	4.120156	-0.823457	-0.672282
H	5.482103	-2.743603	-0.499685
H	6.739626	-1.779953	0.282355
H	6.382928	-1.532074	-1.436477
2SA7DMA			
C	-0.577810	3.698276	2.611253
N	-0.273809	3.816196	1.190306
C	-0.854873	5.006081	0.585217
H	-0.094833	4.510815	3.165227
H	-0.189646	2.751688	2.991538
H	-1.657608	3.736782	2.837398
H	-0.611106	2.992745	0.695055
H	-0.394816	5.906377	1.006900
H	-1.946544	5.096843	0.738714
H	-0.662752	5.004047	-0.490488
C	-1.926958	-3.559616	-2.801326

N	-2.905004	-3.122245	-1.807569
C	-4.278812	-3.381216	-2.223763
H	-1.923169	-4.653133	-2.866955
H	-0.929278	-3.232571	-2.503109
H	-2.126016	-3.167280	-3.813459
H	-2.783028	-2.124979	-1.656117
H	-4.459595	-4.460748	-2.264017
H	-4.525675	-2.966756	-3.216871
H	-4.972363	-2.951761	-1.496618
C	-5.199409	3.162253	-1.843268
N	-4.329771	2.624484	-0.793779
C	-4.930377	2.655729	0.545549
H	-6.088232	2.532775	-1.933765
H	-4.671697	3.143119	-2.798491
H	-5.529210	4.191650	-1.641537
H	-3.452541	3.138699	-0.781375
H	-5.820941	2.021956	0.552228
H	-5.226565	3.667248	0.857669
H	-4.217119	2.247561	1.262567
S	-1.772016	0.417527	-0.341577
O	-1.132720	1.643295	-0.828155
O	-2.107514	0.456463	1.081723
O	-3.143485	0.243362	-1.155892
O	-1.044400	-0.822186	-0.720960
H	-3.671431	1.110358	-1.064719
H	-1.182562	-2.185463	0.450957
C	-2.637286	-2.727011	1.802960
N	-1.257419	-2.826023	1.264184
C	-0.874765	-4.201925	0.852280
H	-2.841545	-1.682015	2.028251
H	-2.716236	-3.339295	2.702465
H	-3.330264	-3.084510	1.042145
H	-0.560299	-2.430509	1.977957
H	0.145385	-4.167827	0.476702
H	-1.565708	-4.526587	0.074938
H	-0.936518	-4.861796	1.719186
C	6.274225	0.595582	-0.289128
N	5.633273	1.294416	-1.417013
C	5.579976	0.452182	-2.625602
H	5.660869	-0.266067	-0.022164
H	6.337672	1.267730	0.570433
H	7.287511	0.244869	-0.532355
H	6.168389	2.132432	-1.627894
H	4.955868	-0.417462	-2.416280

H	6.575018	0.104260	-2.938532
H	5.136324	1.018870	-3.447828
C	2.072348	2.080824	-1.777281
N	2.939837	1.903151	-0.579990
C	2.961501	3.077473	0.330453
H	1.035661	2.190752	-1.461797
H	2.156169	1.187031	-2.392267
H	2.403215	2.960760	-2.331788
H	3.925808	1.687234	-0.893970
H	1.942528	3.329670	0.640052
H	3.410915	3.925478	-0.190100
H	3.565147	2.827342	1.203326
S	2.402436	-1.517598	-0.188760
O	3.761445	-1.573347	-0.695063
O	1.860664	-2.745904	0.375832
O	2.172535	-0.356463	0.728696
O	1.531162	-1.159428	-1.514510
H	2.611509	1.053630	-0.045957
H	0.593745	-0.993515	-1.247741
C	-0.088679	-0.570594	3.867571
N	0.552124	-1.586049	3.027191
C	1.475963	-2.451654	3.764975
H	-0.718140	0.065045	3.242319
H	0.640017	0.059077	4.401081
H	-0.721014	-1.054525	4.619208
H	1.079521	-1.118476	2.285929
H	1.988492	-3.102451	3.055980
H	0.922013	-3.068249	4.480595
H	2.231581	-1.881872	4.326745
2SA8DMA			
C	5.762834	1.667047	-2.665763
N	4.884876	1.035527	-1.690648
C	5.617963	0.348963	-0.633035
H	6.323417	2.483298	-2.196139
H	5.168614	2.096937	-3.476431
H	6.501411	0.977564	-3.113686
H	4.271940	0.361338	-2.158728
H	6.155448	1.076166	-0.012917
H	6.363988	-0.373816	-1.010282
H	4.913307	-0.188874	0.004908
C	0.052519	4.978375	2.139198
N	-0.525046	4.145698	1.082239
C	-1.337762	4.921500	0.137481
H	0.764690	5.692527	1.712552

H	0.587433	4.349266	2.854326
H	-0.706388	5.555980	2.689665
H	-1.133376	3.437813	1.523249
H	-0.705649	5.631263	-0.407041
H	-2.129219	5.499400	0.639253
H	-1.795042	4.238791	-0.579117
C	2.032782	-0.940756	-3.927907
N	2.887572	-1.146206	-2.762182
C	3.512379	-2.464437	-2.746204
H	2.643291	-0.905955	-4.836473
H	1.504021	0.010004	-3.837344
H	1.276016	-1.731837	-4.062232
H	2.335148	-1.026242	-1.916294
H	4.235423	-2.545370	-3.564986
H	2.790388	-3.292298	-2.857283
H	4.043934	-2.602784	-1.803306
C	3.563090	-4.364682	2.988686
N	2.865562	-3.076946	2.970308
C	3.278139	-2.166518	4.046079
H	4.628288	-4.202554	2.805211
H	3.175312	-5.001610	2.191365
H	3.459677	-4.895366	3.946502
H	1.861851	-3.230479	3.028373
H	4.334874	-1.917894	3.918410
H	3.146605	-2.601845	5.047137
H	2.698778	-1.245843	3.970017
S	1.206590	-0.959482	0.925980
O	0.257592	-2.037198	1.217369
O	1.362285	0.016346	1.999245
O	2.635511	-1.658011	0.690951
O	0.968611	-0.305475	-0.393093
H	2.825577	-2.226708	1.512904
H	1.078465	1.529411	-0.278555
C	2.646309	2.687576	0.400398
N	1.344304	2.529977	-0.305257
C	1.381415	2.968991	-1.725329
H	2.562742	2.204210	1.372130
H	2.853745	3.752251	0.518838
H	3.431057	2.215018	-0.195780
H	0.596298	3.089981	0.215838
H	0.404292	2.774483	-2.162526
H	2.161199	2.412894	-2.244484
H	1.608611	4.035292	-1.761264
C	-6.088334	-1.029778	-0.621310

N	-5.533531	-2.323749	-1.059888
C	-5.333691	-2.363653	-2.520228
H	-5.369261	-0.244050	-0.855741
H	-6.253232	-1.048305	0.458675
H	-7.040000	-0.791993	-1.117150
H	-6.180655	-3.062767	-0.798972
H	-4.620990	-1.585022	-2.797828
H	-6.265978	-2.191225	-3.076479
H	-4.932001	-3.337732	-2.809990
C	-2.030057	-3.325413	-0.648833
N	-2.933844	-2.464246	0.159684
C	-2.943704	-2.797754	1.605499
H	-1.025704	-3.252844	-0.235636
H	-2.029963	-2.954774	-1.671710
H	-2.390760	-4.355272	-0.613576
H	-3.912244	-2.502028	-0.240884
H	-1.934410	-2.668312	1.993384
H	-3.279243	-3.826955	1.743759
H	-3.624537	-2.117000	2.115979
S	-2.299543	0.663658	-1.403639
O	-3.430580	0.525030	-2.299395
O	-1.612014	1.948641	-1.400640
O	-2.602444	0.200544	-0.012704
O	-1.240775	-0.446718	-1.956315
H	-2.661914	-1.447828	0.064053
H	-0.440319	-0.428217	-1.375652
C	-1.671192	1.304539	3.466682
N	-2.312176	2.036558	2.376749
C	-3.663108	2.476750	2.705978
H	-0.707274	0.916913	3.132785
H	-2.277827	0.457533	3.834269
H	-1.500819	1.974657	4.316780
H	-2.353017	1.439336	1.550218
H	-4.123653	2.938064	1.829598
H	-3.632045	3.223918	3.506437
H	-4.320082	1.656607	3.045687
3DMA			
C	-2.285316	-1.304237	1.213117
N	-1.617702	-0.848072	-0.000352
C	-2.285520	-1.304540	-1.213584
H	-3.275095	-0.842324	1.291667
H	-1.706398	-1.001671	2.089042
H	-2.425740	-2.398489	1.256778
H	-0.644254	-1.162645	-0.000423

H	-3.275673	-0.843336	-1.291629
H	-2.425205	-2.398887	-1.257341
H	-1.707236	-1.001428	-2.089742
C	0.011235	2.629890	1.213431
N	0.073220	1.823669	0.000179
C	0.012760	2.629046	-1.213694
H	0.906109	3.256133	1.292933
H	-0.016965	1.977147	2.089258
H	-0.866249	3.298638	1.256713
H	-0.685474	1.137364	-0.000003
H	0.907272	3.255967	-1.291887
H	-0.865173	3.297066	-1.259027
H	-0.013223	1.975760	-2.089187
C	2.273025	-1.324911	1.213748
N	1.543907	-0.976706	0.000070
C	2.274377	-1.324408	-1.212935
H	2.370820	-2.412820	1.292659
H	1.720175	-0.976161	2.089331
H	3.289831	-0.896820	1.257782
H	1.327125	0.023129	0.000146
H	2.372408	-2.412276	-1.292138
H	3.291176	-0.896168	-1.255718
H	1.722429	-0.975445	-2.089002
3SA			
S	2.453303	-0.912397	-0.075672
O	1.701196	-0.150044	-1.066277
O	3.861532	-1.036833	-0.154936
O	2.077523	-0.323128	1.349795
O	1.860678	-2.370800	-0.045667
H	1.289198	0.262576	1.283646
H	0.879461	-2.355932	-0.099787
S	-1.976018	-1.376488	-0.074586
O	-0.916118	-2.350134	0.009575
O	-2.002218	-0.452780	-1.175022
O	-3.356678	-2.142931	-0.083850
O	-2.111869	-0.601128	1.283631
H	-3.260607	-2.996996	0.366376
H	-1.449726	0.146467	1.299004
S	-0.276830	2.406685	0.085967
O	-0.202668	1.208464	0.952168
O	-0.350936	3.691197	0.672745
O	0.949162	2.347724	-0.873951
O	-1.541048	2.226462	-0.833039
H	1.270198	1.407820	-1.018765

H	-1.684280	1.282701	-1.083178
3SA1DMA			
S	2.762920	-0.873362	-0.489535
O	4.045736	-1.423948	-0.740599
O	2.476927	-0.232042	0.787222
O	2.458681	0.158452	-1.641743
O	1.699903	-2.020041	-0.704365
H	1.723331	0.776226	-1.396470
H	0.851956	-1.820320	-0.235637
S	-1.980601	-1.788389	0.238944
O	-2.480539	-3.032008	0.700666
O	-0.613854	-1.376995	0.564375
O	-2.142384	-1.748068	-1.325372
O	-2.931636	-0.644301	0.763127
H	-1.839324	-0.867583	-1.673540
H	-2.521305	0.247712	0.582575
S	-0.931992	1.746236	-1.014544
O	-1.410522	0.760144	-1.977148
O	-1.620511	1.629267	0.300167
O	0.512174	1.839044	-0.840994
O	-1.322051	3.191345	-1.602738
H	1.190400	0.615028	1.542453
H	-2.214126	3.141050	-1.976332
C	0.174118	0.381397	3.333801
N	0.537559	1.174865	2.127750
C	1.177331	2.489825	2.408009
H	-0.266485	-0.555492	3.000237
H	-0.539800	0.943652	3.934969
H	1.075491	0.182549	3.911793
H	-0.300619	1.329607	1.539329
H	1.390093	2.968780	1.454631
H	2.102588	2.323991	2.957806
H	0.495592	3.104846	2.994444
3SA2DMA			
S	0.305583	2.815687	-0.607035
O	0.341053	4.037021	-1.337894
O	1.509161	2.255060	-0.035351
O	-0.769877	3.018531	0.537947
O	-0.370055	1.690790	-1.497424
H	-0.844065	2.192239	1.078442
H	0.173812	0.834569	-1.486350
S	-0.562618	-0.484960	2.233167
O	0.860469	-0.250424	2.436203
O	-1.299299	0.635758	1.619604

O	-0.881661	-1.761124	1.586377
O	-1.234524	-0.537498	3.707349
H	-0.020974	-2.456404	0.216063
H	-0.738633	-1.178014	4.236879
S	0.369747	-1.835052	-1.812634
O	1.112903	-2.479262	-2.851294
O	0.539022	-2.793910	-0.521470
O	0.956023	-0.520642	-1.363580
O	-1.076174	-1.673570	-2.027183
H	2.341140	-0.316601	-0.333761
H	-2.138585	-0.788976	-1.135086
C	-3.522050	0.754836	-1.385195
N	-2.875073	-0.302307	-0.561161
C	-3.804961	-1.334824	-0.029559
H	-2.749623	1.441865	-1.723196
H	-4.259498	1.283229	-0.781144
H	-4.006987	0.286514	-2.241072
H	-2.365276	0.126465	0.232327
H	-4.270324	-1.856508	-0.864897
H	-4.566684	-0.854291	0.584260
H	-3.225619	-2.031128	0.573037
C	3.420888	-1.714446	0.753063
N	2.957573	-0.319142	0.510736
C	4.061353	0.670251	0.372229
H	4.076745	-2.013207	-0.063859
H	2.553356	-2.368685	0.773393
H	3.958441	-1.753685	1.699811
H	2.309766	-0.048483	1.269073
H	4.681067	0.385145	-0.477456
H	4.660153	0.664388	1.283051
H	3.623180	1.650164	0.207988
3SA3DMA			
S	3.251574	-0.654750	0.449502
O	4.658055	-0.781369	0.685675
O	2.830598	-0.749579	-0.986233
O	2.568934	-1.922612	1.170826
O	2.614622	0.546906	1.047170
H	1.618464	-1.954673	0.900379
H	1.111132	0.551703	1.787154
S	-2.021300	1.948724	-0.006256
O	-0.614226	2.380583	-0.088382
O	-3.007388	2.982625	0.116447
O	-2.354308	1.199532	-1.397388
O	-2.144642	0.862929	1.031257

H	-1.614447	0.558956	-1.583024
H	-2.935575	-0.538670	0.508919
S	-0.273283	-1.792646	-1.070257
O	-0.320015	-0.452820	-1.693150
O	-1.449685	-2.603572	-1.377407
O	0.955716	-2.547170	-1.729307
O	-0.009484	-1.708828	0.383256
H	1.769065	-2.001437	-1.545085
H	0.749809	1.804303	-1.119814
C	1.312069	1.740986	-3.117746
N	1.629024	1.712897	-1.664593
C	2.568255	2.781346	-1.229601
H	0.650232	0.906700	-3.334115
H	2.238240	1.643947	-3.683673
H	0.824210	2.685130	-3.358699
H	2.029843	0.780834	-1.417568
H	2.104819	3.752811	-1.398315
H	3.490641	2.698493	-1.803875
H	2.781497	2.630784	-0.174528
C	-3.552459	-2.347144	1.329191
N	-3.423003	-1.412233	0.181918
C	-4.706295	-1.028392	-0.464549
H	-2.550886	-2.591358	1.678588
H	-4.055375	-3.256360	1.001015
H	-4.125477	-1.868758	2.123050
H	-2.783612	-1.856163	-0.514593
H	-4.484493	-0.318951	-1.259334
H	-5.351075	-0.554660	0.275134
H	-5.189137	-1.917937	-0.868430
C	0.258126	-0.423268	3.404156
N	0.285966	0.688387	2.420376
C	0.400112	2.039287	3.030098
H	0.138447	-1.356981	2.860476
H	-0.574411	-0.275953	4.092646
H	1.199281	-0.438582	3.952291
H	-0.573862	0.661564	1.832695
H	1.344589	2.108013	3.568605
H	-0.436533	2.200679	3.709619
H	0.364589	2.772081	2.227353
3SA4DMA			
C	-4.302433	-2.735938	-1.539920
N	-3.313966	-2.388807	-0.492664
C	-3.461992	-3.149028	0.773184
H	-4.200161	-3.789667	-1.799222

H	-4.104964	-2.125688	-2.420031
H	-5.309901	-2.534807	-1.175343
H	-3.407600	-1.375012	-0.259877
H	-3.352097	-4.213562	0.567691
H	-4.437271	-2.942180	1.213513
H	-2.670798	-2.822491	1.444427
S	0.185729	-2.266320	-0.620554
O	0.884764	-1.368278	-1.589150
O	-0.485781	-1.408694	0.435870
O	-0.865930	-3.063176	-1.301339
O	1.184424	-3.149375	0.046185
H	-2.330045	-2.575153	-0.857980
H	2.633109	-2.537920	-0.132320
C	4.524838	-2.497684	0.788368
N	3.548101	-1.984108	-0.197853
C	4.030286	-1.983328	-1.602774
H	4.070770	-2.469619	1.778018
H	5.420948	-1.876418	0.780503
H	4.785789	-3.526649	0.540199
H	3.265542	-1.018255	0.078679
H	3.209119	-1.651203	-2.233078
H	4.321593	-2.997072	-1.879038
H	4.881867	-1.308999	-1.697906
S	2.419018	1.619004	-0.192233
O	3.630012	2.338266	-0.484182
O	2.595654	0.451768	0.733219
O	1.297883	2.451216	0.301972
O	1.935358	0.988904	-1.579195
H	0.004157	2.894146	-0.702884
H	1.441744	0.112928	-1.465124
C	-0.596483	4.826602	-1.114090
N	-0.766331	3.358996	-1.239870
C	-0.759656	2.853349	-2.638039
H	-0.620639	5.090006	-0.057995
H	-1.407001	5.333922	-1.637455
H	0.364026	5.116546	-1.538719
H	-1.655377	3.065748	-0.770790
H	-0.914086	1.778351	-2.601693
H	0.204010	3.073257	-3.095325
H	-1.564721	3.333116	-3.195360
S	-2.731814	1.128616	0.543258
O	-3.839510	0.178982	0.366661
O	-3.035516	2.490377	0.088494
O	-2.140657	1.066423	1.890307

O	-1.575654	0.678360	-0.476015
H	-0.490888	0.639458	2.154259
H	-1.108115	-0.169897	-0.131608
C	0.778048	1.682557	3.397667
N	0.451891	0.487631	2.577820
C	0.434606	-0.795131	3.327858
H	0.818323	2.540674	2.731467
H	1.749756	1.539337	3.870112
H	0.004969	1.818644	4.153088
H	1.143159	0.418749	1.804002
H	0.249884	-1.589341	2.607633
H	-0.361073	-0.760406	4.071744
H	1.397511	-0.933894	3.820736
3SA5DMA			
C	5.859489	-1.906249	-1.190501
N	5.376455	-1.502470	0.127096
C	6.314986	-1.838819	1.192898
H	6.729722	-1.303734	-1.472526
H	5.076036	-1.742031	-1.933627
H	6.157573	-2.967052	-1.243073
H	4.487057	-1.966167	0.302800
H	7.234253	-1.253988	1.080182
H	6.600266	-2.904465	1.209756
H	5.876418	-1.591135	2.162801
C	1.099363	4.320428	1.758428
N	1.140270	3.820367	0.381163
C	1.289463	4.898930	-0.606157
H	2.054534	4.789355	2.012192
H	0.935310	3.490229	2.449377
H	0.306260	5.064691	1.918728
H	0.274188	3.318568	0.180747
H	2.281719	5.351530	-0.515145
H	0.541420	5.693208	-0.473639
H	1.171604	4.480617	-1.605012
S	-4.130528	-0.065624	0.537142
O	-5.517711	-0.122891	0.888729
O	-3.832390	-0.206584	-0.924034
O	-3.638077	1.413188	0.930077
O	-3.253778	-1.005268	1.284209
H	-2.747657	1.581877	0.525516
H	-1.764722	-0.616543	1.891446
S	1.404864	-1.885694	0.167748
O	0.088031	-2.528646	0.321644
O	2.547079	-2.742770	0.374726

O	1.519451	-1.404067	-1.358396
O	1.444314	-0.620936	0.971920
H	0.734871	-0.817106	-1.558633
H	2.238966	2.454153	0.100711
S	-0.976603	1.419354	-1.547811
O	-0.658421	-0.012917	-1.747543
O	-0.057048	2.330373	-2.194474
O	-2.388239	1.648200	-2.250528
O	-1.172651	1.720539	-0.102402
H	-3.042703	1.024035	-1.838215
H	-1.357892	-2.357424	-0.721122
C	-1.927743	-2.717075	-2.684325
N	-2.242560	-2.491451	-1.248543
C	-3.005707	-3.596375	-0.609409
H	-1.407464	-1.838030	-3.055858
H	-2.857889	-2.864139	-3.232838
H	-1.295122	-3.599460	-2.777096
H	-2.784603	-1.604154	-1.147345
H	-2.403584	-4.504210	-0.628663
H	-3.936091	-3.748891	-1.155875
H	-3.226865	-3.300908	0.413294
C	3.117358	1.531593	-1.565974
N	2.835044	1.591439	-0.103803
C	4.062269	1.595281	0.739393
H	2.174937	1.622308	-2.103072
H	3.601213	0.584754	-1.795927
H	3.773541	2.361912	-1.829129
H	2.268130	0.766269	0.178302
H	3.763288	1.627246	1.786971
H	4.654767	2.479291	0.500540
H	4.630643	0.680740	0.541545
C	-1.021414	0.820183	3.187653
N	-0.906036	-0.480422	2.482244
C	-0.794359	-1.657612	3.382547
H	-1.067700	1.608294	2.440082
H	-0.154398	0.959367	3.834245
H	-1.935400	0.826245	3.780079
H	-0.078280	-0.467700	1.849213
H	-1.700926	-1.733578	3.981769
H	0.077215	-1.540244	4.026488
H	-0.675253	-2.542045	2.760907
3SA6DMA			
C	0.207672	5.691552	0.919715
N	-0.086358	4.541804	0.070645

C	-1.072508	4.848881	-0.963912
H	0.705964	6.468403	0.330863
H	0.887888	5.397632	1.723351
H	-0.687860	6.145514	1.378036
H	-0.440646	3.777107	0.639065
H	-0.649051	5.562545	-1.678581
H	-2.004047	5.284551	-0.565692
H	-1.332532	3.936093	-1.503076
C	5.961818	1.182864	-2.391787
N	5.481253	0.953766	-1.033298
C	6.573136	0.839803	-0.067160
H	6.438558	2.166708	-2.456248
H	5.122417	1.172707	-3.092188
H	6.698770	0.435348	-2.732845
H	4.931399	0.098715	-1.004470
H	7.062949	1.811697	0.057460
H	7.345006	0.111459	-0.367172
H	6.175266	0.522774	0.897913
C	-6.816163	0.767681	-0.539843
N	-5.644092	0.197684	0.134360
C	-5.971511	-0.387983	1.441005
H	-7.521692	-0.027886	-0.796802
H	-6.505396	1.261401	-1.462706
H	-7.346873	1.502145	0.082145
H	-4.955280	0.936935	0.292917
H	-6.624320	-1.256002	1.307800
H	-6.482696	0.322328	2.105513
H	-5.048506	-0.710026	1.925635
S	3.233217	-1.630623	0.968316
O	4.573233	-1.815755	1.447152
O	3.138532	-1.096523	-0.429776
O	2.580171	-3.097531	0.905912
O	2.353529	-0.823152	1.848762
H	1.690817	-3.013433	0.476499
H	0.724528	-1.153558	2.118477
S	-2.058580	1.110731	0.530538
O	-0.774961	1.593154	1.066620
O	-3.204693	1.961327	0.780683
O	-1.917520	1.092572	-1.073205
O	-2.289707	-0.316575	0.903309
H	-1.153711	0.478764	-1.308190
H	-3.000280	-1.139093	-0.727134
S	0.104987	-1.969429	-1.509954
O	0.076951	-0.485024	-1.501089

O	-0.935357	-2.566807	-2.323249
O	1.487883	-2.354026	-2.208016
O	0.170092	-2.507753	-0.133401
H	2.211713	-1.950075	-1.663294
H	0.955245	1.439700	0.152837
C	1.890555	2.143700	-1.560883
N	1.916157	1.500251	-0.215770
C	2.779068	2.227893	0.759392
H	1.302077	1.514346	-2.224460
H	2.917437	2.217771	-1.915567
H	1.441595	3.130487	-1.448984
H	2.263144	0.526217	-0.307885
H	2.396245	3.241914	0.861979
H	3.794998	2.222395	0.362593
H	2.744132	1.692261	1.705312
C	-3.719605	-1.059036	-2.684261
N	-3.825555	-1.462640	-1.253970
C	-3.963611	-2.929209	-1.053082
H	-3.592511	0.020830	-2.722509
H	-4.634546	-1.353851	-3.199125
H	-2.851969	-1.549975	-3.120435
H	-4.621563	-0.921779	-0.785889
H	-4.039406	-3.129552	0.014999
H	-3.080061	-3.417355	-1.461751
H	-4.864548	-3.277368	-1.558515
C	-0.404397	-2.696013	2.930384
N	-0.220453	-1.269488	2.557913
C	-0.301863	-0.325756	3.703091
H	-0.396073	-3.286555	2.018176
H	-1.356464	-2.811719	3.449306
H	0.414507	-3.002308	3.580150
H	-0.928348	-0.997940	1.846591
H	0.515137	-0.534347	4.392635
H	-1.261585	-0.449437	4.204818
H	-0.221259	0.685518	3.311325
3SA7DMA			
C	-4.104760	3.275418	3.405847
N	-3.645392	3.695849	2.084275
C	-4.413554	4.821579	1.561518
H	-3.899462	4.063041	4.138328
H	-3.565180	2.377125	3.713627
H	-5.184702	3.054830	3.445203
H	-3.721896	2.907385	1.447200
H	-4.235444	5.709371	2.176868

H	-5.502434	4.643854	1.541364
H	-4.089757	5.052717	0.543382
C	5.038883	3.452250	-0.964820
N	5.304526	2.225175	-1.708790
C	6.471663	2.334990	-2.577268
H	5.836919	3.628987	-0.234864
H	4.094403	3.347345	-0.427152
H	4.970995	4.349813	-1.603983
H	4.483494	2.005266	-2.269019
H	7.377530	2.450432	-1.972498
H	6.426655	3.190255	-3.273635
H	6.578901	1.422283	-3.168367
C	4.684015	-4.291202	2.069967
N	4.055048	-3.125538	2.685220
C	4.102195	-3.173802	4.144055
H	5.762344	-4.277497	2.260886
H	4.532487	-4.263602	0.988515
H	4.292699	-5.252738	2.443730
H	3.085185	-3.074619	2.382411
H	5.139560	-3.095135	4.486368
H	3.682290	-4.101345	4.569026
H	3.546050	-2.330180	4.559900
C	-5.016433	-4.204062	-2.734731
N	-3.862412	-3.545158	-2.133303
C	-2.998918	-4.470660	-1.401616
H	-4.683091	-4.896443	-3.514575
H	-5.665144	-3.461100	-3.205749
H	-5.622539	-4.783313	-2.016447
H	-4.172021	-2.821067	-1.492020
H	-2.515364	-5.160108	-2.101592
H	-3.539625	-5.078691	-0.656596
H	-2.219472	-3.912108	-0.880001
S	1.551702	1.130826	-2.016294
O	1.898965	1.533556	-0.620056
O	2.493869	1.592347	-3.006478
O	1.693479	-0.477501	-2.029152
O	0.132336	1.418718	-2.294165
H	1.026200	-0.853949	-1.385423
H	-1.130117	0.191958	-2.305503
S	-3.511203	-0.097137	0.738174
O	-3.691520	-1.029701	-0.375765
O	-2.935962	-0.702690	1.939185
O	-2.898699	1.168022	0.317925
O	-5.005609	0.391759	1.189999

H	0.404965	1.903462	0.436311
H	-5.372075	-0.296759	1.761888
S	0.353144	-1.484837	1.064388
O	-0.150867	-1.314001	-0.323050
O	1.557689	-2.322269	1.110423
O	0.513706	-0.204928	1.753065
O	-0.750793	-2.335896	1.835053
H	2.984780	0.347664	0.169650
H	-1.573156	-1.788252	1.900596
C	-0.250113	2.715284	2.251011
N	-0.417847	2.419037	0.800701
C	-0.630907	3.635862	-0.030019
H	-1.139622	3.249003	2.585452
H	0.638947	3.332953	2.381705
H	-0.133750	1.769111	2.772386
H	-1.237795	1.797789	0.684556
H	0.243541	4.279652	0.060498
H	-1.518956	4.146494	0.337977
H	-0.746917	3.324067	-1.065002
C	-2.975337	0.375461	-3.210617
N	-1.923840	-0.436564	-2.544469
C	-1.420068	-1.576390	-3.363380
H	-3.310519	1.136652	-2.508952
H	-3.807867	-0.273151	-3.477703
H	-2.552105	0.840872	-4.099889
H	-2.317911	-0.795476	-1.659593
H	-0.600100	-2.040994	-2.821720
H	-1.062623	-1.191434	-4.317802
H	-2.234118	-2.292019	-3.484896
C	4.646592	-0.815600	-0.283330
N	3.577280	-0.360387	0.650509
C	4.084573	0.215721	1.923506
H	4.163609	-1.289269	-1.136579
H	5.281029	-1.528590	0.241035
H	5.202729	0.061780	-0.620670
H	2.947351	-1.154556	0.874864
H	4.735623	1.059286	1.696927
H	4.619878	-0.569583	2.454931
H	3.226008	0.541575	2.508738
3SA8DMA			
C	0.452434	5.412425	-2.340871
N	-0.536494	5.072329	-1.320263
C	-0.954903	6.234305	-0.542867
H	-0.007122	6.048675	-3.104606

H	0.809056	4.501695	-2.826566
H	1.330881	5.944720	-1.940756
H	-0.137544	4.375151	-0.696800
H	-1.492973	6.937477	-1.187074
H	-0.116579	6.782918	-0.080194
H	-1.637474	5.922614	0.252055
C	-3.839837	-2.047355	4.599032
N	-3.487058	-0.638394	4.439493
C	-4.302704	0.237255	5.275074
H	-3.583252	-2.382498	5.609440
H	-3.273387	-2.650409	3.886312
H	-4.912278	-2.250713	4.441152
H	-3.606513	-0.383891	3.462673
H	-4.083514	0.051518	6.331507
H	-5.388218	0.100763	5.131417
H	-4.062316	1.282574	5.064699
C	5.102760	2.179867	2.522919
N	5.339737	2.195776	1.083162
C	6.500004	2.999120	0.712595
H	5.911045	1.641186	3.030084
H	4.162421	1.663384	2.725445
H	5.043915	3.186545	2.972461
H	4.510393	2.565325	0.623017
H	7.413120	2.538554	1.104538
H	6.461347	4.034564	1.092837
H	6.587440	3.040816	-0.375723
C	4.686415	-4.448646	-2.514408
N	4.049371	-4.336991	-1.205037
C	4.063171	-5.599138	-0.470156
H	5.759590	-4.629906	-2.392760
H	4.562698	-3.513421	-3.065208
H	4.279900	-5.265116	-3.135178
H	3.086421	-4.033095	-1.329179
H	5.092650	-5.868992	-0.211489
H	3.630763	-6.443009	-1.033965
H	3.499949	-5.491152	0.459904
C	-5.152284	-0.334241	-4.765778
N	-3.952565	-0.510682	-3.956090
C	-3.138439	-1.645562	-4.385010
H	-4.872885	-0.057219	-5.787552
H	-5.760439	0.476646	-4.356896
H	-5.783360	-1.238239	-4.830293
H	-4.206572	-0.644148	-2.981929
H	-2.699994	-1.439309	-5.367083

H	-3.707116	-2.587781	-4.466486
H	-2.324028	-1.802108	-3.675157
S	1.591486	1.928224	-0.001401
O	1.950770	0.946371	1.062631
O	2.531444	3.016535	-0.138973
O	1.702016	1.107253	-1.381106
O	0.176380	2.333908	0.126433
H	1.029001	0.362116	-1.360529
H	-1.160579	1.739998	-0.965260
S	-3.483270	-1.077625	0.469954
O	-3.694249	-0.547770	-0.878689
O	-2.918954	-2.427646	0.500179
O	-2.841598	-0.110427	1.364807
O	-4.962695	-1.228911	1.151897
H	0.472468	0.229720	1.961423
H	-5.346107	-2.054469	0.825061
S	0.365769	-2.061033	-0.640435
O	-0.123063	-0.779807	-1.213866
O	1.568481	-2.545261	-1.329745
O	0.523448	-1.988586	0.811419
O	-0.747075	-3.149061	-0.972895
H	3.023795	-0.366661	0.452859
H	-1.565473	-2.926016	-0.459958
C	-0.124110	-0.910217	3.611560
N	-0.339377	0.164629	2.601665
C	-0.586117	1.502622	3.204007
H	-1.014042	-0.957452	4.240347
H	0.756391	-0.661407	4.204822
H	0.030332	-1.842159	3.074480
H	-1.160287	-0.086270	2.022072
H	0.285312	1.789473	3.791898
H	-1.466743	1.435362	3.840237
H	-0.732515	2.216486	2.397483
C	-2.987709	2.637708	-1.323633
N	-1.961503	1.594910	-1.606168
C	-1.476062	1.602673	-3.017220
H	-3.322637	2.512565	-0.295220
H	-3.827174	2.491182	-2.001470
H	-2.523415	3.614696	-1.467452
H	-2.371521	0.671867	-1.387134
H	-0.664358	0.884131	-3.098256
H	-1.123293	2.605290	-3.253213
H	-2.302623	1.294962	-3.658921
C	4.662139	-0.588897	-0.805214

N	3.604648	-1.147160	0.085491
C	4.129031	-1.943604	1.226267
H	4.168298	-0.104882	-1.646262
H	5.289055	-1.409249	-1.151314
H	5.229519	0.152709	-0.239012
H	2.960921	-1.745272	-0.468687
H	4.803493	-1.321237	1.813367
H	4.641984	-2.812105	0.816053
H	3.281125	-2.264176	1.829751

4DMA

C	-0.195554	3.258121	-0.779933
N	-0.179458	2.193655	0.217309
C	-0.163995	2.710202	1.581572
H	-1.134986	3.817878	-0.717938
H	-0.130511	2.826488	-1.781628
H	0.629371	3.982902	-0.665385
H	0.644660	1.599686	0.071141
H	-1.102137	3.232686	1.797647
H	0.660951	3.417491	1.776395
H	-0.073238	1.881394	2.287963
C	0.193559	-3.257656	-0.779618
N	0.179750	-2.193321	0.217766
C	0.167805	-2.709757	1.582041
H	1.133526	-3.816846	-0.720581
H	0.125199	-2.825957	-1.781061
H	-0.630546	-3.983020	-0.662783
H	-0.644535	-1.599365	0.073415
H	1.105938	-3.233453	1.795157
H	-0.657445	-3.415959	1.779506
H	0.080381	-1.880838	2.288734
C	3.258367	0.193995	0.779470
N	2.194634	0.179878	-0.218537
C	2.711938	0.165736	-1.582487
H	3.983362	-0.630587	0.663667
H	2.825979	0.126533	1.780661
H	3.818066	1.133631	0.720042
H	1.599910	-0.643762	-0.073406
H	3.417904	-0.660116	-1.778312
H	3.236201	1.103308	-1.796642
H	1.883406	0.077638	-2.289538
C	-2.713043	-0.167394	-1.581252
N	-2.195300	-0.180195	-0.217419
C	-3.258814	-0.193241	0.780909
H	-3.238101	-1.104842	-1.794006

H -1.884678 -0.080889 -2.288709
H -3.418433 0.658748 -1.777887
H -1.600722 0.643700 -0.073386
H -3.818853 -1.132711 0.722171
H -3.983509 0.631531 0.664762
H -2.826114 -0.125426 1.781947

4SA

S -1.675947 1.783399 -1.378037
O -0.943518 1.580619 -0.131993
O -1.733535 3.073251 -1.965417
O -1.124545 0.702497 -2.394366
O -3.147066 1.277984 -1.181972
H -0.194339 0.463227 -2.165468
H -3.146860 0.465154 -0.628120
S 1.899532 -1.417316 -1.570229
O 1.370377 -0.042713 -1.526733
O 2.911979 -1.748645 -2.500149
O 2.386595 -1.755805 -0.112866
O 0.687595 -2.384906 -1.816568
H 1.953372 -1.170387 0.560063
H 0.041920 -2.344641 -1.071637
S -1.847409 -1.601601 1.178711
O -0.769160 -2.244615 0.459667
O -2.889547 -0.945893 0.451686
O -2.603312 -2.665640 2.073597
O -1.230026 -0.680724 2.279398
H -1.966244 -3.180954 2.593628
H -0.308999 -0.371948 2.028478
S 1.788021 1.404384 1.666738
O 1.221001 0.037043 1.583309
O 2.734703 1.694918 2.676387
O 2.412581 1.704707 0.258759
O 0.596821 2.402698 1.809574
H 2.014705 1.135591 -0.450817
H -0.068250 2.263884 1.080463

4SA1DMA

S 0.302579 2.654666 -0.576085
O 0.920076 3.917169 -0.758219
O 0.949431 1.627781 0.242122
O -1.131831 2.893923 0.035426
O 0.031722 2.051744 -2.002908
H -1.505667 2.061186 0.416151
H -0.338150 1.130159 -1.964779
S 3.790227 -0.513403 0.280457

O	5.181563	-0.748909	0.417988
O	2.872079	-0.854782	1.357825
O	3.599767	1.017297	-0.053932
O	3.305412	-1.258735	-1.026093
H	2.654313	1.285439	0.054607
H	2.327223	-1.383511	-1.010911
S	-3.440123	0.037646	0.642555
O	-2.099636	0.537322	0.992131
O	-4.569733	0.568412	1.311084
O	-3.611569	0.231292	-0.906138
O	-3.424221	-1.519021	0.850440
H	-2.751082	0.042048	-1.378308
H	-2.771461	-1.947577	0.223521
S	-0.626782	-1.635750	-1.502439
O	0.611065	-1.488664	-0.760904
O	-1.208152	-0.335417	-1.937963
O	-0.174986	-2.401797	-2.835240
O	-1.640069	-2.465594	-0.848575
H	-0.955554	-2.594627	-3.376479
H	-0.459240	-0.221924	1.604184
C	0.496402	0.269664	3.364541
N	0.273673	-0.630231	2.197847
C	-0.104850	-2.027789	2.550553
H	0.755501	1.255469	2.984118
H	1.317451	-0.125019	3.960328
H	-0.415785	0.321689	3.957308
H	1.148771	-0.657971	1.641472
H	-0.225250	-2.589267	1.626679
H	-1.039754	-2.016716	3.109115
H	0.691898	-2.465714	3.149354
4SA2DMA			
S	4.228417	-0.238587	0.285704
O	3.373637	0.864496	-0.125384
O	5.479814	0.027491	0.901240
O	3.391563	-1.166504	1.253067
O	4.499788	-1.149580	-0.972339
H	2.459233	-1.251263	0.916017
H	3.637841	-1.435539	-1.375529
S	-2.597633	1.357291	-1.243285
O	-3.245747	0.804595	-0.050709
O	-1.575087	2.365399	-0.972568
O	-2.145554	0.314380	-2.178424
O	-3.825858	2.115129	-1.974324
H	-0.522674	-0.045259	-2.094906

H	-3.494939	2.497005	-2.799886
S	-1.382124	0.252236	2.664946
O	-0.220353	0.619598	1.634665
O	-1.927748	-1.026456	2.245944
O	-0.924537	0.425203	4.000372
O	-2.407953	1.396956	2.366381
H	-1.755550	-2.426801	-0.580982
H	-2.789995	1.269201	1.449079
S	0.791427	-1.545821	-1.244381
O	-0.338719	-2.426704	-1.524570
O	2.065755	-1.954510	-1.801188
O	0.457140	-0.135402	-1.927956
O	0.906991	-1.251626	0.220935
H	0.169854	2.216723	-0.476821
H	0.114946	-0.185063	1.139670
C	-3.790086	-2.403336	-0.995447
N	-2.648933	-2.473072	-0.040481
C	-2.620022	-3.693635	0.812785
H	-3.665194	-1.512511	-1.605431
H	-4.723251	-2.353456	-0.436076
H	-3.773943	-3.293560	-1.623306
H	-2.642906	-1.651878	0.583414
H	-2.511181	-4.568897	0.173927
H	-3.545107	-3.754184	1.384359
H	-1.774983	-3.613051	1.492430
C	1.626701	3.054458	-1.674581
N	1.163559	2.487221	-0.377642
C	1.304965	3.407454	0.785349
H	1.488149	2.295720	-2.441513
H	2.682359	3.305228	-1.589980
H	1.035786	3.939526	-1.905311
H	1.725401	1.641173	-0.196801
H	0.714324	4.303615	0.600724
H	2.356959	3.660305	0.906823
H	0.936700	2.892687	1.669440
4SA3DMA			
S	-4.767861	-0.817303	-0.502366
O	-6.016461	-0.931299	-1.170582
O	-4.274706	0.496353	-0.115844
O	-4.826863	-1.723898	0.783435
O	-3.664423	-1.498860	-1.402346
H	-3.941625	-1.739099	1.243076
H	-2.758509	-1.351570	-0.996507
S	4.311428	-0.212272	-0.829625

O	5.688742	-0.513905	-1.074461
O	4.057454	0.757045	0.287761
O	3.778174	0.524244	-2.156107
O	3.427471	-1.390360	-0.630955
H	2.868580	0.862388	-1.973498
H	1.890538	-1.531422	-1.288592
S	-1.199374	-1.196970	1.208961
O	0.104941	-1.734422	1.593842
O	-2.355724	-1.838236	1.813410
O	-1.263089	0.312231	1.721579
O	-1.315690	-1.122191	-0.283576
H	-0.399125	0.766718	1.462537
H	-1.543373	2.730948	-0.159383
S	1.128475	2.119656	-0.240819
O	0.958723	1.378282	1.034836
O	0.100837	3.140931	-0.428037
O	2.490538	2.916129	-0.094205
O	1.271506	1.205520	-1.384516
H	3.211625	2.241347	0.043483
H	1.743177	-0.901325	1.913121
C	2.512228	0.208151	3.480263
N	2.677890	-0.654180	2.279184
C	3.441126	-1.907324	2.529449
H	1.967955	1.099789	3.179868
H	3.497219	0.478136	3.859704
H	1.955577	-0.339480	4.240207
H	3.154221	-0.105879	1.526275
H	2.894396	-2.521624	3.244001
H	4.422659	-1.650093	2.926181
H	3.556000	-2.424325	1.580061
C	-2.989924	3.179266	1.270596
N	-2.581284	2.656943	-0.063346
C	-3.207841	3.362984	-1.214682
H	-2.516892	2.565049	2.033588
H	-4.072293	3.104564	1.360373
H	-2.666283	4.215369	1.360478
H	-2.862358	1.664481	-0.105853
H	-2.820501	2.932403	-2.136361
H	-2.947730	4.419487	-1.167911
H	-4.286686	3.227114	-1.168335
C	0.918642	-1.499308	-3.131102
N	0.988500	-1.880064	-1.695251
C	0.920721	-3.343889	-1.441651
H	0.910535	-0.413963	-3.193328

H	0.007206	-1.907703	-3.567720
H	1.792591	-1.895244	-3.646602
H	0.212003	-1.427615	-1.177681
H	1.786604	-3.824300	-1.894963
H	-0.000559	-3.742772	-1.865040
H	0.925486	-3.499835	-0.364810
4SA4DMA			
S	3.911153	0.296477	0.069998
O	5.070019	0.763299	0.772866
O	3.975999	-1.055004	-0.500850
O	2.725639	0.234856	1.198476
O	3.364264	1.262431	-0.938264
H	1.878078	0.162363	0.688634
H	1.326900	-2.944675	0.225945
C	2.948609	-3.813245	1.149569
N	2.310433	-3.170113	-0.028814
C	2.317699	-4.006106	-1.260001
H	2.914022	-3.115024	1.983547
H	3.985938	-4.045052	0.911860
H	2.399977	-4.718710	1.404226
H	2.821729	-2.281003	-0.226774
H	1.854062	-3.430870	-2.057420
H	1.749875	-4.917478	-1.075113
H	3.348420	-4.247241	-1.517636
S	0.266075	-0.125167	-1.670999
O	0.366855	-1.573741	-1.892724
O	-0.995062	0.439666	-2.163935
O	0.529376	0.251990	-0.267915
O	1.389627	0.568080	-2.552096
H	-0.978850	1.066274	1.777796
H	2.220512	0.710327	-2.012272
S	-1.999569	2.995266	0.160195
O	-2.980503	1.891961	0.228831
O	-2.514676	4.322179	0.345137
O	-0.831124	2.675060	1.045440
O	-1.407591	2.975993	-1.338458
H	0.767542	2.942392	0.368731
H	-1.273635	2.040532	-1.642734
S	-1.583094	-3.081742	0.622695
O	-2.328668	-4.212064	1.097267
O	-0.196614	-2.956353	1.106412
O	-1.501684	-3.264276	-0.976055
O	-2.295073	-1.770096	0.812764
H	-0.848286	-2.615573	-1.346870

H	-3.221646	-1.055350	-0.424192
C	-0.080441	-0.211638	3.175521
N	-1.239274	0.242460	2.363800
C	-2.423587	0.619660	3.180666
H	-0.382727	-1.069065	3.775448
H	0.245393	0.602908	3.822236
H	0.725818	-0.506298	2.511396
H	-1.520699	-0.523695	1.710148
H	-2.135478	1.395656	3.889329
H	-2.786087	-0.259992	3.711472
H	-3.185001	1.008714	2.509141
C	-3.882133	-0.771117	-2.398555
N	-3.868630	-0.422457	-0.951592
C	-5.201133	-0.489707	-0.297568
H	-2.876312	-0.637541	-2.788119
H	-4.576630	-0.109996	-2.917256
H	-4.199155	-1.807672	-2.508211
H	-3.474233	0.526160	-0.789626
H	-5.087588	-0.224078	0.750930
H	-5.589470	-1.504261	-0.379448
H	-5.877236	0.213860	-0.782038
C	1.587446	4.362539	-0.904063
N	1.722226	3.282126	0.111873
C	2.423473	3.697530	1.357384
H	1.029121	3.970207	-1.750643
H	2.581136	4.683209	-1.214736
H	1.036158	5.194412	-0.467697
H	2.257363	2.490729	-0.303336
H	1.838975	4.470849	1.853953
H	3.414348	4.070788	1.101950
H	2.525483	2.823406	1.997412

4SA5DMA

C	-4.243893	-0.365002	-2.552672
N	-4.363159	0.484280	-1.359125
C	-5.617490	1.248059	-1.324003
H	-4.992638	-1.162077	-2.520832
H	-3.252267	-0.818559	-2.578588
H	-4.391081	0.200516	-3.483506
H	-3.592510	1.155248	-1.359290
H	-6.466953	0.570175	-1.193000
H	-5.784069	1.822022	-2.246213
H	-5.588466	1.947188	-0.486690
S	-1.995788	2.686261	0.461782
O	-3.225870	3.077099	1.103687

O	-0.806657	3.480628	0.801019
O	-1.715201	1.190936	1.057773
O	-2.114703	2.479394	-1.007196
H	-0.949202	0.817689	0.552436
H	2.362267	2.601843	0.443138
C	2.288943	4.518334	1.192241
N	1.871394	3.495256	0.198567
C	2.173817	3.868508	-1.210621
H	2.030680	4.161644	2.187295
H	1.761476	5.450042	0.991749
H	3.366045	4.665012	1.124198
H	0.845627	3.341139	0.310344
H	1.759883	3.110444	-1.871376
H	3.253767	3.924769	-1.338529
H	1.712795	4.831974	-1.427607
S	0.434446	0.290469	-1.788277
O	1.777135	0.120452	-2.347203
O	-0.473703	-0.804800	-2.153505
O	0.455238	0.550047	-0.333289
O	-0.105176	1.622281	-2.471774
H	0.320827	-1.123937	1.927178
H	-0.890003	1.973551	-1.949024
S	-0.990774	-3.096700	0.662723
O	0.457336	-3.307496	0.458550
O	-1.728885	-4.230565	1.149271
O	-1.204980	-1.843196	1.449400
O	-1.625831	-2.790347	-0.785047
H	-2.881841	-1.035805	1.161146
H	-1.155923	-2.032675	-1.220835
S	4.090020	0.409214	0.371923
O	5.483144	0.310378	0.705181
O	3.326543	1.404475	1.162850
O	4.042160	0.925016	-1.155014
O	3.344581	-0.885041	0.368883
H	3.182546	0.660717	-1.570657
H	2.794047	-1.936426	-1.033542
C	0.996500	0.486500	3.064214
N	1.228370	-0.769763	2.300963
C	1.860399	-1.850359	3.103783
H	1.959518	0.918228	3.326687
H	0.415844	0.251753	3.956305
H	0.435132	1.176744	2.440575
H	1.840586	-0.583156	1.484404
H	1.231364	-2.064323	3.967506

H	2.848915	-1.525749	3.424686
H	1.933633	-2.735690	2.477619
C	2.183766	-2.998796	-2.753905
N	2.489630	-2.891990	-1.301145
C	3.531534	-3.839635	-0.822801
H	1.393673	-2.293159	-2.994789
H	1.863900	-4.018568	-2.968007
H	3.078971	-2.758650	-3.326141
H	1.621426	-3.051920	-0.741756
H	3.730346	-3.627619	0.224781
H	4.443254	-3.690897	-1.400310
H	3.169556	-4.860002	-0.942549
C	-4.537464	-2.244157	0.949233
N	-3.902534	-0.902830	1.046509
C	-4.411453	-0.071594	2.169892
H	-4.097721	-2.776407	0.108646
H	-5.610829	-2.119807	0.803831
H	-4.343443	-2.807203	1.860936
H	-4.054925	-0.372769	0.120310
H	-4.172296	-0.559994	3.114882
H	-5.492884	0.029545	2.074125
H	-3.940386	0.907339	2.118785

4SA6DMA

C	4.941800	-2.564914	2.429920
N	5.140823	-2.425018	0.989454
C	6.486378	-2.811335	0.574158
H	4.971454	-3.623090	2.713023
H	3.962153	-2.163435	2.696497
H	5.703245	-2.039647	3.031147
H	4.978294	-1.449944	0.745219
H	6.632113	-3.885096	0.732448
H	7.286348	-2.283653	1.121051
H	6.616958	-2.611063	-0.492215
C	2.354568	3.848761	-3.337696
N	2.586241	3.626917	-1.905157
C	3.715319	4.404700	-1.379650
H	2.040212	4.882921	-3.507066
H	1.560122	3.184247	-3.681706
H	3.252001	3.666306	-3.946053
H	2.786267	2.639184	-1.760420
H	3.480387	5.472796	-1.417943
H	4.642137	4.242609	-1.947927
H	3.893218	4.120995	-0.341445
S	-1.816009	-3.738300	-0.895122

O	-1.788396	-5.135456	-0.574269
O	-3.108161	-3.173388	-1.306024
O	-1.438324	-2.972364	0.504592
O	-0.729592	-3.291732	-1.825570
H	-1.213775	-2.043313	0.241754
H	-3.854675	-0.432636	0.461868
C	-5.144994	-1.913986	1.069094
N	-4.433292	-1.167048	-0.000777
C	-5.330508	-0.522019	-0.996874
H	-4.401833	-2.375782	1.716313
H	-5.762216	-2.688375	0.615634
H	-5.756373	-1.219867	1.643695
H	-3.809053	-1.839101	-0.500399
H	-4.707884	-0.049220	-1.752284
H	-5.942396	0.225751	-0.493925
H	-5.960041	-1.285487	-1.453041
S	-0.967393	0.163275	-1.591558
O	-2.364626	0.597637	-1.702678
O	-0.009774	1.263163	-1.786036
O	-0.692074	-0.582863	-0.348691
O	-0.681230	-0.830701	-2.796913
H	0.714358	-0.068569	2.015920
H	-0.838801	-1.776983	-2.509308
S	2.805020	0.635999	0.482199
O	2.188854	1.872802	0.964422
O	4.246181	0.552811	0.557052
O	2.116200	-0.563384	1.052609
O	2.500244	0.572553	-1.116314
H	1.826324	-1.967676	-0.054464
H	1.545346	0.788873	-1.295380
S	-2.940377	2.130574	1.410727
O	-3.593987	3.104458	2.241452
O	-3.315403	0.721128	1.653635
O	-3.426228	2.471911	-0.092589
O	-1.452697	2.256332	1.372916
H	-3.002164	1.826706	-0.713427
H	-0.079907	2.937771	0.014830
C	-0.833798	-0.800903	3.216595
N	-0.014048	0.306291	2.660336
C	0.653975	1.131289	3.701903
H	-1.638452	-0.379797	3.816768
H	-0.198854	-1.441950	3.828896
H	-1.261208	-1.374940	2.400221
H	-0.616580	0.942856	2.085396

H	1.272907	0.487125	4.326553
H	-0.105930	1.623543	4.307905
H	1.278637	1.864171	3.198199
C	-0.854232	4.385688	-1.215628
N	0.216936	3.859706	-0.328267
C	0.502796	4.714546	0.852396
H	-0.976774	3.686613	-2.039973
H	-0.557246	5.366141	-1.588582
H	-1.785517	4.453498	-0.656953
H	1.107895	3.729811	-0.897757
H	1.321122	4.257894	1.404912
H	-0.388640	4.763459	1.475015
H	0.787754	5.710608	0.512662
C	2.778094	-2.763886	-1.716217
N	1.773845	-2.840942	-0.617483
C	1.978199	-4.006335	0.289122
H	2.600771	-1.851917	-2.281931
H	2.663658	-3.638083	-2.356408
H	3.767683	-2.739551	-1.262696
H	0.822484	-2.911950	-1.031292
H	2.974856	-3.924472	0.720296
H	1.875942	-4.923170	-0.290266
H	1.206821	-3.982097	1.056479
4SA7DMA			
C	6.216997	-0.310614	-2.829614
N	5.755872	-0.599689	-1.475147
C	6.778987	-1.261316	-0.667012
H	7.017992	0.435512	-2.798266
H	5.397234	0.104147	-3.422018
H	6.608860	-1.194573	-3.361398
H	4.934364	-1.197045	-1.517168
H	7.593804	-0.561534	-0.452239
H	7.218360	-2.145787	-1.158074
H	6.342052	-1.590070	0.277199
C	2.816323	4.198695	3.181109
N	3.057358	4.353211	1.749539
C	3.889110	5.512986	1.444926
H	3.750734	3.947317	3.695317
H	2.107752	3.382967	3.338409
H	2.408131	5.105595	3.659401
H	2.155702	4.449865	1.286982
H	4.899038	5.362163	1.840615
H	3.504461	6.457372	1.867195
H	3.971384	5.635386	0.362117

C	-2.891459	3.499089	-3.806253
N	-2.796724	3.568892	-2.343512
C	-3.259238	4.853457	-1.801471
H	-3.941543	3.530133	-4.111722
H	-2.458601	2.559508	-4.154654
H	-2.371482	4.328874	-4.306174
H	-1.822675	3.444225	-2.073340
H	-4.333403	4.964952	-1.978637
H	-2.750283	5.713226	-2.259428
H	-3.073978	4.873866	-0.727039
S	2.722720	-2.851727	-0.078689
O	3.984999	-3.244711	0.480598
O	1.866318	-3.922817	-0.602993
O	1.887875	-2.192945	1.159944
O	2.816929	-1.724217	-1.064569
H	1.129028	-1.712089	0.739147
H	-1.276102	-3.772274	0.560365
C	-0.382836	-5.419061	1.410875
N	-0.668204	-4.555906	0.235010
C	-1.341613	-5.259007	-0.890069
H	0.141043	-4.822370	2.155132
H	0.249720	-6.249733	1.100917
H	-1.322703	-5.782463	1.823570
H	0.238444	-4.170397	-0.107987
H	-1.458657	-4.550309	-1.706017
H	-2.316738	-5.612370	-0.557221
H	-0.720743	-6.096668	-1.206523
S	-0.551507	-0.909782	-1.455604
O	-1.333193	-2.130215	-1.684570
O	-1.280203	0.311501	-1.828386
O	-0.000723	-0.827091	-0.089162
O	0.690093	-0.943696	-2.447968
H	-0.563107	0.802613	2.095957
H	1.475363	-1.374176	-2.003200
S	-0.350299	2.953772	0.501195
O	-1.779876	2.738969	0.734225
O	0.129508	4.312435	0.617530
O	0.470046	1.968122	1.270201
O	-0.088133	2.588687	-1.063556
H	1.934778	1.231658	0.446947
H	-0.506964	1.713657	-1.285226
S	-3.574529	-2.099995	1.012201
O	-4.842454	-2.400060	1.618914
O	-2.420274	-2.875327	1.514067

O	-3.749662	-2.513573	-0.542901
O	-3.236030	-0.646313	0.985574
H	-2.896856	-2.329492	-1.010107
H	-3.226992	0.813356	-0.467691
C	-0.536192	-0.843738	3.386195
N	-1.241950	0.235651	2.649164
C	-2.015076	1.150081	3.530686
H	-1.270085	-1.462020	3.900423
H	0.151891	-0.396221	4.103762
H	0.012957	-1.457250	2.678883
H	-1.907304	-0.183886	1.956797
H	-1.343852	1.586620	4.270403
H	-2.803214	0.584650	4.026904
H	-2.436864	1.935963	2.909727
C	-4.549034	0.449253	-1.994654
N	-3.949364	1.344370	-0.969874
C	-4.919056	1.856760	0.032016
H	-3.754590	0.133801	-2.667499
H	-5.315777	0.998470	-2.541522
H	-4.977166	-0.423701	-1.505737
H	-3.478212	2.165619	-1.458317
H	-4.381372	2.516291	0.709754
H	-5.335886	1.015033	0.581679
H	-5.707058	2.407717	-0.482061
C	3.261817	1.885596	-1.012113
N	2.861356	0.945185	0.075923
C	3.844821	0.915657	1.198305
H	2.486028	1.883018	-1.774773
H	4.213782	1.538612	-1.411267
H	3.354141	2.878223	-0.575095
H	2.778516	-0.009051	-0.316193
H	3.893243	1.919052	1.620671
H	4.805595	0.609690	0.787638
H	3.504184	0.189021	1.934189

4SA8DMA

C	-0.647328	-5.233086	-1.167148
N	-0.361917	-4.237482	-0.137159
C	-0.853324	-4.642641	1.178329
H	-0.060831	-6.139329	-0.980126
H	-0.368243	-4.841827	-2.147025
H	-1.709832	-5.524093	-1.213565
H	-0.814385	-3.364611	-0.396148
H	-0.302049	-5.524373	1.525081
H	-1.924894	-4.907499	1.180482

H	-0.693227	-3.834580	1.893610
C	-4.110940	2.773601	2.989567
N	-4.087551	1.342643	3.317765
C	-4.682268	1.044890	4.623196
H	-5.147555	3.114864	2.906446
H	-3.616015	2.940029	2.030967
H	-3.616477	3.388647	3.756159
H	-3.121910	1.010159	3.316962
H	-5.754410	1.263358	4.603641
H	-4.233570	1.631834	5.438260
H	-4.548513	-0.014051	4.852678
C	3.835434	4.676276	-2.197686
N	3.551263	4.253768	-0.822864
C	4.238752	5.083405	0.172349
H	3.428232	5.676580	-2.375631
H	3.362732	3.983399	-2.896942
H	4.912201	4.706843	-2.419289
H	3.871662	3.288801	-0.706901
H	3.838860	6.102318	0.154959
H	5.322816	5.143767	-0.002345
H	4.078333	4.664706	1.167546
C	7.163057	-1.426383	0.572704
N	6.033493	-2.274683	0.201611
C	6.393323	-3.275760	-0.796245
H	7.912700	-2.017642	1.109477
H	6.820615	-0.627869	1.233865
H	7.662827	-0.957836	-0.292058
H	5.284686	-1.687621	-0.158765
H	7.101289	-3.992506	-0.366854
H	6.861143	-2.852273	-1.702395
H	5.503589	-3.831662	-1.103745
S	-3.048599	-1.674300	-2.660176
O	-1.780675	-2.057548	-2.035610
O	-2.971488	-0.388652	-3.376387
O	-3.183785	-2.804170	-3.840687
O	-4.225462	-1.812547	-1.816312
H	-4.025321	-2.644465	-4.289440
H	-3.798049	0.049888	0.473567
C	-5.857547	0.017464	0.306007
N	-4.604514	-0.258794	1.053557
C	-4.413316	-1.686467	1.429487
H	-5.892782	1.079672	0.065370
H	-6.714068	-0.250321	0.926029
H	-5.849688	-0.565622	-0.612821

H	-4.541796	0.347048	1.930241
H	-3.487742	-1.759395	1.998587
H	-4.353231	-2.279535	0.519106
H	-5.256217	-2.007810	2.043311
S	3.150266	0.661663	-0.031369
O	4.357936	1.425275	-0.296939
O	3.326307	-0.797364	-0.227394
O	2.879867	0.866398	1.538303
O	1.949377	1.155195	-0.731925
H	1.909394	0.750825	1.777292
H	0.925300	-0.021695	-1.658980
S	-0.374635	-0.562199	2.407815
O	-0.622376	-0.986452	0.866915
O	0.410707	0.687191	2.361443
O	-1.682969	-0.392417	3.024344
O	0.392663	-1.702182	2.926379
H	0.389437	3.078151	-0.789551
H	1.888222	-2.173469	2.308098
S	-2.224923	2.010239	-0.983420
O	-0.912805	2.073322	-1.647509
O	-2.560440	3.193155	-0.211344
O	-3.342181	1.927618	-2.115929
O	-2.357605	0.737756	-0.216950
H	-3.237038	1.068091	-2.613714
H	-1.193844	-0.300966	0.432780
C	0.062720	5.096440	-0.996380
N	0.746224	3.945975	-0.349308
C	0.500749	3.865043	1.117469
H	0.277569	5.076806	-2.063971
H	0.434267	6.024931	-0.561508
H	-1.009784	4.998784	-0.838047
H	1.792618	4.009733	-0.532039
H	-0.572884	3.811101	1.286326
H	0.919843	4.751023	1.595734
H	0.971102	2.965456	1.504207
C	0.543917	0.146403	-3.681128
N	0.555455	-0.633948	-2.413882
C	1.361582	-1.884012	-2.483321
H	-0.053863	1.038609	-3.516352
H	0.101093	-0.464036	-4.466772
H	1.569122	0.412606	-3.937578
H	-0.415593	-0.918510	-2.180883
H	1.206572	-2.445388	-1.564380
H	2.412915	-1.625308	-2.583861

H	1.016120	-2.470790	-3.333564
C	3.882602	-2.190124	2.924806
N	2.817308	-2.466524	1.923425
C	2.745769	-3.884708	1.480602
H	3.849058	-1.129697	3.169052
H	4.842679	-2.440203	2.472923
H	3.697049	-2.786865	3.817867
H	2.990473	-1.857859	1.094483
H	1.910552	-3.994655	0.783963
H	2.579732	-4.517995	2.352490
H	3.691279	-4.147435	1.007237

5DMA

C	-0.048810	-3.860213	0.449811
N	0.016226	-2.434984	0.753784
C	-0.003348	-2.169558	2.188053
H	0.856552	-4.363080	0.806524
H	-0.105584	-4.004236	-0.631866
H	-0.913159	-4.370987	0.909094
H	-0.778376	-1.955367	0.314686
H	0.905426	-2.561725	2.657592
H	-0.865372	-2.621533	2.709249
H	-0.030318	-1.090878	2.359865
C	2.324152	-1.080358	-2.037174
N	2.373399	-0.878215	-0.593487
C	3.648889	-1.289902	-0.017574
H	3.045285	-0.423294	-2.535405
H	1.328541	-0.827029	-2.409330
H	2.551817	-2.115429	-2.346663
H	1.613698	-1.410150	-0.152765
H	4.453724	-0.642540	-0.382369
H	3.927235	-2.330748	-0.258937
H	3.610624	-1.192990	1.070108
C	-2.388390	-1.049035	-2.003120
N	-2.378937	-0.894625	-0.552568
C	-3.673553	-1.197990	0.047705
H	-2.540251	-2.100508	-2.270128
H	-1.424291	-0.737035	-2.411803
H	-3.178592	-0.463424	-2.504606
H	-2.113208	0.068968	-0.318142
H	-3.910397	-2.259344	-0.083501
H	-4.507460	-0.617638	-0.384352
H	-3.638895	-0.994569	1.120677
C	2.125739	2.982178	-0.784057
N	1.576881	2.054499	0.199730

C	2.082360	2.312676	1.544098
H	1.775794	3.999720	-0.579170
H	1.781438	2.705867	-1.783597
H	3.229312	3.008849	-0.797459
H	1.822408	1.094851	-0.070364
H	1.727359	3.285660	1.900666
H	3.184519	2.319786	1.607231
H	1.709223	1.549080	2.230918
C	-2.028205	2.999121	-0.859013
N	-1.576548	2.058882	0.161568
C	-2.044739	2.422837	1.494902
H	-3.117877	2.951155	-0.959540
H	-1.592331	2.732307	-1.824754
H	-1.762163	4.048214	-0.641452
H	-0.550363	2.031004	0.162949
H	-3.136217	2.345534	1.545202
H	-1.772603	3.450270	1.793409
H	-1.627212	1.733803	2.233050
5SA			
S	-3.924222	-1.496927	-0.382422
O	-4.469972	-2.795769	-0.486693
O	-2.874223	-1.226100	0.612601
O	-3.340376	-1.076637	-1.789929
O	-5.100686	-0.487889	-0.127848
H	-2.695363	-0.343191	-1.692337
H	-4.772749	0.442346	-0.097958
S	4.248896	-0.982314	-0.564014
O	5.159297	-1.940554	-1.081888
O	2.920292	-0.856280	-1.149786
O	4.060133	-1.149355	1.010111
O	4.939908	0.420066	-0.589956
H	3.357422	-1.810803	1.192089
H	4.283631	1.141492	-0.444069
S	0.497125	-1.969201	0.782678
O	0.169106	-0.647566	1.294652
O	1.666989	-2.622588	1.297399
O	-0.730705	-2.897475	1.010453
O	0.541913	-1.916475	-0.785457
H	-1.572752	-2.383588	0.914201
H	1.433567	-1.557864	-1.064766
S	-2.381235	2.053594	0.070036
O	-3.797107	1.951118	-0.152860
O	-1.731993	3.328500	0.129068
O	-1.975351	1.306184	1.392740

O	-1.729418	1.162355	-1.077129
H	-2.244651	0.358575	1.338606
H	-0.729370	1.277614	-1.080347
S	1.639577	2.295379	0.035849
O	0.828726	1.576407	-0.931659
O	3.042165	2.420252	-0.215182
O	1.099379	3.757513	0.208646
O	1.393483	1.685846	1.456303
H	0.117339	3.750181	0.264140
H	0.968201	0.784311	1.407712

5SA1DMA

S	3.784419	-1.552807	-0.147410
O	5.141025	-1.882191	0.099432
O	3.387257	-0.917067	-1.390364
O	2.939842	-2.871045	0.060321
O	3.220952	-0.659583	1.051789
H	2.003419	-2.724133	-0.222575
H	2.939736	0.238058	0.768575
S	-2.737091	2.119967	-0.710338
O	-3.387543	3.353596	-0.957120
O	-1.597031	2.065159	0.207347
O	-3.794745	1.084314	-0.170153
O	-2.294724	1.539053	-2.104087
H	-3.347810	0.324722	0.280866
H	-1.882447	0.640419	-2.046056
S	1.824033	2.998579	0.319965
O	2.851251	3.969641	0.401295
O	1.921500	1.780395	1.134994
O	0.463690	3.707766	0.671409
O	1.645638	2.541609	-1.174573
H	-0.323275	3.155140	0.420405
H	1.240503	1.635560	-1.198686
S	-2.822752	-2.399212	0.662978
O	-2.439412	-0.999954	0.922435
O	-3.891082	-2.971340	1.393676
O	-3.126265	-2.519981	-0.872151
O	-1.537926	-3.274310	0.889621
H	-2.460309	-2.006531	-1.405708
H	-0.796819	-2.961046	0.297383
S	0.151687	-1.065817	-1.514318
O	0.553293	0.147544	-0.810296
O	-1.224510	-1.001803	-2.034756
O	1.060069	-1.225808	-2.791024
O	0.362409	-2.271533	-0.669464

H	2.002187	-1.142880	-2.499036
H	-0.896529	-0.121502	1.667641
C	-0.844112	1.168185	3.282370
N	-0.183918	0.239380	2.317565
C	0.514515	-0.912752	2.962493
H	-1.353633	1.943327	2.715478
H	-0.081863	1.607716	3.923425
H	-1.561769	0.606125	3.878086
H	0.498625	0.773628	1.751282
H	1.013432	-1.492630	2.191004
H	-0.219933	-1.522595	3.485715
H	1.257250	-0.528686	3.659387

5SA2DMA

S	4.953864	1.158465	0.634748
O	6.224498	1.708889	0.940407
O	4.284998	1.452660	-0.624189
O	5.073289	-0.403826	0.770099
O	3.953099	1.558935	1.804416
H	4.295517	-0.867144	0.360462
H	3.032855	1.646250	1.445910
S	-5.539085	-0.229969	0.586328
O	-4.974903	0.586625	-0.479953
O	-6.846411	0.036901	1.068973
O	-5.490618	-1.736791	0.133956
O	-4.540318	-0.163549	1.812372
H	-4.575656	-1.979455	-0.166651
H	-3.601129	-0.228378	1.480483
S	2.665719	-2.347580	-1.373613
O	3.683835	-3.164767	-1.926971
O	2.876636	-1.678777	-0.085801
O	2.306243	-1.233013	-2.424554
O	1.368632	-3.221072	-1.248280
H	1.852347	-0.466255	-1.986811
H	0.646827	-2.783908	-0.718135
S	0.929229	1.862787	-0.449083
O	-0.285284	2.654421	-0.442878
O	1.441075	1.527351	0.901594
O	0.793062	0.632192	-1.273498
O	2.017163	2.768874	-1.137088
H	-0.624497	-0.177261	-1.466439
H	2.915566	2.356833	-1.028713
S	-1.783746	-1.403537	-0.151014
O	-2.902187	-2.281551	-0.424859
O	-1.474543	-0.691873	-1.544416

O	-2.083873	-0.324544	0.817738
O	-0.532249	-2.092191	0.250514
H	-3.512657	1.550428	-0.741339
H	0.216739	-1.363922	1.735229
C	-0.163602	-0.194439	3.422236
N	0.753007	-0.769975	2.397032
C	1.898215	-1.542240	2.962261
H	-0.950908	0.348519	2.906636
H	0.404387	0.474286	4.067582
H	-0.594325	-1.004394	4.009456
H	1.101931	0.007928	1.806250
H	1.508294	-2.330225	3.605453
H	2.530815	-0.867464	3.537586
H	2.462018	-1.969514	2.137195
C	-3.013648	2.176953	-2.639102
N	-2.953513	2.317499	-1.155732
C	-3.483958	3.611336	-0.642592
H	-4.050841	2.266048	-2.957681
H	-2.630229	1.193598	-2.902597
H	-2.404789	2.956515	-3.094767
H	-1.969317	2.226718	-0.846201
H	-4.531688	3.700751	-0.924178
H	-2.900648	4.427765	-1.065163
H	-3.391972	3.618147	0.442014

5SA3DMA

S	-6.199232	-0.969685	-0.675339
O	-4.972290	-1.742280	-0.542752
O	-7.318254	-1.525273	-1.348866
O	-6.674130	-0.539938	0.765327
O	-5.831831	0.398544	-1.379161
H	-5.939860	-0.076241	1.246625
H	-4.969943	0.737750	-1.013706
S	6.444575	-0.742664	0.083517
O	5.705220	0.498544	0.002801
O	7.864639	-0.728993	0.104513
O	5.941807	-1.553055	1.353417
O	5.984590	-1.675213	-1.126659
H	4.983491	-1.747754	1.221557
H	5.030717	-1.887838	-0.997769
S	-3.327956	0.982496	1.173188
O	-4.605380	0.839814	1.843797
O	-3.468374	1.072593	-0.315895
O	-2.767953	2.399932	1.643206
O	-2.317601	-0.020716	1.534463

H	-1.910223	2.538360	1.166411
H	-0.615036	0.290263	2.064695
S	2.306072	-1.359713	0.187401
O	1.197973	-2.135160	0.715196
O	3.588636	-2.076351	0.108162
O	1.997026	-1.027243	-1.357067
O	2.444677	-0.040965	0.856608
H	1.140162	-0.519663	-1.380997
H	2.485983	2.136947	-1.257594
S	-0.279097	1.804192	-1.062241
O	-0.286951	0.320226	-1.153327
O	0.846427	2.400886	-1.766604
O	-1.566878	2.301384	-1.851319
O	-0.421089	2.258594	0.330884
H	-2.358215	1.947032	-1.373738
H	-1.654586	-0.947662	-0.714583
C	-1.980329	-2.119660	-2.378470
N	-2.220382	-1.778874	-0.949668
C	-1.919773	-2.886685	0.003736
H	-2.189413	-1.240321	-2.984576
H	-2.641527	-2.936612	-2.663346
H	-0.939051	-2.411941	-2.503632
H	-3.214638	-1.520389	-0.827956
H	-0.853528	-3.102169	-0.026038
H	-2.511593	-3.756198	-0.278037
H	-2.203765	-2.548781	0.997146
C	4.073447	1.501654	-2.414322
N	3.501409	1.959287	-1.114373
C	4.149536	3.180155	-0.561403
H	3.559703	0.587652	-2.703851
H	5.133870	1.308252	-2.279530
H	3.906011	2.278360	-3.159360
H	3.572104	1.201894	-0.419438
H	3.643918	3.452473	0.363687
H	4.053090	3.989447	-1.283954
H	5.195315	2.957955	-0.362570
C	0.367039	1.613676	3.322857
N	0.261829	0.305744	2.619293
C	0.255099	-0.872582	3.530667
H	0.406137	2.399078	2.572797
H	1.273180	1.618634	3.927899
H	-0.507996	1.748617	3.957219
H	1.050202	0.213446	1.944408
H	-0.628861	-0.823536	4.164871

H	1.158143	-0.854565	4.140045
H	0.244195	-1.771582	2.919961
5SA4DMA			
S	0.843927	3.297878	-1.004262
O	1.987374	2.838181	-0.246788
O	0.974466	4.332052	-1.978299
O	0.222164	2.019356	-1.738108
O	-0.313885	3.724150	-0.039748
H	0.678400	1.184104	-1.436259
H	-0.432683	3.061030	0.723599
S	-1.494896	0.872158	1.814284
O	-1.586174	0.327035	0.451897
O	-0.578561	2.053760	1.888950
O	-2.911699	1.509351	2.153320
O	-1.147292	-0.105147	2.829360
H	-3.638663	1.030747	1.670574
H	2.020868	0.542344	2.481065
C	1.634271	0.620964	4.517182
N	1.771628	1.272287	3.186767
C	2.799444	2.344768	3.110360
H	0.797126	-0.071693	4.462015
H	1.436226	1.381392	5.272600
H	2.557266	0.087899	4.741300
H	0.855029	1.641567	2.866145
H	2.793850	2.748122	2.098530
H	3.773451	1.912962	3.337663
H	2.558851	3.128391	3.828861
S	1.017619	-1.630722	-1.792810
O	1.305993	-2.663295	-0.789536
O	1.867585	-1.687731	-2.982463
O	-0.407586	-1.477618	-2.064359
O	1.474807	-0.217066	-1.090821
H	-1.963922	0.963930	-1.330564
H	1.816409	-0.354481	-0.142737
S	-4.955130	-0.837829	0.067373
O	-4.396496	-1.887618	0.923969
O	-4.475050	-0.893223	-1.314309
O	-6.535780	-1.167556	-0.101514
O	-4.888093	0.499799	0.670957
H	-6.947746	-1.079282	0.769773
H	-1.363408	-2.019090	-0.360884
S	3.652149	-1.400457	1.443656
O	2.470743	-0.488642	1.230795
O	4.196910	-1.277337	2.767478

O	3.037782	-2.876704	1.347283
O	4.599714	-1.259272	0.329603
H	2.477431	-2.915214	0.537233
H	4.362094	-0.781533	-1.254055
C	-3.331411	2.450361	-1.735576
N	-2.718819	1.121545	-2.015561
C	-2.214590	0.949136	-3.405658
H	-3.726678	2.434200	-0.722297
H	-4.142126	2.620368	-2.443192
H	-2.569554	3.221413	-1.833047
H	-3.418036	0.377068	-1.803446
H	-1.485310	1.728538	-3.614098
H	-3.057835	1.015383	-4.092811
H	-1.737686	-0.026539	-3.474414
C	-2.127881	-3.886003	-0.753105
N	-1.871318	-2.744615	0.165682
C	-1.113987	-3.103867	1.399718
H	-2.689946	-3.516593	-1.608299
H	-2.710468	-4.638872	-0.223549
H	-1.174445	-4.296289	-1.079541
H	-2.787013	-2.334636	0.445672
H	-0.997397	-2.203396	1.999837
H	-0.142634	-3.497284	1.111221
H	-1.686982	-3.849944	1.949772
C	4.369829	0.962132	-2.384315
N	4.311224	-0.520946	-2.268892
C	5.388500	-1.244078	-2.992803
H	3.578050	1.391911	-1.773909
H	4.236229	1.249220	-3.427015
H	5.338548	1.307273	-2.024044
H	3.388111	-0.872014	-2.604594
H	6.355040	-0.949026	-2.586178
H	5.338546	-1.003064	-4.054357
H	5.242850	-2.313541	-2.850570
5SA5DMA			
S	-3.322520	-3.466759	-0.270327
O	-3.389350	-2.738279	-1.539162
O	-2.002182	-3.987927	0.076085
O	-3.985765	-2.763541	0.835433
O	-4.246904	-4.771749	-0.592087
H	-4.623868	-1.210065	0.355662
H	-4.253332	-5.322856	0.203127
C	-5.856056	-0.620501	-1.200161
N	-4.910068	-0.312961	-0.093052

C	-5.441054	0.637254	0.924814
H	-5.376926	-1.335417	-1.865170
H	-6.090086	0.300165	-1.733462
H	-6.766036	-1.050993	-0.782628
H	-4.032187	0.067331	-0.508077
H	-4.653035	0.882696	1.634495
H	-6.292968	0.177904	1.425896
H	-5.748131	1.554494	0.424155
S	3.213279	-1.704513	1.725831
O	3.708036	-2.326256	2.923627
O	3.721348	-2.300793	0.460406
O	1.735336	-1.564136	1.647413
O	3.790549	-0.200748	1.759279
H	5.196777	0.101618	-0.868564
H	3.281097	0.399798	1.140043
C	6.108591	-1.385681	-1.978917
N	5.684354	-0.810543	-0.679552
C	6.781363	-0.594300	0.297913
H	5.234077	-1.461482	-2.623278
H	6.541563	-2.373236	-1.819006
H	6.842137	-0.728009	-2.444812
H	4.955084	-1.429126	-0.241578
H	6.344290	-0.184010	1.206038
H	7.506931	0.103234	-0.120532
H	7.262600	-1.546866	0.519653
S	-1.322660	0.051792	-1.499871
O	-2.628508	0.729063	-1.275510
O	-0.345071	0.946446	-2.117286
O	-0.853174	-0.664541	-0.318807
O	-1.593010	-1.049101	-2.634377
H	0.631674	-0.035411	1.716451
H	-2.229853	-1.718659	-2.276020
S	2.996958	1.744562	-1.168217
O	2.584334	3.053473	-1.672069
O	4.430739	1.483281	-1.322035
O	2.506469	1.493732	0.204311
O	2.329317	0.627415	-2.103016
H	0.991694	-2.505693	0.360468
H	1.340979	0.732676	-2.102501
S	-2.361473	3.231492	1.323340
O	-2.429683	4.634729	1.649245
O	-2.985538	2.289020	2.242176
O	-3.140491	3.121779	-0.102113
O	-0.964872	2.774659	0.986482

H	-2.879441	2.276186	-0.538028
H	-0.195180	3.633397	-0.205887
C	-1.028936	-0.268499	2.907467
N	0.031147	0.574654	2.289573
C	0.885986	1.292288	3.271419
H	-1.724262	0.380669	3.435549
H	-0.558982	-0.983076	3.581893
H	-1.546547	-0.794407	2.108687
H	-0.407388	1.290000	1.669650
H	1.399040	0.564362	3.898020
H	0.256189	1.943342	3.875979
H	1.613350	1.883284	2.719175
C	-0.606400	4.315092	-2.127252
N	0.247387	4.277939	-0.908771
C	0.438310	5.594642	-0.247389
H	-0.678705	3.300881	-2.516228
H	-0.146747	4.971636	-2.866196
H	-1.596566	4.677336	-1.854799
H	1.167482	3.855061	-1.155500
H	1.131847	5.466756	0.582432
H	-0.521398	5.937677	0.137143
H	0.848111	6.306927	-0.963487
C	1.128831	-3.100388	-1.630185
N	0.665579	-3.298555	-0.230819
C	1.157597	-4.557431	0.390760
H	0.666582	-2.200549	-2.025579
H	0.828934	-3.961128	-2.227979
H	2.211462	-2.995117	-1.616787
H	-0.369045	-3.305042	-0.194971
H	2.245754	-4.540227	0.395244
H	0.780650	-5.405836	-0.178847
H	0.784196	-4.606199	1.411622
5SA6DMA			
C	8.007470	1.660454	-0.100352
N	7.178775	0.989711	-1.098926
C	7.615798	1.274898	-2.463146
H	9.018713	1.240414	-0.111876
H	7.587461	1.501195	0.895571
H	8.098196	2.748162	-0.261002
H	6.214171	1.292089	-0.985377
H	8.603077	0.834532	-2.637767
H	7.688976	2.352611	-2.687170
H	6.918152	0.829237	-3.176380
S	-4.103941	-2.865321	-0.912927

O	-4.011345	-2.022098	-2.100118
O	-2.936589	-3.706500	-0.643517
O	-4.584098	-2.150532	0.279933
O	-5.298341	-3.899393	-1.324494
H	-5.005499	-0.492438	0.095671
H	-5.341963	-4.575385	-0.634159
C	-5.791550	0.899527	-1.240172
N	-5.399457	0.473816	0.131667
C	-6.515001	0.479057	1.112940
H	-4.913628	0.830507	-1.876577
H	-6.152820	1.926998	-1.202121
H	-6.573960	0.235386	-1.605848
H	-4.652654	1.096967	0.508394
H	-6.128295	0.161811	2.079374
H	-7.289645	-0.210773	0.779906
H	-6.914922	1.488716	1.196050
S	2.216446	-2.395694	2.009963
O	2.484003	-3.199810	3.171617
O	2.774173	-2.934216	0.740453
O	0.794915	-2.019354	1.807456
O	2.999718	-1.005758	2.271668
H	4.746573	-0.643898	-0.114900
H	2.625191	-0.280111	1.702503
C	5.498282	-2.072737	-1.401286
N	5.043685	-1.642185	-0.054778
C	6.072743	-1.780843	1.008850
H	4.687846	-1.901032	-2.108588
H	5.752839	-3.132519	-1.375665
H	6.364520	-1.471199	-1.673775
H	4.186122	-2.176502	0.227332
H	5.640404	-1.427499	1.943088
H	6.938456	-1.182166	0.729846
H	6.347590	-2.831197	1.106094
S	-1.433189	0.235119	-1.641256
O	-2.643893	1.063661	-1.500958
O	-0.270765	1.002152	-2.111679
O	-1.158848	-0.588615	-0.463918
O	-1.730514	-0.772229	-2.853491
H	-0.142226	-0.227624	1.622859
H	-2.568473	-1.260628	-2.647287
S	2.803440	1.352131	-0.423789
O	2.601255	2.743290	-0.834947
O	4.218047	0.971164	-0.331922
O	2.039957	1.014645	0.795064

O	2.259461	0.408923	-1.590748
H	0.152154	-2.730872	0.290481
H	1.295804	0.605828	-1.774476
S	-2.884632	3.206785	1.170235
O	-3.164125	4.486360	1.761231
O	-3.734556	2.083320	1.603448
O	-3.158063	3.406961	-0.408578
O	-1.442880	2.801735	1.244529
H	-2.909876	2.561912	-0.872993
H	-0.379786	3.558917	0.139639
C	-1.896357	-0.544706	2.643317
N	-0.736757	0.309956	2.266404
C	0.082819	0.760313	3.422346
H	-2.582654	0.045249	3.248097
H	-1.522291	-1.404977	3.195144
H	-2.387886	-0.872818	1.730872
H	-1.071411	1.153244	1.758271
H	0.470964	-0.113764	3.941379
H	-0.542933	1.356485	4.085437
H	0.906097	1.359193	3.040588
C	-0.256638	4.334722	-1.796061
N	0.288224	4.133110	-0.424193
C	0.542413	5.388398	0.327936
H	-0.372244	3.355311	-2.257147
H	0.446711	4.938559	-2.369305
H	-1.223192	4.830742	-1.725182
H	1.173043	3.581870	-0.501945
H	0.953916	5.132516	1.302918
H	-0.398017	5.921824	0.461558
H	1.253887	6.002825	-0.223167
C	0.493976	-3.239852	-1.702119
N	-0.197088	-3.426996	-0.398439
C	-0.010767	-4.781030	0.188174
H	0.250783	-2.252488	-2.083273
H	0.141174	-3.999154	-2.400001
H	1.564516	-3.332640	-1.533850
H	-1.213340	-3.262932	-0.514885
H	1.053819	-4.953514	0.333643
H	-0.440375	-5.521162	-0.485515
H	-0.523962	-4.814877	1.146973
5SA7DMA			
C	-3.949789	7.036914	1.231726
N	-3.797960	5.880421	0.355837
C	-4.717950	5.907912	-0.776980

H	-3.651287	7.948622	0.703017
H	-3.300090	6.927389	2.103558
H	-4.982346	7.186108	1.591941
H	-3.958909	5.027054	0.886533
H	-4.449027	6.721085	-1.460000
H	-5.771828	6.055241	-0.483953
H	-4.650509	4.964587	-1.323028
C	7.485439	3.346980	-0.290141
N	6.913212	2.366271	-1.209058
C	7.278238	2.630567	-2.598465
H	8.575604	3.245792	-0.267877
H	7.109794	3.169682	0.720399
H	7.254683	4.391574	-0.559755
H	5.899895	2.380782	-1.120249
H	8.354823	2.484195	-2.735048
H	7.037638	3.654529	-2.931094
H	6.757478	1.931580	-3.257394
S	-2.867854	-4.301111	-0.858850
O	-3.065222	-3.523386	-2.090019
O	-1.499548	-4.790174	-0.692792
O	-3.443332	-3.677114	0.331706
O	-3.802092	-5.627656	-1.029745
H	-4.365986	-2.246145	0.099969
H	-3.504344	-6.088669	-1.826324
C	-5.572945	-1.181779	-1.226384
N	-5.031760	-1.442989	0.135568
C	-6.067344	-1.751817	1.155291
H	-4.733663	-0.989477	-1.889172
H	-6.230379	-0.313481	-1.185138
H	-6.125038	-2.059006	-1.561945
H	-4.493694	-0.617555	0.476147
H	-5.573566	-1.925436	2.109287
H	-6.612005	-2.646267	0.855075
H	-6.745997	-0.904750	1.245507
S	3.014738	-2.035552	2.145340
O	3.436514	-2.659219	3.370193
O	3.745724	-2.489472	0.931686
O	1.553277	-2.059986	1.886183
O	3.395338	-0.472938	2.314798
H	5.034053	0.180237	-0.067680
H	2.857890	0.083663	1.686328
C	6.260267	-1.067874	-1.165843
N	5.613305	-0.669138	0.109965
C	6.569556	-0.382983	1.211644

H	5.482630	-1.228974	-1.911485
H	6.824776	-1.987913	-1.012909
H	6.914981	-0.256014	-1.480212
H	4.937808	-1.408692	0.421468
H	5.994532	-0.094605	2.089336
H	7.227844	0.424141	0.894023
H	7.144837	-1.283022	1.429128
S	-1.224049	-0.591922	-1.688293
O	-2.612726	-0.109598	-1.566178
O	-0.308224	0.441034	-2.192096
O	-0.741900	-1.269939	-0.484860
O	-1.239976	-1.682289	-2.861579
H	0.174861	-0.538288	1.572450
H	-1.904987	-2.381455	-2.626988
S	2.599662	1.560873	-0.544664
O	2.058356	2.849055	-0.979064
O	4.065649	1.537608	-0.466237
O	1.957695	1.076953	0.696298
O	2.286891	0.487440	-1.681305
H	1.148246	-2.963565	0.413250
H	1.303367	0.455895	-1.865447
S	-3.414973	1.951500	1.054746
O	-4.111286	3.076564	1.630164
O	-3.866358	0.625773	1.509991
O	-3.736877	2.034661	-0.522366
O	-1.926687	2.041225	1.144555
H	-3.261439	1.284295	-0.974561
H	-1.069947	3.080482	0.006291
C	-1.412319	-1.290272	2.640924
N	-0.539483	-0.163081	2.208458
C	0.132799	0.544012	3.331336
H	-2.226827	-0.889017	3.240876
H	-0.805702	-1.990271	3.211880
H	-1.805452	-1.776569	1.751768
H	-1.097344	0.533287	1.678233
H	0.747262	-0.168312	3.877793
H	-0.628833	0.975273	3.979620
H	0.759593	1.326695	2.911118
C	-1.083424	3.702507	-1.981913
N	-0.516672	3.717436	-0.603740
C	-0.486145	5.067768	0.024831
H	-1.035175	2.682121	-2.358150
H	-0.484012	4.359428	-2.611888
H	-2.113809	4.049683	-1.942965

H	0.451820	3.333829	-0.649734
H	-0.066177	4.970389	1.025453
H	-1.506821	5.458433	0.077848
H	0.150661	5.718554	-0.574610
C	1.671207	-3.327687	-1.569361
N	1.021726	-3.720349	-0.290246
C	1.557636	-4.979148	0.293332
H	1.189802	-2.426369	-1.936234
H	1.544410	-4.134049	-2.291547
H	2.724505	-3.142249	-1.372001
H	0.005100	-3.843444	-0.442815
H	2.620532	-4.846949	0.485643
H	1.381930	-5.796467	-0.404684
H	1.033826	-5.177177	1.226355
5SA8DMA			
C	5.743465	-5.974224	1.931579
N	5.448705	-4.935722	0.950477
C	6.469878	-4.835659	-0.087487
H	5.702744	-6.960201	1.456221
H	4.993824	-5.954513	2.726485
H	6.738554	-5.872356	2.398061
H	5.370929	-4.035859	1.419346
H	6.453042	-5.730690	-0.718928
H	7.493559	-4.729682	0.311264
H	6.263824	-3.968068	-0.717920
C	-7.815219	2.632503	0.512943
N	-7.018732	1.737859	1.346214
C	-7.363952	1.840870	2.763779
H	-8.863904	2.317523	0.524993
H	-7.466400	2.587960	-0.522415
H	-7.784536	3.686859	0.838595
H	-6.032595	1.959322	1.235373
H	-8.365014	1.430514	2.934866
H	-7.358667	2.878055	3.138320
H	-6.646440	1.270604	3.355140
C	-5.796595	-5.315689	-0.968849
N	-5.476759	-4.126237	-1.752526
C	-5.602073	-4.356503	-3.189078
H	-6.859681	-5.556505	-1.073553
H	-5.598303	-5.126063	0.088837
H	-5.222851	-6.209769	-1.267461
H	-4.525332	-3.832550	-1.544412
H	-6.651222	-4.533680	-3.448374
H	-5.020077	-5.221550	-3.549998

H	-5.264919	-3.472171	-3.734917
S	2.232772	4.645471	-1.023068
O	2.770580	3.944029	-2.197283
O	0.773863	4.727150	-1.010519
O	2.834625	4.224213	0.241836
O	2.771000	6.180974	-1.154142
H	4.132096	3.097277	0.153762
H	2.452363	6.526203	-1.999718
C	5.686035	2.329788	-1.008231
N	4.980990	2.505682	0.291048
C	5.807326	3.133113	1.354468
H	4.985816	1.889356	-1.712849
H	6.540763	1.669978	-0.860154
H	6.017287	3.303986	-1.365995
H	4.649280	1.585097	0.651905
H	5.206251	3.214549	2.257900
H	6.118282	4.125312	1.029452
H	6.676985	2.507225	1.550493
S	-3.144520	1.231409	1.822946
O	-3.771223	1.730239	3.019892
O	-3.944851	1.436706	0.584820
O	-1.744427	1.666223	1.600466
O	-3.068629	-0.368459	2.027813
H	-4.465375	-1.512046	-0.355556
H	-2.396913	-0.764185	1.404407
C	-6.133285	-0.753322	-1.326006
N	-5.291561	-0.928709	-0.113287
C	-6.018720	-1.550622	1.027744
H	-5.534941	-0.267882	-2.096473
H	-6.988506	-0.131135	-1.066556
H	-6.441748	-1.742522	-1.663981
H	-4.903290	-0.010079	0.183599
H	-5.314796	-1.671201	1.848654
H	-6.404531	-2.516119	0.703909
H	-6.821557	-0.874301	1.318340
S	1.672875	0.670923	-1.809901
O	3.109578	0.551873	-1.495937
O	1.102358	-0.579873	-2.330861
O	0.895996	1.259168	-0.717483
O	1.575177	1.674263	-3.050336
H	0.052446	0.428287	1.336312
H	2.007997	2.530382	-2.793001
S	-1.642521	-2.182455	-0.767437
O	-0.803946	-3.355599	-1.020701

O	-3.079632	-2.471477	-0.797053
O	-1.232676	-1.463537	0.459839
O	-1.447992	-1.174345	-1.986158
H	-1.508264	2.481468	0.080100
H	-0.477564	-0.959532	-2.111784
S	4.150293	-1.136448	1.289221
O	5.033632	-2.041044	1.983588
O	4.233972	0.274910	1.703395
O	4.624702	-1.199103	-0.248543
O	2.721662	-1.572809	1.266487
H	4.022249	-0.610324	-0.782168
H	2.220267	-2.819144	0.138615
C	1.295263	1.650495	2.437995
N	0.784200	0.306767	2.045398
C	0.242808	-0.486576	3.181548
H	2.143429	1.514591	3.106354
H	0.487442	2.191780	2.925942
H	1.606320	2.175824	1.538589
H	1.542921	-0.248723	1.605769
H	-0.567732	0.070074	3.646393
H	1.046594	-0.667512	3.893857
H	-0.132573	-1.428208	2.788949
C	2.534649	-3.549465	-1.787729
N	1.870817	-3.600611	-0.454812
C	2.081172	-4.880174	0.278488
H	2.304480	-2.589236	-2.246116
H	2.142885	-4.358775	-2.403623
H	3.608350	-3.662943	-1.651620
H	0.848938	-3.444671	-0.593467
H	1.561111	-4.817019	1.233766
H	3.153459	-5.026693	0.439757
H	1.660149	-5.694913	-0.310803
C	-1.960992	2.406903	-1.948861
N	-1.471253	3.123200	-0.740648
C	-2.253132	4.341573	-0.403455
H	-1.381544	1.496823	-2.065936
H	-1.833073	3.049578	-2.819426
H	-3.008929	2.158271	-1.795945
H	-0.483700	3.401838	-0.868534
H	-3.278067	4.046079	-0.187057
H	-2.214966	5.033647	-1.243329
H	-1.803767	4.808264	0.470488
6DMA			
C	-3.958989	0.052987	1.060281

N	-3.050249	-0.248847	-0.041209
C	-3.750651	-0.783426	-1.204718
H	-4.635161	0.867426	0.778598
H	-3.386075	0.380808	1.931018
H	-4.584229	-0.804648	1.364141
H	-2.358401	-0.937498	0.276530
H	-4.406066	-0.018451	-1.635027
H	-4.375955	-1.664167	-0.976897
H	-3.025903	-1.070727	-1.970220
C	0.617268	2.229590	2.322755
N	1.059673	2.472966	0.953885
C	1.690743	3.779457	0.799611
H	1.481251	2.152584	2.991878
H	0.071564	1.284354	2.367991
H	-0.039183	3.022796	2.721486
H	0.248073	2.412820	0.327901
H	2.625384	3.816221	1.369675
H	1.060523	4.617616	1.144798
H	1.935240	3.949423	-0.251765
C	-2.341395	3.476310	-0.689791
N	-1.462192	2.331171	-0.900423
C	-1.065692	2.182729	-2.296481
H	-1.802510	4.407745	-0.894331
H	-2.668181	3.502498	0.352486
H	-3.240635	3.467803	-1.330335
H	-1.942718	1.476915	-0.595259
H	-0.451333	3.035029	-2.606638
H	-1.918747	2.119476	-2.994329
H	-0.463658	1.278322	-2.412096
C	-0.616855	-2.227697	2.323105
N	-1.059025	-2.472670	0.954468
C	-1.689378	-3.779646	0.801429
H	-1.480923	-2.150492	2.992098
H	-0.071653	-1.282124	2.367449
H	0.039987	-3.020157	2.722682
H	-0.247505	-2.412643	0.328359
H	-2.624136	-3.816298	1.371308
H	-1.058800	-4.617109	1.147647
H	-1.933531	-3.950847	-0.249827
C	3.959251	-0.054134	1.060325
N	3.050274	0.247921	-0.040902
C	3.750497	0.782087	-1.204711
H	4.635318	-0.868561	0.778365
H	3.386528	-0.382052	1.931152

H	4.584578	0.803442	1.364172
H	2.358798	0.936904	0.276947
H	4.405666	0.016877	-1.634976
H	4.376019	1.662767	-0.977258
H	3.025619	1.069334	-1.970107
C	2.340810	-3.476160	-0.691200
N	1.461508	-2.330931	-0.900858
C	1.064358	-2.181842	-2.296660
H	1.801857	-4.407494	-0.896018
H	2.668024	-3.502904	0.350930
H	3.239777	-3.467306	-1.332118
H	1.942135	-1.476799	-0.595439
H	0.450092	-3.034140	-2.607016
H	1.917120	-2.117995	-2.994815
H	0.462017	-1.277549	-2.411542

6SA

S	5.315209	-0.525451	1.373512
O	6.161037	-1.267579	2.230659
O	4.617652	-1.158115	0.259681
O	4.219602	0.186064	2.274792
O	6.154744	0.665934	0.773469
H	3.509007	0.560421	1.708493
H	5.618763	1.167037	0.119584
S	-5.468310	0.435926	1.144699
O	-6.404241	1.263678	1.807351
O	-4.459478	0.997906	0.252153
O	-4.698056	-0.408837	2.245553
O	-6.266514	-0.643476	0.321769
H	-3.891933	-0.809660	1.858089
H	-5.639618	-1.210027	-0.181172
S	-2.745969	-1.879479	-0.675041
O	-4.150383	-2.157274	-0.668490
O	-2.170567	-0.998662	-1.665485
O	-2.394231	-1.279926	0.768409
O	-2.030289	-3.251361	-0.690650
H	-1.808087	-0.481859	0.677901
H	-1.047598	-3.177140	-0.861878
S	-1.412790	2.197110	-0.399592
O	-0.417513	3.223568	-0.531082
O	-1.120479	1.060007	0.452867
O	-2.699821	2.926461	0.070583
O	-1.740998	1.673042	-1.843226
H	-3.450980	2.278676	0.208142
H	-1.964598	0.708466	-1.830586

S	2.846616	1.893615	-0.712169
O	4.268058	2.062748	-0.761473
O	2.334220	1.059803	0.383348
O	2.213739	3.299627	-0.672097
O	2.264704	1.336629	-2.053109
H	1.214157	3.264065	-0.617865
H	2.252770	0.339691	-2.053165
S	1.548128	-2.143819	-0.800343
O	2.101463	-1.304381	-1.840281
O	0.574065	-3.141320	-1.141686
O	2.686258	-2.877979	-0.047273
O	0.844934	-1.223859	0.278582
H	3.486621	-2.283348	0.089674
H	1.292080	-0.344321	0.350848

6SA1DMA

S	-5.786347	-0.843401	1.071220
O	-6.869744	-1.193891	1.911850
O	-5.886845	-0.945403	-0.373754
O	-5.369957	0.646691	1.428092
O	-4.525001	-1.695015	1.528017
H	-4.707236	0.964148	0.774461
H	-3.820954	-1.623652	0.842156
S	3.464040	1.911875	-0.119885
O	4.877916	1.662264	-0.096505
O	2.658981	1.582603	1.028177
O	3.286532	3.434278	-0.464890
O	2.870958	1.188411	-1.389252
H	2.359738	3.706970	-0.268264
H	2.116021	0.599050	-1.148011
S	4.588725	-1.992274	0.598524
O	5.141994	-3.187674	1.133845
O	3.343880	-1.484896	1.148926
O	5.704943	-0.892660	0.662474
O	4.404649	-2.083624	-0.978297
H	5.395455	-0.011727	0.339143
H	3.505676	-2.408790	-1.204064
S	-0.399095	2.825168	0.031763
O	-0.483522	1.700431	0.934479
O	0.541346	3.879757	0.266940
O	-0.097902	2.319623	-1.428933
O	-1.828998	3.478203	-0.072054
H	-0.704314	1.578975	-1.696320
H	-2.496859	2.755487	-0.159441
S	0.668285	-1.840419	-1.524683

O	1.766171	-2.729570	-1.741897
O	0.891561	-0.594503	-0.810930
O	0.035539	-1.518104	-2.925446
O	-0.441197	-2.651358	-0.764349
H	-0.665163	-0.822650	-2.818422
H	-1.277856	-2.112003	-0.651413
S	-2.909539	0.025917	-1.273568
O	-1.774637	0.350325	-2.152893
O	-2.634179	-1.167741	-0.436523
O	-3.350012	1.167994	-0.458854
O	-4.066720	-0.348454	-2.267746
H	0.670057	0.437630	1.761767
H	-4.860640	-0.603520	-1.728570
C	1.511536	0.454002	3.650457
N	1.116066	-0.244927	2.393325
C	0.208675	-1.406825	2.605418
H	2.164348	1.281243	3.385967
H	2.035581	-0.250529	4.294644
H	0.615009	0.822567	4.146884
H	1.967325	-0.562336	1.902356
H	0.001741	-1.865774	1.642555
H	-0.716969	-1.058473	3.061694
H	0.702173	-2.126561	3.256605
6SA2DMA			
S	1.380737	-2.870578	1.353184
O	2.176351	-3.640868	2.245521
O	1.936040	-2.383308	0.108339
O	0.070570	-3.690688	1.074062
O	0.763010	-1.602880	2.105558
H	-0.483496	-3.232858	0.391440
H	1.247168	-0.774449	1.839582
S	-4.644564	-1.249449	0.449909
O	-3.858147	-0.731068	1.551719
O	-6.055914	-1.337746	0.570779
O	-4.235887	-0.390062	-0.852209
O	-4.108782	-2.649561	0.005963
H	-3.960381	0.532129	-0.584441
H	-3.127483	-2.611327	-0.171015
S	5.274658	0.965829	0.327882
O	4.482522	0.384128	-0.740862
O	6.673961	0.740454	0.393631
O	5.047140	2.530290	0.310592
O	4.648593	0.507891	1.708173
H	4.080943	2.732769	0.264480

H	3.661035	0.544540	1.666681
S	-2.745296	2.972949	-1.079016
O	-3.624336	3.913463	-1.672079
O	-3.260037	1.976808	-0.134257
O	-2.007587	2.183950	-2.226834
O	-1.612296	3.776668	-0.349300
H	-1.660563	1.311255	-1.897246
H	-0.950541	3.180832	0.103127
S	-1.148702	-1.477637	-1.750245
O	-0.010168	-1.912989	-2.518447
O	-1.542449	-2.383974	-0.645928
O	-1.020736	-0.081801	-1.235900
O	-2.374879	-1.444943	-2.763394
H	0.429846	0.578353	-0.952067
H	-3.173002	-1.133111	-2.285610
S	1.407106	1.745365	0.574587
O	2.319891	2.852075	0.407620
O	1.290700	1.075214	-0.865513
O	1.917235	0.703865	1.498632
O	0.021381	2.125926	0.948205
H	3.168882	-0.731535	-1.460875
H	-1.160969	1.290164	2.056147
C	-1.478318	0.123626	3.760177
N	-1.957911	1.001613	2.651522
C	-2.675170	2.227436	3.110182
H	-0.979033	-0.742430	3.331210
H	-2.337342	-0.190783	4.350606
H	-0.780237	0.685770	4.379138
H	-2.595908	0.450912	2.053657
H	-1.994951	2.832563	3.707694
H	-3.536394	1.928030	3.705336
H	-3.004331	2.777767	2.232756
C	2.871035	-0.366626	-3.466342
N	2.866101	-1.273481	-2.284103
C	3.763932	-2.457438	-2.415604
H	3.888431	-0.017085	-3.630547
H	2.223901	0.480387	-3.251687
H	2.505104	-0.912690	-4.334275
H	1.905264	-1.594390	-2.102646
H	4.787179	-2.104675	-2.531065
H	3.459601	-3.037994	-3.285562
H	3.668628	-3.051477	-1.510602
6SA3DMA			
S	2.794908	3.528602	-0.613038

O	3.041134	4.916267	-0.793260
O	3.894703	2.581232	-0.543877
O	1.930186	3.370403	0.699110
O	1.821251	3.070174	-1.765764
H	1.975183	2.439056	1.061518
H	1.809219	2.068420	-1.855322
S	-3.828446	0.592061	2.309532
O	-3.602012	1.769563	1.496740
O	-4.276052	0.753756	3.653102
O	-4.815116	-0.392422	1.597303
O	-2.504364	-0.296749	2.251141
H	-4.499999	-0.602548	0.670962
H	-1.683144	0.262107	2.325904
S	-3.724818	-0.471977	-2.003488
O	-3.726130	0.975729	-1.930164
O	-3.794228	-1.159427	-0.694910
O	-5.131441	-0.926771	-2.667645
O	-2.667458	-1.044887	-2.847271
H	-5.250859	-0.424161	-3.486023
H	-1.189537	-0.351837	-3.111801
S	2.615050	-3.601409	0.110446
O	3.765819	-4.423524	0.273005
O	1.286758	-4.079275	0.399432
O	2.848969	-2.269390	0.975787
O	2.670282	-3.030842	-1.359098
H	2.012520	-1.939262	1.436657
H	1.851057	-2.470369	-1.524878
S	0.458018	-0.130774	-1.778264
O	1.789658	0.451503	-2.000030
O	-0.263565	0.020234	-3.177906
O	0.527093	-1.581627	-1.477004
O	-0.339388	0.573775	-0.776219
H	-2.389407	-2.182900	-0.243844
H	3.679492	-0.792357	0.134496
S	1.038244	0.280395	2.436261
O	0.829815	-1.147528	2.155092
O	2.083386	0.884414	1.605564
O	-0.211792	1.035316	2.507662
O	1.705291	0.369298	3.912559
H	-1.250958	2.063960	-0.595743
H	1.032719	0.125829	4.565205
C	-1.403750	3.736938	0.641836
N	-1.888981	2.872195	-0.473606
C	-2.009185	3.576336	-1.781730

H	-1.319404	3.126207	1.535639
H	-2.124387	4.537520	0.800808
H	-0.429160	4.139270	0.376880
H	-2.784916	2.445455	-0.202332
H	-2.406189	2.873492	-2.508944
H	-1.020524	3.922907	-2.079088
H	-2.686080	4.422187	-1.668549
C	5.385475	0.006366	0.958555
N	4.399181	-0.113142	-0.151638
C	4.981154	-0.520760	-1.462352
H	4.849507	0.310016	1.855222
H	6.123053	0.761355	0.692461
H	5.863858	-0.959162	1.114964
H	3.937664	0.804126	-0.270232
H	4.177245	-0.540372	-2.193938
H	5.425473	-1.509749	-1.364612
H	5.733667	0.211642	-1.750567
C	-1.708373	-3.382453	1.319648
N	-1.630683	-2.871581	-0.079830
C	-1.733253	-3.930566	-1.125179
H	-1.633646	-2.536948	1.997358
H	-0.886184	-4.074633	1.480791
H	-2.668720	-3.880103	1.451161
H	-0.746746	-2.364328	-0.237321
H	-1.713355	-3.446656	-2.098893
H	-2.675755	-4.460361	-0.993465
H	-0.890391	-4.609401	-1.013594

6SA4DMA

S	-0.638695	3.941338	-1.479308
O	-0.799254	5.325287	-1.780062
O	-1.665677	2.991672	-1.860791
O	0.739694	3.500914	-2.121693
O	-0.327849	3.740662	0.052935
H	0.810068	2.511721	-2.198195
H	-1.127740	3.343352	0.527356
S	-2.800796	-3.284117	-2.229720
O	-3.451820	-2.130882	-1.640396
O	-3.555627	-4.260094	-2.939833
O	-1.671487	-2.789562	-3.218827
O	-1.968736	-4.009146	-1.097555
H	-1.224082	-1.976869	-2.867857
H	-2.025697	-3.542796	-0.216684
S	-2.279270	2.181783	2.602804
O	-0.921579	1.865113	3.007582

O	-3.285407	1.154475	2.892458
O	-2.647974	3.439261	3.561834
O	-2.388883	2.676658	1.215505
H	-3.588753	3.635395	3.448718
H	-2.723669	1.501553	-1.042912
C	-4.554032	0.745762	-0.402175
N	-3.347402	0.717635	-1.277708
C	-3.646565	0.784062	-2.737183
H	-4.227225	0.742801	0.634207
H	-5.149555	-0.138645	-0.619961
H	-5.118149	1.653069	-0.613823
H	-2.836164	-0.152847	-1.081121
H	-2.703803	0.733213	-3.274784
H	-4.145191	1.728466	-2.947337
H	-4.276971	-0.062961	-2.995847
S	4.355296	-0.855361	0.658369
O	5.627630	-1.361823	1.083118
O	4.309369	0.588750	0.335638
O	4.036380	-1.625849	-0.731325
O	3.207054	-1.195651	1.549996
H	3.087366	-1.489516	-0.982903
H	2.059163	0.181953	1.995314
S	0.646332	-0.167251	-1.714762
O	0.337508	0.469874	-0.291464
O	1.492251	-1.346468	-1.513300
O	-0.642937	-0.481176	-2.329576
O	1.372878	0.927756	-2.401068
H	0.801900	-2.867507	1.954507
H	3.134575	1.058613	-2.446312
S	-1.547536	-1.697589	1.796682
O	-0.244453	-1.542084	2.469907
O	-1.752966	-3.070571	1.337385
O	-2.694145	-1.434784	2.843329
O	-1.716223	-0.679830	0.730043
H	-2.881172	-0.455761	2.917562
H	-0.450259	-0.000130	0.138414
C	2.037326	-4.308882	2.790352
N	1.629782	-3.430132	1.664121
C	1.343788	-4.151837	0.390872
H	2.223325	-3.691232	3.667397
H	2.947356	-4.843180	2.519679
H	1.236314	-5.016581	3.000456
H	2.361162	-2.700746	1.513236
H	0.504467	-4.827197	0.543400

H	2.233796	-4.706406	0.094415
H	1.094120	-3.421157	-0.375394
C	1.928838	0.653185	3.995428
N	1.624982	0.929934	2.565340
C	2.091768	2.262801	2.086619
H	1.514230	-0.321086	4.244867
H	1.455109	1.419666	4.605847
H	3.008354	0.655416	4.137361
H	0.602887	0.887780	2.456468
H	1.703257	2.418207	1.083272
H	3.179616	2.267613	2.076892
H	1.692666	3.027350	2.749979
C	5.049167	0.549016	-3.116860
N	4.119588	1.331181	-2.257673
C	4.234413	2.808163	-2.402323
H	4.912598	-0.507433	-2.894826
H	6.073867	0.838291	-2.885700
H	4.831605	0.752079	-4.165063
H	4.273226	1.063057	-1.250770
H	3.467019	3.282095	-1.792927
H	4.082261	3.082070	-3.445912
H	5.223981	3.123516	-2.073726
6SA5DMA			
S	3.981864	-2.543169	-1.389291
O	4.207640	-3.894095	-1.787428
O	5.076818	-1.660548	-1.068286
O	3.086469	-1.905253	-2.522393
O	2.998118	-2.555654	-0.142376
H	2.834527	-0.970137	-2.308508
H	3.272870	-1.877196	0.560839
S	-3.816739	-3.265971	0.185886
O	-3.710459	-2.831050	-1.207945
O	-2.553683	-3.632557	0.822979
O	-4.640321	-2.368106	1.008595
O	-4.665888	-4.648434	0.038818
H	-5.208410	-0.979394	0.135280
H	-4.781632	-5.013856	0.927372
C	-6.195646	-0.700651	-1.665043
N	-5.400201	-0.187546	-0.516616
C	-6.028453	0.949439	0.215126
H	-5.655949	-1.537395	-2.103375
H	-6.321519	0.096768	-2.396610
H	-7.169222	-1.032309	-1.304952
H	-4.459903	0.092074	-0.865115

H	-5.344487	1.300797	0.986563
H	-6.968208	0.610855	0.651074
H	-6.209405	1.763567	-0.485102
S	2.438360	-0.454753	2.550690
O	2.671029	-0.636739	3.954509
O	3.591970	-0.840929	1.670776
O	1.196872	-1.052688	2.017843
O	2.291287	1.132476	2.354995
H	5.144830	1.019298	-0.293495
H	2.252335	1.379703	1.390398
C	6.917373	0.257214	0.530612
N	5.558519	0.851775	0.648986
C	5.514316	2.133756	1.404960
H	6.836660	-0.663928	-0.039848
H	7.303325	0.053705	1.529354
H	7.569992	0.963902	0.018445
H	4.910231	0.173357	1.099402
H	4.487298	2.489552	1.418599
H	6.153447	2.861012	0.905506
H	5.862263	1.961959	2.422906
S	-1.589064	-0.110505	-1.517442
O	-2.901625	0.585885	-1.467240
O	-0.578802	0.691790	-2.208627
O	-1.176353	-0.641483	-0.223516
O	-1.812126	-1.368948	-2.487943
H	-0.271093	0.063872	2.235141
H	-2.484597	-1.961448	-2.067637
S	2.734964	1.895652	-1.455867
O	2.195072	2.901779	-2.364418
O	4.155994	1.611095	-1.607567
O	2.324453	2.151403	-0.062498
O	2.041712	0.480917	-1.868255
H	0.657973	-2.362047	0.427229
H	1.050981	0.570861	-1.980096
S	-2.821995	3.307723	0.847849
O	-2.837534	4.740708	1.016828
O	-3.580819	2.508783	1.805697
O	-3.497882	3.078393	-0.617972
O	-1.441475	2.737007	0.682016
H	-3.206460	2.196041	-0.949725
H	-0.539975	3.445984	-0.624234
C	-2.242368	-0.257247	2.781186
N	-1.083887	0.640387	2.515466
C	-0.717402	1.493580	3.679761

H	-3.107495	0.361326	3.007018
H	-1.997755	-0.904482	3.623372
H	-2.430084	-0.854962	1.894587
H	-1.292098	1.273935	1.716066
H	-0.443706	0.854807	4.518854
H	-1.574946	2.115166	3.930714
H	0.133040	2.110260	3.401320
C	-1.006117	4.099051	-2.546859
N	-0.122451	4.076420	-1.347269
C	0.085081	5.403000	-0.705726
H	-1.078832	3.080763	-2.924874
H	-0.560162	4.747627	-3.300629
H	-1.990849	4.459750	-2.257040
H	0.789845	3.670742	-1.633691
H	0.800634	5.279035	0.105625
H	-0.865580	5.748820	-0.302203
H	0.477257	6.103087	-1.443111
C	0.260938	-3.791194	-1.050532
N	0.144400	-3.246351	0.333539
C	0.616189	-4.184152	1.389530
H	-0.044265	-3.019913	-1.753762
H	-0.406326	-4.648084	-1.131418
H	1.290688	-4.085161	-1.232827
H	-0.853654	-3.038892	0.504148
H	1.655128	-4.436763	1.189074
H	-0.012417	-5.072672	1.369223
H	0.535605	-3.683188	2.351387
6SA6DMA			
S	4.317938	1.301240	-2.282708
O	4.332835	0.026511	-2.977216
O	3.091657	2.076185	-2.385491
O	4.803417	1.197149	-0.876720
O	5.510955	2.216330	-2.937078
H	5.131448	-1.487940	0.511320
H	5.287402	2.346684	-3.869396
C	7.146063	-1.013724	0.435068
N	5.835229	-1.253222	-0.218455
C	5.855494	-2.284397	-1.291147
H	7.016047	-0.261530	1.211321
H	7.858667	-0.655797	-0.307307
H	7.506206	-1.941223	0.879610
H	5.479271	-0.343853	-0.598714
H	4.861902	-2.339002	-1.724511
H	6.135975	-3.244466	-0.858283

H	6.572684	-1.986076	-2.054463
S	-3.799027	-0.085251	-2.482838
O	-4.418770	-0.690298	-3.633690
O	-2.714589	-0.928616	-1.887065
O	-3.335468	1.303196	-2.641409
O	-4.961114	-0.060151	-1.365845
H	-2.769325	-4.001116	-0.791349
H	-4.604641	0.373141	-0.548221
C	-4.107095	-4.016784	-2.377968
N	-3.557541	-3.416902	-1.132285
C	-4.559793	-3.221684	-0.048004
H	-3.283859	-4.189536	-3.069291
H	-4.812895	-3.318781	-2.825558
H	-4.592227	-4.963480	-2.140906
H	-3.157205	-2.478459	-1.376773
H	-4.080353	-2.701772	0.779730
H	-4.935662	-4.193811	0.271483
H	-5.370300	-2.603451	-0.430321
S	-0.294444	-4.053272	0.056240
O	-1.305741	-4.981244	-0.436019
O	-0.823548	-2.719942	0.354610
O	0.167855	-4.697364	1.474360
O	0.930439	-3.999825	-0.769353
H	0.916786	-4.151949	1.794500
H	0.451872	-0.426262	-0.543966
C	-0.059484	1.188634	-1.764514
N	-0.051363	-0.265293	-1.429230
C	0.556725	-1.101411	-2.504394
H	-0.408635	1.748239	-0.901671
H	-0.750686	1.333904	-2.592887
H	0.948451	1.496418	-2.036455
H	-1.033594	-0.566405	-1.295704
H	0.554248	-2.139951	-2.183118
H	1.576940	-0.763565	-2.682780
H	-0.041913	-0.983261	-3.406166
S	-0.551411	3.809185	1.564702
O	-1.723816	3.668476	2.435212
O	-0.928884	3.983751	0.148529
O	0.479544	4.708299	2.026862
O	0.206719	2.337118	1.611995
H	1.985186	2.241571	0.918346
H	-0.474863	1.622645	1.492211
S	2.573686	-1.627456	1.289173
O	1.881638	-2.565662	2.201875

O	3.903446	-1.229005	1.758013
O	2.897406	-2.446542	-0.045542
O	1.723443	-0.485061	0.928601
H	2.129477	-3.044853	-0.318123
H	-1.031186	-1.082220	2.270069
S	-3.076171	0.541894	1.734099
O	-1.639557	0.434675	1.332961
O	-3.616363	-0.725021	2.180023
O	-3.086929	1.469796	3.034838
O	-3.861810	1.239614	0.704619
H	-2.618570	2.326212	2.831853
H	-3.371637	2.658187	-1.527193
C	3.081924	3.907250	0.332227
N	2.980082	2.517650	0.874236
C	3.545629	2.356305	2.242164
H	2.695493	3.895891	-0.683884
H	4.133450	4.191410	0.317565
H	2.492464	4.570022	0.961436
H	3.481956	1.882958	0.228490
H	2.961226	2.963926	2.930796
H	4.583912	2.686456	2.233046
H	3.493034	1.302818	2.510611
C	-0.251973	-0.445882	4.066612
N	-0.582977	-1.522342	3.093650
C	-1.463755	-2.590036	3.642539
H	0.375608	0.288187	3.565908
H	0.280051	-0.882657	4.911298
H	-1.173140	0.030327	4.397646
H	0.298411	-1.938124	2.739969
H	-1.577942	-3.355482	2.880259
H	-2.429343	-2.151735	3.883263
H	-0.992062	-3.014983	4.528808
C	-2.975153	4.482289	-2.388296
N	-3.280011	3.643403	-1.199954
C	-4.504107	4.057964	-0.462442
H	-2.062768	4.110888	-2.849878
H	-2.832284	5.514551	-2.071004
H	-3.797621	4.409733	-3.098430
H	-2.454804	3.685138	-0.559064
H	-5.360694	3.999818	-1.133906
H	-4.373846	5.079813	-0.107059
H	-4.638148	3.378199	0.374791
6SA7DMA			
C	-8.681464	-1.671082	0.328046

N	-7.391543	-2.347212	0.509106
C	-7.518656	-3.776657	0.814031
H	-9.190894	-2.092955	-0.541366
H	-8.509917	-0.610316	0.138673
H	-9.342406	-1.774677	1.199244
H	-6.861058	-1.882006	1.241894
H	-7.978053	-4.287387	-0.035309
H	-8.131712	-3.968559	1.705037
H	-6.526656	-4.204234	0.968449
S	5.605008	0.776858	0.198404
O	6.994218	1.054593	0.443157
O	5.101839	-0.467742	0.887366
O	4.657697	1.871218	0.431173
O	5.534953	0.406605	-1.375950
H	2.197713	0.738045	1.973131
H	4.644645	0.036855	-1.589597
C	3.520654	1.320547	3.440077
N	2.960108	0.291467	2.526506
C	2.429865	-0.906008	3.229538
H	3.923683	2.124400	2.829761
H	4.320432	0.875328	4.031848
H	2.728284	1.689980	4.089767
H	3.700302	0.003867	1.849755
H	2.129110	-1.645439	2.490810
H	1.561247	-0.611356	3.814802
H	3.212510	-1.316089	3.868922
S	-4.376680	-1.196620	-0.756907
O	-3.413067	-2.307115	-0.739281
O	-4.735464	-0.728749	0.603350
O	-3.932326	-0.093645	-1.624444
O	-5.705477	-1.733033	-1.417102
H	-3.139708	2.231052	0.328312
H	-6.378323	-2.026222	-0.687060
C	-4.215419	2.639481	2.034527
N	-4.095675	2.050510	0.673321
C	-5.094680	2.579896	-0.295965
H	-3.409446	2.257053	2.655901
H	-5.188376	2.375646	2.448943
H	-4.118287	3.720461	1.951132
H	-4.202154	1.019064	0.723380
H	-4.967918	2.042944	-1.232343
H	-4.911716	3.641883	-0.434629
H	-6.093354	2.399829	0.102532
S	-0.413630	1.526784	1.781232

O	0.970337	1.888694	1.402267
O	-0.473535	0.457473	2.769207
O	-0.993715	2.811204	2.578395
O	-1.292653	1.337251	0.620130
H	-0.922486	3.605765	1.988918
H	-0.800257	-3.147727	1.057040
C	-2.236247	-4.602852	1.398557
N	-1.816193	-3.179229	1.301002
C	-2.058693	-2.378458	2.533074
H	-2.011323	-5.098673	0.457315
H	-3.305600	-4.642495	1.604611
H	-1.674568	-5.088325	2.194865
H	-2.343170	-2.745870	0.511310
H	-1.623392	-1.386371	2.412236
H	-1.590916	-2.882035	3.379304
H	-3.133498	-2.295371	2.690696
S	1.925205	-0.562419	-1.533144
O	0.860109	-1.416763	-2.128613
O	3.267594	-1.005715	-1.928001
O	1.681175	0.854833	-1.729567
O	1.812670	-0.803757	0.044968
H	1.988626	2.569958	-0.396131
H	1.451094	-1.721045	0.231530
S	-1.344099	4.892293	-0.447039
O	-2.544596	4.088261	-0.590086
O	-0.309360	4.656651	-1.465338
O	-1.903302	6.403180	-0.734164
O	-0.782709	4.928933	0.913000
H	-1.149175	7.005508	-0.679334
H	-0.642980	-0.405261	-2.352197
S	1.306726	-4.361666	-0.165370
O	0.871514	-3.158495	0.639350
O	0.689372	-5.578730	0.290657
O	0.695579	-4.101753	-1.624472
O	2.765159	-4.377920	-0.291994
H	0.834043	-3.155446	-1.879567
H	4.112726	-3.294698	-0.338050
C	2.619334	4.357942	0.447885
N	2.142192	3.540743	-0.702461
C	3.068442	3.557910	-1.868437
H	1.886182	4.273313	1.244524
H	2.701432	5.395218	0.123200
H	3.587965	3.974152	0.759766
H	1.206905	3.896050	-0.989827

H	4.024582	3.149532	-1.548814
H	3.176598	4.586461	-2.212499
H	2.645597	2.933493	-2.650202
C	-1.217250	1.560805	-2.747975
N	-1.452340	0.087058	-2.774542
C	-1.663545	-0.480870	-4.131116
H	-1.091988	1.863685	-1.712753
H	-2.080694	2.062094	-3.182903
H	-0.314672	1.785826	-3.310644
H	-2.303615	-0.109122	-2.207266
H	-1.832403	-1.552410	-4.037175
H	-0.777011	-0.299079	-4.736908
H	-2.535689	-0.009562	-4.582127
C	5.825809	-3.675438	0.743562
N	5.084732	-2.927310	-0.303550
C	5.683322	-3.034078	-1.661635
H	5.320711	-3.531275	1.696677
H	6.842101	-3.288896	0.808033
H	5.833100	-4.735116	0.491831
H	5.039665	-1.924569	-0.001472
H	5.755208	-4.087295	-1.932576
H	6.669982	-2.572974	-1.654161
H	5.032605	-2.511116	-2.356815
6SA8DMA			
C	-5.024450	-4.280294	-2.666923
N	-6.064962	-4.388142	-1.631444
C	-5.818368	-5.491385	-0.689898
H	-4.077929	-4.038250	-2.181640
H	-5.280662	-3.468653	-3.350285
H	-4.905232	-5.208342	-3.241149
H	-6.967743	-4.525110	-2.077425
H	-4.895635	-5.282379	-0.146691
H	-5.719645	-6.462421	-1.192365
H	-6.637386	-5.543989	0.029530
C	9.179595	-1.043568	0.661551
N	8.105831	-0.922341	-0.319546
C	8.614270	-0.796178	-1.683352
H	9.716809	-1.986983	0.514668
H	8.759906	-1.050607	1.670798
H	9.921400	-0.228288	0.606938
H	7.554293	-0.091554	-0.110664
H	9.082620	-1.735100	-1.999151
H	9.363542	0.005212	-1.799403
H	7.786817	-0.578810	-2.362077

S	4.900905	1.272488	-0.200146
O	6.304706	1.609665	-0.117469
O	4.519169	0.094181	0.650476
O	3.957393	2.370063	0.016089
O	4.709377	0.752455	-1.716429
H	1.673642	1.261025	1.897409
H	3.845063	0.277147	-1.797137
C	3.089792	2.058139	3.159174
N	2.507731	0.911060	2.415222
C	2.123087	-0.230658	3.286239
H	3.385533	2.811765	2.434112
H	3.965964	1.718042	3.711338
H	2.340567	2.454247	3.843250
H	3.195288	0.589221	1.700410
H	1.788827	-1.055629	2.661069
H	1.307398	0.084774	3.933041
H	2.992087	-0.536290	3.870059
S	-4.793035	-1.516341	0.018126
O	-3.771628	-2.585886	0.034561
O	-4.865934	-0.760197	1.272539
O	-4.630138	-0.638243	-1.161544
O	-6.194321	-2.228238	-0.115952
H	-3.918082	2.378115	0.453201
H	-6.134086	-3.042466	-0.754117
C	-4.852224	2.699705	2.255506
N	-4.749335	2.011957	0.940552
C	-5.941592	2.189828	0.068549
H	-3.906421	2.588123	2.780772
H	-5.667225	2.253121	2.824356
H	-5.045873	3.757303	2.081460
H	-4.603770	0.993396	1.090702
H	-5.807948	1.568184	-0.813834
H	-6.016572	3.238847	-0.209005
H	-6.827123	1.862437	0.612503
S	-0.938240	1.945393	1.906678
O	0.363624	2.328167	1.311487
O	-0.794666	1.043880	3.041395
O	-1.530488	3.301141	2.568561
O	-1.920004	1.522379	0.903406
H	-1.619386	3.982207	1.855921
H	-1.079728	-2.859773	1.829165
C	-2.363805	-4.282279	2.626042
N	-2.065133	-2.898017	2.171789
C	-2.286481	-1.849971	3.208103

H	-2.107300	-4.974255	1.827085
H	-3.421534	-4.351294	2.878824
H	-1.752652	-4.511507	3.498120
H	-2.670669	-2.694445	1.345375
H	-1.922385	-0.891474	2.841622
H	-1.737069	-2.124882	4.108773
H	-3.352980	-1.783444	3.416749
S	1.199393	-0.449669	-1.433448
O	0.158881	-1.429756	-1.855190
O	2.539810	-0.858642	-1.870642
O	0.851524	0.917851	-1.773428
O	1.198349	-0.506545	0.163815
H	1.134724	2.826349	-0.615303
H	0.931206	-1.420287	0.484959
S	-2.383219	4.839175	-0.745955
O	-3.523089	3.937362	-0.699222
O	-1.394686	4.533740	-1.791190
O	-3.083716	6.245781	-1.198518
O	-1.749058	5.111551	0.551568
H	-2.388523	6.916653	-1.233742
H	-1.399860	-0.569388	-2.097322
S	0.900297	-4.098061	0.422324
O	0.505800	-2.819640	1.125402
O	0.369851	-5.265554	1.077366
O	0.133241	-4.029630	-0.986180
O	2.336337	-4.097146	0.144939
H	0.220397	-3.121983	-1.369036
H	3.663882	-2.977009	-0.059500
C	1.702011	4.743177	-0.074406
N	1.194241	3.751490	-1.062958
C	2.021224	3.670192	-2.299115
H	1.048789	4.717434	0.792725
H	1.680754	5.731527	-0.533499
H	2.719154	4.466076	0.193708
H	0.214926	4.001935	-1.312514
H	3.029559	3.375736	-2.016656
H	2.019762	4.647213	-2.782338
H	1.589030	2.917154	-2.951499
C	-2.197346	1.335025	-2.414161
N	-2.274368	-0.154858	-2.476252
C	-2.475330	-0.697429	-3.842880
H	-2.014770	1.620478	-1.382212
H	-3.141935	1.753229	-2.757849
H	-1.375327	1.674704	-3.038083

H	-3.073776	-0.457533	-1.877114
H	-2.511766	-1.784440	-3.789466
H	-1.642439	-0.391869	-4.474648
H	-3.412387	-0.313944	-4.244994
C	5.555682	-3.075591	0.798957
N	4.597779	-2.550062	-0.212002
C	5.018151	-2.822759	-1.614267
H	5.192328	-2.811535	1.790864
H	6.525577	-2.611508	0.611395
H	5.609425	-4.159939	0.706001
H	4.508199	-1.523698	-0.054870
H	5.082575	-3.901734	-1.753537
H	5.988768	-2.358816	-1.778149
H	4.268937	-2.403033	-2.279867
7DMA			
C	2.784802	-3.691139	-0.668083
N	1.923437	-2.530461	-0.867487
C	1.523368	-2.366859	-2.260857
H	2.230704	-4.612274	-0.878516
H	3.113773	-3.730978	0.373071
H	3.682181	-3.692189	-1.311284
H	2.417980	-1.686262	-0.557462
H	0.882432	-3.199697	-2.569480
H	2.374263	-2.325692	-2.963015
H	0.947704	-1.444928	-2.371511
C	4.441643	-0.317446	1.122312
N	3.583705	0.009049	-0.012806
C	4.351151	0.424456	-1.183125
H	5.046930	-1.201749	0.895361
H	3.825514	-0.548986	1.994357
H	5.135724	0.495364	1.398163
H	2.953129	0.771820	0.258444
H	4.945862	-0.414188	-1.561105
H	5.045988	1.258057	-0.981606
H	3.669543	0.735003	-1.978561
C	-0.271872	-1.813826	2.172557
N	-0.553567	-2.702554	1.050182
C	-0.724955	-4.090250	1.467680
H	-1.141424	-1.756014	2.836385
H	-0.066261	-0.808720	1.797640
H	0.589974	-2.134550	2.783439
H	0.225104	-2.645068	0.383646
H	-1.619349	-4.188667	2.092316
H	0.127534	-4.485652	2.046980

H	-0.861575	-4.725150	0.588840
C	-0.959419	4.179591	-1.221980
N	-0.641558	2.775185	-0.983746
C	-0.354752	2.053275	-2.218869
H	-0.081554	4.703837	-1.614814
H	-1.239283	4.658569	-0.280520
H	-1.783587	4.330258	-1.940761
H	-1.438730	2.327701	-0.516315
H	0.560302	2.441784	-2.679012
H	-1.160034	2.126981	-2.970325
H	-0.193455	0.996399	-1.994419
C	1.459157	2.437805	2.266431
N	1.876262	2.515777	0.870137
C	2.714189	3.682207	0.609883
H	2.329174	2.272961	2.911201
H	0.779223	1.593430	2.400763
H	0.949029	3.348420	2.625883
H	1.040792	2.566162	0.275235
H	3.663302	3.592303	1.149366
H	2.250094	4.636185	0.914963
H	2.942289	3.742223	-0.457074
C	-4.282586	-2.250066	0.238605
N	-3.124819	-1.601530	-0.368174
C	-3.046242	-1.837391	-1.805864
H	-5.207157	-1.799424	-0.138132
H	-4.259920	-2.106526	1.321656
H	-4.337722	-3.334165	0.037935
H	-2.269359	-1.955353	0.076242
H	-3.893369	-1.363040	-2.313196
H	-3.054995	-2.907137	-2.078741
H	-2.129317	-1.394441	-2.201270
C	-3.178598	1.604440	1.771386
N	-3.178508	1.464872	0.318987
C	-4.371943	2.039012	-0.294048
H	-3.112773	2.662062	2.048894
H	-2.307227	1.095134	2.189170
H	-4.081713	1.191874	2.254211
H	-3.125104	0.468210	0.078459
H	-4.386732	3.124255	-0.146299
H	-5.315302	1.637279	0.115073
H	-4.360943	1.849357	-1.370104
7SA			
S	1.624160	0.093228	2.866808
O	2.424918	-0.798813	2.014218

O	1.344019	-0.281871	4.200000
O	2.334812	1.492806	2.872352
O	0.246968	0.333677	2.129428
H	2.414388	1.830736	1.948246
H	0.363772	0.650991	1.209773
S	5.327531	-0.618604	-0.015648
O	6.540071	-1.174318	-0.495024
O	4.095360	-0.777334	-0.788464
O	5.095739	-1.181707	1.434400
O	5.465644	0.925733	0.271049
H	4.196528	-0.946569	1.760208
H	4.925216	1.455936	-0.365946
S	-5.542231	0.262630	1.182838
O	-6.379097	1.029246	2.026395
O	-4.673569	0.896992	0.196282
O	-4.616956	-0.641837	2.101352
O	-6.443143	-0.771488	0.408932
H	-3.858382	-0.981486	1.583072
H	-5.893605	-1.274550	-0.232309
S	-3.066202	-1.860962	-1.174765
O	-4.470234	-2.100073	-1.030747
O	-2.577424	-0.975197	-2.205938
O	-2.520193	-1.299664	0.228650
O	-2.402658	-3.253641	-1.271040
H	-2.049032	-0.434239	0.088232
H	-1.406791	-3.215405	-1.362079
S	-1.852012	2.252539	-0.940039
O	-0.931782	3.321450	-1.190802
O	-1.387303	1.108802	-0.164974
O	-3.080820	2.910217	-0.258743
O	-2.381091	1.728757	-2.319440
H	-3.766636	2.225788	-0.004675
H	-2.483853	0.742835	-2.320591
S	2.348200	2.267468	-1.057775
O	3.765067	2.411530	-1.231309
O	1.861319	1.922847	0.271188
O	1.712395	3.595169	-1.549958
O	1.745669	1.237591	-2.072188
H	0.723462	3.556392	-1.460018
H	1.503699	0.381716	-1.625470
S	1.212162	-2.373419	-0.885670
O	0.901286	-0.953544	-0.832200
O	0.228912	-3.265958	-1.432898
O	2.510149	-2.617452	-1.700321

O	1.521410	-2.855819	0.569594
H	3.235075	-1.984296	-1.411107
H	1.834687	-2.102699	1.142318
7SA1DMA			
S	-2.499128	-1.380629	2.953305
O	-2.015403	-0.121030	2.395338
O	-2.326790	-1.673392	4.329499
O	-4.030836	-1.510632	2.631873
O	-1.856666	-2.539857	2.079998
H	-4.200084	-1.270693	1.689661
H	-1.321272	-2.163719	1.348051
S	4.508472	-2.741250	-0.654249
O	4.757052	-4.100056	-0.964325
O	3.376688	-2.033214	-1.242189
O	4.377904	-2.609512	0.920716
O	5.812562	-1.924054	-0.995634
H	3.995046	-1.733856	1.145839
H	5.728529	-0.984513	-0.711219
S	-4.815054	-1.365370	-1.147830
O	-4.067868	-0.797191	-0.008740
O	-6.121630	-1.855379	-0.904193
O	-4.778842	-0.285684	-2.292494
O	-3.977826	-2.515511	-1.786831
H	-4.671307	0.634958	-1.941292
H	-3.021735	-2.276994	-1.878590
S	-2.690047	2.312862	-0.982675
O	-4.062777	2.179541	-1.400217
O	-1.724938	2.891457	-1.881567
O	-2.712246	3.084087	0.374476
O	-2.107622	0.896761	-0.609550
H	-1.784014	3.087359	0.751935
H	-2.807239	0.308723	-0.218204
S	-0.078228	-1.471615	-1.461638
O	-1.347893	-1.883763	-1.989906
O	0.554712	-0.273775	-1.939350
O	-0.253495	-1.339067	0.121308
O	0.861267	-2.700331	-1.607167
H	0.101514	-0.468038	0.479234
H	1.827649	-2.464401	-1.468249
S	4.162681	1.160317	0.457722
O	5.439537	0.611448	0.104108
O	3.338260	1.765617	-0.558296
O	3.350330	-0.010908	1.149194
O	4.401116	2.176557	1.622349

H	2.356470	0.234779	1.230922
H	3.516231	2.475186	1.972338
S	0.631478	2.010177	1.905945
O	0.921767	0.682783	1.248622
O	1.852963	2.635092	2.374524
O	-0.173755	2.849048	1.016052
O	-0.202867	1.686573	3.197473
H	1.618870	1.996708	-1.480924
H	-0.917494	1.026409	2.994838
C	1.407693	4.041948	-1.691571
N	1.099359	2.637105	-2.093130
C	1.433005	2.318569	-3.512477
H	1.107440	4.170831	-0.654408
H	0.843844	4.717695	-2.332412
H	2.477166	4.209441	-1.801437
H	0.093790	2.470611	-1.936362
H	1.178862	1.277985	-3.695382
H	2.498971	2.479039	-3.665175
H	0.854642	2.972929	-4.162832

7SA2DMA

S	-5.649779	-1.900662	-1.065276
O	-4.445130	-1.827300	-0.251427
O	-6.233284	-3.145939	-1.402877
O	-6.765529	-1.031262	-0.361551
O	-5.359579	-1.114109	-2.417338
H	-6.439686	-0.118793	-0.185166
H	-4.769423	-0.353753	-2.231781
S	3.145369	-4.021815	-0.689241
O	3.633606	-2.662377	-0.845346
O	3.921346	-5.126407	-1.126291
O	2.840381	-4.255070	0.848401
O	1.737642	-4.111518	-1.382664
H	2.464225	-3.443788	1.256360
H	1.255824	-3.243852	-1.359600
S	3.444010	3.036758	-1.815299
O	4.629628	3.111900	-2.598379
O	3.302461	1.985394	-0.819668
O	3.244882	4.419940	-1.100016
O	2.215466	2.925006	-2.804174
H	2.427107	4.377804	-0.533569
H	1.405593	2.668679	-2.299513
S	2.242174	-0.736106	2.602510
O	1.225047	-0.122833	3.420660
O	3.475552	-1.197736	3.146721

O	1.592100	-1.996836	1.872567
O	2.593061	0.231706	1.409025
H	0.672122	-1.786312	1.503743
H	1.883347	0.930128	1.262111
S	-4.194381	1.600416	-0.058827
O	-5.623272	1.524047	-0.171588
O	-3.546101	1.037962	1.100470
O	-3.626724	0.891222	-1.360408
O	-3.789131	3.092617	-0.231652
H	-2.696515	0.506335	-1.215202
H	-2.828878	3.226574	0.034532
S	-0.811030	-1.359480	-0.583030
O	0.399981	-1.785379	-1.252708
O	-0.719596	-1.381013	0.890808
O	-1.266029	-0.015801	-1.055158
O	-1.918596	-2.387234	-1.021034
H	-0.335722	1.368446	-1.160864
H	-2.816590	-2.191593	-0.644811
S	0.067461	2.926123	0.312259
O	0.918503	4.090356	0.168109
O	0.073406	2.275669	-1.179855
O	0.581212	1.876272	1.209945
O	-1.326775	3.231990	0.640301
H	4.266197	0.501101	-0.516950
H	-2.116709	1.003476	2.219691
C	-1.490455	2.075720	3.877728
N	-1.502032	0.848438	3.031701
C	-1.947308	-0.385904	3.740540
H	-1.216587	2.918895	3.248795
H	-0.762189	1.942867	4.675685
H	-2.485950	2.226462	4.293001
H	-0.556245	0.706627	2.655942
H	-2.951900	-0.223444	4.128102
H	-1.250112	-0.594170	4.549267
H	-1.948653	-1.203709	3.024335
C	5.653567	-0.220458	-1.864261
N	4.959753	-0.266234	-0.544450
C	5.865222	-0.154233	0.634242
H	6.118784	0.755432	-1.990862
H	4.913613	-0.376764	-2.646599
H	6.398323	-1.013841	-1.900416
H	4.427747	-1.150907	-0.491282
H	6.383136	0.802977	0.592098
H	6.585479	-0.970794	0.604528

H	5.266031	-0.220117	1.539643
7SA3DMA			
S	-3.777547	-3.737915	-1.239148
O	-4.183743	-5.095654	-1.156874
O	-2.812962	-3.311761	-2.243599
O	-5.083540	-2.879940	-1.385475
O	-3.204189	-3.280116	0.173788
H	-4.897840	-1.908737	-1.362169
H	-2.399252	-2.717470	0.044277
S	2.180534	-2.173618	3.312230
O	2.001307	-2.872110	4.536438
O	3.264459	-2.517273	2.409175
O	0.826092	-2.261972	2.495310
O	2.286121	-0.641524	3.668199
H	0.989406	-2.276889	1.508891
H	2.548303	-0.109265	2.856657
S	-3.755101	0.640093	-0.485245
O	-3.620072	0.446846	0.937031
O	-4.683859	-0.198677	-1.199659
O	-4.120480	2.105063	-0.847186
O	-2.318129	0.550167	-1.145164
H	-3.410816	2.740631	-0.510942
H	-1.813441	-0.237381	-0.783278
S	-1.625158	4.054853	1.089233
O	-2.042595	3.214021	2.195870
O	-2.112674	3.613643	-0.238415
O	-2.392111	5.472098	1.240544
O	-0.191563	4.361305	1.054262
H	-2.215461	5.817628	2.127429
H	1.033462	3.396824	1.646911
S	3.533657	0.717022	-3.056656
O	4.620094	0.381526	-3.912219
O	2.398210	1.474393	-3.519547
O	2.974933	-0.650554	-2.425371
O	4.155737	1.412671	-1.785083
H	1.969883	-0.687840	-2.375815
H	3.411663	1.723209	-1.185310
S	1.747744	1.512564	0.952432
O	2.837819	0.669425	1.463277
O	1.750664	2.763790	1.928934
O	2.037133	2.023107	-0.409019
O	0.424922	0.896662	1.014969
H	-0.843553	3.032610	-1.449365
H	3.676976	-1.320933	-0.796376

S	0.119481	-1.986663	-1.008352
O	0.422938	-0.985296	-2.034524
O	1.252648	-2.275613	-0.126166
O	-1.119495	-1.625510	-0.262881
O	-0.181559	-3.367532	-1.716204
H	-0.801249	0.347448	2.236886
H	-1.117861	-3.384434	-2.052217
C	-2.124171	-0.899360	3.283356
N	-1.510144	0.428805	2.986919
C	-0.847810	1.070218	4.160417
H	-2.626669	-1.252889	2.388415
H	-2.848605	-0.776729	4.087496
H	-1.336084	-1.589431	3.574835
H	-2.211896	1.069283	2.595000
H	-0.469557	2.038688	3.846149
H	-0.030387	0.431898	4.490536
H	-1.581578	1.195879	4.955284
C	4.442059	-3.226814	-0.660944
N	4.239177	-1.853566	-0.117350
C	5.494234	-1.106285	0.180645
H	3.462588	-3.670592	-0.825478
H	5.000394	-3.813646	0.066484
H	4.989072	-3.160499	-1.600170
H	3.686595	-1.931990	0.752397
H	5.219437	-0.131838	0.577489
H	6.066304	-0.988648	-0.738213
H	6.066628	-1.666561	0.918415
C	-0.660281	2.257376	-3.376693
N	-0.092402	2.885304	-2.146456
C	0.584138	4.193687	-2.384589
H	-1.113797	1.309727	-3.100223
H	0.146482	2.097014	-4.086635
H	-1.415224	2.926898	-3.787651
H	0.596369	2.260598	-1.700543
H	0.916941	4.582186	-1.424819
H	-0.130031	4.880336	-2.836910
H	1.430758	4.027254	-3.047563

7SA4DMA

S	-3.076831	-3.859253	-1.845942
O	-3.587009	-4.989074	-2.544130
O	-1.937925	-4.003179	-0.957052
O	-2.727508	-2.778148	-2.947246
O	-4.242306	-3.173225	-1.042963
H	-2.136045	-2.061980	-2.602300

H	-3.987162	-2.982855	-0.080457
S	0.283307	4.046359	-1.593850
O	1.149525	3.560686	-0.523333
O	0.396580	5.403099	-2.012612
O	0.487019	3.148807	-2.865053
O	-1.203319	3.710169	-1.205380
H	0.494209	2.171602	-2.619066
H	-1.327376	3.477420	-0.225687
S	6.404036	-1.138366	-0.353047
O	5.707411	0.129559	-0.446936
O	7.684181	-1.314278	-0.943264
O	6.524380	-1.531517	1.169284
O	5.445849	-2.255861	-0.955729
H	5.636098	-1.430875	1.603081
H	4.514061	-2.063041	-0.698508
S	-3.117613	2.897723	1.627650
O	-1.691324	3.122983	1.250056
O	-3.233176	1.977322	2.742353
O	-3.627274	4.297266	2.259548
O	-3.951378	2.654397	0.455574
H	-3.817718	4.907267	1.532696
H	-3.810218	1.397258	-0.877158
C	-5.000615	0.072793	-1.947800
N	-3.812981	0.965791	-1.818694
C	-3.739668	2.046218	-2.842099
H	-4.936568	-0.693192	-1.180942
H	-4.987250	-0.393797	-2.931632
H	-5.903411	0.668870	-1.821887
H	-2.954031	0.392399	-1.880969
H	-2.850673	2.644231	-2.652913
H	-4.628116	2.670633	-2.760291
H	-3.687980	1.593223	-3.831190
S	2.766427	-1.016397	1.458249
O	4.018081	-1.403134	2.087635
O	2.625706	0.443109	1.254460
O	2.910809	-1.634787	-0.052941
O	1.570402	-1.614307	2.034885
H	2.036377	-1.560352	-0.529584
H	1.101765	1.222621	1.920599
S	-0.162370	-0.285593	-1.529713
O	-0.608274	0.470591	-0.206350
O	0.504746	-1.533082	-1.146388
O	-1.406927	-0.531223	-2.289720
O	0.749866	0.659131	-2.184481

H	-0.970291	-3.570931	0.553035
H	2.623639	2.497758	-0.846982
S	-3.043585	-1.321772	1.704328
O	-1.802541	-1.412608	2.459675
O	-3.648416	-2.621517	1.398703
O	-4.144357	-0.591888	2.589292
O	-2.880840	-0.482236	0.482532
H	-3.877383	0.351190	2.708967
H	-1.463481	0.052947	0.152223
C	-0.638607	-4.354861	2.448303
N	-0.169552	-3.711790	1.186984
C	0.851664	-4.504784	0.445372
H	-1.358082	-3.689006	2.915861
H	0.220421	-4.505799	3.100594
H	-1.101665	-5.309322	2.202378
H	0.229126	-2.786270	1.413541
H	0.436877	-5.485837	0.221470
H	1.744158	-4.594483	1.061887
H	1.080168	-3.984393	-0.480501
C	0.040942	1.005462	3.695572
N	0.481110	1.804976	2.512904
C	1.205967	3.057620	2.862896
H	-0.447011	0.100005	3.341885
H	-0.659457	1.603882	4.276197
H	0.917690	0.753818	4.290684
H	-0.344742	2.071708	1.951291
H	1.423244	3.595753	1.942340
H	2.126464	2.798015	3.384028
H	0.568930	3.665982	3.503040
C	3.824067	1.680302	-2.339099
N	3.559334	2.065370	-0.920270
C	4.562695	3.011763	-0.354359
H	3.048295	0.985533	-2.651364
H	4.803012	1.212234	-2.386374
H	3.788181	2.578407	-2.954785
H	3.521904	1.229096	-0.317276
H	4.286393	3.233258	0.674831
H	4.555849	3.926866	-0.944876
H	5.537988	2.533014	-0.381202
7SA5DMA			
S	3.059739	4.309648	-2.297600
O	4.025214	3.721481	-1.387985
O	3.475379	5.202519	-3.324832
O	2.273115	3.119129	-2.992146

O	1.957079	5.053603	-1.459898
H	2.352752	2.297012	-2.446785
H	1.760937	4.589935	-0.595472
S	-0.571788	-3.916371	-1.437082
O	0.771767	-4.453446	-1.469585
O	-1.672529	-4.698764	-1.905776
O	-0.789350	-3.453877	0.047694
O	-0.612610	-2.569407	-2.262241
H	-1.671029	-2.943990	0.170209
H	0.208121	-2.018053	-2.072826
S	4.458407	-1.891767	1.611684
O	4.430892	-0.579078	2.261453
O	3.251542	-2.698103	1.757354
O	4.941687	-1.829121	0.221626
O	5.555303	-2.771178	2.442569
H	3.915050	-2.830448	-0.789717
H	6.343743	-2.224051	2.562294
C	3.759488	-3.368461	-2.792804
N	3.449840	-3.573999	-1.351754
C	3.862715	-4.897853	-0.811216
H	3.395940	-2.383458	-3.076275
H	3.252769	-4.136156	-3.375782
H	4.837357	-3.433890	-2.936924
H	2.432944	-3.479614	-1.225475
H	3.629486	-4.912586	0.251245
H	4.935143	-5.021133	-0.956800
H	3.310382	-5.679327	-1.329487
S	-2.877726	-0.915325	1.286109
O	-2.947985	0.339958	0.533661
O	-1.781928	-1.021252	2.238722
O	-4.176153	-1.028701	2.168947
O	-2.902441	-2.067224	0.324060
H	-4.993806	-0.898485	1.589785
H	1.529052	-1.882340	2.098740
C	0.481227	-3.308657	3.151601
N	0.752414	-1.893557	2.775422
C	1.107118	-1.020150	3.929339
H	0.216483	-3.855463	2.249290
H	-0.349551	-3.329833	3.855173
H	1.379992	-3.729448	3.598108
H	-0.095516	-1.507471	2.321048
H	1.242360	-0.001945	3.572267
H	2.028931	-1.386591	4.377321
H	0.290276	-1.047552	4.648819

S	0.242587	3.160155	1.225786
O	-0.466651	2.620853	0.046207
O	1.458916	3.897717	0.863861
O	-0.650708	3.858491	2.138418
O	0.747462	1.879850	2.069353
H	-2.308404	3.276569	1.803917
H	1.011372	1.163717	1.438970
S	-6.570752	0.474169	-0.164693
O	-6.215488	0.357429	-1.589997
O	-6.184442	1.712390	0.474033
O	-8.197687	0.527298	-0.120912
O	-6.200819	-0.755911	0.566830
H	-8.527363	-0.291242	-0.516053
H	-3.602338	-1.492188	-1.229154
S	1.507307	0.011900	-1.008256
O	1.455650	-0.146241	0.455118
O	1.586811	-1.273113	-1.721414
O	0.121496	0.604286	-1.482437
O	2.567709	0.952814	-1.407305
H	-0.129083	1.395967	-0.908603
H	4.324195	0.874538	1.192814
C	-4.174098	2.925390	2.667901
N	-3.248314	2.954222	1.501187
C	-3.705827	3.817725	0.374738
H	-3.752268	2.266543	3.425853
H	-5.137670	2.546540	2.334263
H	-4.270108	3.934241	3.068815
H	-3.124829	1.985098	1.146715
H	-3.807192	4.841487	0.734449
H	-4.659273	3.437022	0.014233
H	-2.946812	3.775912	-0.404124
C	-3.129507	-0.384018	-2.921878
N	-4.057568	-1.232102	-2.124383
C	-4.500452	-2.478830	-2.803394
H	-2.813809	0.447816	-2.296444
H	-3.656965	-0.015498	-3.801160
H	-2.262925	-0.974640	-3.209524
H	-4.898084	-0.655091	-1.875447
H	-5.198084	-2.995766	-2.146212
H	-3.636766	-3.115051	-2.992084
H	-4.997119	-2.219828	-3.737991
C	4.513637	2.914551	1.539426
N	4.530662	1.725557	0.637971
C	5.825718	1.511947	-0.068077

H	3.506845	3.037935	1.931629
H	4.778493	3.791738	0.955295
H	5.227242	2.745281	2.345317
H	3.794990	1.813656	-0.077593
H	6.622177	1.453893	0.673093
H	5.986150	2.345188	-0.747767
H	5.762208	0.572549	-0.613070

7SA6DMA

S	4.661309	-2.979433	-2.226059
O	5.388619	-3.519750	-3.324961
O	3.891384	-3.840009	-1.350954
O	5.703155	-2.178514	-1.342601
O	3.706656	-1.857546	-2.788391
H	5.276260	-1.866837	-0.495883
H	2.943536	-1.665946	-2.160079
S	3.132669	4.867121	0.077828
O	4.498962	4.786148	-0.405474
O	2.258409	5.801401	-0.610077
O	2.510171	3.524375	0.265973
O	3.211705	5.366003	1.644607
H	3.730130	2.229335	0.025035
H	3.597458	6.253126	1.638395
C	4.597296	1.568132	-1.734350
N	4.500169	1.584882	-0.245115
C	5.757199	2.002515	0.439081
H	3.625132	1.294729	-2.141650
H	5.343172	0.832114	-2.031029
H	4.879815	2.565520	-2.066550
H	4.274759	0.634679	0.099289
H	5.593546	1.948226	1.514074
H	5.988128	3.023175	0.145562
H	6.552163	1.313917	0.157202
S	3.880085	-1.340357	1.978078
O	3.136672	-0.189430	2.457564
O	3.174158	-2.605619	1.882665
O	4.648001	-1.011093	0.745716
O	5.012854	-1.537358	3.139271
H	1.173872	0.543623	2.087295
H	5.429306	-2.398575	2.997237
C	0.332911	0.075142	3.917258
N	0.627997	1.029221	2.812147
C	1.378782	2.240936	3.245833
H	-0.210052	-0.772442	3.504356
H	-0.274400	0.583194	4.666306

H	1.278006	-0.252995	4.343697
H	-0.253855	1.323619	2.355474
H	1.618158	2.844745	2.372281
H	2.299774	1.918392	3.726088
H	0.759229	2.806452	3.941354
S	0.897204	-0.156288	-1.215191
O	1.239079	0.726205	-2.316240
O	0.716202	0.509760	0.072830
O	-0.563891	-0.741725	-1.640511
O	1.763378	-1.355062	-1.111061
H	-0.873306	-1.433913	-0.995447
H	0.683728	-3.900944	0.800692
C	2.151259	-5.355199	0.856074
N	1.469264	-4.210008	0.194336
C	0.912625	-4.532168	-1.148905
H	2.516018	-5.015675	1.821966
H	2.984861	-5.668011	0.231165
H	1.432239	-6.163765	0.982860
H	2.134588	-3.430751	0.122661
H	0.484145	-3.623632	-1.561371
H	0.137970	-5.288046	-1.028533
H	1.720485	-4.887381	-1.782613
S	-2.749050	1.691298	0.777803
O	-1.760514	2.130887	1.759925
O	-3.205177	0.298044	0.971798
O	-4.008611	2.622675	1.065318
O	-2.340239	1.933572	-0.618414
H	-4.724572	2.419786	0.408160
H	-0.695766	2.791094	-0.720478
S	-1.926386	-2.973201	1.152136
O	-0.874478	-3.858058	1.634202
O	-1.797088	-2.618490	-0.277690
O	-3.282232	-3.429437	1.480420
O	-1.678241	-1.610162	1.968142
H	-2.399152	0.067328	-1.932757
H	-2.229383	-0.877400	1.577290
S	-6.564207	0.702272	-0.831282
O	-5.876045	1.995743	-0.798935
O	-7.461325	0.441562	0.276896
O	-7.454879	0.718890	-2.199898
O	-5.646840	-0.428081	-1.109881
H	-8.123121	1.412044	-2.101033
H	-5.487532	-1.337839	0.467900
C	0.149481	3.844422	-2.296621

N	-0.090394	3.619916	-0.842774
C	-0.745464	4.769115	-0.154091
H	0.594907	2.938895	-2.704622
H	0.822642	4.692839	-2.402589
H	-0.805341	4.051112	-2.780032
H	0.825179	3.430997	-0.390312
H	-1.703419	4.962022	-0.634822
H	-0.086155	5.630775	-0.222680
H	-0.916699	4.490063	0.883434
C	-3.491315	1.015251	-3.410478
N	-3.258460	-0.115758	-2.471623
C	-3.161623	-1.449093	-3.127894
H	-3.559986	1.925803	-2.821376
H	-4.425633	0.842039	-3.942785
H	-2.659224	1.072297	-4.111404
H	-4.053156	-0.142131	-1.801470
H	-2.980621	-2.196376	-2.357507
H	-2.331351	-1.438386	-3.831589
H	-4.100145	-1.651030	-3.642668
C	-5.697761	-1.169828	2.530411
N	-5.574549	-1.973819	1.281342
C	-6.727335	-2.877218	1.027154
H	-4.817895	-0.535605	2.607884
H	-5.752766	-1.849676	3.380168
H	-6.592329	-0.554346	2.461192
H	-4.688060	-2.531319	1.322224
H	-7.625901	-2.271999	0.920183
H	-6.827542	-3.573506	1.859042
H	-6.541085	-3.428514	0.106881
7SA7DMA			
S	-3.702664	-3.063405	-0.552988
O	-2.438290	-3.572434	-0.013619
O	-4.828201	-3.995110	-0.411826
O	-4.023679	-1.723734	-0.014459
O	-3.543686	-2.898512	-2.129152
H	-6.816177	-1.835625	0.990507
H	-2.893779	-2.166461	-2.317820
C	-7.572827	-3.652735	1.649720
N	-7.063639	-2.768080	0.573787
C	-8.023128	-2.537622	-0.537848
H	-6.793815	-3.769670	2.401452
H	-7.822887	-4.627491	1.231426
H	-8.454435	-3.200511	2.103415
H	-6.184038	-3.189272	0.183534

H	-7.571100	-1.833347	-1.233054
H	-8.940891	-2.109085	-0.135785
H	-8.232427	-3.483629	-1.036592
S	4.913784	-3.351266	-0.795177
O	3.852164	-3.322818	-1.783988
O	5.820758	-2.189034	-0.839741
O	4.505169	-3.662951	0.579674
O	5.851049	-4.640106	-1.165336
H	5.343589	-2.611727	1.630235
H	5.976159	-4.637178	-2.124240
C	5.445138	-1.850854	3.572760
N	5.946236	-1.950161	2.175943
C	7.360884	-2.391222	2.051012
H	4.415301	-1.499140	3.542424
H	6.062352	-1.142647	4.125416
H	5.499333	-2.833786	4.040478
H	5.840623	-1.031679	1.701849
H	7.607832	-2.422055	0.992104
H	7.466408	-3.384533	2.486185
H	8.006122	-1.683394	2.570830
S	-6.131382	0.755255	0.799693
O	-6.649334	-0.314115	1.671651
O	-7.041801	1.845054	0.531911
O	-4.783009	1.207007	1.236704
O	-5.894121	0.068223	-0.647700
H	-3.410547	0.166811	1.745124
H	-5.121277	-0.550128	-0.566524
C	-2.014243	1.068892	2.967615
N	-2.452741	-0.046128	2.085452
C	-2.412243	-1.371859	2.757738
H	-2.051158	1.996913	2.403523
H	-0.992063	0.871975	3.284288
H	-2.685121	1.120664	3.825132
H	-1.865944	-0.078606	1.225429
H	-2.663104	-2.135495	2.027599
H	-3.136153	-1.374928	3.573198
H	-1.405271	-1.526918	3.139845
S	-1.567201	0.161220	-1.664778
O	-1.721871	-0.989582	-2.563730
O	-1.063994	-0.235620	-0.338896
O	-0.334943	0.968689	-2.370858
O	-2.681643	1.090948	-1.619510
H	-0.307184	1.905121	-2.026374
H	-3.141871	3.696884	-0.604326

C	-4.763588	4.383950	0.472823
N	-4.130321	3.414328	-0.462589
C	-4.821160	3.312808	-1.780447
H	-4.178679	4.410336	1.390128
H	-5.777326	4.048661	0.683308
H	-4.760696	5.370763	0.011672
H	-4.136978	2.483871	-0.008709
H	-4.298535	2.566452	-2.372238
H	-4.786491	4.287523	-2.266866
H	-5.849820	3.003710	-1.604134
S	1.707615	0.075785	1.380205
O	0.738480	-0.603963	2.222356
O	1.468066	1.526254	1.217499
O	3.081289	-0.014763	2.238835
O	1.983856	-0.596145	0.100209
H	3.838654	0.313188	1.695853
H	0.683975	-1.951359	-0.196548
S	-0.358420	4.080162	-0.348810
O	-1.648007	4.703129	-0.614132
O	0.238280	3.382486	-1.505406
O	0.619167	4.966180	0.299379
O	-0.729448	2.930840	0.716214
H	1.511751	0.627976	-2.196342
H	0.057682	2.339909	0.871801
S	5.553675	1.388952	-0.154578
O	5.438951	0.545519	1.067990
O	6.508511	2.461800	-0.055890
O	6.058446	0.418878	-1.316623
O	4.201097	1.843908	-0.569993
H	5.867457	-0.535045	-1.116806
H	3.325533	3.172235	0.293369
C	0.476302	-3.424265	-1.655046
N	0.281779	-2.901986	-0.271559
C	0.890375	-3.755334	0.786202
H	0.002339	-2.726789	-2.343786
H	-0.015586	-4.393547	-1.726031
H	1.543379	-3.517742	-1.848731
H	-0.736895	-2.832997	-0.107758
H	1.957776	-3.853757	0.593951
H	0.402126	-4.728964	0.771701
H	0.733902	-3.264777	1.744925
C	3.058415	-0.438221	-3.085138
N	2.486417	0.801357	-2.492620
C	2.497545	1.970632	-3.414683

H	3.065171	-1.224266	-2.335186
H	4.079988	-0.233022	-3.402115
H	2.450885	-0.734153	-3.939930
H	3.028639	1.044897	-1.642382
H	2.013999	2.808750	-2.916773
H	1.943688	1.713444	-4.316578
H	3.531206	2.211235	-3.658987
C	3.383556	3.948939	2.202695
N	3.163058	4.094007	0.738826
C	4.058901	5.081536	0.079083
H	2.715277	3.169990	2.562652
H	3.164100	4.898080	2.690835
H	4.420856	3.665582	2.379973
H	2.163759	4.366925	0.565600
H	5.086593	4.725696	0.140977
H	3.948799	6.048063	0.569714
H	3.763313	5.169354	-0.964982
7SA8DMA			
C	9.576456	1.239760	-1.711841
N	8.600627	0.436039	-0.971764
C	9.210092	-0.563923	-0.087873
H	10.169383	1.830397	-1.008592
H	9.050907	1.927980	-2.376295
H	10.266328	0.629061	-2.311468
H	7.969921	-0.029426	-1.621364
H	9.791738	-0.055985	0.685924
H	9.877450	-1.254318	-0.622449
H	8.420021	-1.136929	0.399245
S	-6.601154	1.221784	0.175944
O	-6.557664	-0.215709	0.417977
O	-5.806761	2.051528	1.064158
O	-6.412620	1.560190	-1.260854
O	-8.130111	1.703218	0.508988
H	-5.012937	2.774070	-1.570247
H	-8.718363	1.221975	-0.088716
C	-3.542384	3.496663	-2.882753
N	-4.071462	3.203595	-1.520451
C	-4.123894	4.391954	-0.623783
H	-3.567311	2.575380	-3.460401
H	-2.520711	3.855600	-2.775185
H	-4.169920	4.255291	-3.350652
H	-3.493676	2.443656	-1.107553
H	-4.618727	4.093203	0.297554
H	-4.705070	5.172693	-1.115113

H	-3.106028	4.728443	-0.440540
S	0.292114	4.151953	-0.378715
O	-0.997518	3.573617	-0.710345
O	0.574330	4.261051	1.062468
O	1.443963	3.610754	-1.113041
O	0.111839	5.696535	-0.915135
H	3.283248	2.285918	1.343220
H	0.949969	6.154957	-0.770065
C	3.261817	3.201311	3.221351
N	3.082161	3.221690	1.745611
C	3.964415	4.191753	1.039971
H	2.603681	2.438856	3.629266
H	3.013447	4.184964	3.619881
H	4.300472	2.960108	3.447204
H	2.093103	3.461078	1.521273
H	3.699145	4.175703	-0.013857
H	5.000583	3.880746	1.160175
H	3.803657	5.184844	1.460079
S	-3.384622	-0.311826	-1.857241
O	-3.166372	0.660376	-0.752027
O	-2.260612	-0.447116	-2.760252
O	-3.950384	-1.572123	-1.374501
O	-4.525138	0.374815	-2.793799
H	-4.963297	-2.025780	0.192535
H	-5.313151	0.582901	-2.238390
C	-5.823167	-2.941157	1.868695
N	-5.251329	-2.970099	0.497460
C	-6.173121	-3.496955	-0.541937
H	-5.030912	-2.641399	2.549531
H	-6.177033	-3.939611	2.126548
H	-6.637061	-2.219999	1.888714
H	-4.360903	-3.507635	0.501722
H	-5.668085	-3.425831	-1.502063
H	-7.067983	-2.877190	-0.553649
H	-6.426398	-4.531563	-0.310490
S	2.943232	-2.552115	-1.681161
O	2.819216	-1.541209	-0.611400
O	1.935944	-2.351054	-2.746855
O	4.361555	-2.261936	-2.379026
O	2.985091	-3.924806	-1.197146
H	4.778301	-1.465162	-1.965424
H	-0.685310	-3.171756	-1.282768
C	-0.063796	-5.088771	-1.722547
N	-0.398418	-3.697524	-2.135293

C	-1.470294	-3.599804	-3.161477
H	0.814712	-5.049848	-1.082096
H	0.164448	-5.677236	-2.611145
H	-0.915650	-5.508717	-1.189267
H	0.473181	-3.221193	-2.468164
H	-1.697222	-2.548767	-3.332548
H	-2.361380	-4.099863	-2.784328
H	-1.127379	-4.081237	-4.077621
S	0.721120	-0.303586	2.555411
O	0.993183	-1.760973	2.709657
O	-0.424132	0.134297	3.351867
O	1.920682	0.504015	2.709804
O	0.293244	-0.116554	1.010718
H	1.929698	1.751477	-1.317000
H	-0.138340	-0.953026	0.688836
S	5.357403	0.560957	-0.048942
O	5.503180	-0.432718	1.024060
O	4.121346	1.345273	0.036706
O	6.514549	1.640649	0.162971
O	5.585924	-0.017297	-1.390512
H	7.386649	1.249797	-0.211750
H	2.704035	-2.061244	2.166511
S	-1.887540	-2.995154	1.217140
O	-0.938770	-2.386928	0.243275
O	-2.634536	-4.119559	0.648539
O	-0.962734	-3.651743	2.343896
O	-2.736621	-1.993674	1.854328
H	-0.265244	-2.988484	2.585888
H	-3.074605	0.554327	1.211295
C	0.442086	0.653479	-2.222234
N	1.866767	0.871331	-1.843557
C	2.781210	0.956457	-3.016415
H	-0.166131	0.644117	-1.324201
H	0.365292	-0.296487	-2.739799
H	0.121235	1.469776	-2.865340
H	2.188620	0.099980	-1.226879
H	2.500046	1.825898	-3.609907
H	2.675363	0.042483	-3.597848
H	3.801325	1.049667	-2.652801
C	4.178271	-1.751182	3.567023
N	3.734118	-2.171450	2.212760
C	4.110399	-3.564808	1.853545
H	3.812237	-0.742410	3.739342
H	5.266308	-1.771807	3.602531

H	3.756332	-2.430519	4.307199
H	4.154663	-1.515131	1.525661
H	3.734598	-3.784217	0.855090
H	3.673789	-4.247749	2.582961
H	5.196904	-3.648793	1.870955
C	-2.488668	2.341384	2.086911
N	-2.802848	0.888037	2.150435
C	-3.846248	0.555856	3.160376
H	-2.021200	2.632513	3.026062
H	-3.418098	2.886496	1.938754
H	-1.801815	2.525825	1.264539
H	-1.933952	0.390166	2.417256
H	-4.784058	1.013214	2.854169
H	-3.518518	0.941888	4.125427
H	-3.930127	-0.525150	3.207016

8DMA

C	1.569419	4.385895	-1.205176
N	1.217701	2.991359	-0.955896
C	0.865601	2.281339	-2.181083
H	2.488065	4.443157	-1.798985
H	1.754518	4.894241	-0.255852
H	0.789499	4.947512	-1.748151
H	0.417478	2.959961	-0.313174
H	1.739492	2.205282	-2.837132
H	0.059852	2.768547	-2.756896
H	0.542267	1.266946	-1.935941
C	4.921695	-2.044442	0.082019
N	3.667187	-1.489492	-0.416155
C	3.565772	-1.564282	-1.869967
H	4.962175	-3.121288	-0.114182
H	4.984426	-1.900416	1.163390
H	5.817721	-1.591323	-0.376745
H	3.599351	-0.506927	-0.126772
H	3.513668	-2.610214	-2.191156
H	4.417780	-1.099138	-2.395902
H	2.650358	-1.068187	-2.200174
C	-4.921991	2.044194	0.080540
N	-3.667095	1.489435	-0.416875
C	-3.565001	1.563839	-1.870660
H	-4.962627	3.120998	-0.115859
H	-4.985260	1.900332	1.161902
H	-5.817682	1.590799	-0.378607
H	-3.599157	0.506960	-0.127164
H	-3.512924	2.609688	-2.192123

H	-4.416680	1.098402	-2.396869
H	-2.649346	1.067809	-2.200290
C	-0.955248	2.284072	2.195775
N	-1.274964	2.989370	0.959006
C	-1.705435	4.363088	1.200010
H	-0.075638	2.733069	2.669396
H	-0.719329	1.241126	1.971630
H	-1.774441	2.298637	2.935524
H	-2.026502	2.484298	0.474965
H	-0.879528	4.949582	1.616878
H	-2.554128	4.443483	1.901276
H	-2.000482	4.827906	0.256101
C	-1.569899	-4.385907	-1.204639
N	-1.217845	-2.991261	-0.956526
C	-0.866291	-2.282148	-2.182392
H	-2.488603	-4.443408	-1.798336
H	-1.755108	-4.893426	-0.254892
H	-0.790172	-4.948187	-1.747211
H	-0.417297	-2.959476	-0.314222
H	-1.740478	-2.206536	-2.838097
H	-0.060820	-2.769789	-2.758237
H	-0.542809	-1.267583	-1.938149
C	-3.520564	-1.693870	1.872596
N	-3.637352	-1.541081	0.425970
C	-4.854098	-2.152607	-0.099043
H	-4.316496	-1.134983	2.376683
H	-2.563416	-1.288691	2.208544
H	-3.587591	-2.742384	2.211654
H	-2.823417	-1.979052	-0.021083
H	-5.735255	-1.623862	0.280146
H	-4.965736	-3.216973	0.171386
H	-4.864011	-2.076849	-1.189115
C	3.522211	1.694498	1.871920
N	3.638092	1.541499	0.425234
C	4.854468	2.153060	-0.100617
H	4.318492	1.135714	2.375569
H	2.565299	1.289316	2.208545
H	3.589391	2.743067	2.210769
H	2.823856	1.979396	-0.021340
H	5.735902	1.624373	0.278006
H	4.966228	3.217439	0.169696
H	4.863658	2.077254	-1.190691
C	0.954606	-2.284181	2.195556
N	1.274533	-2.989132	0.958646

C	1.704563	-4.363047	1.199283
H	0.074685	-2.733068	2.668703
H	0.719108	-1.241075	1.971711
H	1.773532	-2.299284	2.935592
H	2.026305	-2.484055	0.474948
H	0.878352	-4.949497	1.615609
H	2.552969	-4.443934	1.900844
H	1.999862	-4.827585	0.255313
8SA			
S	-8.073568	-2.736853	-0.538391
O	-7.411729	-1.820841	-1.435912
O	-9.471982	-2.977728	-0.618033
O	-7.272018	-4.112830	-0.739718
O	-7.747471	-2.344969	0.949215
H	-7.780258	-4.833808	-0.337050
H	-6.833331	-1.967100	1.015360
S	-4.642588	-0.396020	-0.013699
O	-3.216890	-0.180740	0.030450
O	-5.240530	-1.329615	0.907705
O	-5.394705	0.955058	0.195284
O	-4.945435	-0.815733	-1.489353
H	-4.921242	1.721954	-0.236956
H	-5.866692	-1.189111	-1.557194
S	6.045981	-2.684439	-1.862354
O	6.763458	-2.830960	-3.072826
O	6.246297	-1.526018	-0.998091
O	4.497084	-2.754183	-2.203208
O	6.305429	-3.969592	-0.987953
H	3.972335	-2.456688	-1.427278
H	5.833687	-3.904758	-0.127518
S	-2.731063	3.299569	-0.628982
O	-4.121400	3.025665	-0.871137
O	-2.040362	2.693722	0.472615
O	-1.981766	2.948457	-1.980653
O	-2.626316	4.870266	-0.533600
H	-1.023911	2.836366	-1.799077
H	-1.700574	5.102062	-0.299802
S	1.062617	3.794830	0.058533
O	0.148502	4.874438	-0.162626
O	1.197523	3.185746	1.361904
O	0.659869	2.632949	-0.971542
O	2.434098	4.291964	-0.462023
H	0.661991	1.750737	-0.512856
H	3.197885	3.684339	-0.249919

S 0.021669 -0.081904 1.684428
O 0.960147 -0.890367 2.423146
O 0.384556 0.295599 0.332872
O -1.316540 -0.856330 1.718303
O -0.303422 1.199969 2.522093
H -2.013280 -0.513309 1.086946
H 0.160751 1.990899 2.150853
S 3.718927 -2.512421 1.390248
O 4.599599 -3.628131 1.212968
O 3.346634 -1.790442 0.165653
O 2.455332 -3.031604 2.113819
O 4.282029 -1.482284 2.416381
H 1.804180 -2.284312 2.256207
H 4.653443 -0.671387 1.969085
S 4.711640 1.375546 -0.026020
O 5.128108 0.694016 1.179411
O 4.579374 2.804467 -0.016499
O 5.671693 1.021619 -1.192881
O 3.292454 0.831454 -0.462172
H 5.959961 0.058724 -1.162092
H 3.184255 -0.121714 -0.217629

8SA1DMA

S -4.812199 0.694431 0.057257
O -3.448270 0.382132 -0.279807
O -5.266375 2.053406 -0.109255
O -5.806129 -0.205688 -0.747209
O -5.096135 0.218153 1.536963
H -5.390368 -1.081951 -0.954682
H -4.259022 0.246969 2.057985
S -2.036404 3.559866 -0.343535
O -1.866901 2.875118 0.933885
O -1.639257 2.825185 -1.515195
O -3.495244 4.096108 -0.461711
O -1.339177 4.955145 -0.283040
H -4.152843 3.358689 -0.338466
H -0.368921 4.818164 -0.114855
S -3.150276 -2.844635 -0.982991
O -2.042363 -1.987554 -1.305558
O -4.471280 -2.551565 -1.471300
O -2.814716 -4.306335 -1.461110
O -3.269674 -2.987198 0.582257
H -1.835733 -4.434947 -1.443105
H -2.551773 -2.491223 1.049732
S 0.788183 -3.434698 -0.560827

O	0.049391	-4.349960	-1.386130
O	0.854793	-2.036413	-0.901267
O	0.265327	-3.592560	0.921482
O	2.242349	-4.019248	-0.447184
H	-0.037357	-2.734696	1.297563
H	2.793264	-3.380721	0.069564
S	1.926638	3.086237	0.061748
O	1.265172	4.356799	0.187387
O	1.230722	1.968012	-0.521147
O	3.248673	3.354607	-0.736192
O	2.398010	2.713243	1.515899
H	3.613610	2.502060	-1.105609
H	2.759667	1.791164	1.560736
S	-1.373822	-0.286237	2.345613
O	-2.623293	0.219495	2.839120
O	-1.327677	-1.677811	1.909261
O	-0.830479	0.548654	1.161022
O	-0.322037	-0.094006	3.483448
H	-1.240962	1.476410	1.096729
H	0.560345	-0.434701	3.176412
S	5.401551	0.337497	-1.371718
O	4.116502	0.995366	-1.576491
O	6.482787	0.577561	-2.254924
O	5.877778	0.671179	0.101671
O	5.142276	-1.217469	-1.340860
H	5.103729	0.630318	0.718880
H	4.505402	-1.458941	-0.623236
S	3.203504	-1.064176	1.895603
O	1.809534	-1.161798	2.268580
O	3.672794	0.316171	1.639802
O	3.967599	-1.574433	3.212867
O	3.618506	-1.964206	0.801564
H	4.915494	-1.659569	3.030238
H	-0.349686	1.075787	-1.715733
C	-1.536711	0.299081	-3.221418
N	-0.339215	0.252276	-2.330580
C	0.960194	0.212401	-3.066488
H	-2.423956	0.307753	-2.596790
H	-1.530385	-0.584681	-3.856285
H	-1.485680	1.206127	-3.820045
H	-0.398385	-0.573447	-1.719457
H	1.773718	0.196878	-2.347809
H	1.031902	1.101380	-3.691145
H	0.981124	-0.684920	-3.682158

8SA2DMA

S	6.145853	-2.504804	0.165916
O	4.882246	-2.224153	-0.509844
O	6.921887	-3.611464	-0.268221
O	6.996454	-1.165303	0.174687
O	5.880327	-2.680289	1.695465
H	6.778751	-0.592648	-0.597062
H	5.292428	-1.961897	2.042956
S	-4.506540	-3.149969	-2.154918
O	-4.635329	-4.218926	-3.076382
O	-5.084291	-1.843045	-2.421193
O	-5.066010	-3.660048	-0.771890
O	-2.959256	-2.917763	-1.861277
H	-5.098669	-2.919821	-0.124827
H	-2.783168	-1.947478	-1.735048
S	4.689724	0.977933	-1.651648
O	4.291525	1.705865	-0.466232
O	6.067384	0.578084	-1.773356
O	3.769297	-0.287155	-1.824833
O	4.310129	1.807063	-2.908324
H	4.191198	-1.062303	-1.345832
H	3.475151	2.329415	-2.750846
S	3.045707	-0.086224	2.319757
O	2.245395	-0.721483	1.297008
O	4.314383	-0.689540	2.638052
O	3.232970	1.433954	1.960132
O	2.265501	0.045033	3.651892
H	3.628454	1.527780	1.054086
H	1.372969	0.485877	3.524125
S	-4.207436	-1.525771	2.389622
O	-4.871453	-2.608365	3.018708
O	-4.227963	-0.188306	2.948267
O	-2.709290	-1.938809	2.147969
O	-4.801570	-1.426227	0.906915
H	-2.147708	-1.128822	1.959466
H	-4.573525	-0.549348	0.468178
S	-3.252622	0.775671	-1.487912
O	-2.320207	-0.364017	-1.501901
O	-4.128978	0.787446	-0.308967
O	-2.585214	2.080770	-1.651825
O	-4.151159	0.665064	-2.783946
H	-1.183275	2.503809	-2.395054
H	-4.582276	-0.225807	-2.794847
S	-1.020239	1.382288	2.318357

O	-0.063471	1.225676	3.399841
O	-1.264228	0.148857	1.549226
O	-2.418739	1.812343	2.966590
O	-0.746384	2.543605	1.446674
H	-3.021410	1.036479	3.074184
H	0.247469	3.016691	0.228066
S	0.867135	2.609236	-1.792497
O	0.631414	3.531701	-0.538082
O	2.022614	3.121769	-2.480223
O	0.827992	1.233379	-1.372265
O	-0.343416	2.925664	-2.735497
H	1.077897	-0.937132	-0.203324
H	-3.028472	3.274560	-0.359896
C	0.677091	-1.827377	-2.046373
N	0.315870	-1.471813	-0.641431
C	0.023597	-2.658800	0.217004
H	0.871626	-0.908828	-2.591039
H	-0.152966	-2.373412	-2.491298
H	1.569768	-2.450066	-2.029116
H	-0.494447	-0.837605	-0.655348
H	0.890789	-3.316361	0.201417
H	-0.852345	-3.173141	-0.174256
H	-0.154812	-2.314729	1.230965
C	-2.545597	5.241996	0.102709
N	-3.021444	3.880493	0.481843
C	-4.358136	3.841453	1.141468
H	-3.247176	5.681931	-0.604675
H	-1.561330	5.150585	-0.354113
H	-2.481716	5.858853	0.998005
H	-2.305929	3.436103	1.086636
H	-5.092260	4.297174	0.478090
H	-4.306574	4.389146	2.080961
H	-4.616978	2.801821	1.323552
8SA3DMA			
S	-5.678879	-1.346404	-1.006692
O	-5.747784	-0.060190	-0.335083
O	-6.863910	-2.043314	-1.353881
O	-4.818800	-1.197387	-2.312528
O	-4.810564	-2.318384	-0.094392
H	-4.088702	-0.525095	-2.209898
H	-4.196983	-1.817778	0.497530
S	-2.852666	-0.720937	2.732601
O	-2.810590	-1.296903	1.379902
O	-4.026450	-0.987405	3.493141

O	-1.606073	-1.163992	3.534126
O	-2.550379	0.824544	2.591418
H	-0.739283	-0.677737	3.306705
H	-3.155974	1.227937	1.918423
S	2.709789	-3.851976	0.104933
O	3.960214	-3.195923	-0.213523
O	2.591379	-5.269454	0.064729
O	2.229999	-3.401457	1.533413
O	1.588443	-3.234688	-0.839676
H	2.384212	-2.418248	1.685117
H	1.933216	-2.498330	-1.439610
S	4.589690	3.079776	0.545977
O	5.329985	1.851935	0.768887
O	5.268957	4.325277	0.477426
O	3.720005	2.895436	-0.759426
O	3.492889	3.226177	1.678260
H	3.662180	1.931307	-1.035799
H	2.906057	2.423180	1.698655
S	-4.077260	3.239503	-0.002577
O	-5.182286	4.094490	0.254758
O	-2.749612	3.643643	0.404549
O	-4.261612	1.815614	0.730656
O	-4.110593	2.849864	-1.512441
H	-4.935342	1.215411	0.305815
H	-3.530422	2.050441	-1.722985
S	-1.484999	0.230303	-1.862332
O	-2.908700	0.630661	-2.017659
O	-1.315683	-1.205732	-1.779980
O	-0.833901	0.781969	-3.191411
O	-0.841500	0.950912	-0.738664
H	0.160527	0.728782	-3.142413
H	-0.036934	-0.032424	0.216145
S	2.813697	-0.068350	-2.609802
O	2.306554	-1.436831	-2.529794
O	1.807401	0.906039	-3.026641
O	3.592902	0.353150	-1.439462
O	3.950131	-0.082835	-3.766043
H	5.153436	0.089753	0.459835
H	3.531878	-0.332693	-4.602929
S	1.389541	-0.008439	1.870457
O	0.471284	-0.701517	0.775837
O	0.640387	-0.026489	3.126719
O	2.601461	-0.839175	1.903470
O	1.655281	1.363076	1.388958

H	-0.244557	-3.163208	-0.273763
H	0.554007	2.619861	0.512342
C	-1.944097	-4.101922	-1.002113
N	-1.190305	-3.384195	0.071190
C	-1.085028	-4.144608	1.350655
H	-1.940883	-3.476678	-1.890273
H	-2.966748	-4.260731	-0.664882
H	-1.449359	-5.052615	-1.194967
H	-1.636918	-2.477411	0.258119
H	-0.532488	-5.064771	1.168642
H	-2.088767	-4.366533	1.708311
H	-0.555911	-3.535050	2.077950
C	0.224241	4.481090	1.355556
N	0.045712	3.481638	0.262963
C	0.488441	3.951961	-1.083359
H	-0.134672	4.042256	2.284757
H	-0.361302	5.367200	1.118369
H	1.281444	4.725103	1.442921
H	-0.952496	3.228101	0.210890
H	0.319067	3.147660	-1.794637
H	1.549042	4.190652	-1.044942
H	-0.098438	4.828258	-1.354396
C	6.500775	-1.021773	-0.638141
N	5.457554	-0.895350	0.417654
C	5.895370	-1.320584	1.775878
H	6.075929	-0.672398	-1.576449
H	6.792322	-2.067383	-0.722814
H	7.356178	-0.406840	-0.362704
H	4.644364	-1.459884	0.139605
H	6.740322	-0.705741	2.081802
H	6.178677	-2.371345	1.742773
H	5.061095	-1.177168	2.459047
8SA4DMA			
S	0.509116	-4.201408	-3.187172
O	0.587875	-5.117679	-4.270526
O	0.657473	-4.633768	-1.812547
O	1.584008	-3.062607	-3.453119
O	-0.873724	-3.444191	-3.323298
H	1.884261	-2.664426	-2.596397
H	-1.147841	-3.029794	-2.462056
S	3.220746	-1.698052	3.830478
O	3.795551	-2.285067	4.991043
O	2.233146	-2.423740	3.053709
O	2.604304	-0.319372	4.281877

O	4.377271	-1.250191	2.849134
H	1.979048	0.062357	3.611208
H	4.243622	-1.598628	1.918449
S	-1.033143	4.695017	-0.331193
O	-1.705616	3.509794	-0.851949
O	-1.813778	5.855623	-0.052424
O	-0.228265	4.252441	0.954097
O	0.115834	5.118861	-1.299084
H	-0.562686	3.364393	1.305518
H	0.656561	4.327643	-1.600699
S	-6.196609	-1.132464	1.412316
O	-5.570365	0.146080	1.121517
O	-7.424876	-1.181749	2.122032
O	-6.394863	-1.910483	0.057530
O	-5.142150	-2.011946	2.205798
H	-5.533624	-1.950408	-0.439701
H	-4.241368	-1.864596	1.830789
S	2.824302	2.718459	-2.296104
O	1.380245	2.980784	-2.127496
O	3.087231	1.388564	-2.841807
O	3.200579	3.779717	-3.458606
O	3.628596	3.071785	-1.131864
H	4.144762	3.693550	-3.655797
H	3.439248	2.600031	0.593277
C	4.618356	2.120875	2.237761
N	3.370443	2.661333	1.626108
C	3.068116	4.075207	1.990615
H	4.725389	1.081029	1.942384
H	4.537266	2.182603	3.321984
H	5.465258	2.709165	1.887300
H	2.571858	2.066194	1.909985
H	2.141148	4.371982	1.503785
H	3.886559	4.708757	1.652477
H	2.958361	4.145891	3.071977
S	-2.724561	-1.426096	-0.670435
O	-3.968013	-2.077518	-1.049557
O	-2.681665	0.017513	-0.961534
O	-2.735847	-1.544082	0.956421
O	-1.509736	-2.119474	-1.103192
H	-1.940362	-1.088294	1.356262
H	-1.317707	0.707536	-1.946377
S	-0.061949	0.875158	1.783908
O	0.417838	0.907616	0.265485
O	-0.625818	-0.438795	2.070318

O	1.151363	1.148593	2.587504
O	-1.048384	1.964375	1.845553
H	1.519198	-3.233629	1.615855
H	-2.986847	2.419464	0.132152
S	3.290380	-1.185233	-0.501171
O	2.146197	-1.899403	-1.101688
O	4.101509	-2.044046	0.358653
O	4.255882	-0.740103	-1.670556
O	2.847059	0.051234	0.177910
H	3.870246	0.053980	-2.127298
H	1.325154	0.477893	0.188331
C	2.281032	-4.982543	0.844285
N	1.236021	-3.917692	0.898031
C	-0.137766	-4.414964	1.198690
H	3.234712	-4.504425	0.629437
H	2.019847	-5.679433	0.051926
H	2.320520	-5.482163	1.811067
H	1.233922	-3.427497	-0.005971
H	-0.134222	-4.872471	2.186995
H	-0.416454	-5.134915	0.433567
H	-0.823521	-3.571481	1.173209
C	0.067180	-0.092083	-3.274911
N	-0.675442	1.059248	-2.681985
C	-1.454329	1.847459	-3.676174
H	0.548739	-0.636831	-2.468964
H	0.818544	0.290076	-3.962767
H	-0.633460	-0.744303	-3.791594
H	0.003724	1.689213	-2.229288
H	-1.921432	2.682717	-3.159930
H	-2.208044	1.202096	-4.125041
H	-0.774419	2.217229	-4.442373
C	-4.153567	2.962001	1.761074
N	-3.948777	2.261598	0.460689
C	-4.891192	2.684146	-0.613423
H	-3.395248	2.610783	2.457111
H	-5.148659	2.720049	2.127935
H	-4.049177	4.034948	1.603156
H	-4.074078	1.251635	0.601647
H	-4.678709	2.090896	-1.500086
H	-4.738931	3.742247	-0.818550
H	-5.907236	2.490716	-0.277001
8SA5DMA			
S	2.771683	-3.383138	2.226288
O	2.891905	-4.560200	3.016014

O	3.798644	-3.011408	1.278904
O	1.394064	-3.476506	1.440245
O	2.543217	-2.184209	3.226974
H	1.390329	-2.916393	0.617671
H	2.438722	-1.311033	2.741753
S	-6.256805	-0.072834	-2.031572
O	-6.043781	0.999191	-1.073762
O	-7.431293	-0.079178	-2.833544
O	-5.031958	-0.137411	-3.018453
O	-6.150406	-1.442852	-1.251224
H	-4.164914	-0.139274	-2.517799
H	-5.878977	-1.303478	-0.296323
S	-1.054666	3.947502	1.426461
O	-1.526742	5.256203	1.750478
O	-1.844974	2.806216	1.870561
O	-0.852105	3.812325	-0.132747
O	0.406144	3.827146	1.971226
H	-1.376120	3.027295	-0.491116
H	0.952516	3.116112	1.507222
S	-4.055694	-1.358982	1.734032
O	-3.315836	-2.390936	1.012490
O	-3.331995	-0.109115	1.952652
O	-5.427899	-1.161995	1.250710
O	-4.220521	-1.912464	3.267814
H	-4.941431	1.702666	0.163519
H	-4.782369	-2.699728	3.239970
C	-4.613791	3.735670	0.133076
N	-4.591723	2.415202	0.825342
C	-5.415892	2.369035	2.064371
H	-4.029604	3.648595	-0.778956
H	-4.180493	4.489245	0.789004
H	-5.645691	3.983075	-0.110016
H	-3.618872	2.171239	1.055060
H	-5.345716	1.367670	2.478432
H	-6.448425	2.597702	1.804982
H	-5.028911	3.102441	2.770287
S	2.666098	0.931191	1.144291
O	3.240214	0.202290	0.019023
O	1.899322	0.072026	2.085312
O	3.863670	1.457077	2.038754
O	1.863269	2.085565	0.716992
H	4.665120	1.636745	1.468817
H	-1.553746	0.147023	2.420681
C	-0.754539	0.878290	4.194921

N	-0.733103	-0.039635	3.021644
C	-0.762685	-1.483424	3.398547
H	-0.740286	1.900916	3.830078
H	0.120183	0.677967	4.811831
H	-1.666787	0.698062	4.761672
H	0.127194	0.142080	2.475164
H	-0.742079	-2.080573	2.490741
H	-1.683089	-1.681309	3.943847
H	0.111301	-1.711309	4.004747
S	1.204818	-2.049703	-2.281951
O	1.262841	-0.621681	-2.681821
O	0.043519	-2.727513	-2.861591
O	2.459149	-2.749351	-2.353842
O	0.861298	-1.982189	-0.662329
H	4.585949	-1.529265	-0.035821
H	0.281352	-1.193042	-0.493147
S	6.070378	1.982481	-0.869942
O	5.036595	2.942838	-1.263116
O	6.122407	0.788921	-1.714467
O	7.498647	2.686983	-1.178462
O	6.070010	1.696024	0.573220
H	7.558602	3.483331	-0.631402
H	2.453885	1.004229	-2.048172
S	-1.747582	0.561960	-1.360990
O	-0.814025	0.057747	-0.346317
O	-2.319749	1.875566	-1.035518
O	-0.910191	0.833765	-2.683842
O	-2.789583	-0.423833	-1.695054
H	-0.137797	0.196237	-2.746654
H	-2.535453	-2.635049	-0.725468
C	6.524734	-1.644510	0.666221
N	5.527022	-1.603684	-0.440774
C	5.573642	-2.783115	-1.349715
H	6.449836	-0.714386	1.225195
H	7.520709	-1.728213	0.232668
H	6.303969	-2.498245	1.302025
H	5.683603	-0.726342	-0.978247
H	5.435590	-3.683057	-0.754181
H	6.540386	-2.798332	-1.852200
H	4.760107	-2.700812	-2.067208
C	3.373728	1.489280	-3.828163
N	2.816394	1.856225	-2.496757
C	1.754615	2.902655	-2.537030
H	4.203351	0.803042	-3.671604

H	3.736972	2.393525	-4.314532
H	2.595051	1.014397	-4.420789
H	3.600316	2.207153	-1.908586
H	1.422428	3.089081	-1.518606
H	0.920974	2.551429	-3.141268
H	2.182194	3.809153	-2.963847
C	-1.814886	-4.569529	-0.701506
N	-2.245121	-3.339239	-1.421491
C	-3.368792	-3.553997	-2.376383
H	-0.974063	-4.321540	-0.057160
H	-1.507824	-5.315663	-1.432860
H	-2.645049	-4.936362	-0.101390
H	-1.424480	-2.967804	-1.944507
H	-4.240384	-3.906566	-1.827791
H	-3.061566	-4.287924	-3.120096
H	-3.600151	-2.606910	-2.855484
8SA6DMA			
S	4.524264	-2.350230	2.183635
O	3.864129	-3.110008	3.202987
O	5.677761	-2.889928	1.503111
O	3.395514	-2.020979	1.119875
O	4.974972	-0.946183	2.711461
H	3.753109	-1.516795	0.324779
H	4.202983	-0.410235	3.095241
S	-2.859434	-4.105599	-1.909842
O	-2.928421	-5.442656	-2.391988
O	-3.973351	-3.200611	-2.115320
O	-2.532772	-4.117006	-0.359205
O	-1.548843	-3.481110	-2.524739
H	-3.145547	-3.498485	0.130742
H	-1.355405	-2.562327	-2.184896
S	-4.193132	-1.756315	2.105253
O	-2.909044	-1.703675	2.799188
O	-4.911321	-0.481749	2.069795
O	-4.170514	-2.427003	0.801238
O	-5.132073	-2.765747	2.970116
H	-5.001804	-1.817666	-1.099456
H	-5.156955	-2.443206	3.882162
C	-5.867203	-0.989343	-2.782521
N	-5.732814	-1.119525	-1.304158
C	-6.987779	-1.506517	-0.602137
H	-4.889130	-0.746594	-3.190260
H	-6.581495	-0.196943	-3.001876
H	-6.202475	-1.940296	-3.190696

H	-5.393995	-0.216171	-0.927518
H	-6.794519	-1.506636	0.467379
H	-7.284477	-2.501070	-0.931390
H	-7.764999	-0.782071	-0.843076
S	5.427676	-1.457375	-1.856414
O	5.080030	-1.672161	-3.244440
O	6.605397	-0.669740	-1.560591
O	4.221074	-0.890482	-1.100760
O	5.613385	-2.931228	-1.262753
H	2.805829	-1.125290	-2.123915
H	5.812626	-2.898227	-0.298827
C	2.157259	-0.322876	-3.920180
N	2.026659	-1.296298	-2.799312
C	2.069089	-2.724645	-3.231185
H	2.092792	0.684525	-3.511165
H	1.346465	-0.487438	-4.629216
H	3.124574	-0.479359	-4.393009
H	1.128736	-1.131066	-2.309355
H	2.004298	-3.355293	-2.346038
H	3.014800	-2.901309	-3.737535
H	1.220287	-2.924544	-3.883827
S	2.237776	1.087722	2.406752
O	3.015672	0.536640	3.522678
O	0.826009	0.609756	2.445001
O	2.154476	2.655505	2.714772
O	2.852932	0.928800	1.100375
H	1.851464	3.101717	1.875421
H	4.190452	2.547618	-0.353780
C	5.499722	2.348902	-1.922362
N	4.957670	1.906423	-0.607325
C	5.973973	1.869301	0.482345
H	4.683254	2.355024	-2.641470
H	6.277540	1.653542	-2.228705
H	5.889676	3.359695	-1.815307
H	4.545356	0.962014	-0.699611
H	5.486790	1.518994	1.388297
H	6.371063	2.873446	0.627146
H	6.760230	1.176103	0.191277
S	-1.217188	0.042432	-1.154690
O	-0.570175	-1.175280	-1.720006
O	-0.531895	1.258989	-1.607871
O	-2.636020	0.030400	-1.897229
O	-1.451462	-0.041145	0.274654
H	-3.267659	0.650503	-1.439928

H	-1.122504	-1.853189	2.318761
S	1.798921	3.846080	-0.779800
O	3.203648	4.179307	-0.615882
O	1.068142	3.628777	0.488327
O	1.038484	4.735616	-1.669256
O	1.864336	2.407210	-1.515596
H	-0.523856	1.707777	2.329761
H	0.996472	1.943836	-1.421214
S	-4.425101	2.583883	0.049672
O	-4.617177	1.391728	-0.825260
O	-5.160581	3.752011	-0.352390
O	-4.989613	2.156525	1.482311
O	-2.972286	2.830525	0.236351
H	-4.882859	1.185546	1.633509
H	-1.993961	3.787879	-0.930035
C	0.365741	-2.438359	3.642043
N	-0.101513	-2.003250	2.293882
C	0.224293	-2.973036	1.208746
H	0.149051	-1.645737	4.355149
H	1.439498	-2.617265	3.604678
H	-0.160612	-3.350416	3.920567
H	0.315277	-1.070620	2.098834
H	-0.271084	-3.919331	1.420096
H	1.303675	-3.100117	1.175333
H	-0.144381	-2.571055	0.269074
C	-2.197591	1.546642	3.530383
N	-1.398216	2.253503	2.492937
C	-1.063957	3.657389	2.860734
H	-2.408858	0.535989	3.189269
H	-3.131275	2.085897	3.684449
H	-1.620917	1.517406	4.454310
H	-1.927953	2.263980	1.603386
H	-0.503097	4.102758	2.043002
H	-0.451545	3.650190	3.761039
H	-1.990959	4.202746	3.034937
C	-2.038090	3.898846	-2.987734
N	-1.680254	4.459363	-1.655623
C	-2.304975	5.777168	-1.359876
H	-1.579392	2.915693	-3.070646
H	-1.658992	4.562032	-3.764433
H	-3.122226	3.815364	-3.059438
H	-0.634064	4.545899	-1.599009
H	-3.385453	5.651744	-1.300936
H	-2.037751	6.484002	-2.144486

H	-1.923529	6.134155	-0.404583
8SA7DMA			
S	5.645702	-2.874374	2.672897
O	4.533566	-3.029563	1.765446
O	5.863306	-3.787560	3.741911
O	6.985668	-2.813883	1.825528
O	5.562852	-1.419347	3.317364
H	6.859100	-2.204462	1.052336
H	5.426768	-0.747980	2.597083
S	2.784306	3.730042	-0.694773
O	1.520230	3.871784	0.031687
O	3.698756	4.866091	-0.514989
O	3.458659	2.446666	-0.391597
O	2.469624	3.748456	-2.251194
H	6.246211	3.026958	-0.089872
H	1.820817	3.022392	-2.474192
C	6.331483	4.206768	1.594254
N	6.177958	4.045228	0.126591
C	7.176124	4.783906	-0.685382
H	5.576696	3.593942	2.083284
H	6.190053	5.253715	1.861236
H	7.323025	3.869861	1.895499
H	5.207266	4.355042	-0.149539
H	6.966154	4.605520	-1.738793
H	8.177330	4.426489	-0.445830
H	7.097310	5.850219	-0.474353
S	-5.796927	3.041851	0.147108
O	-4.857012	3.280115	-0.933413
O	-6.606026	1.818107	-0.009531
O	-5.257450	3.160491	1.506604
O	-6.870177	4.274495	0.104933
H	-5.846838	1.836403	2.417391
H	-7.124352	4.403555	-0.819213
C	-5.626244	0.714344	4.166014
N	-6.314584	1.023307	2.883942
C	-7.764442	1.328589	3.014040
H	-4.582946	0.492617	3.948961
H	-6.101498	-0.150574	4.628543
H	-5.702576	1.577169	4.827417
H	-6.198079	0.228842	2.225385
H	-8.150552	1.541308	2.019683
H	-7.889754	2.199663	3.656335
H	-8.276505	0.468426	3.444620
S	5.844709	0.223373	0.020743

O	6.659390	1.394143	-0.294858
O	6.529086	-1.051058	-0.158151
O	5.161292	0.345157	1.333996
O	4.658837	0.154852	-1.070424
H	3.221832	0.398849	1.315194
H	4.141688	1.003412	-1.041657
C	1.994556	-0.974751	2.274187
N	2.235087	0.339469	1.606661
C	1.935097	1.507060	2.483444
H	2.242988	-1.776872	1.585092
H	0.943637	-1.019420	2.550267
H	2.633239	-1.040916	3.153407
H	1.656535	0.408300	0.743261
H	2.050705	2.414548	1.896246
H	2.629569	1.498615	3.323576
H	0.910329	1.408590	2.832892
S	0.830015	0.540765	-2.105721
O	0.695312	1.843542	-2.771776
O	0.593271	0.631140	-0.656753
O	-0.430755	-0.272532	-2.720111
O	2.023345	-0.215145	-2.458681
H	-0.342263	-1.256783	-2.546445
H	2.762860	-2.932513	-2.029352
C	4.716342	-3.407530	-1.548451
N	3.705430	-2.517333	-2.188514
C	3.892725	-2.339765	-3.654997
H	4.494314	-3.487303	-0.486282
H	5.704622	-2.972048	-1.679994
H	4.653991	-4.387779	-2.019228
H	3.714545	-1.586599	-1.751450
H	3.129963	-1.650907	-4.007959
H	3.790634	-3.310257	-4.138774
H	4.884651	-1.928071	-3.837178
S	-2.038693	-0.275714	1.220583
O	-1.068183	0.389285	2.071581
O	-1.663572	-1.644989	0.812064
O	-3.315770	-0.475215	2.197486
O	-2.514137	0.538082	0.086969
H	-4.091895	-0.812170	1.688032
H	-1.516953	2.077460	-0.110389
S	0.149590	-3.635491	-1.389825
O	1.428420	-4.058489	-1.946977
O	-0.672202	-2.825829	-2.316452
O	-0.637581	-4.718994	-0.790513

O	0.583032	-2.639932	-0.207802
H	-2.310694	-0.202507	-2.335442
H	-0.223958	-2.200462	0.176182
S	-5.922947	-1.764083	-0.103338
O	-5.737077	-1.150576	1.240908
O	-6.766457	-2.929516	-0.122366
O	-6.629855	-0.652651	-1.004969
O	-4.591918	-1.992178	-0.727401
H	-6.527633	0.258982	-0.623470
H	-3.500750	-3.333104	-0.175770
C	-1.564570	3.821756	-1.261001
N	-1.170902	3.052680	-0.045241
C	-1.683571	3.635686	1.226180
H	-1.133268	3.322030	-2.126521
H	-1.148907	4.825298	-1.178909
H	-2.650932	3.856262	-1.316332
H	-0.138973	3.020015	-0.017454
H	-2.770721	3.680166	1.181091
H	-1.257872	4.630454	1.351383
H	-1.379833	2.982518	2.041606
C	-4.031194	0.803600	-2.913549
N	-3.277178	-0.442091	-2.604980
C	-3.234639	-1.415681	-3.731027
H	-4.048222	1.440933	-2.033274
H	-5.050813	0.534029	-3.185146
H	-3.542974	1.315267	-3.742596
H	-3.712306	-0.905464	-1.782539
H	-2.630691	-2.268716	-3.428658
H	-2.780295	-0.934831	-4.596258
H	-4.253050	-1.726010	-3.960933
C	-3.217269	-4.375889	1.583986
N	-3.177752	-4.278724	0.099571
C	-4.032078	-5.274304	-0.602053
H	-2.593814	-3.580292	1.985293
H	-2.834715	-5.350280	1.886180
H	-4.246532	-4.254369	1.920928
H	-2.186678	-4.386100	-0.228111
H	-5.076815	-5.075850	-0.366270
H	-3.744388	-6.276853	-0.287404
H	-3.872029	-5.170342	-1.673803
8SA8DMA			
S	4.641454	-3.717344	1.756821
O	5.592755	-4.638420	1.186484
O	3.798524	-4.234527	2.848176

O	5.236056	-2.405383	2.135514
O	3.521223	-3.364075	0.635826
H	1.893300	-1.657083	2.979206
H	3.933542	-2.829939	-0.082047
C	3.214807	-1.351556	4.550650
N	2.294493	-2.212354	3.762006
C	1.182413	-2.797995	4.547737
H	3.993575	-1.004156	3.878009
H	3.652609	-1.947431	5.351272
H	2.659744	-0.509105	4.963340
H	2.864868	-3.005706	3.347761
H	0.580624	-3.423580	3.890094
H	0.566924	-2.001127	4.965048
H	1.593681	-3.410882	5.349355
S	-4.350756	-2.844777	-1.469207
O	-3.094029	-3.514573	-1.164127
O	-5.514393	-3.738782	-1.571941
O	-4.611788	-1.712057	-0.546516
O	-4.247737	-2.212057	-2.936090
H	-7.381183	-2.208853	0.566266
H	-3.621574	-1.444507	-2.918999
C	-8.086673	-4.159396	0.636957
N	-7.660401	-2.954877	-0.116075
C	-8.697716	-2.397484	-1.022779
H	-7.255516	-4.494458	1.255340
H	-8.357532	-4.948639	-0.063935
H	-8.938078	-3.910198	1.270046
H	-6.807251	-3.202160	-0.683584
H	-8.297887	-1.492786	-1.475679
H	-9.587185	-2.149943	-0.443564
H	-8.937903	-3.132594	-1.790453
S	4.150554	-1.517959	-2.587702
O	2.757529	-1.918529	-2.775719
O	4.425709	-0.161460	-3.083037
O	4.709892	-1.785179	-1.266413
O	5.033827	-2.519234	-3.529885
H	6.231957	-1.628379	1.144778
H	4.663213	-2.488621	-4.422516
C	7.680421	-0.164049	1.446901
N	6.873642	-1.028045	0.549506
C	7.676288	-1.907237	-0.341193
H	7.001681	0.466449	2.015983
H	8.342104	0.465269	0.851863
H	8.263597	-0.795524	2.116612

H	6.232482	-0.430682	0.007654
H	6.992406	-2.488728	-0.952699
H	8.279231	-2.573038	0.275115
H	8.318136	-1.293059	-0.973378
S	-6.676241	0.316059	1.148837
O	-7.086980	-0.986946	1.697512
O	-7.633023	1.391161	1.283259
O	-5.309022	0.690579	1.609221
O	-6.540725	0.102269	-0.448380
H	-3.882725	-0.372883	1.587249
H	-5.762099	-0.496292	-0.616812
C	-2.362889	0.194791	2.864550
N	-2.895237	-0.650253	1.762080
C	-2.800163	-2.107912	2.034699
H	-2.483530	1.240332	2.594231
H	-1.302892	-0.024258	2.986976
H	-2.919021	-0.025367	3.775882
H	-2.385654	-0.437776	0.877890
H	-3.107003	-2.647062	1.143245
H	-3.451618	-2.354410	2.873428
H	-1.765480	-2.344522	2.280865
S	-2.265728	0.635994	-1.656121
O	-2.504793	-0.122124	-2.882827
O	-1.552407	-0.184456	-0.640796
O	-1.188759	1.751919	-2.137298
O	-3.384751	1.368899	-1.096990
H	-1.206374	2.554910	-1.535232
H	-3.932528	3.707566	0.584211
C	-5.564139	4.001354	1.815292
N	-4.900819	3.339844	0.658018
C	-5.609380	3.542880	-0.638347
H	-4.966416	3.817959	2.706354
H	-6.556688	3.571561	1.935782
H	-5.615843	5.072977	1.626929
H	-4.853693	2.322479	0.856664
H	-5.063213	2.998133	-1.403790
H	-5.629188	4.609436	-0.861343
H	-6.618481	3.146529	-0.543208
S	1.554434	0.313313	1.081678
O	0.838261	-0.684338	1.902089
O	1.086823	1.690177	1.343155
O	3.036397	0.244497	1.697033
O	1.642184	-0.007461	-0.336680
H	3.721640	0.570732	1.052077

H	1.107183	-1.837119	-1.668451
S	-1.157515	4.227542	0.623230
O	-2.503771	4.776272	0.721206
O	-0.738132	3.894356	-0.755204
O	-0.124630	5.010171	1.312418
O	-1.287012	2.824861	1.397892
H	0.665669	1.655988	-2.274317
H	-0.416381	2.338311	1.362808
S	4.967240	2.339629	-0.639639
O	5.063740	1.136078	0.224679
O	5.691711	3.487450	-0.145623
O	5.662938	1.939477	-2.015118
O	3.542840	2.636679	-0.950103
H	5.232572	1.119408	-2.381812
H	2.725749	3.703254	0.291191
C	-0.320842	-2.788057	-2.834740
N	0.175539	-2.253911	-1.533979
C	0.271384	-3.287506	-0.463257
H	-0.462274	-1.954717	-3.519998
H	-1.274194	-3.282346	-2.659520
H	0.420410	-3.480854	-3.228854
H	-0.449401	-1.488534	-1.209654
H	1.007570	-4.033888	-0.756275
H	-0.712984	-3.735600	-0.339669
H	0.601725	-2.793207	0.447211
C	1.690118	1.050376	-3.951724
N	1.527910	1.938434	-2.767136
C	1.411522	3.380584	-3.126072
H	1.813114	0.026162	-3.611521
H	2.581854	1.347895	-4.499375
H	0.801105	1.150835	-4.573644
H	2.311713	1.831509	-2.097940
H	1.122995	3.938245	-2.238740
H	0.635391	3.488999	-3.882270
H	2.371465	3.722692	-3.508392
C	3.117038	4.049051	2.287148
N	2.548796	4.464023	0.974249
C	3.138150	5.718008	0.432099
H	2.652379	3.105604	2.563662
H	2.891989	4.817140	3.026634
H	4.193751	3.926869	2.177201
H	1.513198	4.585621	1.071824
H	4.197624	5.552158	0.243446
H	2.989094	6.521414	1.152659

H 2.627698 5.967170 -0.496798

Coordinate information for SA-MA-DMA system

1MA

O 0.386462 1.694575 0.131780
O 2.089383 -1.469706 0.246714
O -2.877627 -0.185634 -0.934861
O 2.748188 0.572579 -0.429131
O -2.235582 -0.071073 1.215237
C 0.488070 0.305920 0.342879
C -0.561788 -0.443623 -0.488850
C 1.895271 -0.161902 0.005982
C -1.955366 -0.199949 0.052330
H 0.304558 0.080144 1.400476
H -0.383185 -1.522532 -0.441867
H -0.507090 -0.132471 -1.533011
H 1.233373 1.978699 -0.241265
H 3.007256 -1.674248 0.011709
H -3.738635 -0.058187 -0.507998

1MA1DMA

O -1.445704 1.770137 -0.617302
O 0.917955 -0.567141 0.728657
O -4.127788 -1.048288 -0.704284
O 1.122038 1.151838 -0.711327
O -3.690325 0.045397 1.207394
C -1.050082 0.666677 0.165997
C -1.847883 -0.582182 -0.228712
C 0.451664 0.436226 0.014460
C -3.296909 -0.464643 0.190542
H -1.247977 0.872314 1.225563
H -1.435412 -1.460448 0.277534
H -1.784130 -0.743437 -1.305792
H -0.637882 2.074786 -1.058492
H 1.937532 -0.658686 0.596686
H -5.023866 -0.954061 -0.346970
C 3.774494 -0.992150 -1.070125
N 3.547929 -0.754672 0.364332
C 4.129182 0.515076 0.828863
H 3.232690 -0.232182 -1.635591
H 3.379753 -1.972851 -1.342596
H 4.837356 -0.948862 -1.342234
H 3.944926 -1.521660 0.899319
H 3.605432 1.335814 0.335976

H 5.201881 0.593599 0.608518
H 3.981994 0.608800 1.906491

1MA2DMA

O 0.268335 -2.872692 -1.073269
O 2.224883 -0.635329 0.932036
O -2.482151 -1.012916 0.955473
O 2.042580 -0.927259 -1.295613
O -0.784579 0.057137 -0.055434
C 0.794134 -2.379192 0.138541
C -0.338115 -2.011965 1.102427
C 1.745494 -1.218803 -0.149852
C -1.212537 -0.883021 0.591686
H 1.402072 -3.156326 0.625780
H 0.086493 -1.694544 2.059998
H -0.957540 -2.890582 1.285164
H 0.700476 -2.349045 -1.766233
H 2.759672 0.187497 0.641684
H -3.005693 -0.222736 0.592858
C -4.504368 0.847523 -1.325279
N -3.627932 1.155224 -0.192133
C -4.134293 2.230335 0.663404
H -5.456635 0.459549 -0.954361
H -4.040689 0.076078 -1.942603
H -4.714374 1.723634 -1.955936
H -2.697302 1.390457 -0.531349
H -5.068737 1.912728 1.133362
H -4.329136 3.162280 0.112751
H -3.410203 2.437202 1.453759
C 2.303539 2.576143 -0.042801
N 3.336550 1.537218 -0.136706
C 4.695109 2.033631 0.091121
H 2.285435 2.975737 0.974605
H 1.329788 2.130699 -0.253134
H 2.475410 3.411056 -0.736741
H 3.272870 1.088365 -1.048306
H 4.781586 2.400859 1.116982
H 4.971195 2.852835 -0.588461
H 5.408652 1.217719 -0.038974

1MA3DMA

O -0.934339 -2.854271 1.249694
O -3.125051 -0.831857 -0.669602
O 0.906724 -0.696381 -1.832369
O -1.646777 -0.147494 0.885607
O 1.356140 -1.695771 0.129519

C	-1.514340	-2.423870	0.046748
C	-0.519893	-2.474872	-1.142391
C	-2.098453	-1.006813	0.155389
C	0.681871	-1.579976	-0.891851
H	-2.343218	-3.099443	-0.175153
H	-1.015341	-2.192110	-2.070899
H	-0.162245	-3.504836	-1.225221
H	-0.058841	-2.440025	1.300972
H	-3.467187	0.125363	-0.605589
H	1.707673	-0.055303	-1.580915
C	4.142685	0.309915	-1.622266
N	2.868288	0.934238	-1.252584
C	2.681070	2.258821	-1.850503
H	4.167748	0.127691	-2.700456
H	4.230946	-0.651119	-1.112230
H	5.010633	0.930260	-1.358995
H	2.814765	1.003616	-0.224215
H	2.626337	2.171367	-2.939347
H	3.496384	2.953270	-1.603643
H	1.741557	2.686822	-1.495687
C	-4.424157	1.853800	0.971559
N	-4.017615	1.709888	-0.433815
C	-2.903287	2.595729	-0.797350
H	-3.603220	1.512315	1.604400
H	-5.292723	1.221073	1.164641
H	-4.673845	2.890268	1.237902
H	-4.811886	1.900093	-1.037386
H	-2.020987	2.288687	-0.233072
H	-3.112655	3.653166	-0.583225
H	-2.685170	2.487623	-1.861762
C	3.756607	0.571813	2.591918
N	2.566197	0.601004	1.747141
C	1.402174	1.178035	2.422535
H	4.081478	1.594059	2.810968
H	4.572220	0.066218	2.068934
H	3.596757	0.060604	3.555636
H	2.327693	-0.339622	1.440014
H	1.543067	2.256116	2.553957
H	1.224740	0.740237	3.418495
H	0.507977	1.008389	1.821165
1MA4DMA			
O	0.354717	0.490226	0.968953
O	2.849413	-1.838173	-0.090255
O	-1.875897	0.197164	-1.702053

O	3.085098	0.366002	0.265101
O	-1.807344	-1.700592	-0.494700
C	0.851019	-0.605473	0.249528
C	0.261160	-0.698398	-1.176937
C	2.379969	-0.623249	0.156019
C	-1.252328	-0.791385	-1.091060
H	0.546292	-1.506258	0.787005
H	0.636822	-1.602027	-1.664096
H	0.548715	0.173449	-1.767827
H	0.664468	1.340232	0.570728
H	3.864827	-1.814499	-0.177546
H	-2.896810	0.146746	-1.521973
C	-5.208569	1.339099	-1.342192
N	-4.467840	0.092272	-1.146261
C	-5.069683	-1.054991	-1.830268
H	-5.189153	1.622252	-2.398763
H	-4.733989	2.137900	-0.768598
H	-6.260830	1.264143	-1.030093
H	-4.395377	-0.119059	-0.140505
H	-5.059065	-0.888560	-2.911677
H	-6.110075	-1.237382	-1.523916
H	-4.474492	-1.943987	-1.614878
C	5.871326	-0.835855	-1.391059
N	5.541585	-1.744332	-0.284377
C	6.019944	-1.254611	1.016513
H	5.323398	0.097039	-1.246865
H	5.550512	-1.281160	-2.334977
H	6.945209	-0.611267	-1.452108
H	5.940449	-2.660018	-0.468316
H	5.476184	-0.340880	1.262672
H	7.097697	-1.040739	1.020048
H	5.805551	-1.999224	1.785609
C	1.245395	3.834173	-0.882761
N	1.517761	2.940679	0.238303
C	1.593392	3.624593	1.527411
H	0.248031	4.269405	-0.771962
H	1.258911	3.267982	-1.816620
H	1.967332	4.663023	-0.968036
H	2.373936	2.414313	0.084943
H	0.619543	4.059961	1.770183
H	2.341455	4.433466	1.550492
H	1.839453	2.896169	2.301973
C	-2.996966	0.030512	2.531666
N	-3.778860	-0.864351	1.677517

C	-4.704864	-1.703820	2.430098
H	-3.642646	0.814412	2.941883
H	-2.203443	0.497633	1.946352
H	-2.523846	-0.490736	3.380465
H	-3.137230	-1.441851	1.137881
H	-5.475765	-1.081565	2.896403
H	-4.218050	-2.284551	3.231842
H	-5.203188	-2.404827	1.755888

1SA1MA

S	2.591090	0.212789	0.030249
O	3.962168	0.569110	-0.012838
O	1.988123	-0.274142	1.259960
O	1.772273	1.484086	-0.456003
O	2.331185	-0.860138	-1.098302
H	0.807429	1.377659	-0.315995
H	1.437168	-1.269693	-0.964159
O	-2.772109	-1.314532	-1.244046
O	-0.503267	-1.175135	1.520795
O	-2.984420	2.385918	-0.101541
O	-0.206625	-1.632170	-0.669854
O	-1.013776	1.338409	-0.225452
C	-2.422100	-1.203122	0.112667
C	-2.919552	0.141534	0.663508
C	-0.915979	-1.358106	0.287513
C	-2.194110	1.321818	0.058990
H	-2.898212	-2.000730	0.700388
H	-2.759821	0.184011	1.745378
H	-3.988580	0.233976	0.474130
H	-1.970175	-1.580329	-1.717346
H	0.478855	-1.041856	1.531876
H	-2.442075	3.108354	-0.456067

1SA1MA1DMA

S	2.800590	-0.353407	-0.281187
O	2.377757	-0.403427	1.237335
O	4.211114	-0.178752	-0.353430
O	2.422607	-1.756576	-0.831512
O	1.947487	0.646729	-0.933227
H	1.412059	-1.962985	-0.695244
H	0.718522	1.507184	-0.246451
O	-2.518250	0.306291	1.596209
O	-3.775518	-0.606104	-1.609742
O	-0.147934	-0.826957	1.274577
O	-2.275221	0.969601	-1.090526
O	-0.036239	-2.264237	-0.451759

C	-2.975210	-0.610640	0.633322
C	-2.152809	-1.924799	0.611955
C	-2.955867	0.021914	-0.758361
C	-0.652518	-1.668302	0.449433
H	-4.019137	-0.859950	0.847562
H	-2.500690	-2.581980	-0.183712
H	-2.309304	-2.423904	1.572457
H	-1.595801	0.040446	1.791604
H	-3.670908	-0.194944	-2.481754
H	1.376624	-0.618686	1.297600
C	0.229134	2.556651	1.486234
N	-0.030004	2.172090	0.073812
C	-0.061175	3.312464	-0.880126
H	1.173233	3.097619	1.537650
H	0.298438	1.650743	2.082800
H	-0.586647	3.181852	1.847120
H	-0.926010	1.661106	-0.011476
H	0.916543	3.791925	-0.892771
H	-0.828100	4.022753	-0.572623
H	-0.293980	2.922451	-1.868604
1SA1MA2DMA			
S	2.426885	-0.399622	-0.638501
O	1.808389	-1.752386	-1.287171
O	3.815189	-0.673503	-0.419740
O	2.112250	0.680672	-1.595823
O	1.629765	-0.207715	0.617966
H	0.626378	0.922603	-2.188041
H	0.594627	-1.555784	1.086380
O	-3.103238	-1.310977	-0.360756
O	-2.035222	2.031473	0.470255
O	-0.756010	-0.974460	-1.895036
O	-1.646888	0.094457	1.509382
O	-0.337807	1.188828	-2.316019
C	-3.066808	0.102291	-0.467636
C	-2.595697	0.558354	-1.875135
C	-2.187742	0.789692	0.611862
C	-1.142722	0.188754	-2.054527
H	-4.089634	0.460657	-0.323623
H	-2.718223	1.632920	-1.978613
H	-3.192493	0.037254	-2.628477
H	-2.346275	-1.635954	-0.867847
H	-0.545595	2.277220	0.922915
H	0.929230	-1.518263	-1.665957
C	-0.489497	-3.313007	0.713506

N	-0.218868	-2.074617	1.482210
C	0.020919	-2.298637	2.928093
H	0.333710	-4.014598	0.848187
H	-0.571463	-3.059900	-0.340058
H	-1.423150	-3.753031	1.062778
H	-1.007458	-1.360027	1.388315
H	0.894504	-2.936760	3.062719
H	-0.856896	-2.768902	3.370894
H	0.192220	-1.334209	3.401486
C	1.198687	3.367882	0.434612
N	0.494819	2.308120	1.198005
C	0.565551	2.449811	2.671686
H	0.745702	4.333663	0.659262
H	1.102449	3.148201	-0.626227
H	2.254772	3.377482	0.704795
H	0.892380	1.381374	0.937515
H	0.177790	3.427559	2.958505
H	1.597856	2.345327	3.006433
H	-0.059812	1.670633	3.103946

1SA1MA3DMA

S	-1.080956	2.026854	-0.392773
O	-1.010133	1.121510	-1.715858
O	-1.951555	3.121668	-0.728001
O	-1.640563	1.109238	0.660023
O	0.304531	2.387211	-0.039282
H	-2.566777	-1.437920	-0.803347
H	1.695596	1.773773	-0.826303
O	2.753243	-2.021803	-1.271290
O	1.201422	-1.797074	1.971278
O	0.176006	-1.123243	-1.420668
O	2.495817	-0.344804	0.879688
O	-1.467109	-2.521018	-0.795914
C	2.136266	-2.538975	-0.098686
C	0.793101	-3.211741	-0.429575
C	1.941529	-1.466557	1.001200
C	-0.258759	-2.212898	-0.918942
H	2.820427	-3.288955	0.310355
H	0.391451	-3.722117	0.444075
H	0.950648	-3.958282	-1.215620
H	2.023225	-1.559473	-1.713345
H	0.582452	-0.521548	2.513976
H	-0.569922	0.212709	-1.548202
C	2.577392	0.993568	-2.550912
N	2.594437	1.321244	-1.105877

C	3.721699	2.189807	-0.695533
H	2.595236	1.915252	-3.134061
H	1.664771	0.444399	-2.770933
H	3.445287	0.379525	-2.789372
H	2.624986	0.446618	-0.486655
H	3.664161	3.145198	-1.218016
H	4.662934	1.692246	-0.929554
H	3.658888	2.352835	0.378581
C	-0.957343	0.088054	3.829180
N	0.053093	0.395388	2.793874
C	1.044675	1.422105	3.194775
H	-0.457593	-0.281174	4.725154
H	-1.624296	-0.684408	3.448153
H	-1.533904	0.982673	4.067904
H	-0.449076	0.710669	1.938967
H	1.497141	1.126967	4.142611
H	0.557908	2.392319	3.295601
H	1.807567	1.451441	2.421590
C	-3.996822	-0.176678	-1.755584
N	-3.336624	-0.721579	-0.543922
C	-4.256551	-1.372681	0.415850
H	-4.467829	-0.992257	-2.305303
H	-3.237419	0.305794	-2.367050
H	-4.747763	0.559366	-1.465938
H	-2.806983	0.037831	-0.058865
H	-4.787260	-2.183277	-0.083884
H	-4.972081	-0.645679	0.802364
H	-3.667228	-1.787047	1.232505
1SA1MA4DMA			
S	1.950439	-1.813257	-0.772406
O	1.591481	-0.731082	-1.902768
O	2.867903	-2.724860	-1.401777
O	2.559941	-1.009931	0.343083
O	0.676646	-2.392800	-0.306067
H	3.023582	1.797601	-0.783523
H	-0.858039	-1.865884	-0.870906
O	-2.377528	1.986012	-0.534710
O	-0.418533	1.255629	2.395262
O	0.223020	1.281144	-1.091470
O	-1.785009	-0.053598	1.204844
O	1.830439	2.726791	-0.476770
C	-1.643560	2.307741	0.644587
C	-0.392182	3.128678	0.298918
C	-1.263641	1.057074	1.476385

C	0.645293	2.320460	-0.484462
H	-2.308510	2.914419	1.266721
H	0.085516	3.499413	1.204364
H	-0.685246	3.993217	-0.306169
H	-1.700490	1.608000	-1.119916
H	0.360449	-0.021043	2.638018
H	1.082692	0.076564	-1.534743
C	-1.986559	-0.969583	-2.382615
N	-1.830790	-1.517436	-1.012496
C	-2.795360	-2.601614	-0.697943
H	-1.843074	-1.771124	-3.107981
H	-1.232062	-0.202098	-2.539631
H	-2.987873	-0.551907	-2.472968
H	-1.935279	-0.762595	-0.278655
H	-2.655716	-3.425467	-1.398577
H	-3.800092	-2.185984	-0.770732
H	-2.606581	-2.948787	0.316504
C	2.065882	-0.715431	3.682361
N	0.982822	-0.919014	2.695710
C	0.109680	-2.084422	2.976459
H	1.631377	-0.547848	4.668148
H	2.643113	0.161100	3.390922
H	2.718625	-1.588841	3.707489
H	1.421304	-1.022704	1.759679
H	-0.248397	-2.018001	4.004878
H	0.663316	-3.011229	2.827830
H	-0.734890	-2.025973	2.295017
C	4.423974	0.890098	-2.103461
N	3.891344	1.152649	-0.744188
C	4.866707	1.754321	0.192732
H	4.732630	1.832968	-2.556303
H	3.635445	0.426371	-2.692180
H	5.275119	0.211082	-2.041047
H	3.514297	0.268387	-0.333002
H	5.229272	2.697379	-0.216797
H	5.704172	1.073340	0.349851
H	4.362833	1.949660	1.138211
C	-5.951537	0.627654	-1.352524
N	-4.863196	0.132903	-0.516867
C	-5.288202	-0.145062	0.852893
H	-6.700304	-0.158589	-1.498304
H	-5.567299	0.907098	-2.336978
H	-6.471401	1.504514	-0.928716
H	-4.112482	0.821978	-0.488487

H -5.960942 -1.010222 0.871957
H -5.823994 0.697608 1.323960
H -4.409180 -0.371938 1.458441

1SA2MA

S 0.177907 3.117535 0.043790
O 1.588506 3.297703 0.297674
O -0.655919 4.217036 -0.299818
O 0.020941 2.040858 -1.134634
O -0.366691 2.332001 1.291417
H 0.777771 1.370580 -1.083372
H -1.282233 1.973106 1.107438
O 3.887146 -1.638513 -1.362666
O 3.302563 1.209892 0.591255
O 1.547428 -2.960759 -0.382431
O 1.910151 0.269888 -0.914119
O 0.879398 -2.053861 1.563689
C 3.769147 -1.020846 -0.111227
C 3.210819 -1.967654 0.989798
C 2.900735 0.236702 -0.192780
C 1.761855 -2.335445 0.767605
H 4.772626 -0.717445 0.189235
H 3.293214 -1.504303 1.972673
H 3.821198 -2.873526 0.961986
H 3.018546 -1.983364 -1.609099
H 2.694534 1.991758 0.534554
H 0.566963 -3.074539 -0.537516
O -4.435565 -0.886336 1.046442
O -2.355092 0.583886 -1.481754
O -1.709219 -1.922642 0.991370
O -2.620231 1.094632 0.699250
O -1.072208 -2.998976 -0.875879
C -3.895089 -0.729650 -0.234799
C -3.267135 -2.027994 -0.801462
C -2.895592 0.427863 -0.280103
C -1.906594 -2.375626 -0.239806
H -4.726300 -0.459672 -0.893477
H -3.162054 -1.978643 -1.884927
H -3.954702 -2.845849 -0.566771
H -3.701321 -0.891988 1.673232
H -1.642699 1.259398 -1.456416
H -0.760584 -2.068648 1.270110

1SA2MA1DMA

S 1.370363 -2.371996 0.214638
O 0.521402 -2.321260 1.409968

O	2.721735	-2.876003	0.453548
O	0.717566	-3.417146	-0.790369
O	1.408081	-1.072146	-0.500595
H	-0.239776	-3.180617	-0.889613
H	1.023868	0.324196	0.101843
O	-4.427806	-1.942744	-1.373898
O	-2.056821	-1.905977	1.300072
O	-2.920792	0.585483	-0.876246
O	-1.908069	-2.635748	-0.831275
O	-3.530983	1.655740	1.002123
C	-4.026529	-1.864424	-0.029750
C	-4.431673	-0.521890	0.603402
C	-2.536896	-2.169139	0.109044
C	-3.581666	0.681248	0.262851
H	-4.537901	-2.648445	0.550287
H	-4.444815	-0.596294	1.690727
H	-5.453793	-0.305342	0.277538
H	-3.644500	-2.199193	-1.880554
H	-1.069181	-2.090416	1.350906
H	-2.389604	1.409706	-1.034216
O	0.973978	3.943136	-1.501817
O	-1.502569	3.342896	1.013928
O	2.986306	1.660423	0.520143
O	-1.371574	2.785165	-1.163932
O	0.776586	1.264487	0.369694
C	0.429838	4.030922	-0.205516
C	1.435859	3.479394	0.822986
C	-0.915906	3.311593	-0.155551
C	1.822034	2.040057	0.549308
H	0.233531	5.080908	0.052085
H	1.002050	3.537288	1.825513
H	2.342080	4.082959	0.796595
H	0.317296	3.470261	-2.035324
H	-2.331812	2.777017	1.000716
H	3.702186	0.110963	0.159819
C	4.475163	-0.671597	-1.586916
N	4.304182	-0.699231	-0.109544
C	5.568909	-0.647417	0.665183
H	4.972705	0.253990	-1.875355
H	3.484086	-0.723120	-2.032577
H	5.068194	-1.531527	-1.896818
H	3.764654	-1.563242	0.140846
H	6.090889	0.283380	0.445102
H	6.193951	-1.498934	0.397317

H	5.329721	-0.689924	1.726763
1SA2MA2DMA			
S	-1.997576	1.136600	1.376322
O	-1.103395	2.008604	2.140046
O	-3.386955	1.131030	1.773954
O	-2.015388	1.710972	-0.139367
O	-1.442838	-0.241278	1.235731
H	-1.192091	2.238135	-0.312802
H	-3.606823	-0.900869	-0.870378
O	2.476153	3.896109	-1.849514
O	1.221829	2.940522	1.365760
O	2.565640	1.035566	-0.981704
O	0.244119	3.066668	-0.662924
O	4.616589	0.669544	-0.145457
C	2.529605	3.742773	-0.452520
C	3.734391	2.888580	-0.035184
C	1.206331	3.201600	0.082361
C	3.687139	1.421863	-0.404286
H	2.658440	4.728720	0.017980
H	3.872552	2.931711	1.048210
H	4.635493	3.310601	-0.486191
H	1.603829	3.579318	-2.123424
H	0.334877	2.587226	1.677952
H	2.571577	0.048821	-1.136328
O	1.939702	-4.345672	-1.021017
O	4.285632	-1.955281	0.127749
O	0.657759	-1.688310	1.947689
O	2.470337	-1.606444	-1.159468
O	-0.166272	-2.990283	0.310328
C	2.699248	-3.720500	-0.023111
C	1.927677	-3.594974	1.320415
C	3.152809	-2.318353	-0.434980
C	0.690513	-2.733565	1.147541
H	3.589562	-4.328501	0.145551
H	2.569961	-3.184110	2.098731
H	1.610708	-4.600609	1.606856
H	1.058872	-3.943077	-0.995710
H	4.475005	-0.988122	-0.049499
H	-0.134690	-1.114711	1.749560
C	-3.146343	-2.948489	-0.747677
N	-2.736787	-1.525846	-0.851841
C	-1.859080	-1.223142	-2.013148
H	-3.699047	-3.231338	-1.644277
H	-3.786565	-3.063701	0.126520

H	-2.259030	-3.565798	-0.631468
H	-2.221928	-1.234768	0.006290
H	-2.375247	-1.482919	-2.937807
H	-0.937083	-1.794013	-1.917429
H	-1.633341	-0.158710	-1.993136
C	-5.085359	1.210222	-1.719825
N	-4.975692	0.201201	-0.657815
C	-6.261709	-0.432953	-0.345905
H	-5.333969	0.726773	-2.669526
H	-4.129363	1.724298	-1.821673
H	-5.861561	1.959011	-1.508214
H	-4.621032	0.656735	0.185346
H	-6.605586	-1.021748	-1.201540
H	-7.045468	0.298204	-0.102795
H	-6.144115	-1.101992	0.509128

1SA2MA3DMA

S	-1.531181	-0.688782	-1.666215
O	-0.430928	-1.397403	-2.324427
O	-2.806427	-0.725057	-2.338976
O	-1.777370	-1.437063	-0.251739
O	-1.123151	0.694517	-1.268515
H	-0.940793	-1.890674	0.035717
H	-2.732119	0.891187	1.567448
O	2.404972	-3.977253	1.916246
O	1.457222	-2.964470	-1.393466
O	3.332031	-1.338256	1.213399
O	0.454689	-2.634935	0.596787
O	4.947798	-1.231557	-0.343775
C	2.517713	-3.884024	0.520909
C	3.887478	-3.344816	0.055194
C	1.357155	-3.091206	-0.088941
C	4.116037	-1.867660	0.283453
H	2.427423	-4.904480	0.134802
H	4.042920	-3.529250	-1.008013
H	4.662114	-3.890478	0.602388
H	2.239721	-3.085627	2.245967
H	0.716408	-2.396218	-1.760341
H	3.454711	-0.344442	1.250618
O	3.188873	4.057130	1.059858
O	4.951562	1.428535	-0.567647
O	1.088904	1.966061	-1.992015
O	3.464327	1.295015	1.118637
O	0.833250	2.966209	0.004051
C	3.726230	3.395579	-0.050462

C	2.797992	3.455296	-1.292967
C	4.044780	1.928308	0.247402
C	1.467355	2.774178	-1.027129
H	4.667004	3.888056	-0.305194
H	3.278947	3.009617	-2.162952
H	2.601679	4.510819	-1.501045
H	2.275941	3.743062	1.149495
H	5.034858	0.442226	-0.438768
H	0.235566	1.497392	-1.759016
C	-2.069801	2.874824	1.404168
N	-1.822484	1.412351	1.322305
C	-0.709985	0.939841	2.187922
H	-2.317657	3.142041	2.432112
H	-2.907632	3.121474	0.752276
H	-1.178583	3.403908	1.074559
H	-1.590875	1.164358	0.336155
H	-0.949686	1.148302	3.231249
H	0.207215	1.451123	1.900593
H	-0.591989	-0.132599	2.042546
C	-4.033753	-1.257798	2.370210
N	-4.253259	0.119797	1.908151
C	-5.151276	0.866407	2.795045
H	-3.498445	-1.252931	3.325104
H	-3.429451	-1.788592	1.634296
H	-4.975801	-1.805426	2.517868
H	-4.678460	0.078092	0.966760
H	-4.688347	0.997915	3.778238
H	-6.115572	0.359741	2.946632
H	-5.349614	1.855738	2.376021
C	-6.484552	-1.082870	-1.002031
N	-5.429055	-0.073747	-0.915892
C	-5.815972	1.192036	-1.538447
H	-7.347825	-0.772817	-0.404096
H	-6.119344	-2.031600	-0.602849
H	-6.835826	-1.256574	-2.031671
H	-4.597806	-0.420515	-1.393446
H	-6.624340	1.660128	-0.966860
H	-6.162949	1.076298	-2.577461
H	-4.961314	1.872095	-1.544937
1SA2MA4DMA			
S	1.563632	-1.466669	-0.563519
O	0.962360	-2.398938	0.395744
O	3.007289	-1.551335	-0.696362
O	1.000087	-1.841414	-2.008272

O	1.135157	-0.059169	-0.301662
H	0.046805	-2.114522	-1.935397
H	4.192484	1.148177	-0.724066
O	-4.064185	-3.587563	-2.065505
O	-1.359418	-3.629168	0.289161
O	-4.046879	-1.225815	-0.384528
O	-1.540176	-2.682181	-1.749352
O	-4.415808	-1.546183	1.807762
C	-3.419520	-3.896630	-0.858692
C	-4.224191	-3.470301	0.390799
C	-1.994459	-3.338413	-0.825706
C	-4.240680	-1.986603	0.682047
H	-3.328831	-4.987081	-0.820835
H	-3.850232	-3.966724	1.286064
H	-5.259017	-3.791836	0.237385
H	-3.848000	-2.669941	-2.274057
H	-0.459725	-3.188489	0.316807
H	-4.000437	-0.260161	-0.119010
O	-3.140672	3.982701	0.762116
O	-3.827357	0.961807	2.533345
O	-0.710564	0.967048	1.363179
O	-3.744103	1.298784	0.311725
O	0.228984	2.907581	0.721324
C	-3.012007	3.067492	1.799787
C	-1.556661	2.940999	2.348797
C	-3.569395	1.682719	1.463169
C	-0.579436	2.293221	1.389938
H	-3.613501	3.439863	2.634986
H	-1.578190	2.356152	3.270981
H	-1.209348	3.951984	2.557310
H	-2.755368	3.642485	-0.087613
H	-4.101562	0.037010	2.277509
H	-0.055058	0.565368	0.734384
C	3.264897	2.963345	-0.218047
N	3.254273	1.648404	-0.910365
C	3.026738	1.735446	-2.374988
H	4.006602	3.609746	-0.688767
H	3.533695	2.802651	0.825753
H	2.273102	3.407609	-0.257065
H	2.493921	1.048069	-0.526220
H	3.840160	2.296294	-2.836480
H	2.077230	2.233784	-2.566802
H	2.993182	0.724899	-2.778046
C	6.068149	-0.503286	-1.494247

N	5.714528	0.406231	-0.394795
C	6.821626	1.294366	-0.026103
H	6.257286	0.068822	-2.408412
H	5.236152	-1.185242	-1.671524
H	6.971502	-1.091292	-1.277098
H	5.458679	-0.167627	0.423802
H	7.051854	1.974356	-0.852399
H	7.742090	0.744864	0.219414
H	6.542594	1.894533	0.843074
C	-3.577899	3.678614	-2.533562
N	-2.439929	3.141728	-1.786034
C	-1.147911	3.390979	-2.420999
H	-3.505916	4.769489	-2.567606
H	-4.500626	3.419159	-2.012275
H	-3.634857	3.306908	-3.568436
H	-2.575185	2.146824	-1.639536
H	-0.961556	4.468164	-2.448416
H	-1.089258	3.008444	-3.452575
H	-0.363379	2.929310	-1.819892
C	5.607670	-2.433714	2.403816
N	4.708696	-1.426333	1.843362
C	3.844073	-0.817737	2.854912
H	6.329267	-1.956103	3.075114
H	6.166163	-2.916927	1.598963
H	5.083529	-3.215300	2.977916
H	4.122339	-1.845775	1.124588
H	4.445193	-0.216754	3.545538
H	3.282862	-1.555546	3.449725
H	3.118613	-0.161352	2.369436
ISA3MA			
S	3.972804	-0.916547	1.077389
O	4.492691	-0.679407	2.380216
O	2.550852	-0.574546	0.846165
O	4.800209	-0.182605	-0.032219
O	4.190097	-2.398109	0.690694
H	4.537048	0.791111	-0.063327
H	3.552391	-2.708621	-0.035706
O	-0.369607	-5.137252	0.319148
O	-2.368890	-2.806863	-1.528984
O	0.669140	-2.196874	-0.265614
O	-2.213609	-3.264990	0.671267
O	2.472626	-3.317550	-1.004643
C	-0.871483	-4.532774	-0.847064
C	0.296124	-4.034119	-1.716066

C	-1.881581	-3.446050	-0.494596
C	1.262138	-3.156488	-0.956323
H	-1.431422	-5.265900	-1.446224
H	-0.091347	-3.472556	-2.570865
H	0.859372	-4.888554	-2.087950
H	-0.865914	-4.763534	1.061672
H	-3.059581	-2.143162	-1.240941
H	1.337148	-1.631125	0.193897
O	-5.611056	1.189675	-0.356919
O	-3.639351	-1.166987	1.488755
O	-2.621450	1.580773	-0.112822
O	-4.169671	-1.029895	-0.696378
O	-2.669568	3.402235	1.200568
C	-5.054948	0.618186	0.800726
C	-4.267928	1.666137	1.602117
C	-4.225337	-0.612405	0.454138
C	-3.113719	2.311770	0.868583
H	-5.860598	0.253125	1.454174
H	-3.863410	1.214682	2.513343
H	-4.942643	2.465806	1.909673
H	-5.289378	0.668042	-1.105690
H	-3.121218	-1.973628	1.209609
H	-1.886333	2.065796	-0.582291
O	1.624056	3.528715	-2.497836
O	-0.384404	4.408539	0.334086
O	1.831842	2.028492	0.422637
O	-0.649860	2.899127	-1.316507
O	3.991401	2.305813	-0.147490
C	1.312413	4.259742	-1.336543
C	2.484474	4.168586	-0.341744
C	-0.011531	3.780371	-0.749654
C	2.857766	2.740166	-0.021653
H	1.168991	5.322306	-1.578678
H	2.220977	4.682056	0.586911
H	3.359836	4.647992	-0.776654
H	0.858611	2.964480	-2.680875
H	-1.265731	4.055815	0.664657
H	2.096435	1.095563	0.612529
1SA3MA1DMA			
S	0.313283	-2.807564	0.480753
O	-0.655278	-3.902001	0.552510
O	1.718929	-3.246181	0.460331
O	0.124893	-2.101634	-0.938798
O	0.089294	-1.778237	1.513756

H	-0.847651	-1.999473	-1.115247
H	1.517181	-1.275744	2.120667
O	-5.131690	-1.733700	-2.222853
O	-3.224494	-3.469413	0.177440
O	-4.544931	0.793140	-0.974811
O	-2.537346	-1.892305	-1.287377
O	-3.882565	0.504074	1.152969
C	-4.887177	-2.166610	-0.912679
C	-5.331916	-1.137227	0.165975
C	-3.412761	-2.513793	-0.700397
C	-4.513049	0.132275	0.172290
H	-5.476651	-3.071883	-0.762426
H	-5.268645	-1.579277	1.159928
H	-6.371324	-0.880098	-0.053423
H	-4.560024	-0.973875	-2.392298
H	-2.247139	-3.637806	0.338884
H	-3.979290	1.612236	-0.917388
O	5.638369	0.489809	-1.147009
O	3.339246	-2.240075	-1.321999
O	2.432268	0.738040	-0.810048
O	4.342226	-1.203486	0.415557
O	2.575136	2.347754	-2.365146
C	4.807773	-0.439825	-1.803623
C	3.795810	0.299508	-2.697377
C	4.121839	-1.347507	-0.783386
C	2.885406	1.242183	-1.943954
H	5.406703	-1.091486	-2.454504
H	3.163106	-0.431633	-3.209904
H	4.330321	0.881253	-3.447330
H	5.605529	0.253828	-0.208333
H	2.759981	-2.702861	-0.640972
H	1.834701	1.387455	-0.342573
O	-0.239485	4.215901	2.268833
O	1.005818	4.057149	-1.071251
O	-2.362255	2.649365	1.337895
O	0.972042	2.474063	0.529226
O	-3.046248	3.010645	-0.771107
C	-0.217698	4.540594	0.906794
C	-1.625570	4.644697	0.265920
C	0.659918	3.578571	0.101985
C	-2.412101	3.351406	0.214422
H	0.244373	5.527284	0.825674
H	-1.557898	5.030867	-0.750264
H	-2.200015	5.353499	0.870414

H	-0.733916	3.390562	2.361145
H	1.580800	3.406992	-1.578062
H	-2.919231	1.815109	1.262089
C	2.473668	0.305034	3.105942
N	2.475212	-1.056519	2.510763
C	2.846762	-2.150336	3.446974
H	1.803932	0.315873	3.965641
H	2.117428	1.019399	2.364863
H	3.483426	0.566337	3.422460
H	3.126340	-1.096504	1.703616
H	2.131189	-2.176442	4.268138
H	3.852420	-1.977720	3.830180
H	2.808484	-3.086291	2.893373
1SA3MA2DMA			
S	-0.104346	-3.390891	0.524634
O	0.937840	-3.772685	-0.620710
O	-1.314806	-4.116415	0.159732
O	0.472795	-3.807390	1.811114
O	-0.249934	-1.914266	0.464510
H	1.433906	-2.639559	2.454635
H	-0.166100	-1.199498	-1.064599
O	5.782589	-0.225674	-0.440182
O	2.733004	-1.955332	-1.157744
O	4.139174	2.426440	-1.191713
O	3.754393	-1.299332	0.746680
O	2.278814	1.191999	-1.366328
C	4.814031	-0.765981	-1.303262
C	4.310158	0.323261	-2.289424
C	3.651487	-1.405670	-0.504781
C	3.486106	1.362409	-1.584510
H	5.255403	-1.560489	-1.918426
H	3.691968	-0.151621	-3.051328
H	5.181910	0.789357	-2.748215
H	5.436271	-0.409859	0.448387
H	1.677257	-3.090000	-0.677752
H	3.547631	3.036828	-0.669730
O	-5.649865	-0.673411	-1.749885
O	-3.653212	-2.936313	0.124334
O	-4.094124	1.339776	-0.499965
O	-3.067376	-1.620278	-1.616939
O	-3.630322	1.072919	1.678650
C	-5.225817	-1.325987	-0.582739
C	-5.226151	-0.408792	0.669122
C	-3.853292	-1.985952	-0.762977

C	-4.231808	0.728488	0.669449
H	-5.947181	-2.121586	-0.386117
H	-5.053864	-0.993000	1.572603
H	-6.222230	0.041633	0.735078
H	-4.917169	-0.120238	-2.046624
H	-2.737174	-3.341164	0.064131
H	-3.446951	2.090911	-0.418779
O	-0.697604	5.415266	-0.484013
O	-1.934186	3.079414	1.937047
O	0.783876	2.611740	0.260061
O	-2.339440	3.359569	-0.259474
O	2.528716	4.022028	0.284403
C	-0.866012	4.900923	0.815187
C	0.513124	4.647903	1.442781
C	-1.775270	3.675180	0.784609
C	1.383590	3.744482	0.598879
H	-1.388330	5.629539	1.454209
H	0.388903	4.194716	2.430260
H	1.035165	5.596913	1.555600
H	-1.345252	4.963100	-1.043636
H	-2.574287	2.307941	1.849630
H	1.383485	2.077003	-0.339373
C	-0.031895	-1.755685	-3.067145
N	0.094055	-0.745978	-1.976948
C	-0.740360	0.466949	-2.195890
H	-1.065880	-2.093344	-3.091072
H	0.628143	-2.588546	-2.841984
H	0.245379	-1.292577	-4.014433
H	1.079825	-0.476207	-1.856168
H	-1.776905	0.152161	-2.285723
H	-0.405901	0.969979	-3.103026
H	-0.628306	1.137397	-1.347063
C	1.322690	-0.678085	3.139694
N	2.099515	-1.884692	2.763902
C	2.982192	-2.413546	3.830172
H	0.713864	-0.895569	4.017766
H	0.674248	-0.423507	2.303844
H	2.007683	0.142168	3.356511
H	2.692524	-1.668828	1.910955
H	2.384713	-2.691624	4.698690
H	3.713445	-1.654861	4.109662
H	3.499074	-3.292439	3.447640
1SA3MA3DMA			
S	-0.391064	-3.501151	0.313119

O	0.800702	-4.191197	-0.451678
O	-1.603952	-3.881400	-0.430608
O	-0.363518	-3.984953	1.697114
O	-0.136494	-2.038290	0.244269
H	0.972908	-3.178293	2.398082
H	-0.400198	-1.559474	-1.343095
O	5.702359	-1.129727	-0.310599
O	2.626644	-2.650354	-1.273735
O	4.314189	1.646635	-0.470688
O	3.499280	-2.046164	0.721064
O	2.299272	0.855543	-1.048587
C	4.688805	-1.432289	-1.234362
C	4.249654	-0.157455	-2.015742
C	3.487024	-2.110501	-0.537700
C	3.531365	0.832430	-1.142134
H	5.072758	-2.133349	-1.982982
H	3.580695	-0.452331	-2.823815
H	5.153063	0.300574	-2.420463
H	5.286910	-1.270645	0.555268
H	1.544469	-3.518943	-0.719061
H	3.770124	2.237616	0.120130
O	-5.845224	-0.131556	-1.616261
O	-3.898383	-2.703790	-0.068464
O	-3.846072	1.271542	-0.133337
O	-3.472384	-1.425759	-1.881902
O	-3.798951	0.939440	2.085784
C	-5.461798	-1.008210	-0.591402
C	-5.365883	-0.328348	0.794841
C	-4.162213	-1.747088	-0.926016
C	-4.255019	0.681785	0.982210
H	-6.246537	-1.765830	-0.517253
H	-5.261587	-1.071377	1.585415
H	-6.307363	0.205268	0.961634
H	-5.074698	0.410830	-1.824922
H	-3.013223	-3.159623	-0.236210
H	-3.134013	1.948947	0.069803
O	-0.208572	5.201254	0.626393
O	-1.865812	2.702598	2.592772
O	0.976978	1.896420	1.010955
O	-1.952325	3.059327	0.373249
O	2.797289	3.208729	1.115434
C	-0.450127	4.400492	1.734603
C	0.843901	3.826077	2.378657
C	-1.493817	3.306214	1.480512

C	1.646555	2.957229	1.443828
H	-0.901996	5.040950	2.500449
H	0.574094	3.234092	3.257484
H	1.475749	4.658530	2.683515
H	0.107366	4.668406	-0.149887
H	-2.576709	2.025954	2.408375
H	1.491333	1.442168	0.285394
C	-0.516771	0.031653	-2.683470
N	-0.738236	-1.392406	-2.325876
C	-0.084637	-2.376685	-3.232694
H	0.543653	0.258940	-2.590450
H	-1.083823	0.649691	-1.988263
H	-0.868604	0.208558	-3.699880
H	-1.758880	-1.571694	-2.270872
H	0.995822	-2.286346	-3.132037
H	-0.401590	-2.185377	-4.258101
H	-0.390512	-3.373887	-2.922301
C	1.272813	-1.277950	3.162278
N	1.786869	-2.592343	2.699633
C	2.591331	-3.332713	3.700367
H	0.644615	-1.422095	4.041716
H	0.686036	-0.845433	2.354663
H	2.114208	-0.629459	3.406612
H	2.383045	-2.432478	1.835806
H	1.987046	-3.530181	4.586063
H	3.466248	-2.742059	3.971483
H	2.912686	-4.275365	3.259657
C	-0.374771	4.232888	-2.648719
N	0.740267	4.049304	-1.715708
C	1.936752	4.814361	-2.079794
H	-0.683726	5.280976	-2.634301
H	-1.223940	3.635179	-2.315005
H	-0.121733	3.965426	-3.686005
H	0.978560	3.063701	-1.661192
H	1.713256	5.882132	-2.015014
H	2.294840	4.600273	-3.098032
H	2.735170	4.594819	-1.369629
1SA3MA4DMA			
S	-2.221874	2.919154	1.032245
O	-2.400729	4.340077	1.113236
O	-3.355345	2.386039	0.043364
O	-0.921478	2.507239	0.397154
O	-2.382433	2.164051	2.297450
H	0.055214	1.536378	-1.685488

H	-1.244346	0.956058	2.420183
O	-2.173261	-3.179375	-2.315422
O	-0.784326	-3.757959	0.937782
O	-3.618871	-0.241261	-0.186412
O	0.149655	-3.441067	-1.085972
O	-1.484438	-0.934599	-0.102738
C	-2.237820	-3.517356	-0.940050
C	-3.206726	-2.589464	-0.212165
C	-0.834900	-3.526604	-0.352356
C	-2.747595	-1.129068	-0.172950
H	-2.602447	-4.550623	-0.830520
H	-3.319511	-2.929709	0.821755
H	-4.188707	-2.649669	-0.682490
H	-1.248514	-3.291303	-2.578780
H	0.164278	-3.768235	1.247989
H	-3.395782	1.382366	0.026488
O	3.659263	4.097699	-2.427657
O	1.027782	4.101184	-0.048752
O	4.739657	1.830424	-0.965820
O	1.545925	2.568377	-1.620579
O	4.010478	1.802164	1.158195
C	3.118484	4.313412	-1.153339
C	4.085257	3.903615	-0.003004
C	1.787733	3.580990	-0.971741
C	4.275542	2.412468	0.127630
H	2.938235	5.385135	-1.057234
H	3.716664	4.276806	0.951527
H	5.052679	4.360717	-0.226037
H	3.659864	3.144481	-2.581760
H	0.194545	3.533797	0.123652
H	4.801055	0.844385	-0.834675
O	5.528793	-3.482737	-0.444048
O	4.509207	-0.743402	1.649089
O	2.667734	-3.406181	-0.284137
O	4.920277	-0.825303	-0.562755
O	1.747341	-3.659427	1.748453
C	5.208300	-2.831835	0.753371
C	4.135062	-3.562369	1.589332
C	4.860925	-1.356805	0.532939
C	2.731920	-3.542916	1.031182
H	6.124295	-2.830777	1.353739
H	4.087080	-3.165073	2.602740
H	4.436020	-4.612705	1.658724
H	4.796832	-3.343203	-1.056941

H	4.322385	0.225845	1.468084
H	1.712938	-3.425128	-0.594385
C	-1.683013	1.620181	-2.811558
N	-0.630967	0.863099	-2.069295
C	0.087316	-0.129403	-2.909350
H	-1.191996	2.239973	-3.562493
H	-2.217985	2.243026	-2.098874
H	-2.356364	0.903782	-3.287849
H	-1.044886	0.357074	-1.256070
H	0.607672	0.390886	-3.712546
H	-0.642109	-0.825622	-3.317845
H	0.802858	-0.665441	-2.288367
C	0.787257	0.457752	2.368416
N	-0.649998	0.088358	2.362076
C	-1.055968	-0.856175	3.438816
H	1.028968	0.940499	3.315072
H	0.966329	1.154198	1.553592
H	1.396599	-0.438249	2.250573
H	-0.904144	-0.315430	1.433473
H	-0.716727	-0.462270	4.397428
H	-0.598178	-1.828213	3.257466
H	-2.147856	-0.920974	3.441844
C	-4.950729	-0.512965	-3.560061
N	-3.650753	-0.952888	-4.065350
C	-3.690528	-1.327246	-5.474944
H	-5.240812	0.420960	-4.052200
H	-4.880996	-0.321538	-2.487646
H	-5.758981	-1.243656	-3.736068
H	-3.326349	-1.743450	-3.515003
H	-3.908119	-0.445820	-6.086621
H	-4.452905	-2.089762	-5.711055
H	-2.716169	-1.713865	-5.785253
C	-5.481769	-0.417753	2.838956
N	-4.301485	0.067484	3.551000
C	-4.586114	0.412104	4.940121
H	-5.782738	-1.392424	3.238997
H	-5.243300	-0.536174	1.780779
H	-6.350917	0.256941	2.923672
H	-3.934926	0.888294	3.074386
H	-4.845237	-0.491246	5.502919
H	-5.419671	1.125632	5.055945
H	-3.699080	0.853570	5.401312
1SA4MA			
S	4.607970	-0.169298	0.561163

O	4.871603	-1.083902	1.647172
O	5.492624	0.947093	0.341696
O	4.565535	-0.967871	-0.786226
O	3.149074	0.344014	0.773176
H	4.181867	-1.884105	-0.631052
H	2.996258	1.207016	0.265573
O	1.509116	3.213456	-3.276995
O	0.603277	5.006889	-0.311338
O	4.831948	3.165567	-1.172143
O	-0.183011	3.105754	-1.230298
O	2.774724	2.557020	-0.497005
C	1.561171	4.285536	-2.368727
C	3.001494	4.493908	-1.881007
C	0.576041	4.067332	-1.224387
C	3.524073	3.300880	-1.120331
H	1.244895	5.213454	-2.865937
H	3.056517	5.362766	-1.217560
H	3.651428	4.686705	-2.735040
H	0.838072	2.601120	-2.941652
H	-0.069035	4.818036	0.408232
H	5.124457	2.391612	-0.633865
O	2.197464	-5.623935	-0.534553
O	3.278728	-3.268723	1.938531
O	0.388957	-3.160100	0.089031
O	3.542342	-3.345313	-0.302063
O	-1.209038	-4.685926	0.501008
C	2.340062	-5.113491	0.768200
C	0.965279	-5.015376	1.452696
C	3.105388	-3.796609	0.749528
C	-0.064145	-4.277174	0.626495
H	2.955691	-5.795334	1.372362
H	1.064788	-4.513011	2.419413
H	0.577924	-6.018131	1.627671
H	2.646417	-5.003941	-1.126830
H	3.838676	-2.453111	1.891839
H	-0.313270	-2.731533	-0.476040
O	-2.025624	1.803772	3.649855
O	-1.497500	2.300988	0.957866
O	-4.114780	0.724176	2.049998
O	-1.133204	4.428562	1.601345
O	-4.794162	2.257418	0.550448
C	-2.446623	2.992797	3.029370
C	-3.958914	3.002237	2.679772
C	-1.613367	3.319263	1.786524

C	-4.339321	1.967226	1.645817
H	-2.260980	3.801317	3.736626
H	-4.255254	3.981727	2.304015
H	-4.499972	2.791564	3.605698
H	-2.359260	1.058188	3.133061
H	-1.009568	2.572556	0.130691
H	-4.333822	0.068742	1.322899
O	-5.674413	-2.873567	-1.720286
O	-5.073252	0.550190	-1.477656
O	-3.051455	-3.692569	-1.107943
O	-4.630274	-0.992618	0.102937
O	-1.505637	-2.107927	-1.496089
C	-4.990654	-1.730733	-2.159503
C	-3.575258	-2.030171	-2.720025
C	-4.888929	-0.679702	-1.052615
C	-2.602536	-2.601080	-1.709996
H	-5.582368	-1.301019	-2.968666
H	-3.131185	-1.127390	-3.139912
H	-3.700206	-2.767143	-3.518542
H	-5.108255	-3.333520	-1.086176
H	-4.979551	1.202390	-0.725362
H	-2.368650	-4.048838	-0.464641

1SA4MA1DMA

S	0.632533	-2.533313	1.618986
O	-0.531893	-2.532194	2.509371
O	1.838408	-3.080862	2.211868
O	0.234780	-3.470888	0.366389
O	0.848827	-1.216935	0.963436
H	-0.581542	-3.986485	0.581368
H	2.107384	-0.641443	-1.892591
O	5.030522	-1.630692	-2.788178
O	5.336708	1.487444	-1.124799
O	4.337318	-2.530484	1.301742
O	3.466346	0.558947	-1.928550
O	3.394900	-2.366293	-0.724719
C	5.501539	-0.789062	-1.764935
C	5.623926	-1.506536	-0.400039
C	4.646679	0.475839	-1.624824
C	4.332801	-2.170044	0.040469
H	6.497844	-0.450237	-2.057260
H	5.941817	-0.816751	0.382584
H	6.386946	-2.286678	-0.485788
H	4.265370	-2.089774	-2.409052
H	4.712241	2.221405	-0.906774

H	3.433843	-2.835891	1.577286
O	-4.770041	-5.196165	0.062248
O	-2.941730	-2.535101	1.517316
O	-3.874940	-0.962887	-1.884150
O	-2.250801	-4.493015	0.636818
O	-5.307270	-0.986007	-0.151606
C	-4.508842	-3.827006	0.261974
C	-4.602872	-3.077214	-1.090084
C	-3.112603	-3.647497	0.849462
C	-4.627257	-1.573517	-0.981462
H	-5.248249	-3.416906	0.951120
H	-5.549294	-3.386020	-1.543984
H	-3.799806	-3.394669	-1.756829
H	-3.907808	-5.627644	-0.025182
H	-2.011437	-2.484072	1.907050
H	-4.005589	0.024183	-1.826860
O	-4.214616	4.375426	-1.699888
O	-5.214063	1.601570	0.333281
O	-1.959128	3.250964	-0.214020
O	-4.220074	1.692735	-1.686762
O	-1.721164	4.740677	1.447784
C	-4.687372	3.746759	-0.535618
C	-3.934478	4.221479	0.721591
C	-4.677758	2.229070	-0.684942
C	-2.428842	4.100994	0.681787
H	-5.739631	4.022240	-0.394744
H	-4.286143	3.675054	1.602325
H	-4.154553	5.275958	0.895587
H	-3.734515	3.701767	-2.200662
H	-5.244327	0.610793	0.170140
H	-0.964533	3.273151	-0.220568
O	3.376445	3.294670	-0.525233
O	0.874309	4.511421	1.696321
O	1.695203	1.195182	1.818014
O	0.740984	3.376840	-0.246327
O	3.810293	0.525608	1.424290
C	2.897580	3.748288	0.733107
C	3.383949	2.849070	1.890524
C	1.377882	3.858040	0.687412
C	3.009732	1.389243	1.691474
H	3.286047	4.756619	0.901801
H	2.954599	3.217945	2.824659
H	4.470218	2.911062	1.946896
H	2.624460	2.922402	-1.013675

H	-0.127882	4.587034	1.619221
H	1.458286	0.251372	1.622766
C	0.200251	0.143536	-2.028053
N	1.136207	-0.981364	-1.764652
C	0.900632	-2.188021	-2.601312
H	0.300888	0.461686	-3.065279
H	0.454174	0.967721	-1.364304
H	-0.820306	-0.185665	-1.835201
H	1.069882	-1.233585	-0.754330
H	1.083733	-1.939097	-3.646686
H	-0.128442	-2.515819	-2.466323
H	1.578079	-2.967326	-2.264285

1SA4MA2DMA

S	3.090596	1.330630	2.172625
O	2.924802	0.072263	2.906911
O	2.570980	2.516355	2.828998
O	4.661719	1.593530	2.023377
O	2.584759	1.185628	0.772655
H	5.065273	0.749987	1.688321
H	0.368543	-1.378663	0.523261
O	-0.009631	3.697366	-2.329888
O	-2.874105	4.656632	-0.405719
O	1.569837	4.368952	1.147166
O	-2.368463	2.797266	-1.570939
O	-0.299829	3.149973	0.831468
C	-0.804037	4.603912	-1.588064
C	0.002003	5.176607	-0.422471
C	-2.096485	3.921396	-1.153862
C	0.403369	4.109662	0.581658
H	-1.113829	5.443322	-2.228033
H	-0.599868	5.923087	0.104207
H	0.890095	5.680086	-0.805052
H	-0.593377	2.959935	-2.562111
H	-3.715290	4.158902	-0.174020
H	1.827163	3.665715	1.802160
O	6.072822	-2.344755	-1.259149
O	3.810595	-2.079856	1.525360
O	3.856601	-0.984641	-2.155748
O	5.411050	-0.674317	0.804729
O	1.824696	-1.843449	-1.796253
C	5.064425	-2.766796	-0.381951
C	3.754330	-3.127612	-1.119532
C	4.793909	-1.723636	0.712373
C	3.083381	-1.895001	-1.743806

H	5.432384	-3.661499	0.131261
H	3.058897	-3.627618	-0.446882
H	4.012018	-3.826936	-1.920652
H	5.637207	-1.684515	-1.824280
H	3.569565	-1.334620	2.138831
H	3.756441	0.647010	-1.974091
O	-1.585502	-5.785443	-1.318620
O	0.435209	-3.930865	-1.477496
O	-3.345704	-3.691168	-0.493513
O	-0.225711	-3.075955	0.494354
O	-3.513267	-3.276599	1.707383
C	-1.038030	-5.249929	-0.136353
C	-2.072504	-5.056414	0.986456
C	-0.227104	-3.960348	-0.359806
C	-3.036038	-3.914752	0.780308
H	-0.315753	-5.997087	0.209885
H	-1.588516	-4.896097	1.948462
H	-2.664121	-5.975429	1.052811
H	-2.213768	-5.139734	-1.663563
H	1.006541	-3.065864	-1.574665
H	-4.022935	-2.962394	-0.569153
O	-6.951260	0.173634	-1.216661
O	-5.197268	-1.268099	1.557290
O	-4.244330	1.285924	-0.431645
O	-5.194167	-1.750559	-0.642850
O	-5.037479	3.279821	0.230664
C	-6.646333	-0.016230	0.142709
C	-6.281331	1.319313	0.804108
C	-5.582940	-1.094286	0.317284
C	-5.132622	2.062624	0.162612
H	-7.529934	-0.404102	0.672094
H	-6.025423	1.156570	1.855675
H	-7.144623	1.984777	0.779384
H	-6.418845	-0.465972	-1.710598
H	-4.550870	-2.035023	1.623770
H	-3.545237	1.840807	-0.877831
C	-0.490945	0.098068	-0.621657
N	0.236822	-0.353471	0.597764
C	-0.467842	-0.051210	1.877341
H	-1.469815	-0.380300	-0.641289
H	0.094309	-0.214336	-1.485215
H	-0.603488	1.178229	-0.582636
H	1.164575	0.110523	0.620208
H	-1.415615	-0.587621	1.889433

H	-0.623809	1.024106	1.937671
H	0.162723	-0.384057	2.699830
C	5.446915	1.737715	-1.477324
N	3.967350	1.602820	-1.573578
C	3.302498	2.687426	-2.339301
H	5.864787	1.776633	-2.483336
H	5.836086	0.872047	-0.944942
H	5.692032	2.650644	-0.935281
H	3.554383	1.559601	-0.618879
H	3.628673	2.647550	-3.378471
H	3.574156	3.649333	-1.904382
H	2.221970	2.571330	-2.282533

1SA4MA3DMA

S	3.210786	1.581422	-0.616708
O	2.189913	1.690704	0.484598
O	3.142527	2.763826	-1.493387
O	4.570011	1.441580	-0.004171
O	2.925584	0.327611	-1.410834
H	4.484440	1.800695	1.559554
H	0.183719	-1.330894	-1.945551
O	-2.380275	4.847481	-3.109150
O	-2.561583	4.853820	0.477792
O	1.449543	4.684067	-1.240220
O	-3.183464	3.291372	-1.016522
O	-0.137151	3.416258	-2.210350
C	-2.148476	5.331082	-1.815207
C	-0.667365	5.671974	-1.559362
C	-2.686504	4.375317	-0.746653
C	0.244216	4.464684	-1.703546
H	-2.730138	6.252336	-1.710760
H	-0.523235	6.112202	-0.571534
H	-0.353009	6.416037	-2.297200
H	-1.859766	4.033104	-3.176372
H	-2.919157	4.204189	1.144316
H	2.057125	3.879981	-1.353296
O	2.855793	-3.067768	3.486964
O	1.326197	-0.503221	1.519983
O	3.650802	-2.756769	0.796391
O	2.904622	-0.360800	3.113178
O	2.184923	-3.330425	-0.781674
C	1.785412	-2.482259	2.787306
C	1.429989	-3.261086	1.509419
C	2.071140	-0.999987	2.490007
C	2.498825	-3.111402	0.424765

H	0.923870	-2.502581	3.464269
H	0.464191	-2.949390	1.110928
H	1.348318	-4.319500	1.775136
H	3.594094	-3.046601	2.858878
H	1.668769	0.399846	1.194287
H	4.479691	-2.133079	-0.483730
O	-2.906930	-4.348596	-3.185005
O	0.184061	-4.674342	-1.451599
O	-2.844561	-3.900537	1.029553
O	-0.870564	-2.801502	-2.133331
O	-4.037951	-3.267411	-0.763423
C	-2.031875	-4.910271	-2.247114
C	-2.732212	-5.274162	-0.908485
C	-0.823432	-4.011614	-1.949613
C	-3.271137	-4.052209	-0.204768
H	-1.651995	-5.837591	-2.679841
H	-2.046842	-5.808105	-0.251899
H	-3.581029	-5.919059	-1.150167
H	-3.323349	-3.580403	-2.771677
H	0.986188	-4.064311	-1.166741
H	-3.231909	-3.070064	1.434111
O	-6.658692	0.584565	1.778517
O	-5.397032	-1.327178	0.452893
O	-4.123661	1.541139	0.681871
O	-3.920254	-1.717375	2.104198
O	-3.533657	3.064711	2.225529
C	-5.567336	-0.005728	2.439940
C	-4.552355	1.027299	2.965823
C	-4.872235	-1.104366	1.633755
C	-4.021272	1.986543	1.924077
H	-5.980062	-0.519656	3.314199
H	-3.695492	0.510532	3.408884
H	-5.012532	1.629613	3.749763
H	-6.383875	0.771348	0.872944
H	-4.884635	-2.041510	-0.023102
H	-3.760742	2.218334	0.028989
C	0.226781	0.188484	-3.352205
N	0.315221	-0.304949	-1.949793
C	-0.718465	0.285799	-1.052010
H	-0.737676	-0.099483	-3.768846
H	1.030529	-0.265001	-3.929956
H	0.336119	1.271533	-3.343387
H	1.280199	-0.085451	-1.602214
H	-1.701444	-0.019729	-1.408414

H	-0.624247	1.368515	-1.077803
H	-0.553701	-0.091321	-0.045200
C	6.212005	-1.085997	-1.068840
N	4.851732	-1.613511	-1.333146
C	4.757964	-2.504289	-2.515981
H	6.874324	-1.910113	-0.800879
H	6.141568	-0.358635	-0.264250
H	6.586977	-0.585696	-1.962236
H	4.179255	-0.813541	-1.437237
H	5.488676	-3.308282	-2.419070
H	4.959586	-1.931224	-3.421536
H	3.755937	-2.927752	-2.531965
C	5.572638	1.690201	3.351203
N	4.317260	1.931581	2.602876
C	3.697319	3.260382	2.834148
H	6.327285	2.412752	3.039857
H	5.916255	0.679923	3.134530
H	5.388576	1.785164	4.421608
H	3.641323	1.170111	2.830502
H	4.402932	4.040481	2.547682
H	3.437115	3.365448	3.888043
H	2.808354	3.322144	2.209803

1SA4MA4DMA

S	-2.510239	-1.878568	-1.582075
O	-1.807174	-1.875431	-0.248672
O	-2.125038	-3.069418	-2.358784
O	-3.985918	-1.829788	-1.356579
O	-2.112481	-0.622218	-2.327452
H	-4.325950	-2.132900	0.221605
H	0.571793	1.183465	-2.322481
O	3.749638	-4.785245	-2.496826
O	3.025833	-4.663835	1.018871
O	-0.429142	-4.867494	-1.635361
O	3.897197	-3.107204	-0.351576
O	1.257668	-3.502254	-2.232937
C	3.234663	-5.245204	-1.278001
C	1.764116	-5.694638	-1.379613
C	3.421772	-4.217066	-0.158875
C	0.835134	-4.566059	-1.794752
H	3.833747	-6.114032	-0.987712
H	1.410061	-6.119937	-0.439313
H	1.695778	-6.479265	-2.138869
H	3.214153	-4.011878	-2.728005
H	3.159195	-3.966658	1.718825

H	-1.042686	-4.112208	-1.918795
O	-3.393450	2.890057	2.277899
O	-1.309972	0.413207	0.768503
O	-3.548730	2.482707	-0.500729
O	-3.156801	0.196385	2.021225
O	-1.816167	3.138891	-1.739956
C	-2.147746	2.383547	1.852936
C	-1.578807	3.167638	0.660373
C	-2.256931	0.879692	1.550395
C	-2.371241	2.918339	-0.625456
H	-1.465188	2.484797	2.703900
H	-0.529856	2.922390	0.491856
H	-1.629733	4.233478	0.902939
H	-3.956683	2.826840	1.489536
H	-1.520771	-0.534784	0.429634
H	-4.007201	1.749871	-1.927693
O	3.643630	4.368727	-2.960560
O	0.217699	4.568506	-2.014796
O	2.577856	4.115522	1.128562
O	1.503707	2.742513	-2.329483
O	4.224835	3.495664	-0.265770
C	2.541568	4.916523	-2.292748
C	2.882409	5.393956	-0.853416
C	1.347828	3.953311	-2.230389
C	3.296230	4.245958	0.034778
H	2.226784	5.793282	-2.861704
H	2.033503	5.915541	-0.414034
H	3.731384	6.077772	-0.930618
H	3.983470	3.644909	-2.417712
H	-0.595739	3.922615	-1.885882
H	2.894939	3.330573	1.664370
O	6.336353	-0.029038	3.088358
O	5.340025	1.720687	1.374360
O	4.234749	-1.223064	1.427789
O	3.459029	2.056070	2.561831
O	3.399353	-2.743053	2.857420
C	5.071848	0.495224	3.410384
C	4.028912	-0.597137	3.714737
C	4.539703	1.502693	2.389912
C	3.858333	-1.635098	2.628100
H	5.204595	1.073489	4.330639
H	3.052084	-0.136226	3.890926
H	4.308421	-1.129719	4.624283
H	6.326357	-0.261338	2.152185

H	4.924988	2.372320	0.739534
H	4.105572	-1.953007	0.744345
C	0.958914	-0.380359	-3.624453
N	0.511149	0.151229	-2.307382
C	1.337096	-0.335079	-1.164876
H	1.973555	-0.035093	-3.819814
H	0.285933	-0.008122	-4.395206
H	0.921686	-1.467526	-3.586630
H	-0.494151	-0.125325	-2.183088
H	2.358898	0.017088	-1.301168
H	1.308809	-1.421898	-1.153651
H	0.922462	0.071477	-0.245238
C	-5.469019	0.551158	-2.853590
N	-4.120123	1.165440	-2.804892
C	-3.787188	1.999361	-3.986241
H	-6.225448	1.336317	-2.821009
H	-5.564935	-0.125468	-2.008789
H	-5.571425	-0.024036	-3.774093
H	-3.393314	0.413468	-2.689463
H	-4.568055	2.747089	-4.131101
H	-3.716541	1.365072	-4.870315
H	-2.843110	2.499759	-3.782897
C	-5.869825	-1.891727	1.631478
N	-4.447197	-2.129917	1.271557
C	-3.852987	-3.361464	1.848528
H	-6.447377	-2.796212	1.439449
H	-6.246506	-1.081274	1.007934
H	-5.929306	-1.586620	2.678110
H	-3.884560	-1.309755	1.576542
H	-4.403818	-4.229620	1.486340
H	-3.906833	-3.316431	2.936407
H	-2.818176	-3.416805	1.515915
C	-6.320457	1.170687	4.555445
N	-5.257139	0.214179	4.264151
C	-4.487574	-0.141220	5.452064
H	-7.064463	0.711248	5.214731
H	-6.825574	1.454352	3.628789
H	-5.963331	2.092922	5.043674
H	-4.624520	0.613999	3.574617
H	-5.116923	-0.701674	6.151498
H	-4.082391	0.730166	5.994934
H	-3.648712	-0.781304	5.167907
2MA			
O	3.747551	-0.488791	1.148980

O	1.373613	-1.601902	-1.299066
O	1.657069	1.590429	0.829709
O	1.300464	-1.626084	0.952103
O	0.984697	1.897881	-1.293217
C	3.208487	-0.630678	-0.133310
C	3.047362	0.725727	-0.888940
C	1.866966	-1.366474	-0.095357
C	1.801336	1.481707	-0.490027
H	3.912146	-1.236816	-0.709913
H	2.999690	0.567605	-1.964778
H	3.932122	1.320328	-0.648657
H	3.044548	-0.161194	1.724609
H	0.414053	-1.838768	-1.222454
H	0.744925	1.918546	1.037328
O	-3.747461	-0.489304	-1.149087
O	-1.373322	-1.602168	1.298903
O	-1.657562	1.591021	-0.829478
O	-1.299880	-1.625199	-0.952277
O	-0.984989	1.897303	1.293547
C	-3.208376	-0.631085	0.133254
C	-3.047652	0.725377	0.888889
C	-1.866617	-1.366392	0.095253
C	-1.801705	1.481558	0.490198
H	-3.911840	-1.237451	0.709855
H	-3.000114	0.567258	1.964739
H	-3.932530	1.319699	0.648393
H	-3.044013	-0.163373	-1.725126
H	-0.413777	-1.838996	1.222220
H	-0.745448	1.919244	-1.036930
2MA1DMA			
O	3.952678	1.154054	-0.636276
O	1.343012	0.224127	1.618030
O	1.738340	-0.934680	-1.288682
O	1.535736	1.910183	0.127896
O	1.945669	-2.828461	-0.098655
C	3.415573	0.471060	0.470546
C	3.520631	-1.059474	0.284429
C	1.981033	0.938872	0.729242
C	2.332579	-1.709290	-0.389911
H	3.989448	0.727386	1.373275
H	3.646045	-1.565471	1.241056
H	4.416796	-1.244173	-0.314288
H	3.272482	1.780803	-0.920017
H	0.355918	0.460790	1.683809

H	0.843719	-1.309780	-1.511710
O	-3.603056	-1.511078	-0.947436
O	-0.706094	-3.226811	0.180497
O	-2.692932	0.884111	0.014205
O	-0.827665	-1.601735	-1.374514
O	-1.161271	0.751479	1.625161
C	-2.753858	-2.035363	0.032573
C	-2.649894	-1.128392	1.291422
C	-1.335257	-2.272377	-0.488692
C	-2.116405	0.267376	0.964510
H	-3.152377	-3.005000	0.340846
H	-2.023170	-1.595398	2.051288
H	-3.662458	-1.017745	1.690020
H	-3.430991	-0.553358	-0.968159
H	0.258481	-3.229075	-0.048768
H	-1.773060	2.081567	-0.296188
C	-1.021808	3.306144	-1.854862
N	-1.054272	2.883074	-0.436191
C	-1.373780	3.957409	0.533809
H	-1.998440	3.699260	-2.137985
H	-0.789914	2.437925	-2.470599
H	-0.259738	4.072582	-2.000885
H	-0.140182	2.470591	-0.173566
H	-2.357843	4.368047	0.307057
H	-0.621297	4.745107	0.482096
H	-1.381733	3.509127	1.525850
2MA2DMA			
O	-3.801243	0.236553	1.913434
O	-2.487317	0.519617	-1.394555
O	-1.455932	-1.668613	1.785805
O	-1.854956	1.384795	0.591708
O	-1.286671	-2.602194	-0.247220
C	-3.681674	-0.138180	0.564436
C	-3.397313	-1.663499	0.410043
C	-2.582485	0.678047	-0.151470
C	-1.951423	-2.034489	0.617566
H	-4.632235	0.054005	0.056022
H	-3.677764	-2.000249	-0.586413
H	-4.010649	-2.175352	1.156098
H	-2.990453	0.737055	2.092509
H	-1.161010	0.615646	-2.185974
H	-0.469647	-1.799580	1.789373
O	3.926117	-1.114117	1.577119
O	1.360570	-2.655325	-0.403524

O	2.684962	1.193365	0.757625
O	1.227317	-1.690245	1.623576
O	1.773369	1.203602	-1.277581
C	3.322396	-1.570590	0.401980
C	3.378848	-0.522380	-0.741687
C	1.864512	-1.984846	0.626605
C	2.549851	0.723482	-0.412986
H	3.860938	-2.465918	0.077653
H	3.043402	-0.956925	-1.683122
H	4.425807	-0.223985	-0.848398
H	3.568571	-0.219338	1.716562
H	0.377215	-2.771809	-0.275071
H	1.372023	2.037954	1.038717
C	-0.316868	-0.902107	-3.330739
N	-0.304210	0.493387	-2.828163
C	-0.342079	1.522768	-3.890560
H	-1.215214	-1.059742	-3.927523
H	-0.335353	-1.577615	-2.478048
H	0.571020	-1.087228	-3.936827
H	0.549289	0.655457	-2.238219
H	-1.254464	1.408331	-4.476333
H	0.530381	1.422933	-4.537438
H	-0.333472	2.506579	-3.423605
C	0.241531	2.702130	2.678727
N	0.469288	2.586267	1.219560
C	0.567035	3.877538	0.501261
H	1.065872	3.250796	3.135370
H	0.194410	1.698652	3.099177
H	-0.700445	3.218118	2.864422
H	-0.329401	2.044050	0.812162
H	1.347978	4.489211	0.954231
H	-0.389521	4.398778	0.545551
H	0.833469	3.655828	-0.530821
2MA3DMA			
O	0.289520	3.278138	1.204053
O	2.979422	1.291584	-0.057336
O	-1.358484	2.687558	-1.008111
O	1.072253	0.613497	0.915898
O	-0.136338	1.412260	-2.398740
C	1.329177	2.946434	0.298225
C	0.938427	3.207688	-1.183259
C	1.849655	1.493073	0.415369
C	-0.222644	2.343668	-1.613512
H	2.175405	3.596802	0.528525

H	1.794754	2.988124	-1.817352
H	0.654928	4.258160	-1.289155
H	-0.553462	3.153220	0.749742
H	3.027738	-1.569779	-0.219198
H	-2.095830	2.036109	-1.227477
O	-4.974798	-1.001253	-0.505161
O	-1.959261	-0.618178	-2.429866
O	-2.884281	-0.977747	1.282119
O	-3.212510	0.897959	-1.345231
O	-1.131436	-2.325432	0.916410
C	-3.888811	-1.431355	-1.275339
C	-3.035436	-2.498106	-0.547260
C	-3.000895	-0.253973	-1.688718
C	-2.271596	-1.909733	0.649934
H	-4.290583	-1.866030	-2.196744
H	-2.330085	-2.975449	-1.227333
H	-3.727522	-3.262611	-0.181740
H	-4.573768	-0.734925	0.341706
H	-1.353430	0.155807	-2.558976
H	-1.848319	-0.157611	2.070493
C	1.293026	-1.877084	-1.349739
N	2.005582	-1.777307	-0.048910
C	1.885501	-2.996042	0.792190
H	1.727418	-2.684590	-1.940970
H	1.400175	-0.928868	-1.874905
H	0.242175	-2.073333	-1.149469
H	1.624645	-0.927073	0.451321
H	2.352807	-3.834904	0.273575
H	0.830389	-3.192379	0.972515
H	2.406825	-2.821690	1.733883
C	-1.740351	1.684947	3.087706
N	-1.106322	0.443779	2.587434
C	-0.489060	-0.398137	3.638037
H	-2.434086	1.437065	3.891761
H	-2.297099	2.142533	2.270580
H	-0.978534	2.379960	3.437813
H	-0.359342	0.674375	1.890419
H	-1.227893	-0.607576	4.412658
H	0.370477	0.114079	4.071534
H	-0.186049	-1.332193	3.168402
C	5.636045	-1.248890	0.713261
N	4.736606	-0.984795	-0.410082
C	5.396906	-1.115009	-1.709314
H	5.942509	-2.299676	0.712909

H	5.117380	-1.043337	1.652339
H	6.547907	-0.632940	0.685916
H	4.339561	-0.046125	-0.313549
H	5.688876	-2.155841	-1.880809
H	6.301763	-0.493923	-1.793076
H	4.706843	-0.819111	-2.502203
2MA4DMA			
O	-1.980475	-2.329557	-1.640853
O	-0.868290	1.065688	-2.092511
O	0.857487	-2.322418	-1.517847
O	-1.526953	-0.023436	-0.239041
O	1.928577	-0.982248	-2.965569
C	-1.598884	-1.174339	-2.367000
C	-0.411742	-1.446252	-3.323268
C	-1.307982	0.061192	-1.471928
C	0.910885	-1.553961	-2.605252
H	-2.460952	-0.917138	-2.987912
H	-0.321713	-0.645040	-4.052765
H	-0.603534	-2.389415	-3.844468
H	-1.209928	-2.594986	-1.122898
H	0.019214	2.138407	-1.293601
H	1.724713	-2.279116	-1.016693
O	4.594295	-1.311943	2.108965
O	3.916534	-0.333936	-1.273822
O	2.156117	-0.173720	2.552817
O	2.989521	-1.960607	-0.029057
O	1.622705	1.673490	1.420609
C	4.539656	-0.426310	1.029784
C	3.927265	0.946200	1.419800
C	3.743276	-1.007084	-0.141210
C	2.451570	0.824285	1.825713
H	5.561898	-0.265063	0.675498
H	4.033617	1.666531	0.608493
H	4.493978	1.310889	2.281527
H	3.708304	-1.266675	2.513589
H	3.286217	-0.671927	-1.964960
H	0.591824	-0.446307	2.355077
C	1.895205	2.871519	-1.815446
N	0.744767	2.805701	-0.882344
C	0.111353	4.117886	-0.594765
H	1.554455	3.237736	-2.783668
H	2.310067	1.872298	-1.934489
H	2.657410	3.539464	-1.412678
H	1.076746	2.377563	0.014623

H	-0.119659	4.616787	-1.537051
H	0.799206	4.732292	-0.012462
H	-0.815926	3.935976	-0.046018
C	-0.742045	-2.075074	2.429980
N	-0.453163	-0.630657	2.230889
C	-1.178510	0.271150	3.156428
H	-0.517144	-2.345656	3.462246
H	-0.092900	-2.643675	1.764121
H	-1.790826	-2.267971	2.189303
H	-0.716372	-0.372015	1.258093
H	-0.897273	0.032410	4.182427
H	-2.252736	0.146029	3.025730
H	-0.879480	1.292520	2.926439
C	-4.510540	-3.494376	0.772937
N	-3.835260	-2.211862	0.935132
C	-4.766500	-1.108237	1.134821
H	-5.010595	-3.774729	1.706172
H	-3.777731	-4.270188	0.539554
H	-5.272163	-3.494751	-0.026076
H	-3.269182	-2.023192	0.110303
H	-5.257192	-1.198445	2.110318
H	-5.561974	-1.056206	0.370197
H	-4.218091	-0.164381	1.111649
C	-3.667462	3.089240	1.502167
N	-2.885436	2.845175	0.296975
C	-3.661283	3.017814	-0.927944
H	-3.985843	4.136387	1.530436
H	-3.052977	2.909338	2.387942
H	-4.576138	2.466711	1.580398
H	-2.492789	1.905507	0.306926
H	-3.941676	4.070080	-1.046114
H	-4.591132	2.423545	-0.948637
H	-3.049793	2.725488	-1.783572

2SA1MA

S	1.356042	2.385495	-0.045946
O	0.916060	1.340212	-0.991749
O	2.446981	3.219544	-0.393584
O	0.125524	3.292264	0.261586
O	1.633491	1.663547	1.325657
H	-0.710724	2.747747	0.359884
H	1.529823	0.678281	1.252002
S	2.127408	-1.810386	0.109715
O	1.294682	-0.995591	1.018250
O	3.476280	-2.060981	0.466161

O 1.408853 -3.166208 -0.121445
O 2.030667 -1.126713 -1.312176
H 0.420368 -3.033012 -0.279682
H 1.689920 -0.200291 -1.237445
O -4.139148 0.266640 1.021707
O -1.678132 0.653481 -1.550317
O -1.447473 -1.193956 1.158901
O -2.035294 1.777796 0.371419
O -1.132645 -2.691914 -0.489939
C -3.558649 0.025602 -0.230650
C -3.195178 -1.470323 -0.426574
C -2.346204 0.924076 -0.444679
C -1.827272 -1.862830 0.075419
H -4.285603 0.281155 -1.012714
H -3.236197 -1.754210 -1.477450
H -3.950628 -2.048691 0.112203
H -3.535054 0.830094 1.523228
H -0.803021 1.104922 -1.543223
H -0.489035 -1.331865 1.326021

2SA1MA1DMA

S 2.081058 -1.984589 -0.365460
O 3.183627 -0.981191 0.135692
O 2.680544 -3.259682 -0.535419
O 0.932074 -1.846761 0.535105
O 1.661912 -1.449380 -1.781381
H -0.698340 -2.279127 0.146262
H 1.273542 -0.524523 -1.744535
S 1.487421 1.987465 -0.853238
O 0.668202 1.020489 -1.658446
O 2.573360 2.604925 -1.541079
O 0.479776 3.135663 -0.425472
O 1.882415 1.295934 0.420846
H -0.431799 2.766881 -0.285181
H 2.791102 -0.064386 0.255619
O -3.874662 -1.599101 -1.435555
O -2.007678 -0.900964 1.547506
O -1.949632 0.644567 -1.703079
O -1.617331 -2.233366 -0.222615
O -1.936171 2.080259 0.025234
C -3.674596 -1.013279 -0.180680
C -3.774813 0.542299 -0.200615
C -2.347337 -1.401345 0.483682
C -2.475912 1.188136 -0.615271
H -4.477271 -1.383011 0.462850

H	-4.040493	0.932763	0.779630
H	-4.560565	0.800899	-0.914514
H	-3.107574	-1.397538	-1.985790
H	-0.471182	-0.203584	2.145588
H	-0.999482	0.929669	-1.814607
C	-0.398054	1.638217	3.092592
N	0.260563	0.445392	2.490589
C	1.180568	-0.283526	3.407147
H	-0.958370	1.330699	3.974800
H	-1.073498	2.066991	2.354771
H	0.366473	2.364290	3.365871
H	0.803932	0.752024	1.652431
H	0.624049	-0.618579	4.281870
H	1.984874	0.386061	3.709455
H	1.584385	-1.137425	2.868710

2SA1MA2DMA

S	-1.450000	2.229799	-0.278087
O	-2.384888	1.481173	0.606158
O	-1.940768	3.491175	-0.753396
O	-0.103286	2.241889	0.340247
O	-1.319524	1.307205	-1.608349
H	1.367630	2.293005	-0.371234
H	-0.862379	0.462577	-1.380357
S	-0.898039	-2.157046	-0.232280
O	-0.206589	-1.114539	-1.046842
O	-2.163516	-2.578473	-0.817758
O	0.045442	-3.433605	-0.301490
O	-1.011857	-1.746441	1.171790
H	0.967279	-3.142717	-0.076998
H	-3.294742	0.332638	-0.097096
O	4.401509	1.064412	-1.951743
O	2.653179	1.058144	1.181454
O	2.344937	-0.991964	-1.627137
O	2.263576	2.093136	-0.777392
O	2.503842	-2.314016	0.185157
C	4.242604	0.756612	-0.592520
C	4.293179	-0.770469	-0.303286
C	2.967564	1.341721	0.033286
C	2.969772	-1.456345	-0.549757
H	5.090148	1.214440	-0.074444
H	4.580717	-0.973079	0.726991
H	5.050299	-1.197721	-0.966590
H	3.573265	0.846892	-2.396487
H	0.884148	0.842632	1.886784

H	1.375447	-1.214072	-1.577862
C	1.238724	-0.611342	3.309360
N	0.318910	0.250881	2.519391
C	-0.584220	1.106003	3.336296
H	1.890233	0.018734	3.912967
H	1.835419	-1.202389	2.618355
H	0.646603	-1.267985	3.945787
H	-0.250306	-0.372668	1.909740
H	0.016197	1.815271	3.905287
H	-1.150818	0.468688	4.015212
H	-1.256496	1.626017	2.659016
C	-4.907635	-0.843249	0.482935
N	-3.918505	-0.404562	-0.533979
C	-4.505459	0.155547	-1.780154
H	-5.497654	0.015160	0.802549
H	-4.363670	-1.255759	1.331004
H	-5.557237	-1.607626	0.056973
H	-3.304039	-1.213229	-0.759424
H	-5.114258	1.022975	-1.527197
H	-5.115543	-0.603100	-2.270095
H	-3.688085	0.467407	-2.427447
2SA1MA3DMA			
S	1.163612	0.428736	2.198526
O	2.333445	0.308396	1.280985
O	1.499263	0.656382	3.574887
O	0.156366	1.349912	1.619570
O	0.479268	-1.038580	2.170044
H	-1.485658	1.065865	1.934973
H	0.219104	-1.264554	1.244087
S	0.448192	-1.559335	-1.624146
O	-0.091363	-2.024720	-0.302129
O	1.804342	-2.065481	-1.843570
O	-0.429006	-2.307388	-2.722011
O	0.287803	-0.125306	-1.800871
H	-1.373675	-2.031260	-2.593997
H	2.843399	-1.251440	0.926559
O	-4.685652	-0.625278	1.891281
O	-2.665647	1.626381	-0.043675
O	-2.697389	-1.806891	0.129466
O	-2.422972	0.730045	2.005240
O	-2.925280	-1.435676	-2.079559
C	-4.428933	0.223520	0.802283
C	-4.543370	-0.494243	-0.566788
C	-3.076407	0.948259	0.884262

C	-3.315268	-1.297047	-0.934222
H	-5.202576	0.996922	0.830602
H	-4.712826	0.214865	-1.375975
H	-5.405448	-1.165212	-0.513055
H	-3.902149	-1.174398	2.016681
H	-0.535657	1.869667	-0.518091
H	-1.765725	-2.080223	-0.094718
C	-0.730364	2.738956	-2.374131
N	-0.160437	2.691904	-1.003644
C	-0.463681	3.889710	-0.180597
H	-1.813844	2.814291	-2.299640
H	-0.460068	1.817416	-2.883280
H	-0.324761	3.604216	-2.899726
H	0.901191	2.557487	-1.040589
H	-1.543381	4.003867	-0.107192
H	-0.018940	4.767944	-0.649829
H	-0.044532	3.731277	0.810604
C	4.643227	-2.055235	0.285625
N	3.181636	-2.160995	0.518114
C	2.775552	-3.298245	1.385840
H	5.150731	-1.904659	1.238097
H	4.831027	-1.204256	-0.367113
H	5.004264	-2.967257	-0.189397
H	2.684927	-2.228617	-0.402431
H	3.216267	-3.172967	2.374291
H	3.116315	-4.230778	0.935810
H	1.691893	-3.294452	1.466139
C	3.201331	1.714392	-2.133679
N	2.633038	2.332350	-0.930661
C	3.424659	3.466264	-0.444544
H	3.162206	2.420756	-2.968615
H	2.615188	0.833543	-2.395593
H	4.253754	1.419556	-1.999158
H	2.579870	1.630174	-0.189206
H	3.396765	4.282914	-1.172513
H	4.479572	3.205361	-0.273515
H	3.008322	3.828383	0.497502
2SA1MA4DMA			
S	0.311510	1.076445	2.153389
O	1.491791	1.145341	1.249630
O	0.551829	1.563474	3.485562
O	-0.894180	1.622413	1.481679
O	0.032023	-0.503482	2.334444
H	-2.426752	0.928326	1.779258

H	-0.106924	-0.916354	1.441201
S	0.513893	-1.582688	-1.259958
O	-0.284631	-1.776986	-0.001433
O	1.868300	-2.093047	-1.107736
O	-0.176998	-2.565935	-2.318219
O	0.405223	-0.221831	-1.766702
H	-1.144186	-2.356847	-2.346104
H	2.526792	-0.254556	1.446057
O	-5.138856	-1.479405	1.650400
O	-3.565895	1.107255	-0.280480
O	-2.823688	-2.299893	0.130201
O	-3.253617	0.371781	1.820682
O	-2.848189	-1.931051	-2.089622
C	-4.999021	-0.645979	0.529703
C	-4.821387	-1.433595	-0.796462
C	-3.866553	0.384895	0.656346
C	-3.404217	-1.921427	-1.005110
H	-5.932169	-0.080077	0.452690
H	-5.085511	-0.825859	-1.660460
H	-5.496859	-2.292752	-0.756506
H	-4.270307	-1.860705	1.829446
H	-1.442383	1.754235	-0.576144
H	-1.827044	-2.300322	0.029979
C	-1.677433	2.059547	-2.610059
N	-1.246710	2.496589	-1.257467
C	-1.914429	3.729889	-0.771057
H	-2.748383	1.868632	-2.591280
H	-1.139377	1.146161	-2.853133
H	-1.442202	2.845651	-3.328694
H	-0.186966	2.645880	-1.234973
H	-2.990266	3.568525	-0.759565
H	-1.658011	4.560071	-1.430026
H	-1.565121	3.925182	0.240932
C	4.069396	-0.264789	2.788746
N	3.294536	-0.916023	1.702274
C	2.725436	-2.242612	2.071088
H	3.411080	-0.082495	3.637410
H	4.450097	0.688692	2.425724
H	4.897407	-0.909353	3.084726
H	3.893743	-1.030584	0.829646
H	2.017710	-2.111320	2.887119
H	3.538950	-2.904942	2.370057
H	2.214508	-2.640592	1.196814
C	2.186209	2.514188	-2.456108

N	1.534728	2.888467	-1.198424
C	2.014330	4.160270	-0.653425
H	1.897434	3.212815	-3.248088
H	1.866415	1.510059	-2.735156
H	3.284738	2.533575	-2.386387
H	1.669148	2.157621	-0.497488
H	1.734222	4.982992	-1.318639
H	3.107928	4.185596	-0.532893
H	1.560480	4.333084	0.323810
C	5.259920	0.028668	-1.269151
N	4.657616	-1.213420	-0.777390
C	5.498978	-2.386665	-1.036964
H	6.185037	0.234729	-0.722337
H	4.572671	0.860768	-1.104716
H	5.504192	-0.011022	-2.340632
H	3.751519	-1.361982	-1.225488
H	6.403241	-2.344159	-0.422364
H	5.808240	-2.458739	-2.089713
H	4.947019	-3.292727	-0.784460

2SA2MA

S	0.270845	2.993613	0.231074
O	1.543380	3.458362	0.728778
O	-0.908427	3.792129	0.446418
O	0.368057	2.756096	-1.315253
O	0.070780	1.564258	0.836628
H	1.228103	2.275737	-1.517093
H	-0.875085	1.251826	0.671941
O	-4.792602	0.307688	-1.770682
O	-3.723799	-1.937816	0.808610
O	-3.495368	2.808293	0.711477
O	-2.999146	-1.571788	-1.297099
O	-2.394787	0.866963	0.440844
C	-4.849028	-0.289045	-0.498991
C	-4.774313	0.804357	0.579974
C	-3.744314	-1.331724	-0.355101
C	-3.436108	1.503803	0.563265
H	-5.800752	-0.822749	-0.369044
H	-4.904744	0.361437	1.572079
H	-5.573900	1.525007	0.413239
H	-4.098850	-0.151689	-2.265548
H	-2.964753	-2.568960	0.862309
H	-2.592356	3.204221	0.664257
S	-0.255663	-2.961865	0.273061
O	0.929322	-3.779565	0.193836

O -1.469290 -3.511091 0.826557
O 0.052212 -1.668606 1.096756
O -0.531447 -2.458304 -1.185372
H 1.015581 -1.389617 0.981610
H -1.479584 -2.135673 -1.267376
O 5.263355 -0.280960 1.151847
O 3.407491 -2.734269 -0.385026
O 3.760821 1.951878 0.203961
O 2.550053 -0.990319 0.759848
O 2.617559 1.428433 -1.666421
C 4.796224 -0.814888 -0.059420
C 4.652073 0.247968 -1.182466
C 3.461864 -1.534876 0.151199
C 3.567540 1.267189 -0.917319
H 5.532976 -1.549473 -0.384533
H 4.434944 -0.229530 -2.138180
H 5.612960 0.764665 -1.249430
H 4.671201 0.438129 1.409966
H 2.528577 -3.156465 -0.219316
H 2.993825 2.547423 0.396458

2SA2MA1DMA

S -0.045410 -2.266581 -0.568393
O -0.113704 -1.434666 -1.773413
O -0.518412 -1.559120 0.636856
O -1.030159 -3.502401 -0.787205
O 1.266610 -2.897425 -0.353795
H -1.560189 -0.737723 -2.126773
H 2.625912 -2.109752 -0.768435
O 4.255412 0.619457 -2.758505
O 3.382196 2.672331 0.017187
O 3.574185 -0.983133 1.135546
O 2.076131 1.436277 -1.344590
O 3.426511 -1.563292 -1.037617
C 4.453528 1.154248 -1.483462
C 4.991943 0.114116 -0.456018
C 3.172947 1.787447 -0.939019
C 3.932616 -0.879081 -0.029465
H 5.205236 1.940306 -1.579447
H 5.361647 0.614848 0.437704
H 5.812199 -0.412468 -0.949156
H 3.552790 -0.042314 -2.698669
H 2.525178 2.973981 0.404471
H 2.180320 -1.552551 2.005446
S -0.345238 2.759368 0.731359

O -1.534685 3.562592 0.862558
O 0.932827 3.312509 1.111353
O -0.505660 1.443569 1.572928
O -0.309237 2.284279 -0.754958
H -1.425928 1.055699 1.417571
H 0.595917 1.905704 -0.993804
O -5.231284 -0.894185 0.711116
O -3.924361 2.349286 0.094622
O -3.325711 -2.047939 -1.181582
O -2.937019 0.589728 1.106781
O -2.436625 -0.261475 -2.232792
C -4.998704 0.231805 -0.085024
C -4.705732 -0.132260 -1.570556
C -3.843998 1.080446 0.454463
C -3.418247 -0.922312 -1.664265
H -5.903953 0.841330 -0.059175
H -4.640952 0.769680 -2.178146
H -5.531852 -0.756829 -1.913908
H -4.511901 -1.522798 0.555315
H -3.122794 2.846334 0.381725
H -1.923323 -3.112904 -0.962276
C 1.416931 -3.193949 3.010942
N 1.333295 -1.779553 2.563817
C 1.175738 -0.780494 3.651786
H 2.275530 -3.318313 3.671011
H 1.526482 -3.817379 2.125487
H 0.500825 -3.458681 3.538195
H 0.538211 -1.687961 1.876144
H 2.051072 -0.807109 4.300646
H 0.280135 -1.015105 4.226825
H 1.068501 0.205361 3.202851

2SA2MA2DMA

S -0.502404 1.310386 -1.775503
O -0.976210 0.603969 -0.407241
O 0.125701 2.575844 -1.377816
O 0.423154 0.377460 -2.432859
O -1.776793 1.493368 -2.477275
H 1.190293 -2.042311 -1.462947
H -3.085998 0.734277 -1.861695
O -4.547776 -2.522708 -0.867803
O -2.825523 -1.363523 2.061213
O -3.910372 1.633262 0.212053
O -2.034368 -2.396601 0.220512
O -3.785456 0.134843 -1.464286

C	-4.407115	-1.921460	0.392030
C	-5.011400	-0.493556	0.459040
C	-2.945663	-1.929674	0.873326
C	-4.183831	0.545526	-0.267189
H	-4.969795	-2.542720	1.094797
H	-5.118922	-0.166498	1.491209
H	-6.001277	-0.541433	-0.004406
H	-4.111081	-1.941100	-1.503737
H	-1.877073	-1.299897	2.360348
H	-2.475759	2.669533	0.302465
S	0.855313	-0.638738	2.363246
O	2.041687	-1.299179	2.907297
O	-0.389927	-0.946350	3.047483
O	1.047075	0.944408	2.591116
O	0.778243	-0.802351	0.887973
H	1.918166	1.180715	2.179272
H	-0.223058	0.151729	0.080068
O	5.239420	1.868430	-0.627409
O	4.278882	-0.799513	1.564543
O	3.047214	0.601828	-2.030614
O	3.387947	1.253441	1.260566
O	2.918281	-1.628153	-1.776195
C	5.223561	0.558902	-0.136048
C	4.981618	-0.513065	-1.238101
C	4.200820	0.385617	0.991135
C	3.546408	-0.583940	-1.712974
H	6.214475	0.367933	0.284309
H	5.258157	-1.502181	-0.877632
H	5.621007	-0.244492	-2.083374
H	4.333922	2.093252	-0.878435
H	3.491407	-0.966307	2.158210
H	2.075681	0.534335	-2.248945
C	-2.362126	4.704633	-0.001747
N	-1.773446	3.420049	0.458162
C	-1.346896	3.399159	1.885190
H	-3.253994	4.923583	0.584326
H	-2.625902	4.602875	-1.053132
H	-1.628895	5.501335	0.118814
H	-0.963694	3.181589	-0.160178
H	-2.222000	3.536182	2.519540
H	-0.632364	4.204263	2.054867
H	-0.872856	2.442707	2.099089
C	-0.421001	-2.931072	-2.435127
N	0.372701	-2.629254	-1.213787

C 0.868227 -3.823943 -0.478376
H 0.168606 -3.568350 -3.093476
H -0.640626 -1.987837 -2.931470
H -1.342437 -3.426389 -2.135639
H -0.210288 -2.094644 -0.557496
H 1.520077 -4.399548 -1.133765
H 0.013654 -4.419010 -0.161094
H 1.424187 -3.474085 0.388588

2SA2MA3DMA

S -0.334985 0.685674 -2.150109
O -0.832407 0.661564 -0.583972
O 0.783602 1.609765 -2.197665
O 0.044471 -0.716695 -2.436595
O -1.535833 1.130849 -2.848781
H 0.194651 -2.932756 -1.067274
H -3.016127 1.031412 -2.063769
O -5.364854 -1.388761 -0.620035
O -3.351845 -0.457459 2.202882
O -3.458347 2.483387 -0.198505
O -2.912700 -1.879869 0.512230
O -3.839703 0.745411 -1.581777
C -5.026604 -0.686470 0.546416
C -5.138713 0.852319 0.392794
C -3.640248 -1.086580 1.075314
C -4.056072 1.467165 -0.475918
H -5.747771 -0.989921 1.311139
H -5.099457 1.340796 1.364618
H -6.110132 1.060270 -0.066134
H -4.797701 -1.042082 -1.322329
H -2.434540 -0.668518 2.523735
H -0.538346 2.346941 0.038647
S 0.358279 -0.832536 2.457742
O 1.399502 -1.650730 3.085389
O -0.891587 -0.765265 3.193064
O 0.906317 0.690791 2.468321
O 0.200661 -1.167429 1.022141
H 1.794774 0.652282 2.035047
H -0.356165 -0.027933 -0.043314
O 4.900098 0.096930 -1.064131
O 3.611848 -1.840616 1.668287
O 2.621000 -1.092840 -2.205350
O 3.170443 0.278066 1.046439
O 2.021478 -3.076244 -1.332031
C 4.727755 -1.039194 -0.263074

C	4.292185	-2.302465	-1.058208
C	3.754759	-0.786303	0.897147
C	2.860204	-2.219235	-1.545922
H	5.701076	-1.257913	0.186002
H	4.387916	-3.194045	-0.442504
H	4.958130	-2.383421	-1.921509
H	4.090422	0.208396	-1.582712
H	2.832304	-1.741505	2.294375
H	1.638556	-0.977838	-2.392549
C	-0.736869	4.253488	-0.719593
N	-0.268837	3.302949	0.327428
C	-0.836132	3.558117	1.679173
H	-1.817501	4.164218	-0.809675
H	-0.263869	3.977140	-1.659782
H	-0.452990	5.266661	-0.433306
H	0.799068	3.301870	0.354678
H	-1.921282	3.490422	1.616876
H	-0.536677	4.552287	2.012190
H	-0.452697	2.800782	2.361382
C	-1.656700	-3.462162	-1.865297
N	-0.749796	-3.174573	-0.720229
C	-0.615725	-4.280076	0.266319
H	-1.328888	-4.377579	-2.357258
H	-1.595050	-2.622017	-2.553898
H	-2.670517	-3.563944	-1.483955
H	-1.108453	-2.357806	-0.208423
H	-0.215204	-5.159591	-0.235785
H	-1.595892	-4.490408	0.690439
H	0.067107	-3.950575	1.046262
C	3.066768	3.807356	-0.997621
N	2.588687	3.232946	0.270394
C	3.293157	3.784731	1.435449
H	2.835056	4.876154	-1.029108
H	2.558422	3.311848	-1.824849
H	4.151911	3.690677	-1.124112
H	2.774209	2.231086	0.243290
H	3.070611	4.851524	1.530755
H	4.383519	3.670697	1.362759
H	2.954742	3.281919	2.343627
2SA2MA4DMA			
S	0.339076	0.833967	-2.127707
O	-0.044803	1.096950	-0.551971
O	1.732655	1.219553	-2.265445
O	0.103036	-0.611297	-2.333691

O	-0.609474	1.698443	-2.824870
H	-0.579169	-2.476417	-0.788572
H	-1.919291	2.283852	-1.992287
O	-4.976497	1.197558	-0.327219
O	-2.564769	1.278875	2.329961
O	-1.590307	3.892471	-0.221587
O	-2.957848	-0.289349	0.757430
O	-2.755381	2.412331	-1.460915
C	-4.301117	1.727849	0.789278
C	-3.758832	3.156963	0.545718
C	-3.194423	0.780983	1.282183
C	-2.574687	3.212078	-0.403971
H	-5.038081	1.789099	1.595315
H	-3.453976	3.616531	1.483918
H	-4.575337	3.745757	0.116574
H	-4.358306	1.256397	-1.070875
H	-1.824442	0.689790	2.647586
H	0.998129	2.525533	-0.076400
S	0.575772	-0.646857	2.530849
O	1.231634	-1.795723	3.160873
O	-0.503886	-0.062562	3.309258
O	1.687149	0.528155	2.453565
O	0.219229	-0.928213	1.121891
H	2.462030	0.123090	1.991098
H	0.111918	0.292955	0.018530
O	4.937873	-1.721757	-1.167129
O	3.124768	-2.900506	1.697969
O	2.337522	-1.984428	-2.214743
O	3.519628	-0.803933	0.980848
O	1.042429	-3.478084	-1.144219
C	4.376856	-2.671583	-0.302835
C	3.446032	-3.691504	-1.018507
C	3.634118	-2.017107	0.870049
C	2.140371	-3.064536	-1.464380
H	5.209114	-3.236300	0.127707
H	3.213140	-4.523282	-0.357450
H	3.986021	-4.059948	-1.894567
H	4.213624	-1.338635	-1.683099
H	2.473744	-2.477874	2.336092
H	1.475206	-1.491306	-2.365282
C	1.579247	4.301780	-0.948981
N	1.664745	3.286557	0.137335
C	1.348599	3.814828	1.491891
H	0.561252	4.683683	-0.987956

H	1.825292	3.809234	-1.887424
H	2.287594	5.104609	-0.741973
H	2.633346	2.833992	0.122707
H	0.338991	4.222808	1.477550
H	2.067903	4.592381	1.750758
H	1.408715	2.993011	2.204148
C	-2.459855	-2.589535	-1.659267
N	-1.560809	-2.472363	-0.474491
C	-1.723160	-3.555928	0.531898
H	-2.267385	-3.546912	-2.143774
H	-2.210190	-1.778489	-2.340343
H	-3.498820	-2.519564	-1.326393
H	-1.735857	-1.574099	-0.002814
H	-1.490142	-4.509257	0.060772
H	-2.749736	-3.548826	0.893495
H	-1.028294	-3.366097	1.346798
C	4.816302	2.266565	-1.330775
N	4.223734	2.030309	-0.004333
C	5.165322	2.315460	1.086465
H	5.051745	3.328819	-1.446169
H	4.095523	1.980827	-2.096941
H	5.742136	1.694274	-1.480000
H	3.977197	1.042600	0.051691
H	5.404581	3.382864	1.099483
H	6.107021	1.758043	0.987624
H	4.710907	2.054258	2.044315
C	-6.741110	-1.992334	-1.436843
N	-5.647813	-1.978420	-0.470463
C	-6.033580	-2.538494	0.819833
H	-7.009017	-3.025748	-1.680301
H	-6.422976	-1.503759	-2.360849
H	-7.654314	-1.486182	-1.079634
H	-5.335157	-1.019660	-0.334642
H	-6.236566	-3.609926	0.717371
H	-6.935111	-2.072863	1.255309
H	-5.213690	-2.416377	1.531721
2SA3MA			
S	-1.696467	3.496500	-1.033664
O	-2.873038	3.067560	-1.750621
O	-1.068232	4.740936	-1.401792
O	-2.024024	3.607805	0.493502
O	-0.662931	2.331541	-1.141735
H	-2.677908	2.892495	0.767365
H	0.256018	2.652328	-0.862800

O	3.079685	3.628802	2.357735
O	4.838802	2.052464	-0.336369
O	1.456814	5.431785	-0.597968
O	3.554767	1.228075	1.321654
O	1.683307	3.198360	-0.428001
C	3.957857	3.584142	1.260599
C	3.521459	4.600486	0.198838
C	4.082348	2.161442	0.726754
C	2.122215	4.336508	-0.300462
H	4.973643	3.861849	1.579004
H	4.199046	4.562060	-0.659631
H	3.565758	5.605769	0.617474
H	2.812485	2.715152	2.534106
H	4.948718	1.089344	-0.593875
H	0.548479	5.218905	-0.922517
S	-1.281246	-3.821010	-0.432481
O	-0.378781	-4.325807	-1.440309
O	-2.621270	-4.349289	-0.372198
O	-0.651893	-4.038022	0.980802
O	-1.333494	-2.271961	-0.621671
H	0.354761	-3.990344	0.933989
H	-2.198646	-1.884901	-0.269005
O	-5.349162	0.066226	2.444494
O	-4.857971	1.483423	-0.807552
O	-4.973217	-3.042779	0.041539
O	-3.795215	1.798700	1.158619
O	-3.600922	-1.262655	0.145988
C	-5.709902	0.372940	1.120896
C	-5.964920	-0.920917	0.346204
C	-4.668069	1.278068	0.473883
C	-4.721528	-1.759877	0.180975
H	-6.644575	0.955421	1.105295
H	-6.342311	-0.695014	-0.656007
H	-6.726735	-1.506201	0.861732
H	-4.595378	0.629820	2.668586
H	-4.155200	2.070816	-1.183875
H	-4.138121	-3.551146	-0.101126
O	4.617510	-3.951796	1.349189
O	2.315870	-4.171858	-1.390416
O	3.705324	-1.328909	0.572106
O	1.961467	-3.952589	0.826972
O	5.157354	-0.501600	-0.929665
C	4.224092	-3.988297	0.003986
C	4.862018	-2.868435	-0.842673

C	2.704575	-4.031446	-0.139251
C	4.590530	-1.447344	-0.401532
H	4.584907	-4.936708	-0.408487
H	4.550174	-2.950489	-1.887355
H	5.946896	-2.994646	-0.827768
H	3.998860	-3.373514	1.812858
H	1.328931	-4.218355	-1.453789
H	3.603558	-0.371416	0.840406

2SA3MA1DMA

S	1.009071	-2.277010	0.037645
O	0.362473	-3.326481	0.789696
O	2.433448	-2.341467	-0.168069
O	0.385816	-2.192360	-1.403110
O	0.599892	-0.940754	0.725653
H	-0.609540	-2.342434	-1.360724
H	1.011064	-0.132009	0.271079
O	-4.691779	-3.569343	-1.969023
O	-2.200000	-4.140955	0.517474
O	-5.183690	-1.156703	-0.579295
O	-2.182559	-2.728717	-1.243441
O	-4.897718	-1.218299	1.648823
C	-4.223601	-3.891847	-0.692028
C	-5.075805	-3.294916	0.459639
C	-2.749024	-3.524959	-0.510366
C	-5.036863	-1.787322	0.577051
H	-4.287778	-4.978800	-0.600589
H	-4.769169	-3.708684	1.419325
H	-6.112942	-3.585440	0.266842
H	-4.636085	-2.610350	-2.070638
H	-1.261052	-3.854191	0.648689
H	-5.177981	-0.165250	-0.442399
S	0.931331	2.059186	-1.284189
O	1.690082	1.134502	-0.370536
O	0.767704	3.381134	-0.691904
O	1.528504	2.045219	-2.615341
O	-0.493381	1.401828	-1.449735
H	2.834610	0.998731	-2.792566
H	-1.150224	1.811401	-0.811102
O	-4.946215	4.103930	-0.327095
O	-4.655541	1.407349	2.013703
O	-1.242278	4.401942	0.755915
O	-5.199707	1.469717	-0.171924
O	-2.245572	2.476072	0.173669
C	-4.765632	3.537284	0.947807

C	-3.442061	4.020407	1.552213
C	-4.872097	2.017626	0.875196
C	-2.249853	3.560141	0.747284
H	-5.574130	3.859294	1.620461
H	-3.327976	3.631518	2.568879
H	-3.444448	5.109035	1.606694
H	-5.138883	3.369985	-0.928335
H	-4.750638	0.418192	1.903269
H	-0.478065	4.036540	0.234958
O	7.034312	-0.042500	1.234596
O	3.777247	1.454167	1.278901
O	4.718265	-1.775216	1.370713
O	5.068939	0.776500	-0.438213
O	3.520274	-1.736680	3.279544
C	5.939300	0.621716	1.811088
C	5.318709	-0.147347	2.998787
C	4.883724	0.963251	0.752172
C	4.412596	-1.300395	2.606629
H	6.325344	1.571709	2.194297
H	4.725805	0.511613	3.632835
H	6.142965	-0.538385	3.602029
H	6.678721	-0.815358	0.778052
H	3.049331	1.517760	0.607098
H	3.983307	-2.334872	1.055213
C	3.538262	-0.942201	-3.156577
N	3.751544	0.495189	-2.835136
C	4.638903	1.215644	-3.785037
H	3.039871	-1.022169	-4.122195
H	2.922591	-1.390588	-2.379910
H	4.504086	-1.445842	-3.191969
H	4.155399	0.583390	-1.878656
H	4.220698	1.151786	-4.789083
H	5.631703	0.767735	-3.762140
H	4.698715	2.258974	-3.479906
2SA3MA2DMA			
S	-1.597661	-2.341691	-0.302158
O	-0.673082	-3.454229	-0.545825
O	-2.828839	-2.388220	-1.079691
O	-1.862092	-2.177890	1.156652
O	-0.764397	-1.056624	-0.740548
H	-0.332419	-2.462355	2.014237
H	-1.010705	-0.266245	-0.182575
O	5.085412	-3.627027	-0.481241
O	1.718395	-3.410986	-1.656546

O	4.860965	-0.846103	-0.675340
O	2.556428	-3.064131	0.411283
O	4.159191	0.037247	-2.616668
C	4.069421	-3.462222	-1.432228
C	4.353310	-2.345213	-2.464063
C	2.691357	-3.286445	-0.782040
C	4.435456	-0.932714	-1.928510
H	4.018263	-4.398771	-1.993822
H	3.605570	-2.350599	-3.256879
H	5.325001	-2.563069	-2.919840
H	5.109214	-2.822339	0.051735
H	0.813161	-3.337069	-1.239067
H	4.938664	0.111939	-0.395367
S	-0.809194	1.216072	2.120331
O	-1.412673	1.041281	0.760755
O	-0.687511	2.635545	2.455527
O	-1.441668	0.377380	3.116686
O	0.678138	0.629886	1.989630
H	-3.184375	-1.065259	1.836520
H	1.252978	1.303350	1.526550
O	4.917349	3.974579	1.394454
O	4.015383	2.549699	-1.765753
O	1.003883	4.341860	1.303843
O	5.059634	1.700195	0.041182
O	2.160828	2.475944	0.814461
C	4.425100	4.006036	0.076203
C	3.004802	4.581795	0.058662
C	4.510277	2.620751	-0.555883
C	2.015863	3.693193	0.777432
H	5.056613	4.658607	-0.544154
H	2.656990	4.694494	-0.972980
H	3.008155	5.569572	0.519940
H	5.226412	3.070126	1.547955
H	4.083896	1.615745	-2.118986
H	0.358245	3.710546	1.731093
O	-6.202620	1.579965	-2.085585
O	-2.922799	2.437429	-0.911652
O	-4.064939	-0.334597	-2.389847
O	-4.633470	1.409675	0.126733
O	-2.646195	0.065783	-4.097516
C	-4.950170	2.217092	-2.133437
C	-4.125555	1.830951	-3.378894
C	-4.159212	1.978351	-0.841307
C	-3.514136	0.437661	-3.357328

H	-5.155608	3.291058	-2.187531
H	-3.301516	2.527890	-3.535345
H	-4.782945	1.900173	-4.250046
H	-6.024091	0.643409	-1.933531
H	-2.382711	2.102365	-0.148421
H	-3.543999	-1.156143	-2.248985
C	-5.098269	-1.585560	1.257428
N	-4.129183	-0.640738	1.881674
C	-4.474372	-0.246139	3.274513
H	-5.181733	-2.472552	1.884717
H	-4.719654	-1.865687	0.277108
H	-6.063805	-1.089852	1.170013
H	-4.096145	0.212010	1.287809
H	-4.553085	-1.143520	3.888115
H	-5.428431	0.279949	3.263301
H	-3.680930	0.392274	3.653533
C	1.091386	-2.211002	3.535668
N	0.554605	-2.906391	2.333776
C	0.287725	-4.358343	2.523834
H	0.377858	-2.311880	4.352730
H	1.221265	-1.159183	3.292912
H	2.043098	-2.665708	3.809504
H	1.229299	-2.818467	1.545895
H	-0.432890	-4.486780	3.330879
H	1.221078	-4.862988	2.770576
H	-0.119436	-4.747657	1.593211
2SA3MA3DMA			
S	-1.895020	-1.880462	1.527901
O	-1.016113	-2.953338	1.989270
O	-2.978298	-2.296769	0.640975
O	-2.369705	-1.021814	2.629435
O	-0.878628	-0.958044	0.666113
H	0.572941	-0.021250	2.370333
H	-1.277211	-0.061831	0.509655
O	4.529782	-4.047615	1.056231
O	1.013439	-3.902468	0.572630
O	4.251350	-1.357209	0.234710
O	2.294417	-2.818969	2.074495
O	4.427893	-1.255994	-1.996100
C	3.359771	-4.024639	0.273801
C	3.518234	-3.250353	-1.054289
C	2.161330	-3.515032	1.077104
C	4.115477	-1.870112	-0.984005
H	3.136247	-5.060811	0.011259

H	2.550532	-3.114019	-1.565362
H	4.155156	-3.824398	-1.731258
H	4.582528	-3.188460	1.493136
H	0.241450	-3.544864	1.095666
H	4.624547	-0.435219	0.177570
S	-1.085677	2.530917	1.267825
O	-1.822715	1.547147	0.414370
O	-0.786486	3.754033	0.525684
O	-1.680160	2.688411	2.572172
O	0.346277	1.812022	1.546105
H	-3.637055	0.097683	2.252786
H	1.007571	2.092713	0.848985
O	5.027500	3.832174	0.441421
O	4.605885	1.358465	-2.114359
O	1.398497	4.580180	-0.752470
O	5.024707	1.200799	0.093673
O	2.196288	2.560619	-0.172188
C	4.837331	3.380457	-0.878063
C	3.579913	4.022043	-1.476339
C	4.809765	1.856525	-0.921851
C	2.322935	3.650151	-0.724275
H	5.689677	3.679737	-1.505256
H	3.454468	3.704214	-2.516111
H	3.689724	5.106721	-1.471666
H	5.155185	3.039782	0.982202
H	4.598016	0.351676	-2.087703
H	0.573427	4.277432	-0.281587
O	-6.115700	0.039562	-2.807223
O	-3.016167	1.637013	-1.959368
O	-4.008690	-1.629764	-1.745638
O	-4.839794	1.210359	-0.711833
O	-2.169001	-1.905055	-3.015087
C	-4.858449	0.612674	-3.058349
C	-3.875412	-0.362491	-3.748528
C	-4.249236	1.194826	-1.776217
C	-3.238873	-1.384794	-2.822710
H	-5.033073	1.449167	-3.741953
H	-3.060816	0.173951	-4.234305
H	-4.434342	-0.895257	-4.523470
H	-5.980793	-0.624141	-2.119143
H	-2.586175	1.831224	-1.085571
H	-3.506474	-2.108779	-1.045388
C	-5.601454	-0.440090	1.927920
N	-4.519731	0.582320	1.976153

C	-4.785932	1.726167	2.890484
H	-5.777057	-0.817422	2.934765
H	-5.268531	-1.252586	1.285736
H	-6.505543	0.015821	1.527521
H	-4.381968	0.940098	1.013142
H	-4.960023	1.341357	3.895168
H	-5.667755	2.262552	2.540706
H	-3.911860	2.374759	2.887013
C	2.449666	0.164487	3.188525
N	1.135154	-0.526416	3.069532
C	0.371093	-0.604972	4.348215
H	2.282119	1.184969	3.527347
H	2.928851	0.169718	2.212239
H	3.069685	-0.382301	3.896951
H	1.311286	-1.483263	2.698318
H	0.186035	0.407543	4.704793
H	0.962955	-1.162581	5.073076
H	-0.574178	-1.104589	4.151638
C	0.943953	-0.496833	-2.529798
N	0.936729	-1.936852	-2.779114
C	1.205818	-2.254272	-4.179305
H	1.946698	-0.097037	-2.703503
H	0.675529	-0.306932	-1.488834
H	0.241450	0.060875	-3.171239
H	0.012390	-2.286485	-2.544725
H	2.232419	-1.968544	-4.429196
H	0.527338	-1.743027	-4.882195
H	1.108522	-3.331268	-4.337219

2SA3MA4DMA

S	-0.799788	-2.231354	1.089346
O	0.209174	-2.915080	1.910288
O	-0.873524	-2.751467	-0.278663
O	-2.093248	-2.087370	1.746408
O	-0.164467	-0.742712	0.981055
H	1.170886	-0.272339	2.250498
H	-0.830680	-0.027573	0.779116
O	5.833945	-3.309577	0.816461
O	2.336486	-3.929176	0.701014
O	5.003159	-0.787173	-0.080904
O	3.477023	-2.480070	1.994294
O	4.361746	-0.700249	-2.225244
C	4.616137	-3.569797	0.163913
C	4.462373	-2.852228	-1.197493
C	3.415152	-3.270520	1.063189

C	4.601699	-1.350457	-1.216629
H	4.594340	-4.642073	-0.041484
H	3.486475	-3.073780	-1.659674
H	5.230708	-3.235291	-1.876512
H	5.795845	-2.393299	1.117517
H	1.529930	-3.617510	1.202537
H	5.062526	0.202245	-0.188663
S	-1.065268	2.445893	1.717841
O	-1.594871	1.468643	0.724825
O	-1.007360	3.794900	1.122693
O	-1.681130	2.347674	3.016131
O	0.476591	2.010811	1.958434
H	-3.795812	-1.502543	1.851766
H	1.031368	2.339038	1.198432
O	4.750609	4.503835	0.000127
O	4.051661	1.903215	-2.360830
O	0.841203	4.758042	-0.503748
O	5.016421	1.880036	-0.324916
O	2.035814	2.926664	0.019272
C	4.344787	3.985420	-1.243431
C	2.931650	4.472359	-1.578567
C	4.480539	2.466306	-1.261621
C	1.896063	3.977243	-0.595820
H	5.013880	4.346600	-2.038870
H	2.640387	4.124214	-2.574518
H	2.917553	5.562706	-1.593027
H	5.094725	3.754574	0.506896
H	4.191427	0.906846	-2.331383
H	0.166183	4.385087	0.137462
O	-5.727680	-2.024245	-0.752482
O	-5.343821	1.286858	-2.124174
O	-3.145320	-2.579744	-1.673240
O	-5.062921	0.553429	-0.039447
O	-2.448446	-0.664100	-2.636722
C	-5.711768	-1.031622	-1.770883
C	-4.746844	-1.391982	-2.930100
C	-5.360163	0.382526	-1.250676
C	-3.316497	-1.479914	-2.435849
H	-6.722029	-0.974686	-2.186444
H	-4.809461	-0.614564	-3.686812
H	-5.043919	-2.356064	-3.350087
H	-4.881462	-2.493251	-0.793442
H	-4.186060	2.204846	-1.594857
H	-2.250627	-2.590412	-1.239301

C	-5.761501	-1.835547	2.451347
N	-4.643968	-0.949260	2.045135
C	-4.291178	0.086445	3.052052
H	-5.470582	-2.424255	3.322065
H	-6.014244	-2.478967	1.612057
H	-6.626104	-1.218573	2.696851
H	-4.887722	-0.452632	1.121418
H	-4.031188	-0.393832	3.995941
H	-5.148036	0.744737	3.193636
H	-3.444007	0.665220	2.691723
C	2.894731	0.520951	3.120476
N	1.830028	-0.513287	3.008985
C	1.034720	-0.711690	4.252436
H	2.438667	1.468357	3.396788
H	3.391144	0.613621	2.156467
H	3.615291	0.200540	3.871919
H	2.274286	-1.407278	2.715360
H	0.479092	0.201793	4.460283
H	1.711981	-0.941551	5.074538
H	0.352273	-1.541846	4.084052
C	1.127846	-1.927476	-3.405695
N	1.371687	-3.082600	-2.544013
C	1.102680	-4.351663	-3.211946
H	1.851591	-1.920723	-4.226743
H	1.267145	-1.009453	-2.831667
H	0.114617	-1.906058	-3.838036
H	0.772642	-3.012211	-1.725925
H	1.817033	-4.500361	-4.028695
H	0.088379	-4.419813	-3.641600
H	1.227566	-5.172285	-2.501528
C	-2.347541	2.916695	-2.318133
N	-3.338223	2.752480	-1.225317
C	-3.832065	4.018174	-0.627656
H	-2.805613	3.480477	-3.131062
H	-2.067703	1.924362	-2.670225
H	-1.474656	3.448643	-1.941058
H	-2.907482	2.176336	-0.484780
H	-4.284500	4.626402	-1.411061
H	-3.008179	4.546189	-0.151389
H	-4.586903	3.761961	0.114462
2SA4MA			
S	-1.018757	0.815478	-2.152251
O	-1.193916	-0.348183	-2.990618
O	-1.830643	1.976044	-2.337770

O	-1.154261	0.403797	-0.643624
O	0.512795	1.188698	-2.312358
H	-0.778267	-0.518594	-0.489210
H	0.707153	2.033145	-1.839971
O	0.020967	-4.534095	0.753190
O	-0.533972	-2.882292	-2.357167
O	2.627244	-3.636611	0.595289
O	-0.243261	-2.023776	-0.287505
O	3.524822	-3.457850	-1.456144
C	0.122363	-4.373043	-0.649166
C	1.519560	-4.756773	-1.188407
C	-0.260588	-2.957102	-1.076759
C	2.657124	-3.879666	-0.709296
H	-0.611513	-5.045040	-1.092969
H	1.520389	-4.738795	-2.277337
H	1.728560	-5.778366	-0.856429
H	0.690350	-3.969818	1.167632
H	-0.780184	-1.958905	-2.621470
H	3.405128	-3.068757	0.870543
S	1.922307	3.381798	0.258550
O	1.052025	3.497468	-0.914819
O	3.248909	3.936449	0.150426
O	1.209456	4.027115	1.456573
O	2.010025	1.871140	0.611463
H	0.176521	4.071153	1.344570
H	2.967816	1.521092	0.576288
O	6.439681	-0.477071	2.414460
O	5.520472	-1.823706	-0.776145
O	5.697532	2.709741	0.222232
O	4.711107	-2.159144	1.299902
O	4.374689	0.910049	0.483601
C	6.613057	-0.735682	1.043589
C	6.739158	0.587205	0.283013
C	5.497186	-1.633437	0.519626
C	5.484049	1.419465	0.352695
H	7.543404	-1.299724	0.876892
H	6.952208	0.400545	-0.774300
H	7.571072	1.162277	0.690669
H	5.708218	-1.036135	2.713093
H	4.783637	-2.439552	-1.054843
H	4.844273	3.204644	0.215349
O	-3.930767	4.809315	1.578780
O	-1.425773	4.745565	-0.966139
O	-3.547434	2.066141	1.080706

O	-1.289669	4.209548	1.219374
O	-4.844433	1.363892	-0.612618
C	-3.449867	4.716718	0.266472
C	-4.175206	3.655409	-0.593346
C	-1.936549	4.526920	0.228838
C	-4.219215	2.244974	-0.044947
H	-3.638194	5.685721	-0.204943
H	-3.731173	3.591350	-1.589389
H	-5.213708	3.969029	-0.723041
H	-3.647729	4.008879	2.039942
H	-0.488204	4.455797	-1.006964
H	-3.629719	1.117557	1.393118
O	-5.689879	-3.914908	0.195688
O	-2.520908	-4.377416	1.762042
O	-5.190588	-1.120697	0.263852
O	-2.982131	-3.755387	-0.354732
O	-3.913754	-0.409022	1.969237
C	-4.780950	-3.847592	1.258802
C	-4.934682	-2.574391	2.132447
C	-3.334133	-3.990745	0.779960
C	-4.616673	-1.263925	1.447412
H	-4.993990	-4.700946	1.906359
H	-4.305985	-2.643299	3.019454
H	-5.982216	-2.529520	2.446257
H	-5.464445	-3.212364	-0.427341
H	-1.594528	-4.418463	1.419492
H	-5.010157	-0.207753	-0.105221

2SA4MA1DMA

S	-0.839875	-0.250103	2.275194
O	-0.414552	0.887117	3.063664
O	-1.992827	-0.994101	2.669982
O	-1.097827	0.226785	0.788305
O	0.421976	-1.168585	2.167709
H	-0.462009	0.968828	0.547731
H	0.245435	-1.991385	1.611230
O	1.333307	4.481900	-1.041089
O	0.644430	3.182877	2.220407
O	3.689881	3.045801	-0.701176
O	0.461808	2.233360	0.179978
O	4.564051	2.980437	1.368094
C	1.414095	4.434082	0.372225
C	2.857787	4.604815	0.892336
C	0.771238	3.158955	0.916105
C	3.791476	3.461095	0.557055

H	0.814176	5.265130	0.743955
H	2.854773	4.723778	1.974467
H	3.265580	5.514803	0.441734
H	1.903574	3.780374	-1.389568
H	0.244479	2.338356	2.561085
H	4.331577	2.294915	-0.881442
S	1.132319	-3.547453	-0.332137
O	0.032891	-3.262624	0.636774
O	2.253748	-4.254627	0.269327
O	0.599898	-4.155624	-1.551277
O	1.641827	-2.099491	-0.761736
H	-0.665774	-3.326760	-2.248517
H	2.591376	-1.946768	-0.484330
O	6.651548	-1.109727	-1.991819
O	6.031046	0.776375	0.990713
O	4.873849	-3.724576	0.335842
O	5.393809	1.075016	-1.149622
O	4.155461	-1.647638	-0.141190
C	6.809642	-0.783909	-0.632385
C	6.491791	-2.000984	0.242960
C	5.982031	0.445216	-0.276029
C	5.052697	-2.442562	0.116205
H	7.853952	-0.499893	-0.434924
H	6.678356	-1.769295	1.296195
H	7.146515	-2.827206	-0.035405
H	6.071393	-0.434460	-2.371014
H	5.498795	1.603448	1.158007
H	3.907208	-3.955562	0.296692
O	-5.822873	-3.580636	0.067640
O	-2.495485	-3.863561	1.345224
O	-3.976708	-1.138647	-0.163673
O	-3.314655	-3.957039	-0.753413
O	-5.059237	0.170381	1.296862
C	-4.823679	-3.511706	1.058425
C	-4.862204	-2.163708	1.802755
C	-3.453256	-3.800043	0.452882
C	-4.653272	-0.930695	0.955359
H	-5.004501	-4.294227	1.806081
H	-4.089629	-2.137503	2.575877
H	-5.829821	-2.058080	2.294603
H	-5.356832	-3.635390	-0.777982
H	-1.590336	-3.873967	0.944964
H	-3.858061	-0.278690	-0.656575
O	-4.387104	5.223751	-0.454295

O	-1.241464	4.541911	-2.003007
O	-4.627081	2.431866	-0.018193
O	-1.781022	4.571013	0.186532
O	-3.711012	1.099067	-1.574453
C	-3.544576	4.739997	-1.461431
C	-4.034598	3.416281	-2.105351
C	-2.095407	4.611764	-0.981300
C	-4.093100	2.204011	-1.202043
H	-3.548458	5.489740	-2.256288
H	-3.413888	3.160405	-2.963411
H	-5.056283	3.594883	-2.456117
H	-4.313799	4.627822	0.301772
H	-0.317364	4.468621	-1.658370
H	-4.739069	1.579281	0.503757
C	-1.341989	-1.359829	-2.424794
N	-1.535775	-2.831758	-2.568123
C	-1.882737	-3.281714	-3.940127
H	-0.498032	-1.056083	-3.042657
H	-1.128029	-1.135794	-1.381921
H	-2.246117	-0.837003	-2.732890
H	-2.260833	-3.163284	-1.904132
H	-1.077772	-3.008454	-4.621589
H	-2.811407	-2.806220	-4.254331
H	-2.004948	-4.363812	-3.932691

2SA4MA2DMA

S	0.099636	1.358278	1.918831
O	1.335042	0.741334	2.386673
O	-0.464063	2.341739	2.847323
O	0.173151	1.874439	0.536445
O	-0.923469	0.111402	1.848258
H	0.197510	0.645871	-0.659094
H	-1.772634	0.409724	1.433744
O	2.856571	-4.426574	0.124304
O	1.890295	-1.809753	2.367386
O	0.066011	-4.408892	-0.003263
O	2.116286	-1.820024	0.118417
O	-1.094146	-4.673101	1.899727
C	2.461365	-3.857208	1.364690
C	1.305394	-4.632245	2.026274
C	2.143031	-2.365333	1.210121
C	-0.029878	-4.568972	1.315516
H	3.334260	-3.916109	2.014956
H	1.148084	-4.279683	3.044942
H	1.593290	-5.687459	2.078982

H	2.104136	-4.338826	-0.478092
H	1.683303	-0.828949	2.305404
H	-0.846233	-4.345738	-0.416843
S	-3.746921	1.642781	-0.443718
O	-3.221744	0.848190	0.677126
O	-5.208620	1.564861	-0.521331
O	-3.202429	3.000244	-0.503143
O	-3.192335	0.960078	-1.801620
H	-1.720067	3.454729	-1.378488
H	-3.674399	0.099241	-1.890866
O	-4.589192	-4.103585	-2.639535
O	-3.538178	-4.494492	0.774180
O	-6.085321	-0.926335	-0.242891
O	-2.331801	-4.140477	-1.091062
O	-4.398969	-1.466861	-1.633176
C	-4.749216	-4.243689	-1.255757
C	-5.726812	-3.217645	-0.650153
C	-3.404639	-4.273983	-0.519382
C	-5.331074	-1.777307	-0.890870
H	-5.181638	-5.236085	-1.091896
H	-5.846859	-3.369486	0.424146
H	-6.710602	-3.364062	-1.105757
H	-4.183780	-3.237270	-2.781186
H	-2.646408	-4.552787	1.215580
H	-5.788945	0.023512	-0.377639
O	1.381164	5.002246	-2.674764
O	-0.867446	5.014253	0.112185
O	2.621351	2.787514	-1.573367
O	-0.857805	3.762996	-1.752541
O	3.410864	3.013688	0.510931
C	1.028078	5.214816	-1.333717
C	2.124135	4.800074	-0.325048
C	-0.332902	4.638801	-0.915398
C	2.715820	3.424108	-0.519154
H	0.894677	6.293842	-1.219039
H	1.761092	4.886979	0.699391
H	2.967092	5.492846	-0.425921
H	1.668247	4.081984	-2.746397
H	-2.548326	4.075852	1.203487
H	3.730120	1.590638	-2.046499
O	7.266796	-0.658473	0.478140
O	5.043893	-3.123130	-0.903994
O	4.831569	0.789712	-0.149531
O	5.200981	-2.308245	1.192811

O	4.376651	0.897494	-2.344556
C	6.651221	-1.417378	-0.526448
C	6.116929	-0.558620	-1.690698
C	5.555758	-2.327100	0.038251
C	5.046615	0.431534	-1.299977
H	7.420206	-2.075321	-0.942698
H	5.736718	-1.185212	-2.498623
H	6.949358	0.025863	-2.096612
H	6.558378	-0.271362	1.008940
H	4.291466	-3.640289	-0.522782
H	3.850058	2.140676	0.322888
C	-0.690172	-1.176076	-1.198428
N	0.383114	-0.148669	-1.317363
C	0.551253	0.387283	-2.695666
H	-0.724402	-1.510068	-0.166162
H	-0.462303	-2.009454	-1.859963
H	-1.636688	-0.721057	-1.467243
H	1.251142	-0.576486	-0.959263
H	-0.401513	0.801386	-3.021467
H	0.860843	-0.419033	-3.359942
H	1.300606	1.173215	-2.672447
C	-2.219174	5.420124	2.751982
N	-2.482073	4.051746	2.231835
C	-3.687327	3.402642	2.815506
H	-3.087126	6.050422	2.558387
H	-1.350963	5.816747	2.234624
H	-2.036345	5.358606	3.824297
H	-1.650830	3.439740	2.424806
H	-4.574237	3.971357	2.538146
H	-3.579876	3.378275	3.899354
H	-3.758400	2.389802	2.426804
2SA4MA3DMA			
S	0.355946	-1.111320	1.757867
O	-0.822656	-0.940291	2.609167
O	1.353174	-2.019220	2.338202
O	0.048852	-1.419916	0.358119
O	1.012124	0.369396	1.761658
H	0.274698	0.369270	-1.384959
H	1.840660	0.344755	1.226927
O	-4.792480	2.570920	0.150295
O	-2.673866	0.816182	2.441389
O	-2.582870	4.239070	0.182354
O	-2.700127	0.831195	0.181376
O	-1.644060	4.735306	2.159838

C	-4.213006	2.255596	1.409342
C	-3.714804	3.511434	2.153245
C	-3.103547	1.203508	1.272351
C	-2.539125	4.216791	1.515212
H	-5.005667	1.792418	1.996571
H	-3.431070	3.256542	3.172826
H	-4.541877	4.227939	2.194522
H	-4.109101	3.006664	-0.377990
H	-1.936368	0.117299	2.406033
H	-1.795689	4.735825	-0.189002
S	3.417554	0.405231	-1.089989
O	3.337336	0.223558	0.365547
O	4.458361	1.358679	-1.485258
O	3.437600	-0.841855	-1.843813
O	2.009011	1.104239	-1.525036
H	2.448130	-2.290771	-1.785036
H	2.059959	2.075616	-1.289630
O	1.567197	6.440904	-2.225872
O	0.606208	5.752494	1.156659
O	4.373175	3.950175	-0.950908
O	-0.472057	5.491033	-0.804114
O	2.141818	3.664167	-0.891208
C	1.713879	6.466152	-0.827036
C	3.048855	5.832997	-0.425686
C	0.510291	5.825677	-0.146376
C	3.141609	4.370012	-0.793455
H	1.724395	7.507043	-0.469440
H	3.193812	5.912040	0.656227
H	3.864572	6.373951	-0.906546
H	0.687793	6.079680	-2.404284
H	-0.228683	5.372578	1.555509
H	4.406731	2.967444	-1.144223
O	0.776423	-5.610404	-1.880929
O	3.070087	-3.673219	-0.006525
O	-1.319913	-3.949736	-1.239950
O	1.864236	-3.088878	-1.808354
O	-1.946160	-4.023102	0.910717
C	1.268428	-5.121165	-0.658341
C	0.175343	-4.899328	0.414724
C	2.161657	-3.879995	-0.789334
C	-1.089397	-4.224921	-0.059327
H	1.940936	-5.888453	-0.269610
H	0.564319	-4.324404	1.259300
H	-0.136861	-5.871725	0.808980

H	0.088527	-4.993425	-2.167525
H	4.745128	-2.154902	1.447224
H	-2.754483	-3.369593	-1.839264
O	-7.111152	-2.725696	0.289328
O	-5.938068	0.401669	-1.046900
O	-4.249410	-2.984665	-0.075942
O	-5.990010	-0.356545	1.075292
O	-3.607755	-3.020108	-2.226677
C	-6.773074	-1.796897	-0.704869
C	-5.842062	-2.383551	-1.784448
C	-6.192861	-0.511808	-0.104973
C	-4.492977	-2.818299	-1.264292
H	-7.705352	-1.514353	-1.203730
H	-5.693341	-1.676990	-2.602379
H	-6.320707	-3.273122	-2.206825
H	-6.353831	-2.779323	0.887015
H	-5.541186	1.202074	-0.619712
H	-2.775021	-3.592473	0.570141
C	-1.118996	1.554589	-2.336385
N	-0.701602	0.276967	-1.702486
C	-0.789576	-0.907145	-2.603530
H	-1.011646	2.358257	-1.611467
H	-2.161131	1.473813	-2.639269
H	-0.482635	1.745153	-3.199467
H	-1.264381	0.119906	-0.850649
H	-0.170258	-0.721473	-3.480412
H	-1.828272	-1.052545	-2.896744
H	-0.423520	-1.775122	-2.062985
C	4.192149	-3.464704	2.987012
N	4.095023	-2.157551	2.291086
C	4.384809	-0.988150	3.158306
H	5.205566	-3.601272	3.366033
H	3.945728	-4.242447	2.268184
H	3.478045	-3.483217	3.809631
H	3.119875	-2.069001	1.950176
H	5.387885	-1.085608	3.575037
H	3.646675	-0.948166	3.958406
H	4.315066	-0.089912	2.549404
C	6.835260	-1.125505	-0.086501
N	5.846021	-2.203199	0.039268
C	6.424988	-3.531727	-0.190139
H	7.574205	-1.209919	0.716111
H	6.337630	-0.159020	-0.004437
H	7.371949	-1.154366	-1.045365

H	5.104950	-2.052841	-0.642531
H	7.143046	-3.764215	0.602300
H	6.952968	-3.603755	-1.152168
H	5.628552	-4.276132	-0.172682
2SA4MA4DMA			
S	-0.012328	-0.962144	-1.727414
O	1.237719	-0.751392	-2.450582
O	-1.002417	-1.728880	-2.484673
O	0.167144	-1.490930	-0.360640
O	-0.593387	0.532619	-1.553883
H	0.366870	-0.798896	2.657307
H	-1.516398	0.474864	-1.207435
O	4.745356	3.122698	-0.170373
O	2.690241	1.387241	-2.534638
O	2.218409	4.380818	-0.007598
O	2.893063	1.175452	-0.298064
O	1.318221	5.186951	-1.900700
C	4.142185	2.887572	-1.439708
C	3.478387	4.147734	-2.022113
C	3.169603	1.706232	-1.356070
C	2.225934	4.619797	-1.316011
H	4.951220	2.581900	-2.103135
H	3.216766	3.983998	-3.066747
H	4.204850	4.966232	-1.981051
H	4.024394	3.321564	0.444275
H	2.092035	0.579200	-2.471566
H	1.358458	4.692971	0.402846
S	-3.861767	0.235461	0.536360
O	-3.156916	0.303732	-0.750602
O	-5.066629	1.075718	0.555638
O	-4.092620	-1.135477	0.999500
O	-2.872751	0.841277	1.651946
H	-2.834225	-2.298821	1.178774
H	-2.907911	1.834177	1.592496
O	-2.220242	5.996839	2.542809
O	-1.007220	5.952061	-0.836962
O	-4.818536	3.685755	0.159145
O	-0.083877	5.167848	1.060511
O	-2.924663	3.491351	1.358806
C	-2.269929	6.203695	1.157426
C	-3.553273	5.647473	0.511247
C	-1.001022	5.704935	0.458103
C	-3.733972	4.161727	0.719160
H	-2.275585	7.287765	1.005194

H	-3.577061	5.851656	-0.561684
H	-4.418112	6.150798	0.951945
H	-2.062696	5.052648	2.673096
H	-0.148531	5.658887	-1.254858
H	-4.916329	2.697732	0.309794
O	-0.379548	-4.918240	1.992277
O	-2.581074	-3.808045	-0.612211
O	1.848077	-3.719651	1.068054
O	-2.114676	-2.944302	1.406836
O	2.200117	-3.679007	-1.142922
C	-0.848097	-4.865430	0.665800
C	0.267159	-4.808590	-0.410232
C	-1.924261	-3.794930	0.410463
C	1.492501	-3.981583	-0.088441
H	-1.396834	-5.796145	0.485241
H	-0.143987	-4.472993	-1.361536
H	0.652767	-5.822739	-0.566057
H	0.467089	-4.443469	2.010713
H	-4.460570	-2.312628	-2.172435
H	3.478344	-3.399296	1.465062
O	7.346141	-1.985437	-1.146985
O	6.078552	0.856060	0.650461
O	4.470091	-2.362926	-0.380138
O	6.076333	0.345899	-1.546769
O	4.399851	-3.138008	1.727390
C	7.082904	-1.203223	-0.010507
C	6.363061	-2.003345	1.084885
C	6.346546	0.080279	-0.397745
C	4.990259	-2.510378	0.712672
H	8.041392	-0.880133	0.416838
H	6.271228	-1.410799	1.998438
H	6.972348	-2.876392	1.337230
H	6.753702	-1.663126	-1.841120
H	5.608980	1.676892	0.350070
H	2.999069	-3.138183	-0.897296
C	0.471936	1.172419	1.920202
N	0.968430	-0.228520	1.989156
C	2.383633	-0.332141	2.430310
H	-0.558981	1.153873	1.578578
H	1.091788	1.726984	1.219999
H	0.525810	1.619341	2.913715
H	0.843243	-0.664029	1.050280
H	2.475291	0.106358	3.425032
H	3.015393	0.196879	1.721175

H	2.663090	-1.381921	2.470626
C	-3.464583	-3.404142	-3.656635
N	-3.655913	-2.170541	-2.853394
C	-3.896463	-0.951351	-3.666884
H	-4.360454	-3.595452	-4.248483
H	-3.275864	-4.225704	-2.969939
H	-2.603046	-3.269235	-4.309115
H	-2.784686	-2.023986	-2.312986
H	-4.801922	-1.084442	-4.259953
H	-3.038562	-0.787078	-4.317261
H	-4.003812	-0.108604	-2.987521
C	-7.039996	-1.751727	-1.253140
N	-5.840952	-2.575483	-1.057598
C	-6.146762	-4.002046	-0.907380
H	-7.490878	-1.973248	-2.225384
H	-6.764875	-0.696271	-1.226199
H	-7.802363	-1.925521	-0.480051
H	-5.360996	-2.248882	-0.219653
H	-6.576727	-4.389274	-1.836291
H	-6.864882	-4.199722	-0.098110
H	-5.224326	-4.546023	-0.698642
C	0.279661	-2.593838	4.758257
N	-0.542045	-1.870505	3.781457
C	-1.693740	-1.201670	4.404083
H	0.720002	-1.887276	5.467944
H	1.092187	-3.113610	4.246655
H	-0.295239	-3.335693	5.330207
H	-0.900561	-2.536908	3.098139
H	-1.341568	-0.423779	5.088287
H	-2.322421	-1.896954	4.978406
H	-2.305134	-0.730225	3.634159
3MA			
O	0.528021	4.646752	1.363323
O	2.027803	2.526561	-1.115413
O	-1.243111	2.497286	0.700156
O	1.954631	2.348565	1.128820
O	-2.246755	2.650896	-1.303956
C	0.843651	4.210872	0.069284
C	-0.387635	4.091338	-0.855367
C	1.671136	2.923893	0.090096
C	-1.385865	3.007004	-0.513904
H	1.490558	4.978151	-0.368165
H	-0.085154	3.933926	-1.891594
H	-0.925670	5.043270	-0.816210

H	0.194851	3.882511	1.849422
H	2.555267	1.680256	-1.061947
H	-1.920364	1.780820	0.859359
O	-3.901904	-1.876850	1.637966
O	-3.727022	0.445414	-1.083888
O	-1.394889	-1.544741	-0.694408
O	-2.983761	0.516782	1.040708
O	-1.538169	-3.745428	-0.265196
C	-4.128079	-1.449534	0.316718
C	-3.557101	-2.487481	-0.671033
C	-3.544656	-0.054355	0.110735
C	-2.063152	-2.672496	-0.516849
H	-5.206741	-1.367955	0.122499
H	-3.766017	-2.168021	-1.695495
H	-4.039163	-3.445970	-0.486368
H	-3.473871	-1.138881	2.095873
H	-3.239669	1.314588	-1.173126
H	-0.414572	-1.689105	-0.555887
O	4.158007	-2.272222	-1.305526
O	3.126442	-0.040465	1.301217
O	1.046502	-4.040423	0.433352
O	3.363197	0.226007	-0.923767
O	1.165131	-1.897958	-0.229413
C	3.979720	-1.876014	0.032899
C	3.099789	-2.896452	0.761271
C	3.431083	-0.452811	0.094842
C	1.675908	-2.901303	0.257850
H	4.950138	-1.844378	0.551012
H	3.063876	-2.669327	1.831578
H	3.530246	-3.891905	0.648653
H	3.979339	-1.490734	-1.848225
H	2.731522	0.877162	1.265807
H	0.093661	-3.961776	0.141763
3MA1DMA			
O	-2.298469	-3.867869	1.672379
O	-2.758089	-2.000774	-1.342283
O	-0.056721	-2.326960	0.354437
O	-3.123762	-1.483296	0.820067
O	1.116483	-3.892412	-0.737168
C	-2.460417	-3.717136	0.282270
C	-1.230562	-4.247833	-0.458136
C	-2.802406	-2.269911	-0.064457
C	0.058353	-3.478761	-0.283055
H	-3.321846	-4.309497	-0.066316

H	-1.426982	-4.279827	-1.533072
H	-1.039839	-5.275532	-0.141496
H	-2.646377	-3.057795	2.071892
H	-2.937752	-1.017486	-1.509507
H	0.830574	-1.875629	0.396172
O	4.756611	0.296250	0.660004
O	3.292884	-2.401619	-1.020129
O	2.931243	2.140823	-0.073595
O	2.280452	-1.047489	0.453024
O	1.821462	1.640619	-1.960699
C	4.380022	-0.340160	-0.534420
C	3.966480	0.663657	-1.643336
C	3.217346	-1.309062	-0.305674
C	2.839393	1.568976	-1.163080
H	5.224346	-0.932855	-0.892487
H	3.676303	0.142300	-2.555520
H	4.837617	1.288058	-1.860051
H	4.253134	1.130797	0.690379
H	2.485739	-2.985681	-0.889651
H	0.554657	1.697619	1.424350
O	-2.791538	3.966873	0.875154
O	-0.165635	3.006841	-1.326992
O	-3.555787	1.175915	0.336304
O	-0.623657	2.484127	0.825360
O	-3.072454	0.535553	-1.759353
C	-2.240863	3.717855	-0.394194
C	-3.199047	2.882479	-1.292297
C	-0.869433	3.018667	-0.293105
C	-3.272770	1.421362	-0.932960
H	-2.093253	4.675145	-0.900917
H	-2.887002	2.941766	-2.333861
H	-4.195845	3.319605	-1.185235
H	-2.387879	3.301786	1.451452
H	1.034689	2.238457	-1.594221
H	-3.480269	0.205250	0.515766
C	1.989664	2.101949	2.890237
N	1.199583	1.137522	2.082464
C	0.348433	0.223481	2.886669
H	1.302744	2.705162	3.482738
H	2.541850	2.737952	2.203575
H	2.674576	1.562737	3.545576
H	1.826956	0.580323	1.488750
H	-0.324026	0.821323	3.500533
H	0.973309	-0.405971	3.520806

H -0.241839 -0.396695 2.214245
3MA2DMA
O 1.118973 4.230175 2.061849
O 3.334517 2.848046 -0.385654
O -0.661547 2.903261 0.307235
O 2.228795 1.857078 1.307506
O -0.652929 3.520543 -1.849740
C 1.800469 4.184858 0.838098
C 0.916845 4.568378 -0.372856
C 2.484067 2.833264 0.616212
C -0.203999 3.611582 -0.719071
H 2.597699 4.930535 0.896601
H 1.519694 4.696986 -1.272009
H 0.453569 5.533327 -0.142982
H 0.511006 3.480605 2.073151
H 3.739847 1.938127 -0.526119
H -1.374681 2.266804 -0.002743
O -4.233187 -0.904188 -0.950668
O -2.427448 1.668234 -2.660805
O -1.988609 -2.277044 -0.797313
O -2.430484 1.121701 -0.480849
O -0.475465 -1.975216 -2.436026
C -3.612917 -0.297905 -2.058455
C -2.725254 -1.296940 -2.842959
C -2.768451 0.907868 -1.642594
C -1.623563 -1.905867 -1.958827
H -4.390801 0.084398 -2.726368
H -2.272684 -0.816444 -3.708836
H -3.375602 -2.104532 -3.192027
H -3.580311 -1.582400 -0.661567
H -1.806380 2.391884 -2.372814
H -1.283471 -2.062032 0.693525
O 3.891037 -3.481841 1.112313
O 1.822827 -2.618819 -1.665120
O 3.143924 -0.608392 0.810260
O 1.329415 -3.254610 0.444950
O 4.326407 0.433929 -0.783146
C 3.625141 -3.178431 -0.236410
C 4.427299 -1.952832 -0.703118
C 2.116725 -3.016812 -0.460133
C 3.960198 -0.595847 -0.229618
H 3.940834 -4.018409 -0.872324
H 4.453974 -1.906039 -1.792327
H 5.459499 -2.075500 -0.359893

H	3.021254	-3.539186	1.534538
H	0.818248	-2.443781	-1.842269
H	2.860277	0.320829	1.030313
C	-1.147028	-3.080654	2.497580
N	-1.236836	-1.820647	1.718985
C	-0.124009	-0.870107	1.974789
H	-0.230768	-3.596470	2.219328
H	-2.006141	-3.703302	2.249894
H	-1.152161	-2.853155	3.564522
H	-2.157378	-1.332855	1.917357
H	0.819878	-1.354921	1.739723
H	-0.144284	-0.561929	3.021065
H	-0.257575	0.002288	1.337373
C	-4.876655	-1.209758	2.489634
N	-3.720295	-0.406907	2.075884
C	-3.592347	0.829852	2.853482
H	-4.730117	-1.575760	3.510241
H	-4.982841	-2.069277	1.825609
H	-5.817512	-0.641532	2.465066
H	-3.831150	-0.165531	1.089980
H	-3.365342	0.593013	3.897322
H	-4.508755	1.437873	2.838786
H	-2.776850	1.432517	2.450947
3MA3DMA			
O	-4.384734	-1.866608	-2.654055
O	-2.260869	-3.410547	-0.204610
O	-3.418027	-0.054676	-0.615459
O	-1.772997	-2.458454	-2.185603
O	-4.442927	-0.252711	1.372386
C	-4.082688	-2.595978	-1.493835
C	-4.728527	-2.014413	-0.221231
C	-2.574946	-2.810232	-1.333978
C	-4.183380	-0.688774	0.263159
H	-4.511355	-3.593497	-1.639572
H	-4.648230	-2.713036	0.612523
H	-5.794242	-1.869813	-0.421710
H	-3.827385	-1.079260	-2.646300
H	-1.266109	-3.477941	-0.109278
H	-3.067550	0.799483	-0.217266
O	-1.234096	4.553999	1.267448
O	-3.273882	1.897051	2.480203
O	0.846489	2.912682	1.037728
O	-2.415682	2.161377	0.419743
O	1.021556	1.236857	2.526563

C	-1.671910	3.622374	2.222100
C	-0.495261	3.003796	3.019513
C	-2.495732	2.493121	1.598478
C	0.544245	2.323159	2.116050
H	-2.338098	4.133259	2.923147
H	-0.856942	2.289493	3.758281
H	0.002790	3.821863	3.549459
H	-0.366306	4.204755	0.976844
H	-3.742572	1.118357	2.073384
H	1.509849	2.367312	-2.067759
O	3.212814	-1.130877	-2.089554
O	2.599037	-0.157795	1.248452
O	0.875328	-2.734430	-2.001797
O	1.287151	0.063905	-0.565670
O	0.374183	-3.434338	0.072146
C	3.149957	-1.431012	-0.701444
C	2.661229	-2.876821	-0.435774
C	2.247260	-0.415331	0.020776
C	1.195605	-3.053565	-0.748228
H	4.165442	-1.342455	-0.315084
H	2.837919	-3.144506	0.609429
H	3.241445	-3.539682	-1.084707
H	2.342612	-1.350887	-2.452420
H	1.904420	0.508541	1.744351
H	-0.117709	-2.696834	-2.104712
C	0.329698	4.078410	-1.800363
N	0.558696	2.617644	-1.666751
C	-0.495555	1.793208	-2.311746
H	0.301981	4.348683	-2.856544
H	1.142277	4.604507	-1.302114
H	-0.613482	4.336147	-1.319898
H	0.625768	2.398257	-0.648538
H	-0.494240	1.989314	-3.385160
H	-1.458192	2.061751	-1.882093
H	-0.276154	0.748249	-2.112648
C	3.638022	2.258319	-3.937854
N	3.197148	1.979255	-2.566994
C	4.077907	2.586273	-1.558737
H	3.561716	3.330268	-4.142071
H	2.996271	1.729691	-4.646043
H	4.678112	1.952788	-4.121835
H	3.200951	0.967333	-2.425880
H	4.071071	3.674318	-1.671608
H	5.119476	2.245567	-1.643809

H	3.710344	2.348360	-0.558684
C	1.979604	-3.314296	3.566387
N	3.205420	-2.850526	2.923376
C	4.390874	-3.037332	3.750839
H	2.034137	-4.396933	3.720094
H	1.127884	-3.114417	2.913516
H	1.788508	-2.845964	4.547009
H	3.107442	-1.869323	2.679298
H	4.579073	-4.106901	3.889851
H	4.312447	-2.581173	4.753332
H	5.262602	-2.609193	3.249759
3MA4DMA			
O	-4.231056	-1.462404	-2.603679
O	-2.463978	-3.158756	-0.008372
O	-3.513832	0.143429	-0.383087
O	-1.831492	-2.748063	-2.124534
O	-4.054620	-0.617563	1.667651
C	-4.141445	-2.348948	-1.515320
C	-4.841128	-1.821261	-0.248710
C	-2.683876	-2.767529	-1.251592
C	-4.095808	-0.699312	0.451975
H	-4.656183	-3.264442	-1.827890
H	-4.989020	-2.614982	0.481573
H	-5.824133	-1.447532	-0.551416
H	-3.928956	-0.603984	-2.276841
H	-1.488436	-3.335355	0.136060
H	-2.976698	0.939894	0.042122
O	-1.068905	4.669820	-0.224966
O	-2.093654	2.485559	2.438150
O	1.224429	3.072527	-0.153679
O	-2.104923	2.129259	0.213007
O	1.633983	2.182506	1.869029
C	-1.163620	4.187032	1.097018
C	0.230046	4.101392	1.771054
C	-1.865201	2.815436	1.243732
C	1.094984	3.065778	1.072789
H	-1.770122	4.899620	1.661561
H	0.125035	3.853309	2.824549
H	0.714660	5.077653	1.676134
H	-0.279419	4.245756	-0.592756
H	-1.943590	1.057414	2.858982
H	1.084911	1.371100	-2.892976
O	3.024021	-1.605915	-2.072838
O	2.837571	0.217334	0.847089

O	0.755056	-3.192816	-1.718799
O	1.087624	-0.267696	-0.485058
O	0.151538	-3.348683	0.438247
C	3.030894	-1.647628	-0.643708
C	2.481132	-2.989475	-0.103449
C	2.240933	-0.456325	-0.045819
C	1.018247	-3.187537	-0.408954
H	4.074016	-1.563379	-0.341554
H	2.643408	-3.035298	0.974424
H	3.041278	-3.798162	-0.583795
H	2.173980	-1.970664	-2.356539
H	2.131950	1.412493	1.363933
H	-0.229095	-3.134604	-1.877107
C	-0.435157	2.827380	-2.832444
N	0.124676	1.507769	-2.444474
C	-0.758536	0.364598	-2.789581
H	-0.712276	2.796337	-3.886706
H	0.328251	3.586836	-2.676624
H	-1.302305	3.046078	-2.211113
H	0.321765	1.479257	-1.432802
H	-0.903773	0.334084	-3.869627
H	-1.714859	0.491424	-2.287911
H	-0.285487	-0.544701	-2.436301
C	3.065651	1.017530	-4.833142
N	2.763172	1.148564	-3.404190
C	3.574986	2.184333	-2.746761
H	2.781348	1.933753	-5.358849
H	2.494215	0.189141	-5.257851
H	4.132378	0.834397	-5.027276
H	2.952659	0.252834	-2.948080
H	3.365716	3.157263	-3.200975
H	4.653535	1.993352	-2.838042
H	3.310447	2.240375	-1.689965
C	3.466521	-1.781929	4.158573
N	4.051041	-1.863707	2.827308
C	5.501419	-1.999695	2.858688
H	3.614942	-2.728309	4.689784
H	2.389888	-1.613355	4.077454
H	3.892898	-0.979154	4.786655
H	3.792887	-1.040274	2.286556
H	5.776013	-2.961924	3.304166
H	6.012142	-1.209012	3.436888
H	5.896740	-1.981749	1.840087
C	-0.543215	-0.493888	2.566262

N	-1.809050	0.018204	3.153709
C	-1.899914	-0.102031	4.625472
H	0.292835	0.055972	2.995994
H	-0.546739	-0.321514	1.491005
H	-0.440856	-1.561061	2.764215
H	-2.621188	-0.433642	2.706048
H	-1.096843	0.477093	5.081017
H	-1.811561	-1.147898	4.923160
H	-2.860823	0.293904	4.952385

3SA1MA

S	1.217595	-2.689695	0.721777
O	1.130932	-1.866564	-0.502724
O	1.992740	-3.874736	0.707111
O	1.780511	-1.773031	1.864525
O	-0.247217	-3.014963	1.147559
H	1.267821	-0.931351	1.919473
H	-0.923632	-2.394222	0.730086
S	-0.005962	1.710718	1.375503
O	0.124698	0.374491	1.901792
O	-0.199895	1.811605	-0.070342
O	-1.148471	2.481154	2.089322
O	1.184193	2.614232	1.821269
H	-2.020221	2.148307	1.708522
H	1.994831	2.264650	1.356844
S	3.154820	1.084258	-1.100587
O	2.866640	1.222175	0.322677
O	4.276313	1.730617	-1.677183
O	3.273468	-0.444442	-1.436789
O	1.847777	1.530922	-1.884585
H	2.517812	-0.965816	-1.066216
H	1.086872	1.598883	-1.263313
O	-4.849167	-0.648952	0.094029
O	-2.745618	1.908605	-1.290175
O	-1.110215	-1.475944	-2.046459
O	-3.197238	1.388508	0.857781
O	-2.080448	-1.576148	-0.021926
C	-4.218911	0.085837	-0.910635
C	-3.373521	-0.783536	-1.878378
C	-3.349805	1.206847	-0.335252
C	-2.124546	-1.322161	-1.224699
H	-5.008265	0.558449	-1.502392
H	-3.098416	-0.230408	-2.775257
H	-3.992478	-1.635016	-2.176624
H	-4.158181	-1.007812	0.666866

H	-2.022139	2.434636	-0.905817
H	-0.298576	-1.746931	-1.552550
3SA1MA1DMA			
S	-0.097409	-2.534249	-1.295307
O	0.211613	-2.292740	0.124321
O	-0.741208	-3.743608	-1.666372
O	-0.973613	-1.350485	-1.816365
O	1.256031	-2.399416	-2.066957
H	-0.549523	-0.436031	-1.667114
H	1.925200	-1.844624	-1.553313
S	-0.413107	2.091721	-0.689963
O	-0.016824	0.983795	-1.571840
O	-0.124163	1.767758	0.739592
O	0.500705	3.316891	-1.058397
O	-1.781067	2.553456	-0.886475
H	1.452592	3.045403	-0.923280
H	-3.087133	1.493276	-1.177980
S	-2.353290	-0.562684	2.236776
O	-2.821268	-0.752509	0.867876
O	-3.198178	-0.913112	3.324255
O	-0.985411	-1.338391	2.354302
O	-1.947823	0.939302	2.437923
H	-0.685028	-1.676129	1.474064
H	-1.268996	1.250806	1.766473
O	5.274050	0.949136	-0.680636
O	2.452181	1.436102	1.464019
O	2.686406	-2.062468	1.278088
O	2.938541	2.349664	-0.540232
O	3.032918	-1.049718	-0.698859
C	4.592510	0.958901	0.543244
C	4.422997	-0.450283	1.158072
C	3.238550	1.673083	0.424969
C	3.318317	-1.222776	0.484891
H	5.205603	1.547422	1.233309
H	4.213448	-0.399856	2.225643
H	5.364827	-0.988167	1.016631
H	4.665914	0.602792	-1.345957
H	1.520442	1.720381	1.277738
H	1.872903	-2.396316	0.835846
C	-5.085536	1.613035	-0.649468
N	-3.896539	0.838082	-1.096291
C	-4.080388	0.075580	-2.362465
H	-5.353676	2.335356	-1.419445
H	-4.829327	2.135878	0.270599

H -5.915391 0.930470 -0.470166
H -3.608420 0.187359 -0.338323
H -4.282733 0.773591 -3.174093
H -4.916125 -0.613628 -2.245947
H -3.169720 -0.485666 -2.564132

3SA1MA2DMA

S 2.023226 2.035483 -1.004751
O 1.636145 2.388860 0.398645
O 3.399189 2.290694 -1.334677
O 1.600221 0.644840 -1.296236
O 1.160740 3.000925 -1.928833
H 0.263042 -0.047060 -1.857899
H 0.252095 3.124511 -1.551439
S -0.353365 -1.986497 -1.239950
O -0.491431 -0.666783 -2.097659
O -0.670306 -1.583226 0.179940
O -1.395205 -2.872646 -1.753753
O 1.008160 -2.485664 -1.353184
H -2.736467 -2.901160 -0.750084
H 2.659979 -1.531754 -1.387603
S 1.970890 -0.594629 2.517836
O 3.086904 -0.557470 1.586080
O 2.253084 -0.667777 3.911457
O 1.023879 0.615652 2.201058
O 1.042619 -1.828548 2.180851
H 1.376133 1.227818 1.478148
H 0.489435 -1.690989 1.360700
O -3.905920 2.446724 -1.122210
O -1.865918 0.765353 0.498149
O -0.572923 3.540261 1.303635
O -3.910185 -0.175025 0.480455
O -1.281968 3.353356 -0.820270
C -3.742290 2.224611 0.266915
C -2.907771 3.328123 0.943652
C -3.178561 0.805323 0.449734
C -1.502399 3.408812 0.388622
H -4.743043 2.214346 0.700887
H -2.861446 3.185360 2.023814
H -3.408591 4.279982 0.742779
H -3.032093 2.694454 -1.466757
H -1.481977 -0.154702 0.441897
H 0.323112 3.356589 0.914333
C 3.999957 -2.883490 -0.604783
N 3.597366 -1.495616 -0.959022

C	4.559480	-0.766711	-1.831926
H	4.115207	-3.467476	-1.516941
H	3.216546	-3.316052	0.012553
H	4.938926	-2.850648	-0.053958
H	3.442796	-0.974321	-0.075955
H	4.631171	-1.284562	-2.788116
H	5.533194	-0.754174	-1.342932
H	4.202737	0.252352	-1.967058
C	-4.793675	-3.249476	-0.754200
N	-3.537278	-2.843528	-0.073511
C	-3.196116	-3.635005	1.138004
H	-4.713679	-4.287987	-1.074333
H	-4.940102	-2.607728	-1.621491
H	-5.632174	-3.133285	-0.068143
H	-3.607273	-1.833639	0.186536
H	-3.085673	-4.683702	0.863563
H	-3.987722	-3.524560	1.878793
H	-2.255185	-3.256646	1.532600

3SA1MA3DMA

S	-4.003668	1.736277	-0.104133
O	-4.775880	0.451467	-0.555723
O	-4.903226	2.835439	-0.208249
O	-3.330171	1.479537	1.162483
O	-2.884165	1.924993	-1.203650
H	-2.081932	0.160424	1.604185
H	-2.033236	1.454803	-0.927321
S	0.437844	0.296608	-1.084972
O	-0.641693	1.040038	-0.305486
O	-0.179155	-0.692225	-1.980130
O	1.222382	1.316232	-1.836303
O	1.314391	-0.385177	-0.076574
H	2.732372	1.457268	-1.453830
H	1.418290	-2.068350	-0.298451
S	-2.569544	-2.806795	-0.250152
O	-1.331329	-2.802910	0.606866
O	-3.273264	-4.053967	-0.272277
O	-3.360803	-1.614479	0.124636
O	-2.044986	-2.581209	-1.742369
H	-4.248088	-0.385750	-0.382307
H	-1.461731	-1.778995	-1.793801
O	3.364642	-0.296699	1.788607
O	6.239580	-0.464470	-0.381158
O	2.903014	2.961214	0.425094
O	4.391147	-1.737409	-0.334456

O	3.649744	1.406848	-1.024750
C	4.631318	0.053293	1.302492
C	4.773433	1.574187	1.034992
C	5.030386	-0.813685	0.102427
C	3.681165	2.069874	0.112478
H	5.351213	-0.198643	2.089602
H	5.748613	1.780030	0.587007
H	4.690781	2.111542	1.978491
H	2.715235	-0.268508	1.058719
H	6.427975	-1.051722	-1.128326
H	1.285196	3.470847	-0.183810
C	-0.420972	-0.046536	2.834718
N	-1.674141	-0.559349	2.224122
C	-2.723442	-0.963022	3.198611
H	-0.648560	0.843545	3.421271
H	0.276227	0.188907	2.034406
H	0.001620	-0.813547	3.483762
H	-1.465187	-1.379282	1.609444
H	-3.000089	-0.101217	3.804336
H	-2.335550	-1.762586	3.829266
H	-3.582120	-1.314361	2.632308
C	1.484481	-3.569050	-1.736395
N	1.231883	-3.097497	-0.349309
C	2.023435	-3.798334	0.693836
H	2.541079	-3.430503	-1.962539
H	0.876868	-2.970811	-2.411164
H	1.212219	-4.621339	-1.816084
H	0.217331	-3.160762	-0.111980
H	3.080383	-3.619600	0.509909
H	1.793392	-4.863354	0.665601
H	1.753144	-3.390032	1.666355
C	-0.199023	4.381901	0.948983
N	0.258159	3.619567	-0.240313
C	-0.117088	4.221891	-1.549368
H	0.199496	5.395416	0.908326
H	0.170166	3.882267	1.843166
H	-1.288034	4.408115	0.962503
H	-0.136328	2.645296	-0.206856
H	0.308343	5.222668	-1.624394
H	-1.203478	4.264754	-1.618370
H	0.274999	3.576103	-2.331948
3SA1MA4DMA			
S	4.823703	-0.748817	-0.666743
O	5.118946	0.754359	-0.999301

O	5.997308	-1.490591	-0.986142
O	4.265844	-0.845351	0.677767
O	3.696025	-1.161485	-1.684096
H	2.803142	-0.030919	1.427553
H	2.773811	-1.024830	-1.282733
S	0.096934	-0.531891	-1.009430
O	1.426971	-1.106477	-0.509247
O	0.367820	0.538817	-1.982337
O	-0.653582	-1.664512	-1.637740
O	-0.638133	-0.023333	0.174023
H	-1.949120	-2.062740	-0.905941
H	-2.227338	1.793028	0.316119
S	2.108736	3.123520	-0.103489
O	1.039974	2.585828	0.806367
O	2.307043	4.541285	-0.003294
O	3.312653	2.285204	0.080876
O	1.570562	2.873071	-1.585338
H	4.399070	1.369415	-0.666019
H	1.228914	1.942445	-1.696132
O	-2.239965	-0.128615	2.372214
O	-5.415256	-0.702198	0.785447
O	-1.418662	-3.388244	1.044765
O	-3.860031	0.859574	0.377245
O	-2.755690	-2.159632	-0.286882
C	-3.472263	-0.763376	2.148429
C	-3.343973	-2.301100	1.994088
C	-4.256267	-0.119286	0.994040
C	-2.406713	-2.684824	0.868253
H	-4.079679	-0.587022	3.042984
H	-4.333112	-2.719692	1.793209
H	-2.954946	-2.724653	2.919052
H	-1.697876	-0.177742	1.558746
H	-5.883114	-0.314826	-0.052895
H	0.034253	-3.747197	0.030377
C	1.315452	-0.461883	2.812619
N	2.247580	0.476289	2.138323
C	3.199191	1.164288	3.051375
H	1.893598	-1.230435	3.326322
H	0.671087	-0.899681	2.056198
H	0.707607	0.086880	3.531386
H	1.707802	1.205398	1.615335
H	3.807205	0.418672	3.562359
H	2.635740	1.753878	3.774199
H	3.827742	1.813069	2.446847

C	-1.770144	3.081256	-1.235835
N	-1.648835	2.638877	0.180703
C	-2.043434	3.662015	1.181095
H	-2.812005	3.323758	-1.443238
H	-1.427598	2.267367	-1.871728
H	-1.134434	3.951112	-1.391722
H	-0.654173	2.383506	0.359731
H	-3.068758	3.977863	0.990957
H	-1.361605	4.507975	1.109916
H	-1.975580	3.214378	2.171216
C	1.887842	-4.402990	0.702310
N	1.017112	-3.752012	-0.307275
C	1.104126	-4.332369	-1.673453
H	1.655246	-5.466548	0.758436
H	1.703530	-3.939485	1.670029
H	2.931448	-4.262448	0.422547
H	1.254832	-2.721120	-0.371770
H	0.802232	-5.379780	-1.647378
H	2.131441	-4.247841	-2.027168
H	0.445128	-3.753942	-2.317332
C	-6.764468	1.646785	-1.356111
N	-6.543025	0.195485	-1.435573
C	-5.599187	-0.184827	-2.500684
H	-5.835730	2.120321	-1.033485
H	-7.533787	1.857074	-0.610570
H	-7.072541	2.080777	-2.316306
H	-7.431447	-0.271006	-1.594537
H	-4.614378	0.215815	-2.256194
H	-5.903128	0.191949	-3.485677
H	-5.518862	-1.271987	-2.542720
3SA2MA			
S	-0.501826	0.189184	2.202607
O	0.355336	0.211867	3.337269
O	0.067307	-0.167580	0.908590
O	-1.782675	-0.624966	2.463078
O	-1.194004	1.648933	2.041452
H	-1.941553	-1.345904	1.750786
H	-0.534509	2.267359	1.645730
O	-1.587211	-5.162491	0.176532
O	-2.654611	-2.057271	-1.232185
O	1.195345	-2.496472	-1.828478
O	-2.023743	-2.572895	0.873597
O	0.945938	-3.814681	-0.025168
C	-1.798669	-4.235878	-0.846596

C	-0.593844	-4.093189	-1.818248
C	-2.188826	-2.860481	-0.303345
C	0.606476	-3.386030	-1.230739
H	-2.642569	-4.602865	-1.435671
H	-0.884095	-3.553212	-2.718078
H	-0.293459	-5.108002	-2.094091
H	-0.878978	-4.825749	0.740520
H	-2.815174	-1.140950	-0.893883
H	1.728868	-3.297516	0.324792
S	0.211563	2.742315	-1.002252
O	0.592717	2.899462	0.408501
O	-1.017896	3.357784	-1.408216
O	1.339562	3.277077	-1.903918
O	0.210247	1.212909	-1.333924
H	2.231130	2.868749	-1.617713
H	0.083277	0.659852	-0.509787
O	5.631516	0.458792	-0.931760
O	3.137774	1.998652	1.138013
O	3.112185	-0.965269	-0.858365
O	3.490544	2.119264	-1.085587
O	3.008318	-2.386488	0.879569
C	4.948841	0.740087	0.257654
C	4.504576	-0.523590	1.026459
C	3.782216	1.697136	0.022254
C	3.466630	-1.390180	0.345218
H	5.654134	1.273939	0.903260
H	4.107807	-0.264447	2.010487
H	5.386988	-1.146792	1.191953
H	4.973498	0.201906	-1.589935
H	2.327006	2.515971	0.944088
H	2.402334	-1.558104	-1.247510
S	-3.936054	1.461890	-0.316595
O	-5.286238	1.053751	-0.461720
O	-2.846732	0.498374	-0.425293
O	-3.688604	2.615737	-1.357556
O	-3.756167	2.182688	1.082009
H	-2.735844	2.861230	-1.404686
H	-2.903457	1.915657	1.492131
3SA2MA1DMA			
S	0.300172	0.210326	-2.329121
O	1.224530	-0.287968	-3.291935
O	0.973253	0.207987	-0.908929
O	0.102327	1.742946	-2.624680
O	-1.013512	-0.403394	-2.210135

H	-0.552235	2.123993	-1.982009
H	-1.296085	-3.186074	-1.044655
O	-0.199386	4.441728	-1.416360
O	-1.979841	3.263321	1.440247
O	1.906607	2.652208	1.618269
O	-1.547654	2.242916	-0.511437
O	2.265607	3.528531	-0.424082
C	-0.563854	4.421893	-0.063050
C	0.624360	4.568048	0.922286
C	-1.410112	3.184730	0.267113
C	1.666707	3.482471	0.758811
H	-1.228562	5.273872	0.113862
H	0.258418	4.544593	1.946796
H	1.095246	5.533977	0.724459
H	0.706137	4.111439	-1.510471
H	-2.521345	2.450063	1.639488
H	2.938876	2.780498	-0.524949
S	-0.575512	-2.191192	1.315078
O	-0.043421	-3.017179	0.187016
O	-1.969600	-2.512460	1.594708
O	0.211388	-2.633757	2.603036
O	-0.325404	-0.762662	1.081072
H	1.191614	-2.572933	2.423339
H	0.391774	-0.185977	-0.176486
O	5.346939	-1.625625	1.690107
O	2.595553	-2.771604	-0.303246
O	3.348109	0.440814	1.148350
O	2.787568	-2.435917	1.918105
O	3.966776	1.565530	-0.695307
C	4.655970	-1.902874	0.500355
C	4.654163	-0.712090	-0.480918
C	3.242760	-2.403323	0.786620
C	3.960635	0.548223	-0.015943
H	5.180199	-2.724188	-0.000820
H	4.181206	-0.992359	-1.426087
H	5.688967	-0.446261	-0.708377
H	4.691050	-1.327781	2.333980
H	1.643315	-2.968540	-0.100000
H	2.845110	1.273839	1.362997
S	-4.181070	0.265902	0.982629
O	-5.517272	0.630598	0.655258
O	-3.416978	1.089417	1.904428
O	-4.213679	-1.210293	1.491650
O	-3.309107	0.100108	-0.342440

H	-3.295086	-1.589735	1.637661
H	-2.631778	0.819248	-0.404032
C	-1.398589	-3.684083	-3.060041
N	-1.924271	-2.988036	-1.853406
C	-3.336575	-3.311792	-1.506512
H	-1.409731	-4.759652	-2.888265
H	-0.380451	-3.343329	-3.240951
H	-2.023711	-3.436021	-3.916817
H	-1.804639	-1.968838	-1.995831
H	-3.418236	-4.381029	-1.315233
H	-3.980988	-3.028096	-2.337549
H	-3.611834	-2.754233	-0.615472

3SA2MA2DMA

S	0.414846	0.486378	-2.026405
O	-0.520737	0.088510	-3.052292
O	0.291045	-0.223151	-0.739073
O	1.856803	0.159069	-2.586120
O	0.372773	1.972122	-1.803334
H	2.519076	0.127055	-1.852846
H	-1.126103	2.657273	-2.137754
O	5.569021	-2.158895	-0.475878
O	3.749746	0.160941	1.535569
O	1.711910	-3.211278	1.230763
O	3.745833	-0.138322	-0.699940
O	2.948075	-3.308862	-0.643577
C	4.937757	-1.704568	0.686956
C	4.071643	-2.792758	1.383250
C	4.086230	-0.459568	0.422746
C	2.790426	-3.126589	0.654207
H	5.726898	-1.425527	1.388672
H	3.805927	-2.484949	2.393490
H	4.684352	-3.697415	1.435181
H	4.889709	-2.249529	-1.156559
H	3.132938	0.919289	1.360837
H	2.064712	-3.461837	-1.097267
S	-2.156701	1.722745	1.148744
O	-3.005245	1.391999	-0.032058
O	-1.453781	2.982659	0.900825
O	-2.877667	1.644413	2.415023
O	-1.097046	0.547747	1.289286
H	-2.763191	0.030345	3.033888
H	-0.543037	0.366712	0.459977
O	-3.187787	-4.530241	-0.593486
O	-3.292128	-0.996811	-1.141961

O	-0.625456	-3.318844	0.005787
O	-3.358259	-2.185152	0.771995
O	0.621625	-3.623146	-1.836307
C	-3.047078	-3.339472	-1.327341
C	-1.722805	-3.263992	-2.116224
C	-3.248210	-2.109625	-0.441557
C	-0.459464	-3.425384	-1.304664
H	-3.858442	-3.324702	-2.061109
H	-1.631326	-2.301450	-2.630635
H	-1.714442	-4.042694	-2.880854
H	-2.663373	-4.421019	0.209369
H	-3.275443	-0.176997	-0.578783
H	0.264317	-3.325165	0.467979
S	2.043298	3.539120	0.956310
O	3.178322	4.293105	1.363226
O	1.959883	2.112717	1.235321
O	0.777841	4.225345	1.597220
O	1.850133	3.736324	-0.591669
H	-0.042120	3.686861	1.432068
H	1.350233	2.969813	-1.006801
C	-2.196714	4.440984	-1.965111
N	-2.124750	2.974802	-2.204331
C	-2.693208	2.516256	-3.501138
H	-1.629056	4.956966	-2.738821
H	-1.770884	4.644566	-0.985187
H	-3.238180	4.761031	-1.992418
H	-2.586650	2.471703	-1.421518
H	-2.183690	3.033575	-4.313455
H	-3.759695	2.739505	-3.528059
H	-2.514831	1.446387	-3.587953
C	-1.503984	-1.484803	3.740454
N	-2.805158	-0.999463	3.203296
C	-3.983751	-1.305498	4.054858
H	-1.320160	-1.018233	4.707794
H	-0.721750	-1.205992	3.039013
H	-1.544424	-2.568090	3.849570
H	-2.961502	-1.408422	2.259236
H	-3.851532	-0.846304	5.034013
H	-4.083760	-2.385284	4.159103
H	-4.872609	-0.898601	3.575515
3SA2MA3DMA			
S	0.048475	0.488881	1.453822
O	-0.133548	1.838505	1.946185
O	-0.263421	0.310188	0.023912

O	1.602269	0.221511	1.640963
O	-0.686645	-0.531413	2.255706
H	1.864136	-0.725523	1.569585
H	-2.032228	0.475860	3.025061
O	5.835953	-1.913565	2.069972
O	3.394470	-3.263596	-0.139328
O	4.082889	0.123962	-1.163211
O	3.186605	-1.900247	1.644883
O	5.256534	0.750400	0.646459
C	5.376876	-2.338225	0.817315
C	5.773868	-1.355417	-0.330518
C	3.858845	-2.504246	0.825360
C	4.961602	-0.081767	-0.328400
H	5.845267	-3.299461	0.595379
H	5.628398	-1.840220	-1.295271
H	6.828965	-1.118619	-0.183805
H	5.157118	-1.329940	2.436613
H	2.397384	-3.199185	-0.179567
H	4.655538	1.551561	0.620365
S	-3.926089	0.889934	-0.191216
O	-3.311478	1.996700	0.589473
O	-4.300473	-0.218818	0.718531
O	-4.934553	1.264578	-1.144304
O	-2.716769	0.295497	-1.089725
H	-0.518068	-1.007438	-2.155291
H	-1.874775	0.292316	-0.562845
O	1.408398	4.486224	-2.441943
O	-1.301073	3.735012	-0.266634
O	2.395270	2.165584	-1.162418
O	-0.543266	2.576168	-2.052133
O	3.644333	2.889638	0.551234
C	0.744427	4.441177	-1.201637
C	1.693769	4.152290	-0.012936
C	-0.437502	3.466499	-1.232773
C	2.674633	3.013070	-0.180439
H	0.321279	5.434450	-1.036108
H	1.114972	3.927168	0.888821
H	2.291505	5.040637	0.199230
H	1.562180	3.568107	-2.696691
H	-2.005606	3.052492	-0.167573
H	3.057099	1.415136	-1.156648
S	-0.503242	-3.229285	-0.464827
O	-0.641522	-4.652575	-0.611778
O	0.859252	-2.685425	-0.386640

O	-1.291826	-2.452837	-1.476921
O	-1.219574	-2.899244	0.945909
H	-2.959922	-2.483798	-1.072460
H	-0.937442	-2.030097	1.326619
C	-3.970312	0.398569	3.784346
N	-2.810062	1.138794	3.218485
C	-2.318062	2.249936	4.079807
H	-3.671947	-0.069087	4.722472
H	-4.284895	-0.343706	3.056150
H	-4.784649	1.100547	3.961912
H	-3.058701	1.514667	2.274925
H	-2.029391	1.845772	5.049919
H	-3.117578	2.979855	4.204311
H	-1.456982	2.695795	3.589976
C	1.309058	-0.608325	-3.038926
N	-0.090336	-0.228706	-2.703244
C	-0.949115	0.071139	-3.879905
H	1.289687	-1.500111	-3.664294
H	1.843648	-0.820131	-2.117434
H	1.784707	0.214332	-3.570796
H	-0.082990	0.596711	-2.087061
H	-1.011875	-0.818292	-4.506358
H	-0.512682	0.899612	-4.434743
H	-1.932625	0.355773	-3.513631
C	-4.837383	-2.323208	-1.955665
N	-3.963223	-2.539816	-0.772650
C	-4.189670	-3.830693	-0.068736
H	-4.636443	-3.097689	-2.695558
H	-4.624954	-1.338940	-2.367552
H	-5.880788	-2.364624	-1.644661
H	-4.100606	-1.740239	-0.115085
H	-3.976287	-4.652680	-0.750820
H	-5.225543	-3.878461	0.267305
H	-3.506679	-3.881702	0.776128

3SA2MA4DMA

S	0.072904	1.602209	-1.475773
O	0.872345	0.535758	-2.042611
O	-0.347227	1.052962	0.073024
O	0.736481	2.845585	-1.142759
O	-1.230221	1.799964	-2.136682
H	-1.100938	3.259524	1.136071
H	-2.533697	0.805134	-2.511236
O	3.111146	4.728148	1.612246
O	1.615815	1.730424	1.687638

O	4.553435	0.677684	1.337402
O	0.455976	3.613597	2.084951
O	4.213579	2.557349	0.159838
C	2.839577	3.644002	2.476085
C	4.012988	2.649859	2.550795
C	1.501184	2.992863	2.071181
C	4.265244	1.957619	1.230675
H	2.684762	4.081102	3.465701
H	3.851471	1.898257	3.323891
H	4.909072	3.222199	2.809595
H	3.355861	4.345937	0.755477
H	0.812364	1.440298	1.164769
H	4.092978	1.818007	-1.404558
S	-1.652393	-2.549959	-0.284205
O	-1.484714	-2.206859	-1.700979
O	-3.177365	-2.925674	-0.046348
O	-0.919127	-3.727241	0.153552
O	-1.386647	-1.360281	0.585993
H	0.772600	-3.337581	0.832162
H	-0.676710	0.120775	0.053036
O	4.346865	-2.878737	-2.421165
O	0.894596	-2.332354	-3.064968
O	4.256137	-0.488288	-1.018500
O	1.915540	-2.685306	-1.092353
O	3.924867	1.345933	-2.262076
C	3.264498	-2.236105	-3.053110
C	3.520876	-0.733489	-3.306738
C	1.953960	-2.444209	-2.282180
C	3.922561	0.049128	-2.078933
H	3.135425	-2.715680	-4.025555
H	2.640045	-0.250312	-3.732276
H	4.338014	-0.633269	-4.028882
H	4.495451	-2.389446	-1.599540
H	0.066091	-2.334381	-2.523005
H	4.566796	0.261903	0.428224
S	-4.468870	0.492774	0.609563
O	-5.712218	0.671779	1.301767
O	-3.919113	1.706862	-0.029208
O	-3.403686	0.052968	1.739613
O	-4.448888	-0.623020	-0.393018
H	-2.665152	-0.455230	1.322861
H	-3.743516	-2.110905	-0.156378
C	2.535990	-4.236244	1.434971
N	1.409073	-3.291525	1.648605

C	1.831793	-1.879428	1.858433
H	3.072393	-3.936972	0.537726
H	2.129611	-5.238163	1.299047
H	3.192179	-4.217671	2.305872
H	0.822309	-3.611324	2.467837
H	2.377724	-1.541563	0.981844
H	2.459842	-1.820025	2.747461
H	0.936456	-1.275150	1.986137
C	-2.817896	3.899719	2.070420
N	-2.061342	3.513319	0.850129
C	-1.972373	4.580701	-0.184573
H	-2.314962	4.737609	2.550811
H	-2.845594	3.043426	2.741942
H	-3.834703	4.165896	1.787365
H	-2.533448	2.679323	0.443982
H	-1.468057	5.444856	0.246105
H	-2.980356	4.845730	-0.501849
H	-1.394146	4.191934	-1.019144
C	-4.328396	1.545008	-3.206654
N	-3.459139	0.409231	-2.801744
C	-3.260685	-0.616299	-3.859410
H	-3.861491	2.070737	-4.038987
H	-4.434562	2.203341	-2.348333
H	-5.304455	1.161899	-3.504940
H	-3.858657	-0.028329	-1.943870
H	-2.756476	-0.156369	-4.709091
H	-4.231771	-1.003459	-4.169030
H	-2.650540	-1.416154	-3.446783
C	0.130991	-3.791878	5.176872
N	-0.270428	-4.200029	3.823786
C	-1.653232	-3.799416	3.499387
H	0.147151	-2.700716	5.234894
H	1.135691	-4.161073	5.395535
H	-0.553078	-4.159097	5.954840
H	-0.215891	-5.213646	3.765734
H	-1.718908	-2.709751	3.477262
H	-2.378947	-4.173101	4.234315
H	-1.914716	-4.166914	2.507973
3SA3MA			
S	-1.375151	0.695402	1.764449
O	-1.040454	2.023833	2.214090
O	-2.721909	0.215584	1.946679
O	-1.021052	0.514422	0.258951
O	-0.376292	-0.262283	2.517957

H	-0.336794	1.197173	-0.055322
H	-0.420305	-1.177362	2.149982
O	1.487318	4.178644	-2.459445
O	0.259163	3.991932	0.853973
O	3.836034	2.831218	-1.676019
O	0.623339	2.313107	-0.608795
O	4.424349	3.108927	0.474523
C	1.505429	4.502752	-1.100000
C	2.933302	4.705514	-0.522766
C	0.737107	3.481041	-0.260052
C	3.802476	3.468712	-0.514386
H	0.981351	5.454652	-0.996401
H	2.885990	5.086221	0.497022
H	3.422742	5.451986	-1.155205
H	1.969414	3.350048	-2.576186
H	-0.211526	3.307190	1.387984
H	4.429182	2.029818	-1.620235
S	0.938844	-3.018946	0.600855
O	-0.302610	-2.748732	1.327225
O	1.938153	-3.830140	1.246302
O	0.578908	-3.699657	-0.741670
O	1.526239	-1.632011	0.241680
H	-0.351854	-3.441346	-1.080769
H	2.552120	-1.645755	0.213208
O	6.591404	-1.680730	-1.656303
O	5.938662	0.944974	0.690358
O	4.680510	-3.465213	1.285346
O	5.437439	0.704437	-1.493676
O	4.061951	-1.577291	0.231945
C	6.749924	-0.991867	-0.440949
C	6.379741	-1.915921	0.722767
C	5.952614	0.309270	-0.454306
C	4.925073	-2.308401	0.710737
H	7.800523	-0.694460	-0.303395
H	6.575964	-1.420121	1.678827
H	6.993925	-2.816013	0.684224
H	6.118179	-1.083181	-2.253213
H	5.390845	1.781519	0.621415
H	3.714146	-3.655540	1.289534
O	-4.117552	-3.286130	-2.894800
O	-2.822526	-3.491178	0.440313
O	-3.941327	-0.901393	-0.972713
O	-1.800585	-3.253165	-1.555025
O	-6.149852	-0.629160	-0.622884

C	-4.164798	-3.605924	-1.527588
C	-5.305558	-2.846354	-0.848012
C	-2.807989	-3.405097	-0.870639
C	-5.176612	-1.339017	-0.819509
H	-4.372147	-4.681644	-1.398899
H	-5.409988	-3.175535	0.190051
H	-6.240947	-3.084619	-1.355512
H	-3.190516	-3.146045	-3.129218
H	-1.931719	-3.307491	0.816025
H	-3.889917	0.085610	-0.872993
S	-4.925608	2.492188	0.183774
O	-3.900916	1.773822	-0.564501
O	-4.957281	3.911966	0.159525
O	-6.336757	1.975902	-0.254345
O	-4.829197	1.995749	1.691882
H	-6.304112	0.985257	-0.403217
H	-4.089445	1.353616	1.790686
3SA3MA1DMA			
S	4.124235	-2.172390	-0.791205
O	3.954456	-3.591621	-0.945907
O	5.349186	-1.673791	-0.199906
O	3.984500	-1.409887	-2.144778
O	2.894007	-1.692540	0.058451
H	3.029286	-1.323433	-2.474340
H	2.993457	-0.710014	0.260367
O	2.432858	3.496170	-0.795871
O	2.095366	2.476126	2.617637
O	5.477032	0.998311	0.420203
O	0.535694	2.752517	1.018679
O	3.234003	0.809474	0.461137
C	2.778069	3.510293	0.566350
C	4.186255	2.952761	0.827366
C	1.686418	2.851785	1.418936
C	4.262194	1.474264	0.546623
H	2.784693	4.564131	0.869712
H	4.485541	3.111078	1.867639
H	4.905081	3.477939	0.196419
H	2.208276	2.587757	-1.064486
H	1.395940	1.950334	3.070629
H	5.468043	0.025735	0.215578
S	-1.228975	1.637170	3.760095
O	-1.196170	2.625422	4.781186
O	-0.003049	0.849583	3.527624
O	-2.411547	0.666902	4.039237

O	-1.634947	2.236448	2.364785
H	-2.416209	-0.066866	3.352143
H	-0.800383	2.401124	1.822052
O	-2.775592	-3.905746	1.725228
O	-0.156808	-1.730309	2.380880
O	1.779854	-4.603874	0.568991
O	-2.326001	-1.209711	2.221435
O	0.493232	-3.250973	-0.666841
C	-1.610025	-3.289551	1.235534
C	-0.438350	-4.270038	1.310660
C	-1.385214	-1.977735	1.996307
C	0.652346	-3.967765	0.306256
H	-1.730419	-2.992727	0.185287
H	-0.840996	-5.257752	1.067784
H	-0.008711	-4.339913	2.309943
H	-3.525543	-3.548341	1.220237
H	-0.080424	-0.839727	2.802711
H	2.475412	-4.336804	-0.073189
S	0.621076	-0.040898	-2.457502
O	-0.545050	0.153609	-3.332260
O	1.591010	-0.993482	-2.996141
O	1.192265	1.257237	-2.060931
O	0.061350	-0.662727	-1.093589
H	-0.010753	2.507828	-2.234810
H	0.257904	-1.631740	-1.037179
O	-5.761779	1.374267	-1.228217
O	-3.080557	-0.363704	-2.845817
O	-4.219905	-0.481607	0.356214
O	-3.191724	1.750912	-2.072239
O	-4.515715	-2.664175	-0.095756
C	-5.192139	0.398182	-2.061675
C	-5.467030	-1.043595	-1.592538
C	-3.702478	0.671187	-2.319106
C	-4.691758	-1.498124	-0.377274
H	-5.682673	0.515124	-3.034690
H	-5.260625	-1.764036	-2.383981
H	-6.531906	-1.116408	-1.351252
H	-5.248184	1.389828	-0.411400
H	-2.110620	-0.175729	-3.006667
H	-3.657683	-0.826516	1.087436
C	-0.807393	4.357769	-1.672080
N	-0.805323	3.126376	-2.506724
C	-0.711171	3.372251	-3.971777
H	0.124229	4.896118	-1.837469

H -0.864035 4.064807 -0.626856
H -1.664505 4.972563 -1.945186
H -1.664758 2.568547 -2.321693
H 0.210438 3.913140 -4.183217
H -1.571718 3.958100 -4.293664
H -0.698339 2.406338 -4.471984

3SA3MA2DMA

S 4.160487 0.752353 -2.198021
O 3.955915 0.967026 -3.605877
O 5.294080 -0.046272 -1.780579
O 4.283447 2.094278 -1.413326
O 2.830416 0.110677 -1.664864
H 3.399971 2.567365 -1.260661
H 2.961053 -0.163919 -0.702980
O 2.469330 0.284224 3.346696
O 2.234576 -3.002580 2.092392
O 5.482642 -1.042013 0.773713
O 0.580547 -1.689055 2.869512
O 3.293717 -0.531091 0.766829
C 2.853954 -1.079581 3.384112
C 4.254381 -1.304054 2.797191
C 1.763323 -1.960177 2.742828
C 4.305142 -0.928193 1.339066
H 2.881569 -1.353164 4.443424
H 4.568956 -2.344992 2.899564
H 4.980010 -0.689746 3.336881
H 2.375313 0.532425 2.412027
H 1.505826 -3.424103 1.547797
H 5.453813 -0.720882 -0.165038
S -0.939009 -4.343394 1.121108
O -0.587012 -5.408138 2.015484
O 0.265473 -3.696878 0.488865
O -1.956688 -4.661993 0.111276
O -1.614626 -3.140781 1.959180
H -2.910776 -3.703159 -0.735899
H -0.881678 -2.589960 2.325224
O -2.798815 -1.083379 -2.950824
O -0.112274 -2.111170 -1.548892
O 1.668611 -0.371731 -4.544429
O -1.530899 -0.854261 -0.349859
O 0.641205 1.212652 -3.348740
C -1.485544 -0.536793 -2.727755
C -0.591862 -0.773015 -3.938507
C -1.002491 -1.165855 -1.412512

C	0.630165	0.125678	-3.899033
H	-1.571485	0.537357	-2.559426
H	-1.165257	-0.513202	-4.834070
H	-0.283986	-1.813503	-4.026675
H	-3.428639	-0.413052	-2.607227
H	0.043081	-2.644635	-0.699945
H	2.452303	0.203012	-4.384150
S	0.949409	2.915005	-0.058038
O	0.260664	3.992903	0.669224
O	2.107626	3.357006	-0.835841
O	1.235433	1.773407	0.828352
O	-0.158127	2.434167	-1.111219
H	0.242701	1.914697	2.276154
H	0.249742	2.042340	-1.920878
O	-5.146134	2.838886	1.764662
O	-2.304279	4.356978	0.212502
O	-3.043911	1.290337	0.097841
O	-2.618828	3.460308	2.260532
O	-4.280293	0.834701	-1.723790
C	-4.482051	3.581912	0.769158
C	-4.651824	2.909529	-0.597023
C	-3.017188	3.791518	1.150241
C	-3.983348	1.563805	-0.786804
H	-4.923255	4.587273	0.691999
H	-4.247607	3.559753	-1.378912
H	-5.715185	2.781473	-0.805605
H	-4.516271	2.754107	2.494839
H	-1.320513	4.316263	0.408600
H	-2.521978	0.468662	-0.132073
C	-0.880302	1.057013	3.818107
N	-0.266729	2.227110	3.130780
C	0.687526	3.008942	3.964663
H	-0.105500	0.324068	4.026638
H	-1.619236	0.619323	3.149339
H	-1.365776	1.398940	4.732051
H	-1.023375	2.846720	2.789446
H	1.506894	2.354903	4.257573
H	0.166164	3.388693	4.843243
H	1.057731	3.835897	3.361607
C	-4.451369	-4.227750	-2.025805
N	-3.709834	-3.214454	-1.230581
C	-4.523439	-2.533717	-0.184751
H	-4.803633	-5.011634	-1.357052
H	-3.773545	-4.658120	-2.761268

H -5.294076 -3.754922 -2.529908
H -3.314973 -2.500375 -1.872162
H -4.943628 -3.289506 0.476943
H -5.315298 -1.952555 -0.656025
H -3.862517 -1.885085 0.384813

3SA3MA3DMA

S -0.093816 1.770080 -0.610057
O -1.122365 0.752851 -0.807302
O 0.362060 2.396401 -1.867160
O -0.453907 2.782134 0.399243
O 1.147358 0.951901 -0.029741
H -1.505946 3.942131 -0.177179
H 1.992639 1.414077 -0.282928
O 5.658821 4.223430 0.175942
O 6.328098 0.917295 -1.005474
O 2.745386 3.365711 -2.460975
O 5.893898 1.736225 1.054831
O 3.421900 2.133121 -0.710497
C 6.019625 3.259413 -0.786460
C 5.066075 3.325803 -1.984323
C 6.062180 1.868932 -0.153776
C 3.658648 2.890761 -1.645485
H 7.034910 3.460646 -1.156620
H 5.423464 2.670956 -2.785178
H 5.044495 4.343191 -2.377095
H 5.585006 3.741442 1.012277
H 6.239308 -0.000989 -0.600905
H 1.843075 2.995303 -2.229578
S 6.476974 -2.423857 0.746638
O 7.876068 -2.127996 0.826119
O 5.702702 -1.416181 -0.084210
O 6.343043 -3.792971 -0.047367
O 5.757655 -2.588496 2.025092
H 5.391221 -3.947006 -0.268751
H 5.059845 -1.151620 2.457923
O 1.158700 -4.768568 -0.973818
O 3.145122 -1.854616 -0.337729
O -1.604330 -2.619487 -2.392002
O 3.674596 -4.021065 -0.639944
O -1.433877 -3.006550 -0.184930
C 1.361965 -3.440195 -0.545267
C 0.553147 -2.486376 -1.425232
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H	1.013402	-3.317450	0.491704
H	0.830756	-2.603874	-2.473250
H	0.734402	-1.449814	-1.126456
H	2.019569	-5.207101	-0.923948
H	4.143923	-1.713617	-0.295992
H	-2.571429	-2.773663	-2.231359
S	-4.529660	1.919722	-0.225836
O	-4.128755	2.772905	-1.345346
O	-5.915425	1.428194	-0.284138
O	-3.686860	0.578733	-0.281536
O	-4.253647	2.567852	1.080309
H	-2.713377	0.733109	-0.460177
H	-5.307628	1.822553	2.171663
O	-6.835557	-3.760240	-1.806192
O	-3.916515	-3.658937	0.270825
O	-6.364610	-1.169100	-0.526258
O	-4.222636	-3.187491	-1.911502
O	-6.666270	-1.123797	1.702436
C	-6.099429	-3.947242	-0.626158
C	-6.734830	-3.236239	0.586189
C	-4.636101	-3.554018	-0.821557
C	-6.581562	-1.732191	0.639588
H	-6.095877	-5.019874	-0.392624
H	-6.333421	-3.629885	1.520396
H	-7.806625	-3.457327	0.568477
H	-6.323911	-3.156698	-2.361727
H	-2.958177	-3.391801	0.093608
H	-6.203110	-0.184952	-0.446428
C	3.273721	-0.061665	2.673330
N	4.756632	-0.177113	2.726198
C	5.357274	0.144995	4.045960
H	2.838913	-0.725361	3.420529
H	2.928870	-0.350531	1.682732
H	2.981611	0.968412	2.874295
H	5.177829	0.452939	2.013366
H	4.965862	-0.541804	4.795774
H	5.114412	1.172366	4.316220
H	6.437000	0.026252	3.972324
C	-2.763044	5.525963	0.347599
N	-2.195811	4.582615	-0.647838
C	-1.535626	5.218152	-1.818186
H	-1.960596	6.126118	0.776599
H	-3.254938	4.937136	1.119519
H	-3.489632	6.174626	-0.142236

H	-2.957669	3.943963	-0.975610
H	-0.735060	5.869962	-1.468415
H	-2.269783	5.796330	-2.379099
H	-1.113386	4.429988	-2.438875
C	-5.595151	1.019968	4.084233
N	-6.066463	1.337631	2.714168
C	-7.291753	2.175215	2.650007
H	-5.376424	1.944129	4.619360
H	-4.691605	0.416830	4.009130
H	-6.365055	0.457151	4.611275
H	-6.259086	0.441892	2.206387
H	-7.105758	3.129025	3.143597
H	-8.113378	1.654308	3.141396
H	-7.523973	2.337949	1.599489

3SA3MA4DMA

S	3.751151	2.140121	0.008371
O	4.907129	1.574072	0.626184
O	3.623942	3.584969	-0.080121
O	3.648297	1.521494	-1.424596
O	2.480868	1.593628	0.770519
H	2.783738	1.808373	-1.894309
H	1.682899	2.190212	0.631619
O	-2.203373	3.999801	-1.503909
O	-2.399131	3.488515	2.045513
O	1.393059	5.101426	-0.022364
O	-2.929376	2.108677	0.354091
O	0.374113	3.158555	0.480192
C	-2.198239	4.363523	-0.151348
C	-0.946460	5.154297	0.264230
C	-2.520998	3.186438	0.774793
C	0.338709	4.360649	0.241515
H	-3.045409	5.048300	-0.019927
H	-1.069173	5.525722	1.286350
H	-0.839972	6.016737	-0.393740
H	-1.557427	3.285842	-1.671528
H	-2.561556	2.681333	2.620272
H	2.220083	4.554896	-0.031822
S	-3.755513	0.338602	3.433364
O	-4.864348	0.913965	4.136025
O	-2.550680	1.241206	3.366389
O	-3.363914	-1.007022	3.875697
O	-4.177410	0.164291	1.882867
H	-2.342865	-2.182990	3.383705
H	-3.658582	0.810592	1.349584

O	0.582955	-2.900586	1.864484
O	-0.226724	0.236893	2.743889
O	4.463119	-1.525079	2.765518
O	-1.327094	-0.982839	1.228021
O	3.604452	-1.959430	0.733834
C	0.968641	-1.529461	1.628868
C	2.153787	-1.171555	2.502136
C	-0.296355	-0.698150	1.834709
C	3.475197	-1.612535	1.894615
H	1.252513	-1.403739	0.582028
H	2.050829	-1.599004	3.501805
H	2.220662	-0.088612	2.621662
H	0.390133	-3.303236	0.992629
H	-1.134749	0.641547	2.925170
H	5.375447	-1.610379	2.308581
S	0.385514	1.131446	-2.488783
O	0.395306	0.530839	-3.966701
O	1.444219	2.154407	-2.525022
O	-0.941669	1.695701	-2.253507
O	0.705446	0.009796	-1.584428
H	-3.019713	1.363815	-1.503523
H	1.683750	-1.245948	-2.232707
O	-3.711116	-3.450990	-3.220136
O	-0.566791	-1.881186	-3.920454
O	-1.964786	-2.500320	-0.869024
O	-2.676766	-1.129696	-3.747921
O	-0.172182	-3.818010	-0.572866
C	-2.338296	-3.469146	-3.542208
C	-1.554107	-4.239797	-2.470101
C	-1.812473	-2.032230	-3.751212
C	-1.165219	-3.491217	-1.215404
H	-2.183147	-4.000455	-4.493166
H	-0.632430	-4.653574	-2.880002
H	-2.172545	-5.090249	-2.163291
H	-3.968097	-2.526905	-3.369171
H	-0.117261	-0.346637	-3.989754
H	-1.603622	-1.977974	-0.095503
C	-4.741765	0.220007	-1.544238
N	-3.610475	0.910882	-2.216251
C	-4.020690	1.928344	-3.221356
H	-5.317898	0.943955	-0.970363
H	-4.341655	-0.539236	-0.875427
H	-5.369808	-0.248838	-2.300428
H	-3.027618	0.202105	-2.711080

H	-4.602468	2.706153	-2.730797
H	-4.607015	1.434412	-3.995430
H	-3.119227	2.359608	-3.647787
C	-1.645499	-3.659055	4.655891
N	-1.903005	-3.137003	3.288294
C	-2.839092	-3.964971	2.481792
H	-2.584514	-3.685098	5.206422
H	-0.952350	-2.986718	5.158829
H	-1.212885	-4.657310	4.592197
H	-0.999799	-3.042702	2.777117
H	-3.794288	-4.021189	3.001391
H	-2.421791	-4.962407	2.343945
H	-2.981932	-3.479932	1.518227
C	3.089322	-1.272401	-3.753379
N	2.089228	-1.959460	-2.886002
C	2.644918	-3.119102	-2.129208
H	3.876843	-0.869877	-3.117918
H	2.588768	-0.462798	-4.279646
H	3.503322	-1.991069	-4.460332
H	1.262701	-2.240864	-3.438617
H	3.354317	-2.751250	-1.390313
H	3.127162	-3.797614	-2.833678
H	1.828383	-3.624046	-1.617395
C	6.958058	-1.397273	0.273916
N	6.934886	-1.443518	1.743670
C	7.444038	-0.205676	2.356532
H	6.303568	-0.591391	-0.059597
H	6.573354	-2.337839	-0.123174
H	7.967395	-1.221244	-0.124234
H	7.496320	-2.228419	2.061624
H	6.789658	0.619638	2.073200
H	8.468412	0.033229	2.038714
H	7.425442	-0.304683	3.443702
3SA4MA			
S	-1.152117	3.952091	-0.775228
O	-1.054182	2.814908	-1.679993
O	-0.104935	4.918803	-0.770132
O	-2.513190	4.680041	-1.050240
O	-1.462711	3.420960	0.676913
H	-3.230902	3.988340	-1.058275
H	-0.815549	2.735208	1.014082
S	1.742609	0.770328	-2.113852
O	1.772733	-0.638055	-2.400480
O	1.499409	1.206512	-0.763339

O	3.089844	1.423359	-2.661497
O	0.740885	1.477162	-3.085221
H	3.841396	0.947107	-2.246869
H	0.139078	2.080906	-2.571792
S	4.901484	-1.101502	-0.376691
O	5.032672	0.193609	-1.039566
O	5.149810	-2.281805	-1.161793
O	5.866549	-1.112914	0.846280
O	3.498057	-1.153924	0.279652
H	5.621889	-0.338732	1.443392
H	2.929596	-1.945561	-0.038185
O	-0.383424	-4.339431	-0.003663
O	-1.300611	-2.276721	-2.793968
O	3.041396	-3.631701	-2.421145
O	-1.208014	-1.800747	-0.595489
O	2.012985	-3.039087	-0.513208
C	-0.504007	-3.988039	-1.357530
C	0.777301	-4.253078	-2.174342
C	-1.026902	-2.557023	-1.536350
C	2.001809	-3.570629	-1.623811
H	-1.286317	-4.628713	-1.774777
H	0.651015	-3.949014	-3.215121
H	0.979570	-5.328644	-2.174450
H	0.314257	-3.780448	0.368431
H	-1.711464	-1.374941	-2.872764
H	3.823152	-3.187279	-2.020359
O	3.476058	2.390921	4.024083
O	4.438214	2.376107	0.575382
O	1.786581	0.522533	2.630897
O	4.903339	0.917512	2.232404
O	-0.024033	1.579500	1.869973
C	3.430755	2.777173	2.677989
C	1.996833	2.844050	2.103133
C	4.342632	1.915403	1.810197
C	1.171811	1.583577	2.188482
H	3.831631	3.794204	2.623476
H	2.017413	3.141988	1.051360
H	1.444450	3.617087	2.643273
H	3.462346	1.425703	4.047137
H	4.872772	1.716946	-0.006812
H	1.181348	-0.287665	2.632468
O	-4.218163	2.627043	-0.962784
O	-2.720877	0.374039	-0.645776
O	-5.614385	0.633508	0.518026

O	-2.712961	0.040863	-2.876218
O	-5.602258	-1.275058	-0.673839
C	-4.283729	1.604379	-1.946346
C	-5.622001	0.821564	-1.847575
C	-3.119879	0.608293	-1.878013
C	-5.638467	-0.057963	-0.616763
H	-4.234756	2.098260	-2.915319
H	-5.746697	0.185730	-2.722779
H	-6.429060	1.555651	-1.802882
H	-4.337473	2.230963	-0.086336
H	-2.062419	-0.380393	-0.624822
H	-5.435338	0.023249	1.289399
O	-3.260150	-1.864911	4.483539
O	-4.228370	-2.686994	1.132146
O	-1.705654	-0.530718	2.246561
O	-4.792714	-0.978181	2.485667
O	0.218640	-1.578843	2.730198
C	-3.249097	-2.624653	3.299042
C	-1.811234	-2.845545	2.797125
C	-4.164300	-2.003482	2.252067
C	-0.999005	-1.590324	2.596965
H	-3.669332	-3.619660	3.500651
H	-1.810334	-3.385245	1.844011
H	-1.274105	-3.459243	3.520795
H	-3.786136	-1.073995	4.299481
H	-4.824181	-2.228778	0.480906
H	-1.106926	0.243776	2.092448
3SA4MA1DMA			
S	-2.087279	3.998774	-0.570361
O	-1.741280	2.883446	-1.433983
O	-1.237849	5.143846	-0.545249
O	-3.544654	4.474394	-0.904714
O	-2.338792	3.433474	0.883779
H	-4.145638	3.679539	-0.876444
H	-1.653491	2.751455	1.154527
S	1.004010	0.794032	-2.393822
O	0.925908	-0.543607	-2.909372
O	0.904274	1.002619	-0.969957
O	2.305775	1.499705	-2.954123
O	-0.066232	1.673945	-3.137527
H	3.106931	1.081181	-2.544707
H	-0.573304	2.223379	-2.491418
S	5.025839	-0.746651	-1.327138
O	4.430327	0.597019	-1.547857

O	4.842478	-1.630450	-2.467709
O	6.390335	-0.655384	-0.810730
O	4.219965	-1.378316	-0.087006
H	6.439703	-0.543253	0.853687
H	3.377108	-1.816634	-0.403669
O	-0.139087	-4.058828	0.023621
O	-1.753868	-2.381235	-2.706972
O	2.710147	-3.155915	-3.014657
O	-1.417386	-1.720695	-0.580840
O	2.070588	-2.675892	-0.912425
C	-0.517278	-3.844919	-1.311944
C	0.639671	-4.015756	-2.315344
C	-1.260934	-2.517304	-1.493423
C	1.872016	-3.196320	-2.010580
H	-1.260861	-4.611952	-1.550257
H	0.312112	-3.785338	-3.329606
H	0.954118	-5.064446	-2.306802
H	0.573443	-3.428382	0.211508
H	-2.261918	-1.532943	-2.789809
H	3.503052	-2.593099	-2.809778
O	2.721462	3.159365	3.499410
O	3.643764	2.469568	0.116860
O	1.362192	0.817012	2.243363
O	4.350967	1.583964	2.071438
O	-0.662956	1.633043	1.788249
C	2.652989	3.279990	2.099526
C	1.220632	3.098260	1.566146
C	3.644179	2.340590	1.416793
C	0.564732	1.778913	1.880840
H	2.960494	4.296685	1.827735
H	1.210056	3.195085	0.476669
H	0.587966	3.890491	1.970342
H	3.114287	2.295243	3.679404
H	4.114181	1.740862	-0.376649
H	0.866574	-0.055029	2.378861
O	-4.978951	2.232447	-0.704422
O	-3.185434	0.213168	-0.544470
O	-5.998180	0.051827	0.884587
O	-3.389222	-0.201680	-2.752385
O	-5.840052	-1.821461	-0.351705
C	-5.017653	1.202791	-1.683095
C	-6.239384	0.268245	-1.466578
C	-3.744398	0.350326	-1.726488
C	-6.030283	-0.620324	-0.260317

H	-5.119722	1.694797	-2.649078
H	-6.375067	-0.369261	-2.338895
H	-7.117572	0.901605	-1.326548
H	-4.925683	1.830008	0.175353
H	-2.433406	-0.455114	-0.579488
H	-5.696007	-0.547579	1.624995
O	-3.167406	-2.244401	4.649177
O	-4.196742	-3.098817	1.324039
O	-1.952817	-0.687189	2.321085
O	-4.894884	-1.509386	2.757729
O	0.130430	-1.445866	2.669335
C	-3.118031	-2.967865	3.442017
C	-1.690451	-2.986524	2.870160
C	-4.157659	-2.441735	2.460541
C	-1.079762	-1.631020	2.618772
H	-3.397332	-4.013095	3.633614
H	-1.647214	-3.530570	1.920611
H	-1.037303	-3.507642	3.570828
H	-3.792822	-1.519331	4.509654
H	-4.878234	-2.699118	0.718964
H	-1.488075	0.164976	2.114100
C	6.026847	-1.531313	2.648845
N	6.353800	-0.306207	1.872776
C	7.581389	0.405439	2.312720
H	6.855692	-2.234829	2.574204
H	5.129269	-1.969070	2.218241
H	5.857532	-1.264561	3.691834
H	5.550436	0.355539	1.913650
H	8.437920	-0.262009	2.223521
H	7.465249	0.727694	3.347092
H	7.727498	1.273080	1.671346

3SA4MA2DMA

S	-3.761652	0.061549	-2.261789
O	-4.009549	-1.335004	-2.033257
O	-4.802357	1.031177	-2.283244
O	-2.688504	0.544604	-1.160825
O	-2.955841	0.255979	-3.615330
H	-2.230749	-0.242538	-0.788057
H	-2.155782	-0.311305	-3.596758
S	0.736845	-0.225893	-2.996768
O	0.316241	1.054427	-3.523619
O	1.763354	-0.976685	-3.635998
O	1.118557	-0.067630	-1.483857
O	-0.609123	-1.082529	-2.935787

H	0.645387	0.722462	-1.064839
H	-0.520117	-1.892406	-2.329455
O	-0.678545	3.951923	1.399605
O	-0.783329	3.103614	-2.082251
O	-3.019278	2.639018	1.485863
O	-0.011035	1.944654	-0.308103
O	-4.660425	3.194991	0.058763
C	-1.063079	4.091574	0.041944
C	-2.571848	4.357611	-0.122822
C	-0.567601	2.916060	-0.802154
C	-3.523756	3.330722	0.461841
H	-0.518772	4.958863	-0.337009
H	-2.823140	4.474280	-1.176510
H	-2.799856	5.306162	0.374496
H	-1.257007	3.279739	1.793317
H	-0.436639	2.355626	-2.629737
H	-3.718048	2.031511	1.876461
S	-1.091593	-3.146946	0.002970
O	-0.310457	-3.001451	-1.252201
O	-2.266632	-3.990722	-0.126796
O	-0.230491	-3.461814	1.134106
O	-1.644800	-1.633015	0.255685
H	1.009298	-2.342053	1.829144
H	-2.538923	-1.695386	0.725502
O	-6.026097	-1.123982	3.510426
O	-6.152740	1.012292	0.641193
O	-4.883929	-3.475305	0.384494
O	-4.855792	1.038611	2.485005
O	-4.005858	-1.604546	1.268101
C	-6.480496	-0.710252	2.244904
C	-6.385884	-1.850749	1.218132
C	-5.737043	0.542266	1.790197
C	-4.970088	-2.304666	0.965327
H	-7.537933	-0.427324	2.321110
H	-6.801991	-1.539043	0.254728
H	-6.975330	-2.700264	1.567103
H	-5.217489	-0.622876	3.685292
H	-5.642561	1.824736	0.372577
H	-3.940630	-3.692358	0.170137
O	5.536281	-3.564638	-0.365062
O	2.291415	-3.669240	-1.673667
O	5.892744	-0.812644	-0.459302
O	2.947239	-2.593599	0.192870
O	4.320565	0.190435	-1.708607

C	4.616296	-3.309894	-1.403910
C	4.971166	-2.064756	-2.259090
C	3.191297	-3.155272	-0.859368
C	5.013686	-0.780259	-1.462713
H	4.622963	-4.177262	-2.066073
H	4.243529	-1.938481	-3.060362
H	5.961904	-2.232636	-2.691215
H	5.884100	-2.716761	-0.057808
H	1.369589	-3.473987	-1.371544
H	5.856772	0.043074	0.066498
O	4.754422	5.199232	0.132179
O	1.953120	3.906171	1.964303
O	3.975862	2.289252	-0.120565
O	2.098424	4.934310	-0.035600
O	5.710369	1.388477	0.984662
C	4.095013	4.701178	1.269863
C	4.803493	3.447091	1.791639
C	2.607262	4.509602	0.979848
C	4.879717	2.280317	0.833879
H	4.133356	5.445682	2.080697
H	4.308638	3.092759	2.700997
H	5.829721	3.698204	2.064683
H	4.063440	5.357786	-0.528475
H	0.984289	3.884674	1.744523
H	4.101154	1.512666	-0.738425
C	1.433461	-0.319753	1.910940
N	1.406431	-1.677478	2.519058
C	0.593683	-1.767346	3.757434
H	0.420511	-0.017940	1.650158
H	2.039559	-0.365833	1.009978
H	1.860205	0.387817	2.622057
H	2.406686	-1.998345	2.718066
H	-0.432516	-1.476707	3.537418
H	1.013871	-1.106932	4.516322
H	0.604983	-2.796541	4.112588
C	5.088488	-1.686825	3.438421
N	4.056477	-2.595047	2.923233
C	4.102360	-3.921377	3.551940
H	4.883960	-1.448254	4.486065
H	5.085355	-0.757232	2.865893
H	6.097507	-2.119402	3.383453
H	4.180869	-2.711430	1.918073
H	3.868598	-3.835294	4.616953
H	5.086451	-4.399902	3.456614

H 3.359581 -4.571792 3.085727
3SA4MA3DMA
S -4.007083 0.362707 0.562921
O -2.688999 -0.146086 -0.164898
O -4.941920 -0.720649 0.681149
O -3.613338 1.051265 1.771554
O -4.580012 1.347116 -0.501677
H -2.284225 0.206372 4.274803
H -3.875497 1.956771 -0.883695
S 0.321360 0.567211 1.832411
O 0.982998 0.095956 3.222541
O -0.171250 1.897122 2.089965
O 1.373907 0.451264 0.811859
O -0.762115 -0.438542 1.584333
H 2.019702 -0.970797 0.562633
H -1.921166 -0.184594 0.484140
O 3.542915 -4.284080 0.037023
O 2.412454 -2.087714 2.636932
O 0.897718 -5.017267 -0.250942
O 2.374560 -1.902724 0.388936
O -0.363502 -4.531726 1.544793
C 3.105669 -3.969484 1.348395
C 1.999841 -4.935662 1.843331
C 2.613544 -2.529811 1.516465
C 0.715992 -4.810459 1.049416
H 3.972484 -4.071066 2.001331
H 1.779310 -4.730644 2.888710
H 2.375804 -5.957211 1.742721
H 2.758857 -4.465967 -0.503234
H 1.586167 -0.674595 3.041930
H 0.037207 -4.892780 -0.767583
S -1.915100 2.415925 -2.708253
O -2.758721 2.884148 -1.569900
O -2.590101 1.478276 -3.600378
O -1.658390 3.698590 -3.602361
O -0.611914 1.944544 -2.228917
H -1.175634 4.358947 -3.035108
H -0.138576 0.479959 -2.821531
O -3.323137 -4.681826 -3.378683
O -2.632621 -4.098383 0.093476
O -4.064938 -0.685364 -2.971346
O -1.287501 -4.679576 -1.611954
O -2.211399 -1.966290 -2.975225
C -3.612135 -4.237916 -2.077049

C	-4.251975	-2.839908	-2.054685
C	-2.383036	-4.349750	-1.176676
C	-3.399512	-1.786191	-2.718407
H	-4.344146	-4.937890	-1.661908
H	-4.453003	-2.498636	-1.033842
H	-5.214256	-2.879327	-2.568883
H	-2.503266	-4.245889	-3.642721
H	-1.812398	-4.228751	0.638137
H	-3.480554	0.062479	-3.259124
O	1.669021	6.435971	-0.567704
O	-1.221057	4.423128	0.071330
O	1.884658	3.336326	-0.673410
O	-0.334495	5.243967	-1.837824
O	3.345324	3.304049	1.032839
C	0.742333	5.747345	0.238940
C	1.455053	4.761513	1.177487
C	-0.330733	5.091098	-0.623561
C	2.331424	3.736338	0.499154
H	0.207199	6.465169	0.877480
H	0.718989	4.196446	1.757727
H	2.085269	5.316799	1.872135
H	1.396840	6.278537	-1.483397
H	-1.841903	3.914923	-0.512309
H	2.441573	2.599646	-1.032953
O	7.398927	0.104973	-0.105960
O	5.201548	-2.492437	-1.228145
O	5.025153	1.609088	-0.002345
O	5.512097	-1.684349	0.852443
O	3.565190	1.406166	-1.695769
C	6.586509	-0.576910	-1.019587
C	5.718200	0.357083	-1.901226
C	5.717877	-1.638406	-0.337166
C	4.653686	1.164418	-1.185760
H	7.260050	-1.108546	-1.696747
H	5.233883	-0.210157	-2.695397
H	6.396941	1.080163	-2.365978
H	6.816556	0.525249	0.539930
H	4.625193	-3.136921	-0.752033
H	4.323203	2.211598	0.408426
C	-1.318923	-1.567939	4.925705
N	-2.232642	-0.847547	4.001892
C	-3.594078	-1.439581	3.926663
H	-1.748770	-1.568856	5.927635
H	-0.357481	-1.059987	4.926276

H	-1.188717	-2.593943	4.579725
H	-1.795749	-0.819393	3.061969
H	-4.046010	-1.413593	4.918676
H	-3.524723	-2.472445	3.584052
H	-4.192475	-0.863067	3.226730
C	0.340472	-0.060661	-4.751759
N	0.083920	-0.411195	-3.330109
C	1.208075	-1.105279	-2.646429
H	1.212630	0.589825	-4.804007
H	-0.533700	0.462769	-5.135176
H	0.517501	-0.970588	-5.325015
H	-0.780807	-0.983123	-3.265149
H	2.057420	-0.426473	-2.574073
H	1.476814	-1.999196	-3.209395
H	0.885314	-1.385281	-1.646934
C	-3.491682	2.525250	4.740060
N	-2.197799	1.885517	4.464221
C	-1.129842	2.339836	5.366886
H	-3.859201	2.208378	5.720651
H	-4.208413	2.225128	3.976054
H	-3.421467	3.621504	4.744048
H	-1.918318	2.102998	3.507589
H	-1.342119	2.008066	6.387608
H	-1.033478	3.433893	5.379912
H	-0.179079	1.914158	5.044818

3SA4MA4DMA

S	3.409042	0.742026	1.388185
O	4.098138	1.348622	0.265361
O	2.218519	1.441097	1.861604
O	2.778128	-0.684027	0.722039
O	4.290488	0.237886	2.442324
H	1.828076	-0.715320	0.930741
H	3.511375	-2.093543	1.504884
S	-1.118890	-1.342995	1.841199
O	-0.905921	-0.484262	2.985448
O	-1.936073	-2.507634	1.946675
O	-1.655359	-0.470217	0.645617
O	0.329044	-1.765516	1.367520
H	-1.348677	0.494956	0.738837
H	0.321745	-2.491027	0.633401
O	-0.830319	4.720974	0.457108
O	-0.445421	2.224131	2.969880
O	1.500601	3.910445	-0.516130
O	-0.933804	2.003343	0.780137

O	3.317210	4.282438	0.741457
C	-0.293881	4.169568	1.649463
C	1.210867	4.480070	1.803534
C	-0.586029	2.670910	1.747024
C	2.031247	4.178265	0.568682
H	-0.832309	4.628013	2.479829
H	1.636190	3.918542	2.636115
H	1.333827	5.545004	2.023311
H	-0.224630	4.438923	-0.253921
H	-0.567527	1.245909	3.009555
H	2.291348	3.248064	-1.802049
S	1.311079	-3.261357	-1.622396
O	0.433055	-3.535906	-0.435991
O	2.732947	-3.304741	-1.256058
O	0.920900	-4.024224	-2.778445
O	0.978638	-1.704731	-1.910002
H	-1.025160	-0.170504	-2.942438
H	1.801833	-1.231707	-2.213863
O	4.208310	1.575252	-4.478267
O	4.587783	3.546884	-1.549649
O	4.682421	-1.480534	-1.634237
O	2.739023	2.714662	-2.514344
O	3.107547	-0.322730	-2.723770
C	4.860254	1.880236	-3.265632
C	5.324644	0.621822	-2.498761
C	4.048688	2.803549	-2.351915
C	4.255199	-0.423324	-2.287806
H	5.753825	2.451011	-3.523985
H	5.716019	0.889418	-1.515127
H	6.132506	0.144105	-3.061261
H	3.469672	0.996121	-4.246892
H	3.814411	4.020418	-0.085989
H	3.944392	-2.137344	-1.522899
O	-5.190014	-4.585639	-1.449103
O	-1.975222	-4.799551	-0.272263
O	-5.836816	-2.025190	-0.549525
O	-2.801142	-2.997307	-1.334137
O	-4.823192	-1.377111	1.342803
C	-4.343872	-4.550050	-0.321770
C	-4.923547	-3.729728	0.856613
C	-2.953652	-4.027817	-0.700490
C	-5.168142	-2.262113	0.580035
H	-4.230073	-5.580592	0.015753
H	-4.267469	-3.789251	1.724369

H	-5.889818	-4.177279	1.111057
H	-5.471137	-3.678838	-1.628462
H	-1.095784	-4.384732	-0.461150
H	-5.987597	-1.039964	-0.658709
O	-6.308836	3.614960	1.876366
O	-3.416519	4.309627	-0.131107
O	-4.885753	1.236059	0.863483
O	-3.656420	3.948786	2.080689
O	-6.180411	0.591579	-0.853494
C	-5.616501	3.922465	0.692309
C	-5.961562	2.931742	-0.429439
C	-4.117638	4.044868	0.964058
C	-5.691321	1.470188	-0.149139
H	-5.927957	4.915616	0.337338
H	-5.418127	3.198075	-1.340883
H	-7.025263	3.008550	-0.663413
H	-5.628558	3.470777	2.551138
H	-2.460618	4.443577	0.111518
H	-4.822132	0.253821	1.041322
C	-3.102528	-0.247923	-2.695731
N	-1.781185	-0.916493	-2.835441
C	-1.705211	-1.866773	-3.980576
H	-3.325324	0.299968	-3.610977
H	-3.055724	0.439920	-1.853498
H	-3.860771	-1.002799	-2.506189
H	-1.607289	-1.454413	-1.979758
H	-1.821549	-1.309539	-4.910030
H	-2.498689	-2.603581	-3.875509
H	-0.739478	-2.367303	-3.950783
C	0.525994	1.176104	-4.703055
N	0.036368	1.217416	-3.315692
C	-0.618152	2.497650	-2.999568
H	-0.317125	1.274031	-5.392822
H	1.011848	0.216372	-4.889148
H	1.241617	1.979417	-4.916037
H	0.847634	1.123468	-2.708234
H	-1.539733	2.591289	-3.581072
H	0.018293	3.360203	-3.235529
H	-0.870432	2.527083	-1.938416
C	3.340861	-4.134966	1.898657
N	3.981642	-2.809253	2.096812
C	5.435048	-2.770134	1.786893
H	3.417506	-4.421900	0.851542
H	2.288182	-4.056767	2.166834

H	3.831076	-4.869506	2.538258
H	3.826790	-2.465523	3.100975
H	5.590855	-3.045840	0.744533
H	5.962480	-3.467367	2.438716
H	5.780474	-1.751494	1.953601
C	2.161330	-1.621746	5.072596
N	3.556682	-1.622019	4.612407
C	4.511622	-1.851770	5.700750
H	1.887750	-2.619321	5.428432
H	1.498213	-1.354992	4.248580
H	1.990487	-0.911112	5.893184
H	3.759376	-0.725427	4.166082
H	4.384704	-2.862262	6.100331
H	4.385907	-1.142840	6.531540
H	5.531749	-1.756897	5.322558

4MA

O	-0.972568	-5.569179	0.028921
O	-2.723231	-2.887490	-1.577310
O	0.431815	-2.803777	-0.418850
O	-2.522486	-3.486240	0.585426
O	2.023640	-4.004766	-1.456510
C	-1.443742	-4.830960	-1.072182
C	-0.272582	-4.438601	-1.986992
C	-2.275673	-3.642636	-0.605224
C	0.848331	-3.735054	-1.256275
H	-2.131616	-5.446016	-1.671011
H	-0.631628	-3.784571	-2.787012
H	0.149673	-5.334400	-2.440325
H	-1.343605	-5.150641	0.819193
H	-3.315168	-2.164529	-1.219185
H	1.201709	-2.392571	0.065803
O	4.401862	-1.164744	2.851058
O	4.083866	-3.046372	-0.117259
O	4.037080	1.350373	1.494194
O	2.523588	-1.776950	0.900521
O	4.222170	1.024292	-0.722423
C	4.821866	-1.544770	1.570521
C	5.476658	-0.388345	0.763867
C	3.680272	-2.149438	0.752063
C	4.518893	0.730944	0.427272
H	5.579738	-2.318062	1.704458
H	5.890758	-0.768924	-0.169361
H	6.280493	0.015807	1.383701
H	3.740978	-0.467102	2.756498

H	3.310145	-3.396638	-0.652487
H	3.439415	2.103717	1.220078
O	-5.830228	1.092502	-0.035427
O	-3.798436	-1.371317	1.589836
O	-2.719658	1.570933	0.430046
O	-4.323234	-1.024360	-0.573955
O	-3.296035	3.403322	1.597360
C	-5.272274	0.427229	1.071473
C	-4.546439	1.429968	1.976323
C	-4.387043	-0.725091	0.613339
C	-3.430820	2.144428	1.248975
H	-6.068919	-0.039002	1.669743
H	-4.114480	0.913047	2.838629
H	-5.260445	2.165544	2.346152
H	-5.531382	0.614816	-0.822569
H	-3.294412	-2.158198	1.236803
H	-1.514283	2.258309	-0.494472
O	0.493617	4.240332	-2.869445
O	-1.390511	4.536120	0.127351
O	2.664280	3.040208	-1.472958
O	-0.828998	2.711125	-1.067029
O	2.551127	3.426935	0.738200
C	0.257384	4.777930	-1.597764
C	1.546462	5.011648	-0.764371
C	-0.753071	3.986473	-0.761238
C	2.300032	3.749677	-0.413131
H	-0.200445	5.756670	-1.752667
H	1.301768	5.526177	0.163834
H	2.205686	5.642985	-1.366205
H	1.020868	3.437817	-2.768649
H	-2.555091	3.830793	1.080113
H	3.209433	2.246973	-1.194978

4MA1DMA

O	-3.560433	4.666623	0.247403
O	-3.809581	1.327629	1.526361
O	-1.118276	2.879532	0.012208
O	-4.111124	2.180650	-0.536697
O	0.097293	4.210958	1.353048
C	-3.507468	3.670802	1.238759
C	-2.159892	3.712573	1.979461
C	-3.827444	2.302131	0.648711
C	-0.947416	3.636487	1.078835
H	-4.291142	3.855136	1.986938
H	-2.103129	2.887918	2.696867

H	-2.082712	4.643706	2.540507
H	-3.729846	4.211794	-0.590138
H	-4.092692	0.465305	1.103472
H	-0.314694	2.916560	-0.579006
O	3.023008	2.651024	-3.254212
O	2.347465	4.075537	-0.036101
O	3.146697	1.000404	-0.551250
O	1.032079	3.059892	-1.556271
O	5.213378	0.404570	-1.198164
C	3.344969	3.358468	-2.081148
C	4.556142	2.707997	-1.395684
C	2.122688	3.471902	-1.175848
C	4.345084	1.250365	-1.052180
H	3.624550	4.393472	-2.328023
H	4.790540	3.246131	-0.472091
H	5.420943	2.769134	-2.055214
H	2.071016	2.478514	-3.216811
H	1.501970	4.141704	0.499999
H	3.036913	0.020206	-0.366171
O	-4.930186	-3.455093	-0.416403
O	-4.257584	-0.197827	-1.753183
O	-1.999820	-2.495347	-0.561634
O	-4.571167	-0.928509	0.354443
O	-1.402028	-3.965090	-2.152221
C	-4.694540	-2.516207	-1.436278
C	-3.539729	-2.970848	-2.339210
C	-4.480637	-1.125518	-0.851456
C	-2.237561	-3.124338	-1.587702
H	-5.589806	-2.433892	-2.068167
H	-3.382011	-2.251110	-3.148524
H	-3.795450	-3.926986	-2.797577
H	-4.796137	-2.991417	0.422131
H	-4.196389	0.701366	-1.324543
H	-0.691110	-2.772789	0.445560
O	2.343941	-3.433965	2.476407
O	0.819204	-4.131016	-0.712480
O	4.963572	-2.168892	-0.468964
O	0.090403	-2.938643	1.044381
O	2.854903	-1.548203	-0.007453
C	2.238329	-4.024064	1.218605
C	3.492779	-3.833688	0.344787
C	0.978467	-3.680785	0.417430
C	3.738538	-2.401761	-0.052697
H	2.149976	-5.105532	1.386026

H	3.401459	-4.414254	-0.578533
H	4.367256	-4.204279	0.881623
H	2.117581	-2.468251	2.468763
H	-0.547786	-4.013859	-1.629141
H	5.065800	-1.217525	-0.754616
C	0.526270	-1.128412	3.996685
N	1.431640	-0.837263	2.883782
C	2.276259	0.334372	3.112873
H	1.114068	-1.395118	4.879065
H	-0.095807	-1.984760	3.734947
H	-0.122925	-0.279651	4.262994
H	0.891166	-0.713676	2.034045
H	2.968196	0.129410	3.934326
H	1.703922	1.239689	3.370699
H	2.861804	0.543174	2.216713
4MA2DMA			
O	0.198785	5.456432	0.140947
O	-1.785859	2.863402	1.605023
O	1.231485	2.470820	0.606110
O	-1.710019	3.714834	-0.477421
O	2.947004	3.460965	1.663911
C	-0.379774	4.752580	1.214353
C	0.723044	4.219011	2.133602
C	-1.347745	3.692704	0.696414
C	1.750619	3.357753	1.437286
H	-1.007360	5.424710	1.822499
H	0.272734	3.625914	2.934868
H	1.255375	5.055476	2.584610
H	-0.342327	5.257055	-0.636545
H	-2.425629	2.201626	1.195015
H	1.951639	1.921964	0.190583
O	5.066457	-0.183988	-2.234154
O	4.877896	2.070457	0.514172
O	4.447419	-2.372682	-0.626220
O	3.194814	1.075192	-0.600866
O	4.496317	-1.794312	1.546549
C	5.479423	0.365037	-1.010595
C	5.988720	-0.693280	0.005756
C	4.385695	1.214251	-0.352395
C	4.909037	-1.676658	0.405810
H	6.311213	1.041373	-1.222052
H	6.358110	-0.202056	0.904271
H	6.804997	-1.240429	-0.472606
H	4.637392	-1.031707	-2.050722

H	4.147082	2.591482	0.962879
H	3.678594	-2.972442	-0.341741
O	-5.589453	-0.498999	0.054710
O	-3.929289	2.356522	-1.336493
O	-2.456720	-0.237141	-2.665458
O	-3.468656	1.179904	0.522224
O	-3.333660	-2.129672	-1.822822
C	-5.207365	0.376908	-0.946704
C	-4.812061	-0.323457	-2.291580
C	-4.111233	1.346152	-0.505562
C	-3.416782	-0.899688	-2.287723
H	-6.077472	0.997653	-1.190884
H	-4.858170	0.408711	-3.097790
H	-5.550471	-1.109009	-2.451482
H	-4.826976	-0.882377	0.573905
H	-3.134104	2.878918	-1.059271
H	0.404569	-0.420754	-1.374999
O	-0.868102	-2.409855	2.156407
O	-0.826591	-2.664132	-1.357435
O	2.180880	-3.112330	2.152643
O	0.265896	-1.283223	0.040485
O	2.424413	-3.820589	0.033707
C	-0.724686	-3.204627	0.993224
C	0.371597	-4.296948	1.161555
C	-0.416360	-2.310022	-0.223273
C	1.761938	-3.729780	1.064594
H	-1.669570	-3.723953	0.825937
H	0.261105	-5.037404	0.369362
H	0.222086	-4.761687	2.137592
H	-0.271810	-1.656768	2.016082
H	-2.369025	-2.405443	-1.725639
H	3.056087	-2.678309	1.980296
C	-4.464373	-1.040040	3.097786
N	-4.028681	-1.771409	1.905373
C	-4.545768	-3.141024	1.864555
H	-5.550039	-0.914419	3.068875
H	-4.012817	-0.047014	3.092672
H	-4.197912	-1.547890	4.037019
H	-3.010708	-1.799503	1.900636
H	-5.637643	-3.113011	1.813896
H	-4.257294	-3.741024	2.741260
H	-4.187188	-3.638531	0.961113
C	0.452880	1.337055	-2.576487
N	0.307501	-0.127902	-2.390779

C	1.259765	-0.942680	-3.186769
H	1.470044	1.627742	-2.321928
H	-0.256300	1.849120	-1.929060
H	0.240392	1.588285	-3.616114
H	-0.671228	-0.397127	-2.605826
H	2.273995	-0.667833	-2.899399
H	1.108960	-0.749171	-4.249281
H	1.064352	-1.989328	-2.961418
4MA3DMA			
O	-1.312228	6.041360	-0.082823
O	1.268580	3.916253	-1.385838
O	-1.742970	2.993956	-0.479628
O	0.826865	4.654976	0.693339
O	-3.415579	3.386781	-1.926520
C	-0.532960	5.462226	-1.100019
C	-1.436429	4.722069	-2.092022
C	0.582230	4.609487	-0.504570
C	-2.307552	3.644875	-1.483917
H	-0.007826	6.246957	-1.668227
H	-0.826878	4.261544	-2.875469
H	-2.103822	5.436078	-2.574446
H	-0.860046	5.853548	0.752170
H	2.022212	3.419464	-0.931579
H	-2.391290	2.341880	-0.071651
O	-5.011647	-0.571750	1.944196
O	-4.937741	1.346033	-1.094871
O	-4.701739	-3.511850	-0.407235
O	-3.440099	1.268969	0.581645
O	-3.340304	-1.744508	-0.669023
C	-5.398665	-0.160228	0.673139
C	-5.670515	-1.352009	-0.275507
C	-4.469993	0.878773	0.047839
C	-4.454737	-2.224034	-0.466869
H	-6.357830	0.363580	0.775555
H	-5.980612	-0.984665	-1.258470
H	-6.478053	-1.953440	0.139890
H	-4.029457	-0.638430	2.064193
H	-4.368438	2.092394	-1.429011
H	-3.858970	-4.045031	-0.511414
O	5.378175	1.069117	0.551907
O	2.830905	3.222684	1.851944
O	2.028359	0.105456	1.226542
O	3.155789	2.518641	-0.258764
O	3.168964	-1.615990	2.107342

C	4.544033	1.612080	1.525543
C	3.973893	0.581325	2.528603
C	3.425855	2.481442	0.937180
C	2.960380	-0.347872	1.887948
H	5.156861	2.308759	2.108608
H	3.461392	1.116531	3.332998
H	4.797646	0.011391	2.956306
H	4.999747	0.271400	0.105161
H	2.095001	3.754890	1.452783
H	1.640368	-1.129536	-1.360415
O	0.974294	-4.754471	-2.318455
O	1.797843	-3.329001	0.852051
O	-1.089887	-3.133152	-0.586770
O	2.141093	-2.657288	-1.276507
O	-2.443386	-4.915922	-0.520411
C	1.185326	-4.809912	-0.922341
C	-0.091751	-5.271358	-0.217731
C	1.740314	-3.473489	-0.386523
C	-1.319539	-4.433150	-0.473923
H	1.962029	-5.554913	-0.687418
H	0.086235	-5.259271	0.862503
H	-0.337248	-6.293234	-0.507582
H	1.433964	-3.944596	-2.589486
H	2.530858	-2.235757	1.572665
H	-1.954975	-2.641106	-0.678356
C	5.685068	-1.102708	-2.083650
N	5.023334	-1.360581	-0.801344
C	5.859203	-2.178909	0.087180
H	6.560893	-0.468928	-1.920990
H	5.008313	-0.569481	-2.754830
H	6.016116	-2.022393	-2.589233
H	4.144328	-1.850098	-0.968206
H	6.745539	-1.607802	0.375923
H	6.191712	-3.115341	-0.385282
H	5.297937	-2.418970	0.989988
C	1.973295	0.558840	-2.558041
N	1.309932	-0.121933	-1.417703
C	-0.175208	-0.086442	-1.467111
H	1.778674	-0.006942	-3.469045
H	3.041822	0.606556	-2.361786
H	1.581695	1.570065	-2.655819
H	1.622363	0.274331	-0.517043
H	-0.516456	-0.586598	-2.372423
H	-0.507920	0.950103	-1.453955

H	-0.562828	-0.608222	-0.597329
C	-1.176768	-0.776772	2.519247
N	-2.518875	-0.836321	3.103310
C	-2.759912	0.232740	4.077707
H	-1.082867	0.140747	1.935522
H	-1.020178	-1.625653	1.852015
H	-0.376554	-0.779875	3.274028
H	-2.643430	-1.734235	3.561487
H	-2.744600	1.193121	3.557710
H	-2.010830	0.261794	4.883656
H	-3.751055	0.107061	4.516523
4MA4DMA			
O	-6.057293	-1.728466	0.155052
O	-2.752167	-2.968465	0.791004
O	-4.668204	0.634019	0.219056
O	-3.683431	-2.240889	-1.123735
O	-3.389639	1.081304	1.998054
C	-4.951133	-2.077741	0.940125
C	-4.588308	-0.990170	1.976572
C	-3.730979	-2.435679	0.083555
C	-4.179800	0.343583	1.348938
H	-5.213086	-2.990189	1.484403
H	-3.796402	-1.335296	2.641654
H	-5.478759	-0.807810	2.586482
H	-5.849865	-0.840548	-0.179984
H	-1.960395	-3.163090	0.216807
H	-4.045321	1.669580	-0.841872
O	-1.542296	4.048260	-1.742577
O	-2.455327	3.158400	0.753530
O	0.505245	2.465017	-2.261046
O	-0.375903	2.274071	0.853624
O	2.502297	2.761276	-1.285848
C	-0.792376	4.227809	-0.524612
C	0.716509	4.301340	-0.773673
C	-1.161268	3.104098	0.458682
C	1.335198	3.079271	-1.446344
H	-1.137213	5.170794	-0.094464
H	1.238618	4.467324	0.168758
H	0.920025	5.162133	-1.420532
H	-0.985371	3.445326	-2.272308
H	-2.762983	2.373999	1.317221
H	0.844588	1.521617	-2.711700
O	1.809274	-3.584684	-2.049786
O	-1.615694	-2.706496	-2.696595

O	1.373922	-0.873450	-1.566826
O	-0.635849	-3.451430	-0.814737
O	0.975271	0.377313	-3.393365
C	0.692766	-3.253261	-2.838234
C	0.922921	-1.972933	-3.656389
C	-0.584011	-3.150618	-1.995313
C	1.099194	-0.724146	-2.787522
H	0.534005	-4.087958	-3.529074
H	0.106101	-1.795319	-4.355543
H	1.834217	-2.104617	-4.248200
H	1.942943	-2.817225	-1.469129
H	-2.417015	-2.605207	-2.105213
H	0.822581	-0.786928	0.105711
O	0.447159	-1.949216	3.541979
O	2.416448	0.225710	1.509090
O	-1.373424	0.094850	3.370206
O	0.595683	-1.002126	1.043603
O	-0.792183	2.161266	4.054194
C	1.268713	-0.825912	3.342556
C	0.845265	0.402521	4.176484
C	1.475891	-0.468524	1.864115
C	-0.515528	1.005781	3.860218
H	2.263941	-1.115329	3.691035
H	1.580417	1.202418	4.083379
H	0.828136	0.089086	5.225412
H	-0.447024	-1.687335	3.279728
H	4.624898	1.099500	-0.245578
H	-2.191543	0.534282	3.006590
C	-2.949747	1.064356	-2.490401
N	-3.717594	2.109286	-1.756606
C	-4.906427	2.616213	-2.485813
H	-3.564916	0.170242	-2.576407
H	-2.052782	0.827964	-1.921270
H	-2.666550	1.435098	-3.475249
H	-3.083480	2.897785	-1.537831
H	-5.579856	1.784816	-2.690670
H	-4.593866	3.082341	-3.420220
H	-5.413317	3.349077	-1.859656
C	4.385565	0.043057	-2.041964
N	4.250220	0.153267	-0.568767
C	4.918368	-0.935609	0.195854
H	5.435939	0.163716	-2.310409
H	3.782816	0.826311	-2.495899
H	4.030907	-0.934299	-2.363186

H	3.255628	0.170681	-0.296687
H	5.953468	-1.019267	-0.137039
H	4.385332	-1.877536	0.048713
H	4.883425	-0.675990	1.251558
C	4.821515	2.812245	1.788683
N	4.966801	2.727556	0.329966
C	6.115863	3.480749	-0.177420
H	5.693186	2.360852	2.272097
H	3.931978	2.258778	2.092838
H	4.738660	3.848973	2.146040
H	4.112396	3.071905	-0.110394
H	7.045327	3.029786	0.182416
H	6.109569	4.534326	0.139402
H	6.121677	3.451819	-1.269163
C	3.990999	-5.000926	0.042498
N	3.048633	-4.049228	0.624652
C	2.883588	-4.221820	2.066846
H	5.006856	-4.781408	0.390289
H	3.968919	-4.908177	-1.044587
H	3.773958	-6.050665	0.305052
H	2.149115	-4.171742	0.169745
H	3.800083	-3.918044	2.585370
H	2.674004	-5.265465	2.357981
H	2.061836	-3.599474	2.425205

4SA1MA

S	-0.523242	-1.498994	2.092453
O	-1.636913	-1.179354	2.938306
O	0.176530	-0.421356	1.414474
O	0.505499	-2.279722	2.974857
O	-0.988006	-2.541088	1.029961
H	1.321935	-2.439424	2.432393
H	-0.589345	-2.355629	0.129607
S	-3.654801	0.702623	0.559889
O	-2.530892	0.104729	-0.161491
O	-4.922600	0.064226	0.518911
O	-3.160238	0.953356	2.042686
O	-3.828112	2.184436	0.090303
H	-2.733818	0.141241	2.409987
H	-2.957678	2.586349	-0.147044
S	-0.100661	2.519058	-0.613485
O	-1.369092	3.187108	-0.668756
O	0.135019	1.363978	-1.445315
O	0.995904	3.592891	-0.850049
O	0.229206	2.109814	0.888232

H	1.896517	3.143969	-0.814033
H	0.043358	1.140692	1.053972
S	-0.849105	-1.873595	-2.526833
O	0.007803	-1.949506	-1.328187
O	-0.777459	-2.901077	-3.497693
O	-2.329698	-1.761771	-2.038322
O	-0.534771	-0.506929	-3.230471
H	-2.460272	-1.066869	-1.333027
H	-0.342541	0.210766	-2.577851
O	5.134106	0.307595	-1.059054
O	3.025984	1.564179	1.564258
O	2.624652	-1.115409	-0.716492
O	3.192725	2.162615	-0.602542
O	2.442668	-2.378743	1.126918
C	4.682966	0.461183	0.255523
C	4.309253	-0.870725	0.944840
C	3.556034	1.493112	0.344636
C	3.033157	-1.536462	0.478034
H	5.522593	0.883110	0.818756
H	4.224666	-0.744213	2.024716
H	5.129160	-1.572151	0.763123
H	4.371838	0.097149	-1.612630
H	2.237279	2.136415	1.552881
H	1.754249	-1.509327	-0.955716
4SA1MA1DMA			
S	-1.494936	2.897392	-0.239612
O	-2.886553	3.251037	-0.159058
O	-0.835093	2.378410	0.932402
O	-1.292540	1.904171	-1.435228
O	-0.739645	4.182920	-0.742955
H	-0.919569	1.020792	-1.129608
H	0.228494	4.013232	-0.687721
S	0.217852	-1.481049	-1.321269
O	1.668215	-1.256383	-1.533787
O	-0.388692	-0.363448	-0.569508
O	-0.374685	-1.443554	-2.784319
O	-0.093314	-2.772364	-0.717417
H	-1.353073	-1.606946	-2.710002
H	-1.321117	0.168554	1.977351
S	4.439338	-1.605558	0.486431
O	5.491321	-2.288210	1.147286
O	4.703369	-0.443987	-0.349427
O	3.653181	-2.664797	-0.363075
O	3.375877	-1.140637	1.583423

H	2.920525	-2.235700	-0.878442
H	2.959893	-0.295583	1.285969
S	2.497888	1.990205	-0.348343
O	2.116227	1.093601	0.740451
O	1.950327	3.311749	-0.373504
O	4.054987	2.153898	-0.337759
O	2.175832	1.303714	-1.708576
H	4.474939	1.253103	-0.324340
H	2.045069	0.304277	-1.638271
O	-4.711954	-2.141697	1.752896
O	-4.619969	1.049197	0.165971
O	-2.792813	-2.890521	-0.206385
O	-3.063167	0.046717	1.451247
O	-2.966474	-1.777294	-2.155959
C	-4.989169	-1.226086	0.729787
C	-4.871726	-1.840168	-0.693361
C	-4.113273	0.028951	0.838900
C	-3.453974	-2.161069	-1.109391
H	-6.026727	-0.911925	0.859850
H	-5.286362	-1.163877	-1.439222
H	-5.452974	-2.766512	-0.687331
H	-3.828584	-2.497214	1.593431
H	-4.015961	1.828387	0.163263
H	-1.838864	-2.985244	-0.457605
C	-0.159043	0.924270	3.523899
N	-0.353376	0.062343	2.323391
C	-0.070284	-1.382761	2.557400
H	-0.833898	0.588175	4.310009
H	-0.382123	1.949674	3.243163
H	0.874330	0.839177	3.856905
H	0.229038	0.417511	1.554369
H	-0.732518	-1.744376	3.342775
H	0.970190	-1.501857	2.856416
H	-0.250027	-1.924883	1.632842
4SA1MA2DMA			
S	-1.124176	2.962658	0.057043
O	-2.415356	2.687095	0.698366
O	0.003014	2.395583	0.823208
O	-1.117118	2.217357	-1.365668
O	-0.905860	4.365468	-0.297801
H	-0.987362	1.248941	-1.208698
H	0.772601	4.503408	-0.480598
S	-0.233351	-1.567357	-1.226042
O	1.254504	-1.584287	-1.309651

O	-0.729583	-0.333392	-0.609766
O	-0.673565	-1.566282	-2.747019
O	-0.759464	-2.774564	-0.593613
H	-1.665192	-1.654217	-2.763724
H	-2.000246	0.213676	2.003414
S	3.743937	-3.284446	0.378600
O	4.468793	-4.422329	0.815584
O	4.414552	-2.209756	-0.341823
O	2.550921	-3.790562	-0.500916
O	3.042561	-2.632420	1.647949
H	2.043003	-3.023009	-0.883312
H	2.901223	-1.667400	1.500186
S	3.247215	0.876196	0.186771
O	2.643460	0.034792	1.203871
O	3.348358	2.290614	0.414573
O	4.709474	0.387085	-0.090063
O	2.490609	0.679814	-1.164522
H	4.719732	-0.608531	-0.175632
H	2.002536	-0.211840	-1.221324
O	-5.691209	-2.002269	1.248270
O	-4.472591	1.134161	0.032251
O	-3.460629	-2.711764	-0.415259
O	-3.645746	-0.257439	1.603274
O	-3.327375	-1.681733	-2.413686
C	-5.564575	-0.955888	0.326261
C	-5.341809	-1.448523	-1.130509
C	-4.457498	0.022171	0.736353
C	-3.945168	-1.960471	-1.400806
H	-6.509499	-0.407474	0.339688
H	-5.537484	-0.652399	-1.847333
H	-6.054710	-2.260190	-1.301667
H	-4.819331	-2.407937	1.337594
H	-3.708708	1.731231	0.267804
H	-2.489794	-2.879798	-0.539195
C	-1.265202	1.261709	3.616407
N	-1.068318	0.388544	2.428049
C	-0.409584	-0.913768	2.717807
H	-1.886040	0.740298	4.344171
H	-1.759699	2.171661	3.283753
H	-0.295046	1.499864	4.050460
H	-0.527487	0.933840	1.726190
H	-0.978502	-1.434256	3.487640
H	0.608059	-0.731923	3.058862
H	-0.397549	-1.505840	1.806109

C	1.962013	4.107992	-2.131064
N	1.798582	4.391896	-0.677485
C	2.555521	5.572028	-0.187032
H	1.612951	4.968159	-2.700933
H	1.360952	3.234697	-2.374813
H	3.011616	3.909970	-2.342711
H	2.103997	3.558202	-0.150233
H	2.228718	6.458826	-0.728957
H	3.620637	5.406720	-0.343832
H	2.356587	5.696567	0.876213

4SA1MA3DMA

S	1.667130	2.519182	-0.910121
O	3.087442	2.168932	-1.016884
O	0.791087	1.844980	-1.855921
O	1.198398	1.967005	0.572597
O	1.443087	3.963056	-0.787961
H	0.771529	1.060630	0.469815
H	-0.196957	4.268331	-0.501646
S	0.024374	-1.080682	1.745501
O	-1.592045	-1.058122	1.903727
O	0.294456	-0.469279	0.421019
O	0.577855	-0.294699	2.833154
O	0.321675	-2.511697	1.765544
H	3.065705	0.083540	2.328552
H	0.542763	-0.456375	-2.031453
S	-4.412979	-2.590539	0.365329
O	-5.336870	-3.661583	0.239636
O	-4.787626	-1.343203	1.011873
O	-3.137765	-3.156880	1.100227
O	-3.892794	-2.236023	-1.089234
H	-2.569805	-2.424034	1.452112
H	-3.522875	-1.307364	-1.102677
S	-3.143341	1.313673	-0.281898
O	-2.761998	0.140493	-1.114363
O	-3.006861	2.580766	-0.986928
O	-4.707876	1.177897	-0.028804
O	-2.468533	1.292067	1.023359
H	-4.878841	0.307446	0.405443
H	-1.939361	-0.154246	1.653119
O	3.562445	-3.590632	-2.108806
O	4.322055	-0.118873	-1.580524
O	2.579984	-3.226764	0.578933
O	2.392557	-1.122390	-2.163803
O	3.620475	-1.547623	1.653631

C	4.310897	-2.498417	-1.649716
C	4.751235	-2.647751	-0.165761
C	3.560449	-1.172233	-1.844581
C	3.606655	-2.415712	0.798616
H	5.216809	-2.458867	-2.259637
H	5.540459	-1.937126	0.071587
H	5.129185	-3.666048	-0.045697
H	2.808406	-3.693220	-1.513314
H	3.782701	0.719121	-1.560729
H	1.778804	-2.973027	1.126597
C	-0.597251	-0.266706	-3.736445
N	-0.387384	-0.757318	-2.348792
C	-0.496254	-2.234560	-2.193776
H	0.146302	-0.725347	-4.386823
H	-0.473433	0.813191	-3.731406
H	-1.602010	-0.535117	-4.059792
H	-1.076818	-0.302740	-1.727568
H	0.268628	-2.704027	-2.808727
H	-1.492590	-2.555232	-2.494359
H	-0.329534	-2.474739	-1.146734
C	2.848483	1.492563	3.840682
N	3.150898	1.107375	2.434167
C	4.498590	1.523351	1.954341
H	3.591891	1.042803	4.498192
H	1.856669	1.120860	4.082748
H	2.888166	2.578224	3.925108
H	2.428978	1.506877	1.800595
H	5.256659	1.041383	2.569779
H	4.581344	2.606960	2.026493
H	4.602231	1.220099	0.916443
C	-1.263239	4.500822	1.261354
N	-1.188254	4.472945	-0.224542
C	-1.635870	5.722303	-0.890372
H	-0.606723	5.285487	1.636590
H	-0.945267	3.529397	1.632247
H	-2.292399	4.687922	1.565129
H	-1.786880	3.685798	-0.561107
H	-1.017456	6.554030	-0.553874
H	-2.681021	5.907172	-0.644458
H	-1.530382	5.599700	-1.967171
4SA1MA4DMA			
S	2.976114	-2.056572	-1.283895
O	4.202828	-1.447424	-1.807191
O	3.151525	-3.107675	-0.300767

O	2.008187	-1.022930	-0.822713
O	2.301498	-2.703522	-2.604364
H	-0.380027	-0.000820	-0.178335
H	1.425834	-3.055744	-2.335103
S	-0.890640	2.063589	0.057247
O	-2.305886	1.739334	0.394040
O	-0.059071	0.729385	0.406610
O	-0.736001	2.293590	-1.377358
O	-0.307105	3.058735	0.941646
H	1.140272	1.772621	-2.168085
H	2.657218	-1.504601	1.493891
S	-3.418742	-1.035666	2.349783
O	-4.300903	-1.442207	3.388612
O	-3.724917	-1.392800	0.963097
O	-3.276244	0.516931	2.442238
O	-1.972627	-1.575932	2.661477
H	-2.792959	0.941121	1.656138
H	-1.510935	-1.927748	1.837626
S	-1.089883	-2.506988	-0.760018
O	-0.623586	-2.542611	0.652306
O	-0.316632	-3.306325	-1.677014
O	-2.543279	-3.193335	-0.752969
O	-1.312676	-1.102990	-1.182599
H	-3.081960	-2.726256	-0.075844
H	-3.143610	-0.175470	-1.149642
O	4.576053	2.059202	2.918954
O	5.170593	0.565065	-0.299803
O	2.326173	3.145734	1.505778
O	4.034678	-0.207822	1.488540
O	2.638649	3.133513	-0.719391
C	5.037736	1.991426	1.596121
C	4.569587	3.187488	0.727487
C	4.685532	0.650078	0.930065
C	3.087918	3.159409	0.406223
H	6.129770	2.034966	1.645663
H	5.115308	3.204229	-0.213587
H	4.790950	4.097909	1.290662
H	3.621394	2.204834	2.885605
H	4.867624	-0.263468	-0.767407
H	1.361915	3.122296	1.256876
C	2.325693	-3.163235	2.687952
N	1.875011	-1.905608	2.031913
C	1.379111	-0.862229	2.974061
H	3.131201	-2.925192	3.381470

H	2.682739	-3.833509	1.910764
H	1.485854	-3.603432	3.224422
H	1.142941	-2.127474	1.340732
H	2.202173	-0.569251	3.622873
H	0.549381	-1.264324	3.553319
H	1.042445	-0.010639	2.387788
C	0.711550	0.285733	-3.549812
N	1.635153	0.989262	-2.617385
C	2.898003	1.448024	-3.262534
H	0.383073	0.981110	-4.322059
H	-0.134033	-0.085450	-2.976679
H	1.244800	-0.554164	-3.992102
H	1.861214	0.307879	-1.847022
H	2.652400	2.081246	-4.115411
H	3.456499	0.570466	-3.583081
H	3.464389	2.014158	-2.530035
C	-3.305501	0.738944	-2.979148
N	-3.907821	0.183753	-1.737503
C	-4.895487	-0.901874	-1.973125
H	-2.824630	-0.066529	-3.532183
H	-2.565241	1.484873	-2.692895
H	-4.093148	1.188203	-3.584336
H	-4.378969	0.986031	-1.203626
H	-4.402447	-1.740553	-2.462811
H	-5.699914	-0.519784	-2.601523
H	-5.288406	-1.222266	-1.010787
C	-6.094513	2.074344	0.606277
N	-5.081209	2.383833	-0.412888
C	-5.471611	3.504628	-1.276860
H	-6.369859	2.953138	1.205201
H	-5.711798	1.307030	1.279558
H	-7.000188	1.696838	0.123456
H	-4.202505	2.611573	0.050438
H	-5.733485	4.406316	-0.706191
H	-6.341112	3.224255	-1.878384
H	-4.649876	3.753362	-1.951455
4SA2MA			
S	-2.688578	2.058471	-1.443048
O	-2.745639	2.399142	-0.050567
O	-3.903202	1.676200	-2.125739
O	-2.043552	3.227217	-2.257813
O	-1.592412	0.936584	-1.693855
H	-1.293044	3.615289	-1.727556
H	-1.949177	0.057405	-1.411557

S	-4.212231	-1.667941	-1.036454
O	-2.753301	-1.486830	-1.150075
O	-4.701929	-2.999725	-1.072660
O	-4.693601	-0.863058	0.221168
O	-4.913882	-0.842543	-2.158658
H	-4.112428	-0.982748	1.021640
H	-4.601301	0.101990	-2.167149
S	0.197344	-3.203816	0.142418
O	1.247372	-4.165143	-0.082586
O	-0.672779	-3.354985	1.284236
O	0.810408	-1.770232	0.238213
O	-0.656699	-3.196103	-1.169966
H	1.739807	-1.726702	-0.164043
H	-1.478365	-2.642114	-1.088176
O	6.116649	-1.940710	0.617520
O	3.941267	-3.725438	-0.495465
O	5.129383	0.674715	0.317510
O	3.225648	-1.594222	-0.593986
O	4.365696	1.217116	-1.725471
C	5.594788	-2.016782	-0.695553
C	5.768485	-0.719889	-1.503980
C	4.122948	-2.432181	-0.606858
C	4.999422	0.477443	-0.990744
H	6.141701	-2.819205	-1.192499
H	5.477768	-0.868768	-2.544291
H	6.833018	-0.466245	-1.480410
H	5.793922	-1.118267	1.012026
H	2.985821	-3.938890	-0.363711
H	4.592332	1.461455	0.611110
S	-1.909968	-0.392674	2.580024
O	-1.739973	0.798666	3.372192
O	-3.217517	-0.990163	2.452336
O	-1.420235	-0.156299	1.118713
O	-0.903069	-1.440220	3.169942
H	-0.679771	0.528900	1.059341
H	-0.833126	-2.222751	2.561384
O	0.148618	4.009592	-0.902935
O	-0.753665	3.168590	2.327074
O	2.725320	3.115229	-0.981617
O	0.245425	1.787608	0.847053
O	3.613829	2.784762	1.057340
C	0.394305	4.153642	0.491955
C	1.882610	4.444203	0.790012
C	-0.060397	2.901737	1.246649

C	2.830481	3.355845	0.320836
H	-0.205040	4.996612	0.833024
H	2.027990	4.584962	1.861008
H	2.148420	5.370952	0.273921
H	0.876367	3.492181	-1.287710
H	-1.071061	2.342255	2.767451
H	3.359951	2.386970	-1.269977

4SA2MA1DMA

S	-4.481422	-3.056943	-0.540299
O	-5.387380	-4.130034	-0.344692
O	-4.766682	-1.978953	0.576491
O	-3.047732	-3.312255	-0.570031
O	-4.874035	-2.324454	-1.885513
H	-1.623365	-2.898165	-1.487424
H	-4.208508	-1.613714	-2.082154
S	-2.413375	0.342879	-1.137222
O	-2.893057	-0.548093	-2.195042
O	-0.978982	0.064107	-0.845792
O	-2.515170	1.813015	-1.645589
O	-3.257782	0.271253	0.073624
H	-1.617267	2.248512	-1.775778
H	-4.185760	-1.185524	0.462656
O	1.919401	3.523230	-3.602233
O	0.662643	3.801215	-0.264245
O	4.677558	1.718418	-1.409874
O	-0.241217	2.963535	-2.158971
O	2.470261	1.335931	-1.539264
C	1.911482	3.986716	-2.274630
C	3.219932	3.602632	-1.576671
C	0.662322	3.511358	-1.539134
C	3.528175	2.125502	-1.516129
H	1.849958	5.086143	-2.255500
H	3.210560	3.970549	-0.546098
H	4.056476	4.082710	-2.085163
H	1.046795	3.137766	-3.764163
H	-0.154918	3.487579	0.207033
H	2.746594	0.385910	-1.463977
S	0.402047	-0.302949	2.416897
O	0.420686	-1.724788	2.109921
O	-0.758890	0.194762	3.100254
O	1.656668	0.073136	3.252930
O	0.688861	0.510570	1.110168
H	2.468300	-0.406630	2.897933
H	-0.039115	0.403948	0.423658

O	6.110930	-2.355484	1.585164
O	2.657096	-3.205093	1.774281
O	5.404140	-0.711267	-0.790802
O	3.686024	-1.251388	2.237298
O	3.279267	-1.265668	-1.273772
C	4.944075	-2.985980	1.150640
C	4.762228	-2.949978	-0.399931
C	3.696584	-2.393168	1.802742
C	4.406281	-1.563904	-0.886626
H	5.019334	-4.033763	1.447363
H	3.974470	-3.640056	-0.698429
H	5.713443	-3.261932	-0.833989
H	6.056800	-1.417696	1.360731
H	1.833838	-2.724289	2.042070
H	5.120494	0.217743	-1.066390
S	-2.430060	3.187999	2.006407
O	-2.756717	4.555620	2.199817
O	-1.403541	2.795051	1.046117
O	-2.016848	2.605484	3.411737
O	-3.737008	2.403814	1.629991
H	-1.558352	1.738246	3.311237
H	-3.538586	1.625778	1.041947
C	0.335402	-3.338180	-0.971273
N	-0.673687	-2.585788	-1.768882
C	-0.515468	-2.688578	-3.244791
H	0.298845	-4.389721	-1.253337
H	0.082682	-3.225515	0.080699
H	1.321640	-2.917252	-1.163842
H	-0.648426	-1.586430	-1.491966
H	-0.629132	-3.729540	-3.545167
H	0.473836	-2.326500	-3.522169
H	-1.283886	-2.075234	-3.711106
4SA2MA2DMA			
S	-3.878416	-2.571469	-1.440868
O	-4.818348	-3.425646	-0.762255
O	-2.791862	-2.041808	-0.558097
O	-3.270862	-3.087244	-2.678814
O	-4.747793	-1.270704	-1.846075
H	-1.740941	-2.434001	-2.768165
H	-4.132852	-0.584707	-2.186435
S	-1.978572	1.177883	-1.455390
O	-2.736348	0.550363	-2.521460
O	-0.696540	0.427608	-1.199061
O	-1.551324	2.602238	-1.971695

O	-2.730350	1.377415	-0.209288
H	-0.573656	2.772074	-1.880658
H	-3.016932	-0.465522	2.157995
O	3.404333	3.183600	-3.253627
O	1.930575	3.761636	-0.045305
O	5.385665	0.790515	-0.687442
O	1.043050	3.141946	-2.028974
O	3.214164	0.943552	-1.232444
C	3.377188	3.638433	-1.923131
C	4.482837	2.961750	-1.106579
C	1.984326	3.470573	-1.321823
C	4.407036	1.456617	-1.001724
H	3.573482	4.721397	-1.890232
H	4.484388	3.354184	-0.085281
H	5.453146	3.202591	-1.543313
H	2.487649	2.980670	-3.488967
H	1.017488	3.656824	0.328788
H	3.239816	-0.046094	-1.146839
S	-0.102346	-0.370758	2.158604
O	-0.387929	-1.775065	1.898846
O	-1.236472	0.386755	2.661815
O	1.033104	-0.246511	3.212817
O	0.534728	0.296879	0.933381
H	1.774840	-0.893400	2.986089
H	-0.070698	0.373260	0.061449
O	5.077640	-3.579336	2.308694
O	1.582352	-3.619369	1.633999
O	5.366992	-1.743004	-0.027748
O	2.863704	-1.978098	2.506097
O	3.335906	-1.752125	-0.990771
C	3.943004	-3.906325	1.563221
C	4.153856	-3.773203	0.023390
C	2.731446	-3.069828	1.971366
C	4.247562	-2.326681	-0.403466
H	3.717092	-4.953551	1.772807
H	3.323553	-4.238514	-0.505803
H	5.084710	-4.291155	-0.212563
H	5.288357	-2.649017	2.158255
H	0.830129	-2.993446	1.788738
H	5.377748	-0.771341	-0.301530
S	-1.490023	3.898586	1.864919
O	-1.476022	5.274106	2.215852
O	-0.463101	3.333594	1.001011
O	-1.471963	3.078823	3.220896

O	-2.877292	3.548441	1.226265
H	-1.318359	2.123132	3.039368
H	-2.799154	2.753686	0.616117
C	0.085410	-3.030831	-1.991098
N	-0.762774	-2.043875	-2.710997
C	-0.288327	-1.671764	-4.067466
H	0.121433	-3.953647	-2.569673
H	-0.382789	-3.218450	-1.027036
H	1.088355	-2.626332	-1.853730
H	-0.833682	-1.190423	-2.133819
H	-0.274314	-2.559643	-4.698936
H	0.712341	-1.245841	-3.999015
H	-0.977313	-0.935755	-4.478296
C	-3.848989	-2.324260	2.565004
N	-3.710578	-1.093495	1.739206
C	-4.989165	-0.367042	1.496643
H	-4.304566	-2.077083	3.523897
H	-2.856207	-2.743965	2.715540
H	-4.467777	-3.031895	2.015038
H	-3.307377	-1.397871	0.800454
H	-5.419176	-0.059469	2.450003
H	-5.667662	-1.034273	0.968261
H	-4.773064	0.498195	0.874812

4SA2MA3DMA

S	1.646300	-1.673007	-1.788345
O	2.985692	-1.558593	-2.291660
O	0.630347	-2.273699	-2.607821
O	1.635429	-2.491975	-0.434401
O	1.235552	-0.223271	-1.344068
H	2.281350	-2.088872	0.230408
H	0.379997	-0.210849	-0.805977
S	-2.582532	-3.984100	-1.479912
O	-3.897221	-4.409978	-1.886639
O	-2.578703	-2.960588	-0.396031
O	-1.611728	-5.040539	-1.140022
O	-2.004064	-3.225826	-2.788973
H	-0.889728	-4.587349	0.286618
H	-1.065289	-2.989025	-2.648053
S	-1.052981	-0.373329	1.539518
O	-2.441854	-0.392280	1.982362
O	-0.272556	-1.554049	1.985961
O	-0.919220	-0.136105	0.094458
O	-0.418536	0.877268	2.299089
H	-3.395196	-1.529814	-0.618552

H	0.562595	0.875946	2.162995
O	-5.289730	4.153492	0.144366
O	-3.576354	1.973591	2.404864
O	-2.334737	3.330929	-0.200852
O	-4.737728	1.573909	0.512277
O	-1.359021	5.290711	0.294524
C	-4.603788	3.823106	1.328533
C	-3.343175	4.684102	1.483160
C	-4.302429	2.326746	1.370148
C	-2.254757	4.471012	0.454179
H	-5.243699	4.029496	2.199234
H	-2.886745	4.499259	2.460287
H	-3.621208	5.738642	1.451618
H	-5.425634	3.318362	-0.325402
H	-3.246701	1.038227	2.314448
H	-1.558475	3.217838	-0.822111
S	3.013335	-0.555186	2.359072
O	3.334644	-1.510254	1.247176
O	4.178118	-0.203326	3.121643
O	2.230684	0.589774	1.822366
O	2.028848	-1.326988	3.333566
H	2.619343	1.798206	0.663346
H	1.136592	-1.417212	2.900663
O	3.561625	4.857114	-1.443922
O	4.392187	1.696658	-0.970174
O	0.795076	4.900775	-1.170066
O	2.550900	2.544438	0.013216
O	-0.263454	3.031824	-1.827494
C	3.294230	3.584508	-1.993587
C	1.927459	3.485365	-2.707582
C	3.469216	2.494269	-0.929668
C	0.712502	3.765031	-1.850074
H	4.073607	3.396877	-2.732637
H	1.799014	2.496363	-3.148779
H	1.934516	4.227277	-3.512571
H	2.765138	5.151400	-0.980130
H	5.123141	0.266471	-0.392857
H	-0.030969	5.052869	-0.615268
C	-3.409561	-0.135549	-2.155348
N	-4.027124	-0.756476	-0.950324
C	-5.368430	-1.355452	-1.192436
H	-3.267254	-0.906252	-2.911000
H	-2.446018	0.275619	-1.863519
H	-4.061289	0.655877	-2.524048

H	-4.107513	-0.041651	-0.212459
H	-5.262923	-2.184313	-1.890536
H	-6.039746	-0.592053	-1.584170
H	-5.751148	-1.734627	-0.246166
C	6.069224	-1.358561	-1.274446
N	5.602202	-0.603330	-0.078764
C	6.672970	-0.244491	0.892840
H	6.791519	-0.749127	-1.816798
H	5.206015	-1.569359	-1.902183
H	6.538377	-2.286910	-0.949091
H	4.853539	-1.129503	0.415783
H	7.379454	0.429738	0.409883
H	7.182828	-1.152924	1.212250
H	6.210697	0.232719	1.754710
C	-1.625675	-4.595059	2.222566
N	-0.547562	-4.298622	1.241630
C	0.751392	-4.955503	1.532641
H	-1.828705	-5.665446	2.212621
H	-2.509700	-4.043428	1.912511
H	-1.309896	-4.275848	3.215086
H	-0.424366	-3.274013	1.215975
H	0.604594	-6.034647	1.568089
H	1.133890	-4.599373	2.489284
H	1.448794	-4.700888	0.737887
4SA2MA4DMA			
S	-1.229012	1.527261	-1.857296
O	-2.534052	1.309117	-2.424688
O	-0.244073	2.234932	-2.628623
O	-1.351097	2.309863	-0.493513
O	-0.714021	0.109468	-1.430326
H	-1.985622	1.824787	0.142138
H	0.093072	0.145031	-0.818060
S	2.825427	4.091499	-1.348798
O	4.138788	4.578238	-1.685998
O	2.814079	3.039559	-0.293029
O	1.799767	5.100133	-1.024352
O	2.334963	3.348294	-2.702154
H	1.045313	4.571295	0.363918
H	1.407290	3.054616	-2.601909
S	1.379578	0.365676	1.609679
O	2.749791	0.472200	2.097977
O	0.514938	1.501763	2.011510
O	1.314942	0.108663	0.161910
O	0.796533	-0.911464	2.360425

H	3.730708	1.662457	-0.480806
H	-0.184734	-0.957179	2.220369
O	5.890656	-3.899042	0.288023
O	3.980877	-1.849416	2.513494
O	2.925305	-3.169256	-0.197695
O	5.209800	-1.356197	0.687040
O	2.016701	-5.190847	0.154950
C	5.124957	-3.630556	1.438685
C	3.890141	-4.540738	1.494392
C	4.765516	-2.147692	1.504876
C	2.859695	-4.338826	0.404780
H	5.720931	-3.840728	2.338989
H	3.368246	-4.394783	2.445047
H	4.208591	-5.583452	1.456671
H	6.013502	-3.046496	-0.153317
H	3.616476	-0.925969	2.430746
H	2.176659	-3.060663	-0.854223
S	-2.739103	0.314848	2.226020
O	-3.026720	1.154777	1.032747
O	-3.931908	-0.050514	2.946733
O	-1.847138	-0.817887	1.863191
O	-1.880741	1.218426	3.221449
H	-2.064889	-1.988444	0.640511
H	-0.965172	1.322568	2.853417
O	-2.853520	-4.823619	-1.772817
O	-3.714400	-1.682723	-1.035587
O	-0.085988	-4.805950	-1.405853
O	-1.950098	-2.679062	-0.062274
O	0.929304	-2.864110	-1.897062
C	-2.604110	-3.498752	-2.194802
C	-1.224010	-3.309641	-2.864901
C	-2.821839	-2.509454	-1.042547
C	-0.023664	-3.621687	-1.999150
H	-3.368602	-3.264063	-2.936127
H	-1.112870	-2.285076	-3.220861
H	-1.190577	-3.986058	-3.725183
H	-2.074544	-5.127305	-1.286629
H	-4.217521	0.442323	-0.961244
H	0.719908	-4.961476	-0.825802
C	3.843596	0.285253	-2.025163
N	4.406253	0.923021	-0.802086
C	5.723744	1.584407	-1.010088
H	3.679669	1.056500	-2.776040
H	2.895755	-0.175982	-1.757695

H	4.540347	-0.469383	-2.388712
H	4.504494	0.207529	-0.066723
H	5.596721	2.412950	-1.704918
H	6.437412	0.854969	-1.391558
H	6.067959	1.972904	-0.052881
C	-5.201536	2.262459	-0.937936
N	-5.181515	0.781218	-1.051870
C	-5.736075	0.270459	-2.331482
H	-4.600848	2.687840	-1.739344
H	-4.776261	2.531752	0.025955
H	-6.232736	2.609129	-1.010146
H	-5.708827	0.355742	-0.214455
H	-5.155953	0.681820	-3.156316
H	-6.779942	0.573892	-2.415769
H	-5.648329	-0.812752	-2.329375
C	1.698660	4.586314	2.329107
N	0.681902	4.245834	1.298335
C	-0.665296	4.817707	1.544337
H	1.841122	5.666351	2.343641
H	2.624947	4.090016	2.050452
H	1.359727	4.232141	3.301836
H	0.620790	3.215913	1.253869
H	-0.586646	5.902848	1.605049
H	-1.065991	4.419074	2.476433
H	-1.311165	4.536584	0.715490
C	-7.586379	0.409265	1.775774
N	-6.436085	-0.309745	1.214478
C	-6.701952	-1.744463	1.031940
H	-8.416166	0.398973	1.062884
H	-7.311506	1.447963	1.970430
H	-7.943314	-0.032977	2.716165
H	-5.648831	-0.213236	1.858907
H	-7.510751	-1.880992	0.308047
H	-6.995891	-2.238898	1.967511
H	-5.806274	-2.230006	0.643185
4SA3MA			
S	2.736965	4.318756	1.859865
O	3.498252	3.076785	1.897163
O	3.141212	5.431018	2.641777
O	2.598544	4.738983	0.335542
O	1.248970	3.997266	2.244775
H	3.152096	4.157990	-0.235638
H	0.896804	3.255770	1.695986
S	0.335882	0.853323	0.099578

O	0.879558	-0.020134	1.087817
O	0.123884	2.257456	0.485026
O	1.216656	0.836085	-1.205965
O	-0.991015	0.305435	-0.464166
H	2.179016	0.825513	-0.976761
H	-1.706319	1.026372	-0.597115
O	-4.849471	3.178024	-2.945116
O	-5.744183	1.899321	0.274246
O	-1.851364	3.978518	-0.359839
O	-5.799757	0.970769	-1.783597
O	-2.854383	2.010965	-0.778330
C	-5.248732	3.286965	-1.601902
C	-4.166368	4.020982	-0.812671
C	-5.604042	1.917466	-1.033057
C	-2.890648	3.233227	-0.664363
H	-6.174387	3.879527	-1.519734
H	-4.518692	4.254308	0.196817
H	-3.942200	4.969323	-1.303185
H	-5.137140	2.308998	-3.257345
H	-5.919439	0.981160	0.596696
H	-1.069197	3.413603	-0.161469
S	-7.007332	-1.518643	0.264728
O	-8.354948	-1.143651	0.514241
O	-5.951515	-0.740174	0.949719
O	-6.817581	-3.017933	0.591835
O	-6.649306	-1.486508	-1.267362
H	-5.839050	-3.279014	0.566555
H	-6.340007	-0.564392	-1.510655
O	-1.966178	-4.911138	0.497375
O	-3.355442	-1.651486	1.009800
O	1.335350	-3.554904	2.093351
O	-4.301850	-3.638815	0.539090
O	0.835892	-3.496047	-0.097315
C	-1.922606	-3.503102	0.483723
C	-0.893473	-3.040166	1.508953
C	-3.313930	-2.929632	0.704856
C	0.511121	-3.398484	1.080322
H	-1.609064	-3.127104	-0.503517
H	-1.097385	-3.486775	2.483120
H	-0.917603	-1.953009	1.616891
H	-2.839833	-5.178193	0.185091
H	-4.288840	-1.326857	1.048684
H	2.258472	-3.715458	1.763175
S	4.921232	1.881815	-0.815896

O	4.152737	3.038688	-1.194447
O	5.983455	1.414026	-1.663615
O	5.535743	2.069507	0.605433
O	3.869109	0.712734	-0.632834
H	4.851628	2.479748	1.211525
H	4.328976	-0.217663	-0.632336
O	6.407678	-4.075728	0.542494
O	3.199019	-4.139254	-1.043079
O	6.597709	-1.259483	-2.185881
O	3.823221	-3.978714	1.116592
O	4.900742	-1.566016	-0.742913
C	5.522977	-4.331168	-0.520348
C	5.929776	-3.486278	-1.730207
C	4.078150	-4.110380	-0.073889
C	5.768846	-2.008264	-1.493357
H	5.580976	-5.387557	-0.825118
H	5.306679	-3.741233	-2.593694
H	6.966424	-3.697916	-1.992925
H	5.862347	-3.998706	1.339313
H	2.280035	-3.932028	-0.687839
H	6.435427	-0.302196	-2.021836

4SA3MA1DMA

S	-1.814032	5.139682	1.557038
O	-1.793442	6.382390	2.244015
O	-0.574320	5.073685	0.590349
O	-1.875439	3.896904	2.311427
O	-3.049547	5.188190	0.576093
H	-1.384870	2.259538	2.507953
H	-3.139763	4.339985	0.083812
S	0.527440	1.529205	-0.457249
O	-0.634991	0.668393	-0.093870
O	0.601009	1.826163	-1.880422
O	0.598183	2.693917	0.430101
O	1.758716	0.595301	-0.081655
H	-0.199490	4.155950	0.496856
H	2.547643	0.834253	-0.651660
O	6.562958	2.516334	-2.347694
O	5.957681	-1.009114	-2.124101
O	2.763298	1.865255	-3.498917
O	6.643921	0.509539	-0.602255
O	3.786142	1.075618	-1.658931
C	6.325724	1.229678	-2.860869
C	5.038273	1.237514	-3.690594
C	6.300336	0.201212	-1.736275

C	3.799064	1.400215	-2.842290
H	7.149823	0.925679	-3.524355
H	4.932317	0.297805	-4.241697
H	5.088256	2.043811	-4.423005
H	6.786936	2.413465	-1.412417
H	5.879667	-1.612148	-1.348515
H	1.959760	1.897762	-2.915886
S	6.150355	-2.263363	1.408147
O	7.411809	-2.911778	1.490175
O	5.378150	-2.435968	0.158608
O	5.266066	-2.719174	2.601260
O	6.249205	-0.722414	1.670023
H	4.300967	-2.465964	2.470795
H	6.442007	-0.238045	0.807289
O	0.085269	-1.963877	2.367466
O	2.676871	-2.590777	-0.018032
O	-2.097638	-4.719106	0.883313
O	2.712939	-2.252310	2.209830
O	-1.864099	-2.864113	-0.365630
C	0.594374	-2.376176	1.108484
C	0.068833	-3.769179	0.717398
C	2.113000	-2.387625	1.147336
C	-1.402084	-3.730524	0.365874
H	0.276620	-1.644773	0.362887
H	0.239677	-4.486518	1.521428
H	0.595413	-4.117837	-0.176466
H	0.753173	-2.203587	3.025993
H	3.665148	-2.569995	0.051563
H	-3.052759	-4.659557	0.595238
S	-3.813981	1.585660	-0.930949
O	-3.136956	2.850112	-0.827124
O	-5.001708	1.477471	-1.744255
O	-2.832508	0.493383	-1.446513
O	-4.163401	1.149442	0.542647
H	-1.931098	0.558258	-0.987674
H	-4.881707	0.437092	0.525536
O	-6.674461	-3.474010	-2.582686
O	-4.289527	-2.867728	-1.417777
O	-6.640775	-0.693970	-1.651937
O	-4.648142	-4.513065	0.080373
O	-5.940076	-0.741515	0.488970
C	-6.512184	-3.664520	-1.202063
C	-7.233505	-2.578754	-0.347679
C	-5.041258	-3.743340	-0.783509

C	-6.551268	-1.238178	-0.448153
H	-6.962157	-4.627450	-0.960911
H	-7.248408	-2.873596	0.701156
H	-8.254436	-2.504641	-0.727591
H	-6.332755	-2.601007	-2.814453
H	-3.357997	-2.861801	-1.049065
H	-6.094623	0.130038	-1.710374
C	0.233220	1.303754	3.373514
N	-1.072441	1.281184	2.653737
C	-2.141460	0.497830	3.332255
H	0.075864	1.693810	4.378320
H	0.910653	1.949066	2.819263
H	0.624575	0.290039	3.406188
H	-0.925823	0.906217	1.698651
H	-2.308992	0.912009	4.325816
H	-1.820963	-0.540616	3.394834
H	-3.049983	0.578685	2.739112
4SA3MA2DMA			
S	-3.136636	4.956258	0.934534
O	-3.349570	6.269111	1.440494
O	-1.597650	4.832791	0.551162
O	-3.476404	3.792779	1.728793
O	-3.873930	4.873837	-0.450977
H	-3.789093	1.384281	1.679512
H	-3.751501	3.977361	-0.867928
S	0.311432	1.623838	0.266685
O	-0.183864	0.415020	-0.601123
O	1.017226	2.569450	-0.608605
O	-0.866807	2.228550	0.913111
O	1.244539	1.023154	1.249054
H	-1.320333	3.886642	0.600741
H	2.709673	1.964334	1.282746
O	6.516359	1.930683	-3.357621
O	5.394649	-1.316404	-2.317357
O	2.296165	1.724593	-2.794128
O	6.748562	0.175262	-1.310712
O	4.165431	1.931039	-1.556769
C	5.808516	0.725866	-3.465115
C	4.307195	0.935777	-3.737793
C	6.038681	-0.165201	-2.244512
C	3.580271	1.587970	-2.583403
H	6.227811	0.189553	-4.322209
H	3.805911	-0.008108	-3.964606
H	4.197934	1.574722	-4.617833

H	6.330841	2.287512	-2.480308
H	5.539715	-1.852116	-1.501681
H	1.818653	2.088863	-1.997176
S	6.421584	-2.238057	1.232576
O	7.658167	-2.912000	1.416891
O	5.573699	-2.639503	0.092965
O	5.578582	-2.341848	2.530209
O	6.613084	-0.678343	1.121089
H	4.605809	-2.094850	2.360228
H	6.757548	-0.398754	0.158808
O	0.379856	-1.474072	2.163863
O	2.908559	-3.274603	0.351267
O	-1.311005	-3.392231	-0.361684
O	3.094549	-1.820500	2.059540
O	-2.142509	-4.085898	1.609905
C	0.891377	-2.350792	1.196162
C	0.227848	-3.721963	1.395648
C	2.412945	-2.459250	1.268187
C	-1.202404	-3.744521	0.902981
H	0.675604	-2.002365	0.177537
H	0.236386	-3.980518	2.454097
H	0.775346	-4.480042	0.830604
H	0.727387	-0.583246	1.975008
H	3.890323	-3.206755	0.316686
H	-2.256022	-3.472829	-0.674948
S	-3.781861	1.173551	-1.380267
O	-3.319427	2.536599	-1.576202
O	-4.660342	0.645458	-2.420832
O	-2.689554	0.239924	-1.032610
O	-4.705172	1.253743	-0.039979
H	-1.176067	0.460700	-0.833571
H	-5.325532	0.472366	-0.048143
O	-6.118308	-4.437386	-2.465858
O	-4.649580	-4.503473	0.774341
O	-6.085970	-1.563398	-2.138877
O	-3.817753	-3.731385	-1.170897
O	-6.151957	-0.960256	0.029235
C	-6.148808	-4.298042	-1.074206
C	-7.024065	-3.102841	-0.597696
C	-4.739646	-4.163579	-0.495015
C	-6.386246	-1.759514	-0.868593
H	-6.593456	-5.210425	-0.672451
H	-7.217341	-3.170491	0.472074
H	-7.968427	-3.169616	-1.143406

H	-5.675982	-3.659026	-2.830036
H	-3.718549	-4.348941	1.106299
H	-5.568333	-0.713565	-2.266055
C	-3.258858	1.496764	3.697404
N	-3.045400	1.026271	2.300586
C	-2.960527	-0.458031	2.154515
H	-4.193325	1.079446	4.071129
H	-3.308398	2.582048	3.683555
H	-2.429903	1.151838	4.314566
H	-2.188579	1.460584	1.913684
H	-3.871772	-0.902958	2.552082
H	-2.086019	-0.824842	2.689229
H	-2.867182	-0.683341	1.095047
C	3.220710	3.981819	1.316652
N	3.556510	2.546219	1.099293
C	4.697802	2.049077	1.915155
H	2.950755	4.131189	2.361503
H	2.380191	4.235123	0.674449
H	4.087287	4.593371	1.067281
H	3.752061	2.391083	0.089411
H	4.461711	2.171828	2.971602
H	5.592686	2.618922	1.667597
H	4.866380	0.997360	1.695543
4SA3MA3DMA			
S	4.308004	4.613581	-1.256701
O	4.724574	5.836307	-1.854195
O	2.801668	4.797874	-0.784432
O	4.381141	3.368989	-1.996282
O	5.107267	4.465787	0.088346
H	4.283099	0.943856	-1.775638
H	4.848723	3.631080	0.567413
S	0.348021	1.918416	-0.332337
O	0.669708	0.702771	0.613452
O	-0.284575	2.968199	0.471110
O	1.616338	2.345995	-0.950025
O	-0.597579	1.374645	-1.336730
H	2.349138	3.920641	-0.759250
H	-2.078598	2.279834	-1.322866
O	-5.528133	3.182878	3.409098
O	-4.908081	-0.290094	2.820180
O	-1.507913	2.640559	2.890569
O	-6.227241	1.209566	1.764233
O	-3.271965	2.190916	1.575736
C	-5.033524	1.902422	3.723339

C	-3.519869	1.967905	3.946050
C	-5.437013	0.895764	2.646973
C	-2.756635	2.288187	2.683807
H	-5.489337	1.535545	4.655420
H	-3.146547	1.012393	4.325758
H	-3.293801	2.724070	4.700299
H	-6.146938	3.056353	2.675905
H	-5.185052	-0.932638	2.102583
H	-1.027078	2.758340	2.030705
S	-6.843176	-1.845647	0.200091
O	-7.902867	-2.021884	1.147452
O	-5.476710	-1.915558	0.819585
O	-6.905880	-2.660953	-1.020233
O	-6.905695	-0.331782	-0.391986
H	-6.076365	-2.205004	-2.278461
H	-6.754823	0.282038	0.371080
O	-0.391435	-1.322242	-2.018164
O	-3.065714	-2.543670	0.042957
O	1.132642	-3.185210	0.616856
O	-3.122776	-1.180070	-1.748483
O	1.685971	-4.311508	-1.249944
C	-0.983020	-1.998423	-0.937655
C	-0.555513	-3.471259	-1.007118
C	-2.510409	-1.867879	-0.937566
C	0.875736	-3.691566	-0.571432
H	-0.655668	-1.584672	0.024660
H	-0.662777	-3.836314	-2.028663
H	-1.186980	-4.064256	-0.341227
H	-0.508753	-0.365755	-1.873836
H	-4.036796	-2.333788	0.181805
H	2.060768	-3.410100	0.907846
S	4.401660	0.905265	1.272202
O	4.210221	2.340395	1.387160
O	5.234384	0.293575	2.305590
O	3.142254	0.168452	1.048121
O	5.246014	0.727192	-0.114247
H	1.655520	0.616967	0.837907
H	5.705646	-0.157089	-0.080290
O	5.760028	-4.930788	2.683873
O	4.123717	-5.079085	-0.461781
O	6.221573	-2.143490	2.122029
O	3.572935	-3.909656	1.382384
O	6.246672	-1.726034	-0.090175
C	5.747893	-4.919731	1.284638

C	6.784265	-3.933993	0.672628
C	4.354738	-4.596425	0.741531
C	6.400191	-2.483688	0.859738
H	6.015340	-5.925336	0.955503
H	6.901180	-4.113521	-0.395478
H	7.733813	-4.123094	1.179411
H	5.494989	-4.051854	2.986662
H	3.217017	-4.795575	-0.777085
H	5.863379	-1.208630	2.204457
C	3.708858	1.029963	-3.783594
N	3.458633	0.706742	-2.352328
C	3.082539	-0.715818	-2.096527
H	4.526538	0.408894	-4.148150
H	3.972980	2.081715	-3.850408
H	2.804941	0.819169	-4.354399
H	2.723754	1.332511	-1.974024
H	3.865517	-1.362223	-2.491130
H	2.128220	-0.932969	-2.573958
H	2.996438	-0.850471	-1.021170
C	-2.751410	4.253100	-1.302774
N	-2.932373	2.802480	-1.031614
C	-4.142520	2.192828	-1.638927
H	-2.661360	4.413529	-2.377014
H	-1.843068	4.578235	-0.799632
H	-3.611243	4.800251	-0.916960
H	-2.970326	2.645782	0.001888
H	-4.114289	2.336069	-2.719462
H	-5.030161	2.666620	-1.221434
H	-4.147095	1.130111	-1.403165
C	-5.133920	-2.951614	-3.998643
N	-5.484377	-1.837182	-3.082169
C	-6.217058	-0.712464	-3.719376
H	-6.046468	-3.363536	-4.428089
H	-4.622954	-3.725122	-3.427383
H	-4.479642	-2.586747	-4.790224
H	-4.619248	-1.492524	-2.620087
H	-7.121436	-1.099385	-4.188015
H	-5.585262	-0.236943	-4.469882
H	-6.494592	-0.007057	-2.938220
4SA3MA4DMA			
S	-4.258237	4.421996	0.582855
O	-4.707219	5.723901	0.947050
O	-2.747312	4.533198	0.128268
O	-4.348284	3.338774	1.548351

O	-5.021798	4.015913	-0.726870
H	-4.324025	0.751402	2.532644
H	-4.591250	3.238596	-1.194204
S	-0.247039	1.737553	0.046449
O	-0.359419	0.395520	-0.758079
O	0.413339	2.743932	-0.796586
O	-1.602130	2.127603	0.456889
O	0.610316	1.382080	1.209085
H	-2.303062	3.646031	0.175690
H	2.060164	2.341443	1.170990
O	5.765447	3.172763	-3.367815
O	5.419977	-0.311309	-2.638848
O	1.795453	2.351224	-3.095178
O	6.517770	1.354329	-1.577869
O	3.477728	2.057485	-1.637202
C	5.409096	1.838816	-3.646095
C	3.914860	1.753358	-3.970416
C	5.824225	0.925993	-2.493496
C	3.041274	2.079926	-2.783274
H	5.960335	1.472647	-4.525320
H	3.654149	0.745488	-4.306505
H	3.677265	2.437403	-4.787082
H	6.333309	3.137005	-2.584951
H	5.695470	-0.888580	-1.867424
H	1.246715	2.481883	-2.276667
S	7.272442	-1.552318	0.200148
O	8.406453	-1.703795	-0.661828
O	5.962232	-1.763663	-0.502844
O	7.307092	-2.285214	1.472895
O	7.183851	-0.005890	0.696029
H	6.356929	-1.796761	2.634140
H	7.029485	0.548487	-0.110765
O	0.642648	-1.323747	1.912759
O	3.533643	-2.482456	0.126880
O	-0.583492	-3.376288	-0.734176
O	3.373115	-1.018719	1.830081
O	-1.201331	-4.444510	1.146845
C	1.351693	-2.003852	0.908315
C	1.003590	-3.495857	1.008136
C	2.864853	-1.785465	1.017666
C	-0.381210	-3.812379	0.491123
H	1.075304	-1.645873	-0.091288
H	1.061567	-3.816987	2.048288
H	1.710538	-4.074946	0.409495

H	0.679880	-0.368435	1.721764
H	4.499777	-2.224266	0.052200
H	-1.484329	-3.646804	-1.066296
S	-3.807564	0.667792	-1.942384
O	-3.771529	2.121041	-2.022382
O	-4.821224	0.024773	-2.781807
O	-2.486127	0.040644	-2.089991
O	-4.277076	0.379435	-0.412135
H	-1.231390	0.324475	-1.297430
H	-4.744000	-0.499015	-0.391726
O	-5.122828	-5.269178	-2.904029
O	-3.562991	-5.305209	0.282597
O	-5.695137	-2.422084	-2.467278
O	-2.966514	-4.207177	-1.592152
O	-5.443049	-2.003535	-0.270097
C	-5.142506	-5.205927	-1.506445
C	-6.177798	-4.180294	-0.955853
C	-3.762025	-4.870468	-0.942572
C	-5.748053	-2.751137	-1.194694
H	-5.432423	-6.194278	-1.146058
H	-6.310868	-4.319090	0.116462
H	-7.118445	-4.373125	-1.475681
H	-4.799915	-4.420790	-3.235649
H	-2.672017	-4.992033	0.620046
H	-5.346752	-1.484258	-2.596754
C	-2.505908	1.385681	3.349836
N	-3.280084	0.603417	2.350126
C	-2.955399	-0.849088	2.338828
H	-2.713626	0.991333	4.345123
H	-2.820202	2.424163	3.275113
H	-1.444357	1.304688	3.123987
H	-3.103133	1.001097	1.418385
H	-3.174806	-1.266708	3.321749
H	-1.898945	-0.990141	2.109754
H	-3.568870	-1.341897	1.587554
C	2.634676	4.336224	0.978715
N	2.902868	2.877968	0.870412
C	4.108137	2.404338	1.596329
H	2.479114	4.600532	2.024611
H	1.739950	4.556655	0.400244
H	3.485785	4.887657	0.579742
H	3.009429	2.621558	-0.138520
H	4.013141	2.651702	2.654080
H	4.990358	2.886522	1.176662

H	4.183474	1.325846	1.469340
C	5.323856	-2.487363	4.324399
N	5.672608	-1.418293	3.355085
C	6.260589	-0.195275	3.959561
H	6.220357	-2.788046	4.865626
H	4.930813	-3.341276	3.774764
H	4.570675	-2.121684	5.022193
H	4.827592	-1.176209	2.798749
H	7.149978	-0.471195	4.525392
H	5.532992	0.276902	4.620078
H	6.546219	0.474393	3.150409
C	-6.921528	0.718729	1.802988
N	-5.997344	1.238504	2.821685
C	-6.533420	1.133951	4.181944
H	-7.014252	-0.365865	1.903012
H	-6.519914	0.940245	0.814732
H	-7.924269	1.160931	1.884902
H	-5.801637	2.213538	2.600222
H	-6.643979	0.080646	4.455139
H	-7.516327	1.614419	4.290424
H	-5.844768	1.600841	4.889916
4SA4MA			
S	0.910934	-2.791311	3.911149
O	1.730366	-1.652592	3.523143
O	1.254075	-3.617033	5.009032
O	-0.549397	-2.240008	4.154716
O	0.758989	-3.727573	2.639353
H	-0.758973	-1.529619	3.504171
H	0.683405	-3.168223	1.834026
S	4.402418	-0.940563	1.334374
O	3.368709	-0.084309	0.754149
O	5.754876	-0.592600	1.070228
O	4.231291	-1.058800	2.877853
O	4.070417	-2.423302	0.892596
H	3.310501	-1.333850	3.139555
H	3.646097	-2.422164	-0.001796
S	-0.213295	-0.534970	0.925596
O	-1.048603	-0.397717	2.120613
O	0.343614	-1.835639	0.657933
O	-1.043637	-0.113808	-0.305990
O	0.894994	0.547235	1.044072
H	-1.544271	0.756631	-0.118063
H	1.838645	0.209337	0.913560
O	-3.308705	4.573741	0.180064

O	-2.329684	2.033118	2.493598
O	-0.590152	5.076705	-0.022982
O	-2.158400	2.124114	0.243060
O	0.628478	4.607106	1.806784
C	-2.880188	4.078617	1.434773
C	-1.744107	4.931331	2.048613
C	-2.438961	2.621553	1.324922
C	-0.440921	4.854768	1.279043
H	-3.743720	4.108844	2.098115
H	-1.547954	4.616422	3.072089
H	-2.082420	5.971301	2.055612
H	-2.522796	4.683318	-0.377936
H	-1.962093	1.123179	2.402851
H	0.286553	4.982730	-0.504570
S	2.655972	-1.491865	-2.525772
O	2.712341	-2.492879	-1.454079
O	3.917843	-1.053637	-3.063551
O	1.798242	-2.068887	-3.666523
O	1.846647	-0.275237	-2.009261
H	1.047658	-2.686510	-3.330734
H	2.404090	0.592668	-1.970484
O	3.804322	4.760960	-2.921179
O	2.977497	4.306400	0.536735
O	5.239266	1.249122	-2.355173
O	1.729523	4.848287	-1.259256
O	3.154257	1.886138	-1.793781
C	4.086714	4.592812	-1.554100
C	4.986108	3.369641	-1.356926
C	2.802230	4.563940	-0.735358
C	4.363252	2.096430	-1.867282
H	4.640241	5.464321	-1.171125
H	5.202300	3.222248	-0.294098
H	5.933721	3.530702	-1.870482
H	2.852994	4.922124	-2.992573
H	2.116928	4.382699	1.033283
H	4.807543	0.410627	-2.639214
O	-2.037809	-5.563098	-2.748032
O	0.798095	-4.392549	-0.942967
O	-3.300119	-3.196451	-1.988774
O	-0.066688	-3.624402	-2.876567
O	-3.135727	-2.590599	0.164767
C	-1.310986	-5.259418	-1.595421
C	-2.174599	-4.667488	-0.453563
C	-0.125726	-4.337002	-1.884473

C	-2.915467	-3.406299	-0.840272
H	-0.883992	-6.195343	-1.226994
H	-1.581774	-4.487845	0.443297
H	-2.936414	-5.412279	-0.201175
H	-2.501396	-4.754950	-3.012783
H	1.507808	-3.730948	-1.115178
H	-4.469724	-2.022174	-2.416944
O	-7.281814	0.429156	0.399813
O	-5.226793	3.013926	-1.001375
O	-4.584269	-0.498419	-0.635418
O	-5.358454	2.170065	1.082990
O	-5.212275	-1.388252	-2.599386
C	-6.818153	1.289279	-0.611056
C	-6.405987	0.503448	-1.861938
C	-5.710554	2.192991	-0.078527
C	-5.310564	-0.507166	-1.622692
H	-7.629997	1.965683	-0.913533
H	-6.069021	1.185902	-2.647921
H	-7.273199	-0.030771	-2.255428
H	-6.700326	0.571913	1.160809
H	-4.535135	3.591737	-0.594054
H	-3.654824	-1.789263	-0.139947

4SA4MA1DMA

S	0.651516	-3.400154	4.159874
O	2.003232	-2.883682	4.037488
O	0.339202	-4.325546	5.187375
O	-0.356807	-2.192029	4.287295
O	0.260435	-4.063024	2.769626
H	-0.347684	-1.610368	3.483942
H	0.604344	-3.503328	2.031338
S	4.016309	-0.797154	1.896474
O	3.505694	0.167276	0.928185
O	5.388124	-0.727494	2.261157
O	3.054822	-0.656056	3.133508
O	3.740086	-2.256693	1.361278
H	2.780544	-1.525023	3.539622
H	2.805917	-2.311564	1.041067
S	0.107553	-1.075135	0.747810
O	-0.501673	-0.673738	2.036780
O	1.063925	-2.184994	0.962271
O	-0.853015	-1.295765	-0.312326
O	0.956158	0.179878	0.236191
H	-0.028352	0.342539	-1.891735
H	1.893733	0.187196	0.584731

O	-2.439796	4.743909	0.660721
O	-1.473566	1.783451	2.430005
O	0.354556	4.739410	0.397237
O	-1.834573	2.132802	0.229483
O	1.557622	4.126044	2.192626
C	-2.023260	3.976142	1.779347
C	-0.787915	4.579037	2.481997
C	-1.778379	2.516308	1.384933
C	0.497180	4.454865	1.694708
H	-2.860868	3.975530	2.476649
H	-0.630123	4.100323	3.446468
H	-0.985372	5.642568	2.647852
H	-1.682615	4.815547	0.062291
H	-1.219392	0.852777	2.190392
H	1.227045	4.627612	-0.082146
S	2.297681	-1.702737	-3.104316
O	2.192513	-2.534185	-1.925606
O	3.604284	-1.508241	-3.680788
O	1.321201	-2.210472	-4.191209
O	1.697511	-0.273934	-2.791265
H	0.519817	-2.694148	-3.768496
H	2.441126	0.369428	-2.479326
O	4.724041	4.099360	-2.544967
O	3.817090	3.568742	0.876680
O	5.348801	0.287738	-2.437596
O	2.643904	4.332159	-0.888932
O	3.431629	1.375076	-1.984887
C	4.933376	3.693948	-1.214145
C	5.501610	2.267249	-1.164915
C	3.668561	3.875778	-0.383919
C	4.655381	1.271201	-1.910091
H	5.678751	4.348666	-0.741834
H	5.573345	1.917357	-0.129812
H	6.505454	2.261185	-1.589534
H	3.794241	4.356897	-2.611671
H	2.984448	3.752906	1.394740
H	4.771144	-0.367056	-2.894199
O	-2.996859	-4.862663	-2.865499
O	0.111487	-4.198352	-1.238799
O	-3.634543	-2.359768	-1.761471
O	-0.723296	-3.345308	-3.151059
O	-3.884697	-2.386682	0.467389
C	-2.116688	-4.778452	-1.781225
C	-2.772201	-4.226621	-0.495961

C	-0.835792	-4.019386	-2.133393
C	-3.458623	-2.892056	-0.662081
H	-1.792663	-5.799072	-1.558939
H	-2.053970	-4.154886	0.322665
H	-3.542881	-4.934648	-0.175397
H	-3.282506	-3.959972	-3.061326
H	0.892962	-3.627620	-1.425696
H	-4.602758	-1.009368	-2.044590
O	-7.331042	1.667756	1.003024
O	-4.766572	3.743732	-0.430936
O	-5.220344	-0.085031	0.016256
O	-4.933814	2.822763	1.619317
O	-5.151304	-0.196603	-2.224744
C	-6.669016	2.380249	-0.005847
C	-6.442185	1.543266	-1.279867
C	-5.363963	2.998123	0.504234
C	-5.544198	0.346699	-1.082947
H	-7.319281	3.215590	-0.284263
H	-6.038949	2.155902	-2.088159
H	-7.410771	1.161440	-1.618286
H	-6.662236	1.143048	1.461838
H	-3.932825	4.120724	-0.057092
H	-4.349656	-1.518455	0.315608
C	-0.311146	2.264298	-2.586553
N	-0.824570	0.959061	-2.089099
C	-1.740901	0.258245	-3.033319
H	0.223289	2.100225	-3.520561
H	0.363864	2.679671	-1.841732
H	-1.153282	2.936198	-2.743042
H	-1.287829	1.116142	-1.178487
H	-1.219918	0.113990	-3.978689
H	-2.633692	0.863731	-3.180423
H	-2.005730	-0.704274	-2.603735
4SA4MA2DMA			
S	-0.672362	-3.251413	3.434845
O	0.535403	-2.429757	3.281365
O	-0.730861	-4.220176	4.467810
O	-1.880974	-2.261636	3.606513
O	-0.936474	-3.979342	2.067157
H	-1.811185	-1.498732	2.957416
H	-0.930851	-3.329462	1.309948
S	3.656423	-2.962516	1.286012
O	3.351317	-1.637034	0.789596
O	5.002227	-3.429672	1.277923

O	3.163009	-3.096081	2.791234
O	2.694413	-3.991624	0.573884
H	2.192137	-2.955150	2.863920
H	2.252861	-3.596883	-0.231544
S	-0.990431	-0.643289	0.581923
O	-1.465690	-0.281147	1.920953
O	-1.209604	-2.044149	0.230562
O	-1.471905	0.275744	-0.472239
O	0.580996	-0.410739	0.702257
H	-1.219415	1.898405	-0.070526
H	1.052487	-0.632521	-0.149643
O	-0.906471	5.511953	0.038304
O	-0.049788	2.595317	1.929045
O	1.855628	4.822895	-0.224363
O	-1.141570	2.889935	-0.024759
O	2.993591	4.374868	1.662162
C	-0.553292	4.828308	1.232590
C	0.781114	5.310758	1.831129
C	-0.557637	3.303936	1.078309
C	1.994644	4.789996	1.096703
H	-1.358573	5.044979	1.937663
H	0.867717	5.004115	2.871174
H	0.791548	6.403909	1.791224
H	-0.209064	5.344922	-0.610885
H	0.556385	0.978081	2.650210
H	2.676682	4.465255	-0.680684
S	1.846065	-2.104956	-2.494394
O	1.329884	-3.094886	-1.524764
O	3.258650	-2.270375	-2.801657
O	0.968679	-1.921035	-3.635916
O	1.746406	-0.682257	-1.663928
H	-0.668827	-1.062601	-3.479542
H	2.640940	-0.216047	-1.642773
O	5.822476	2.774659	-3.021162
O	5.020877	3.098124	0.459017
O	5.461256	-0.921893	-2.097170
O	4.010588	3.857776	-1.403845
O	3.967687	0.663123	-1.531121
C	6.045288	2.618198	-1.640794
C	6.301720	1.142471	-1.314251
C	4.903873	3.231505	-0.840844
C	5.122937	0.266476	-1.667248
H	6.941113	3.181539	-1.339462
H	6.500870	1.019095	-0.245376

H	7.180852	0.801040	-1.860162
H	5.006286	3.284951	-3.115198
H	4.283634	3.580828	0.924231
H	4.659353	-1.467644	-2.311435
O	-4.457303	-4.255341	-2.641953
O	-1.156939	-4.395855	-1.377924
O	-4.565221	-1.648944	-1.559658
O	-2.021958	-2.904287	-2.821322
O	-4.392187	-1.511894	0.669179
C	-3.527921	-4.340074	-1.589589
C	-4.034032	-3.642905	-0.304217
C	-2.156052	-3.795021	-2.009819
C	-4.343269	-2.172752	-0.467301
H	-3.402021	-5.399307	-1.360276
H	-3.339952	-3.768845	0.526764
H	-4.972982	-4.127261	-0.014018
H	-4.576426	-3.313257	-2.821398
H	-0.307137	-3.935751	-1.573993
H	-4.906443	-0.051453	-1.835673
O	-6.299453	3.473079	1.188980
O	-3.546972	4.858353	-0.671348
O	-5.018983	1.119840	0.190561
O	-3.638757	4.133976	1.462952
O	-5.118099	0.903916	-2.040641
C	-5.612383	3.946007	0.063667
C	-5.722488	3.005414	-1.153310
C	-4.156626	4.308189	0.386376
C	-5.239635	1.593290	-0.918091
H	-6.093621	4.886853	-0.220889
H	-5.199511	3.418362	-2.017361
H	-6.778778	2.921753	-1.429992
H	-5.812451	2.703300	1.511382
H	-2.614846	5.077159	-0.439435
H	-4.609998	-0.554947	0.511416
C	-0.410763	0.988243	-3.593710
N	-1.255050	-0.214605	-3.349237
C	-2.470011	-0.288016	-4.211254
H	-0.057123	0.963722	-4.623144
H	0.436113	0.955223	-2.913770
H	-1.008207	1.882547	-3.419850
H	-1.526036	-0.222613	-2.353766
H	-2.156556	-0.273720	-5.254422
H	-3.108747	0.567825	-3.996645
H	-2.980896	-1.218052	-3.982847

C	2.531425	0.624918	3.168764
N	1.064448	0.430765	3.362573
C	0.557757	0.818898	4.706323
H	2.752563	1.689723	3.229549
H	2.805660	0.227866	2.193611
H	3.065047	0.078338	3.945244
H	0.826464	-0.556756	3.190162
H	0.766061	1.874546	4.870854
H	1.051453	0.212051	5.463957
H	-0.516413	0.645756	4.732376

4SA4MA3DMA

S	-4.225984	-2.034289	1.467517
O	-3.110861	-2.152677	2.405708
O	-5.497847	-2.563869	1.808995
O	-4.400914	-0.502538	1.148028
O	-3.781257	-2.680114	0.103315
H	-3.520717	-0.071134	0.935898
H	-2.915280	-2.288926	-0.202094
S	-0.386275	-4.383460	2.764364
O	0.168769	-3.047419	2.854569
O	0.293638	-5.468361	3.390946
O	-1.859871	-4.379821	3.334481
O	-0.705392	-4.700729	1.247461
H	-2.372149	-3.630498	2.941346
H	-0.039102	-4.316859	0.619526
S	-1.072748	-0.188976	-0.116520
O	-2.064097	0.617243	0.600655
O	-1.636891	-1.364823	-0.778624
O	-0.218684	0.604495	-1.023287
O	-0.125288	-0.707802	1.060349
H	0.357352	2.081280	-0.464794
H	0.634684	-1.232901	0.703839
O	1.481278	5.460489	0.089944
O	0.977767	2.362568	1.833803
O	3.833940	3.765718	0.053575
O	0.719934	2.996498	-0.317233
O	4.764831	3.254997	2.034473
C	1.472448	4.632251	1.247125
C	2.809857	4.649805	2.008899
C	1.021334	3.196581	0.956039
C	3.905089	3.820334	1.380219
H	0.704413	5.052662	1.897981
H	2.675723	4.282022	3.025128
H	3.154336	5.686764	2.069622

H	2.071518	5.047018	-0.554471
H	-1.344434	0.517075	3.711839
H	4.522238	3.133651	-0.303658
S	2.097886	-3.224623	-0.944605
O	0.725230	-3.723451	-0.794407
O	3.120265	-4.069789	-0.338627
O	2.414892	-2.765608	-2.291356
O	2.064527	-1.864547	-0.015149
H	1.789444	-1.230499	-2.923761
H	3.006262	-1.573546	0.132875
O	6.727124	-0.042855	-2.137665
O	6.393308	1.341805	1.149004
O	5.609074	-3.125522	-0.223093
O	5.535792	1.941200	-0.845541
O	4.623590	-1.122902	0.085150
C	7.081379	0.119909	-0.782382
C	7.012161	-1.233718	-0.075208
C	6.230777	1.210734	-0.141512
C	5.619066	-1.825162	-0.073219
H	8.118517	0.481530	-0.694286
H	7.326431	-1.118652	0.966219
H	7.697896	-1.928022	-0.559897
H	6.310152	0.784868	-2.412736
H	5.822267	2.082221	1.502112
H	4.679983	-3.496898	-0.236799
O	-2.480067	-1.828890	-5.553453
O	-1.409437	-3.625874	-2.662319
O	-2.952332	0.276588	-3.761380
O	-0.439303	-1.878380	-3.693954
O	-4.358670	-0.160326	-2.071397
C	-2.670802	-2.539295	-4.355884
C	-3.819722	-1.964198	-3.498154
C	-1.374082	-2.634059	-3.541772
C	-3.651735	-0.510465	-3.120500
H	-2.947216	-3.559525	-4.630624
H	-3.980124	-2.550570	-2.592909
H	-4.741532	-2.024339	-4.087308
H	-2.320536	-0.909604	-5.297801
H	-0.607595	-3.607537	-2.091667
H	-2.859630	1.931412	-3.499659
O	-4.400450	4.598041	0.253959
O	-1.149032	5.692038	-0.838331
O	-3.976445	2.455818	-1.507340
O	-1.710764	4.430281	0.943817

O	-2.841072	2.924785	-3.382990
C	-3.450886	5.194688	-0.583922
C	-3.570581	4.759822	-2.064443
C	-2.014123	5.035982	-0.057554
C	-3.471568	3.267499	-2.281662
H	-3.643379	6.272243	-0.558125
H	-2.829118	5.268606	-2.677526
H	-4.565627	5.052900	-2.415538
H	-4.379233	3.645470	0.080963
H	-0.226057	5.584311	-0.507570
H	-4.219540	0.800377	-1.853183
C	2.734389	0.533816	-2.388634
N	1.662040	-0.211604	-3.102459
C	1.624745	0.038382	-4.570679
H	3.704450	0.171117	-2.722605
H	2.631363	0.352710	-1.323931
H	2.630869	1.598011	-2.595624
H	0.752362	0.010315	-2.672933
H	2.575761	-0.274271	-5.000492
H	1.471231	1.103265	-4.745279
H	0.807373	-0.541817	-4.988356
C	0.605592	-0.119685	4.165326
N	-0.831570	-0.410097	3.903964
C	-1.508301	-1.136845	5.009736
H	0.686215	0.444610	5.094653
H	0.989435	0.471335	3.336793
H	1.143446	-1.062664	4.244360
H	-0.880849	-0.972189	3.046519
H	-1.491531	-0.514080	5.904216
H	-0.986267	-2.073776	5.193118
H	-2.533403	-1.343653	4.711549
C	-3.533024	2.147149	3.498869
N	-2.065323	2.080009	3.398685
C	-1.418950	3.184520	4.122042
H	-3.831414	2.066554	4.547787
H	-3.980114	1.316419	2.952382
H	-3.929368	3.087497	3.095543
H	-1.818874	2.160304	2.413250
H	-1.615135	3.085424	5.193871
H	-1.786000	4.164391	3.791873
H	-0.342276	3.140611	3.953857
4SA4MA4DMA			
S	-0.870059	-3.831737	3.524321
O	0.567507	-3.628373	3.393712

O	-1.370828	-4.759919	4.475942
O	-1.539065	-2.433898	3.797951
O	-1.424010	-4.250679	2.102649
H	-1.217986	-1.761131	3.129643
H	-1.177363	-3.567427	1.408885
S	4.461354	-2.006045	0.173440
O	4.075490	-0.694466	-0.331342
O	5.861131	-2.300944	0.307073
O	3.687319	-2.337787	1.431043
O	3.881641	-3.105446	-0.886236
H	2.863373	-3.749209	1.301560
H	3.213969	-2.693796	-1.477857
S	-0.518195	-1.089289	0.527164
O	-0.596943	-0.779309	1.965157
O	-0.813107	-2.500895	0.247733
O	-1.273306	-0.165672	-0.332956
O	1.021596	-0.857392	0.226187
H	-1.616618	1.431550	0.152400
H	1.219318	-0.559209	-0.705310
O	-2.183012	5.044705	0.177077
O	-0.524294	2.449512	1.988356
O	0.594435	5.203138	-0.058199
O	-1.860312	2.393861	0.179843
O	1.834210	4.992398	1.803698
C	-1.699276	4.455903	1.380500
C	-0.554690	5.265261	2.014592
C	-1.290570	2.986378	1.216435
C	0.751065	5.138607	1.263515
H	-2.556226	4.447087	2.058194
H	-0.381563	4.947261	3.040056
H	-0.848615	6.319163	2.022706
H	-1.428904	5.139558	-0.421967
H	1.361029	-0.334394	2.460456
H	1.480256	5.135851	-0.528949
S	1.943060	-0.989527	-3.334545
O	1.817478	-2.267469	-2.605586
O	3.288455	-0.702621	-3.801726
O	0.885134	-0.781385	-4.315178
O	1.626276	0.127410	-2.162110
H	-0.577743	-0.058505	-3.735962
H	2.390735	0.784949	-2.075879
O	4.917696	4.596257	-2.966267
O	4.065685	4.246771	0.500595
O	5.231540	0.865861	-2.798592

O	2.912122	4.997993	-1.280299
O	3.481134	1.919681	-1.853776
C	5.159197	4.251495	-1.623079
C	5.677802	2.809906	-1.535512
C	3.919847	4.509815	-0.777084
C	4.684793	1.814227	-2.086800
H	5.936592	4.907232	-1.205364
H	5.877735	2.536909	-0.495081
H	6.611901	2.734414	-2.090942
H	4.003221	4.907814	-3.013305
H	3.253655	4.526331	1.007085
H	4.550746	0.215193	-3.108319
O	-3.513295	-4.373767	-3.570288
O	-0.326212	-4.008851	-2.501002
O	-4.707735	-2.254087	-2.163397
O	-1.674120	-2.251941	-2.861933
O	-4.135768	-2.075574	-0.003506
C	-2.694376	-4.389998	-2.419515
C	-3.484375	-4.056791	-1.135385
C	-1.511659	-3.428783	-2.609963
C	-4.154426	-2.701629	-1.155732
H	-2.299272	-5.402006	-2.326945
H	-2.859042	-4.133411	-0.248043
H	-4.285011	-4.799145	-1.047927
H	-4.030705	-3.555921	-3.529228
H	0.390963	-3.335859	-2.624158
H	-5.405521	-0.756284	-2.302470
O	-7.205015	2.243877	1.047730
O	-4.585439	4.013307	-0.676281
O	-5.380973	0.325758	-0.211973
O	-4.714230	3.294842	1.457957
O	-5.816919	0.149003	-2.408367
C	-6.588179	2.910372	-0.021704
C	-6.601285	2.089676	-1.322513
C	-5.189352	3.410770	0.354153
C	-5.868006	0.773624	-1.243044
H	-7.180988	3.811762	-0.212618
H	-6.190443	2.666104	-2.154065
H	-7.639338	1.857898	-1.579699
H	-6.540717	1.662342	1.438449
H	-3.706824	4.357579	-0.383889
H	-4.599061	-1.195816	-0.068152
C	-1.055640	1.854413	-3.062608
N	-1.403364	0.430971	-3.321202

C	-2.581794	0.245274	-4.214654
H	-0.862874	2.344711	-4.016163
H	-0.160332	1.879562	-2.447759
H	-1.880996	2.340104	-2.544250
H	-1.558260	-0.060262	-2.430188
H	-2.363925	0.706701	-5.177166
H	-3.455960	0.713381	-3.763853
H	-2.747623	-0.821414	-4.329325
C	2.930023	1.003328	2.344601
N	2.352702	-0.316584	2.725890
C	2.474271	-0.644127	4.175294
H	2.358259	1.791313	2.830112
H	2.888255	1.094001	1.262240
H	3.970363	1.031791	2.666035
H	2.823224	-1.065106	2.159875
H	1.967877	0.138380	4.743127
H	3.532243	-0.700446	4.429506
H	1.999981	-1.610262	4.344670
C	-0.681685	1.151689	5.829979
N	0.286283	1.841854	4.979705
C	0.683721	3.139129	5.518158
H	-0.217454	0.897224	6.788144
H	-0.996677	0.220583	5.354342
H	-1.583142	1.749114	6.046566
H	-0.111384	1.974749	4.054146
H	1.246075	3.000570	6.447016
H	-0.168404	3.803374	5.747595
H	1.335648	3.652009	4.806662
C	1.659105	-5.103488	0.219512
N	2.364039	-4.668295	1.457196
C	3.366171	-5.639837	1.967669
H	2.395617	-5.247965	-0.567292
H	0.959149	-4.325615	-0.076953
H	1.120761	-6.029946	0.420415
H	1.671022	-4.457591	2.192833
H	4.130149	-5.786217	1.205622
H	2.876923	-6.585772	2.199311
H	3.825504	-5.226379	2.863803

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